RUSSIAN ACADEMY OF SCIENCES
URALS DIVISION
Institute of Electrophysics

Multiple Bands - A Key to High - Temperature Superconductivity in Iron Arsenides?

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Outline of the talk

- Crystal structure and phase diagram
- Electronic structure and ARPES
  - Rare-Earth Puzzle?
  - Fermi surfaces
- Cooper pairing in multi-band system
  - Gaps relations on different Fermi surface sheets
  - Effective coupling constant – from weak to strong coupling?
- Conclusions

REFeAs superconductors

$RE^{3+}O^{2-}Fe^{2+}As^{3-}$

$LaO_{1-x}F_xFeAs$ T_c=26K

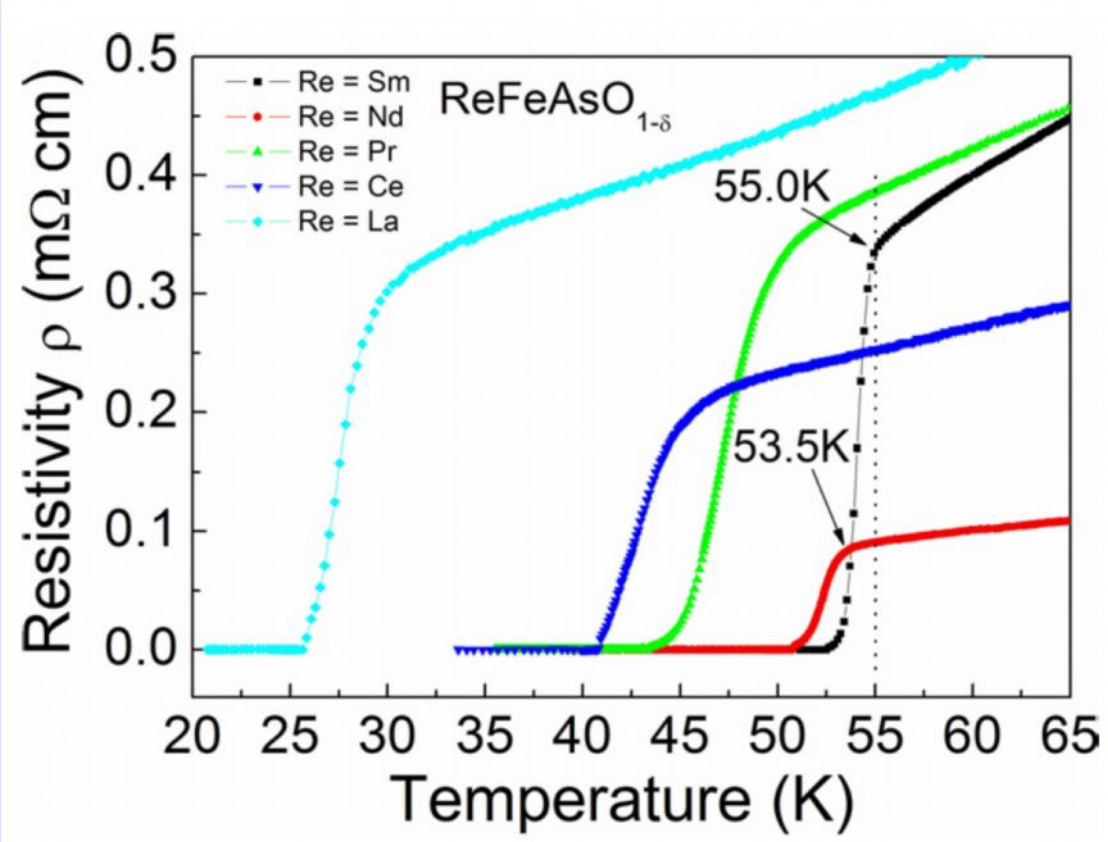
$CeO_{1-x}F_xFeAs$ T_c=41K

$SmO_{1-x}F_xFeAs$ T_c=43K

$NdO_{1-x}F_xFeAs$ T_c=52K

$PrO_{1-x}F_xFeAs$ T_c=52K

$SmFeAsO_{1-\delta}$ T_c=55K



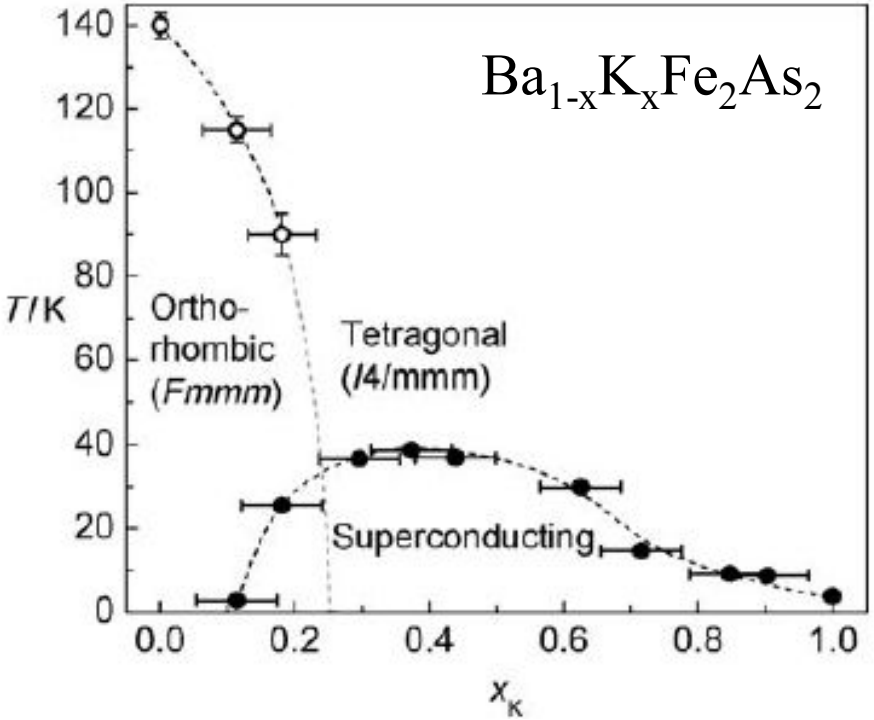
Why T_c is different? Chemical pressure?

Z. Ren *et al.* EPL **83,** 17002 (2008)

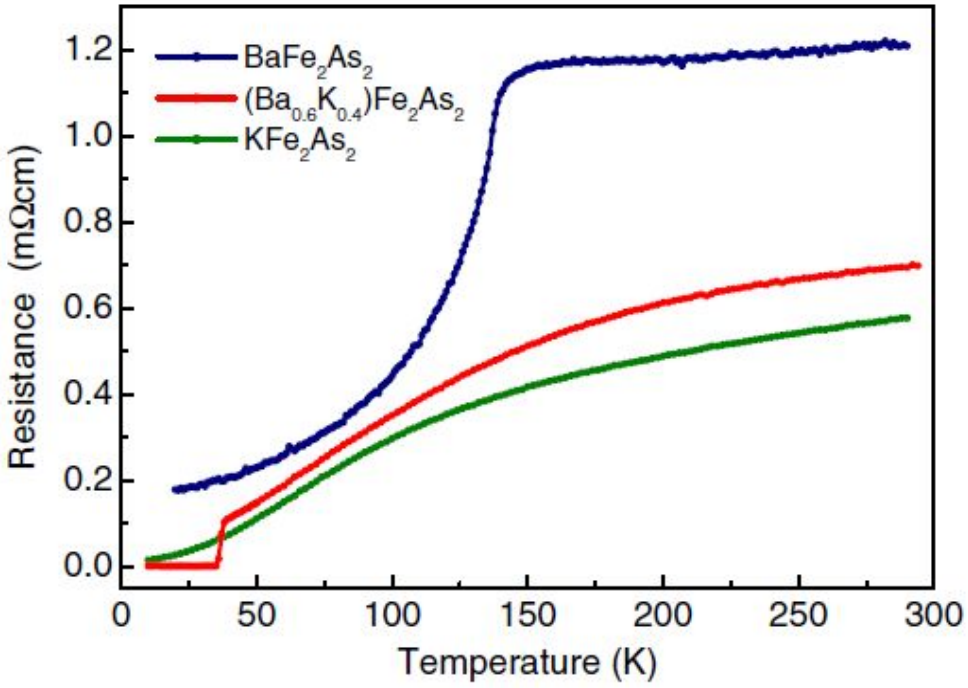
AFe_2As_2 (A=Ba, Sr, …) superconductors

$(Ba_{1-x}K_x)Fe_2As_2$	T_c=38K	M. Rotter et al., PRL **101**, 107006 (2008)
$(Sr_{1-x}K_x)Fe_2As_2$	T_c=38K	G. Wu et al., Europhysics Letters **84**, 27010(2008)
$(Sr_{1-x}K/Cs_x)Fe_2As_2$	T_c=37K	K. Sasmal et al., PRL **101**, 107007 (2008)
$(Ca_{1-x}Na_x)Fe_2As_2$	T_c=20K	G. Wu et al., J. Phys.:Cond. Mat. **20**, 422201 (2008)
$(Eu_{1-x}K_x)Fe_2As_2$	T_c=32K	H.S. Jeevan et al., Phys. Rev. B **78**, 092406 (2008)

122: $A^{2+}Fe^{2+}{}_2As^{3-}{}_2$



M. Rotter et al., Angew. Chem. In. Ed. **47**, 7949 (2008)



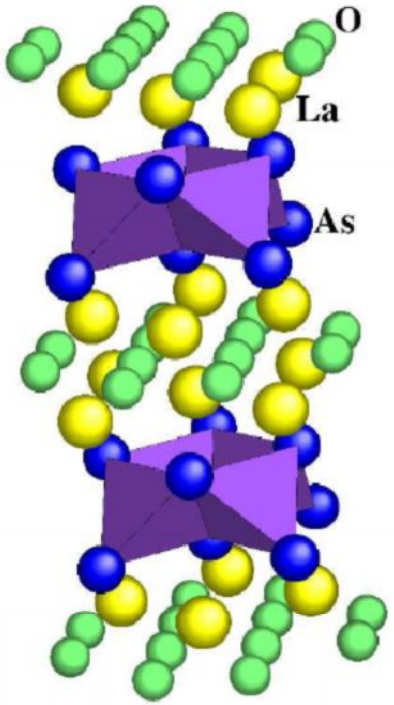
M. Rotter et al., PRL **101**, 107006 (2008)

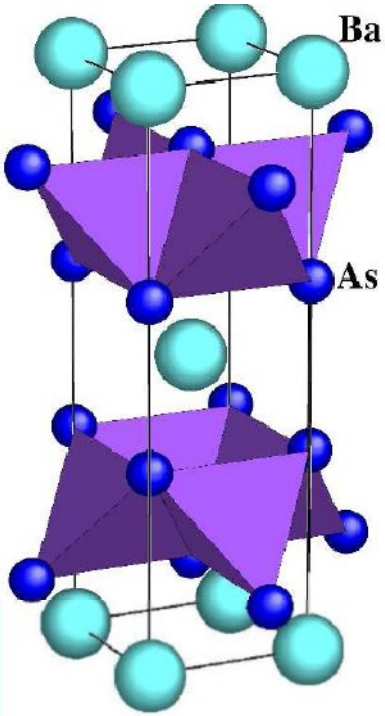
Crystal structure of $ReOFeAs$ and $BaFe_2As_2$

150 K

T(*P*4/*nmm*) → O(*Cmma*)

La ¼, ¼, z_{La}
Fe ¾, ¼, ½
As ¼, ¼, z_{As}
O ¾, ¼, 0





140 K

T(*I*4/*mmm*) → O (*Fmmm*)

Ba 0, 0, 0
Fe ½, 0 ¼
As 0, 0, z_{As}

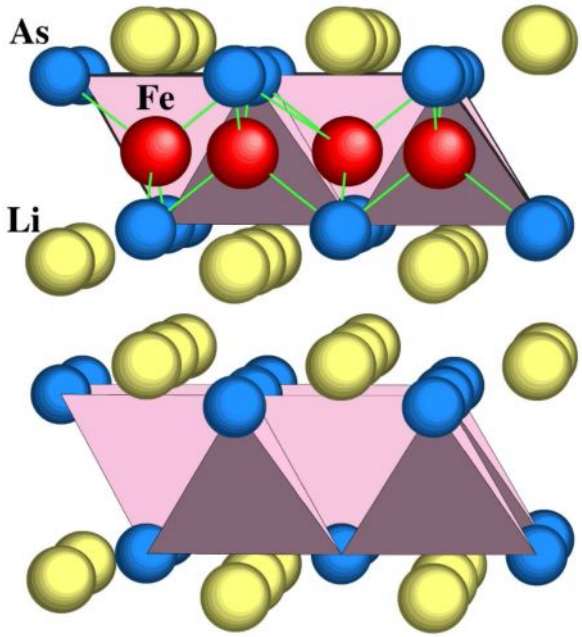
LaOFeAs

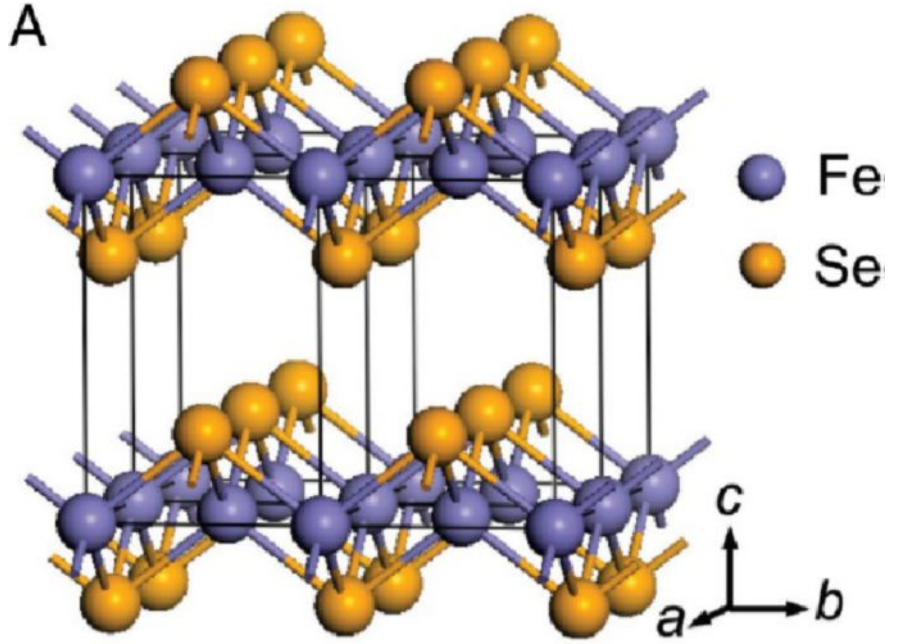
- ZrCuSiAs-type structure
- *P4/nmm*, *a*=4.03 Å, *c*=8.74 Å
- Charge $(LaO)^{+}(FeAs)^{-}$
- Distance of FeAs layers 8.74 Å
- *d*(Fe-As)=2.41 Å,
- As-Fe-As=113.6°; 107.5°

$BaFe_2As_2$

- $ThCr_2Si_2$-type structure
- *I4/mmm*, *a*=3.91 Å, *c*=13.21 Å
- Charge $(Ba)^{2+}[(FeAs)^{-}]_2$
- Distance of FeAs layers 6.61 Å
- *d*(Fe-As)=2.39 Å,
- As-Fe-As=109.9°; 109.3°

Crystal structure of LiFeAs and FeSe





LiFeAs (Superconducting without doping)

- PbFCl-type structure
- *P4/nmm*, *a*=3.79 Å, *c*=6.36 Å
- Li (¼, ¼, z_{Li}) Fe(¾, ¼, ½) As (¼, ¼, z_{As})
- *d*(Fe-As)=2.42 Å
- As-Fe-As=103.1°; 112.7°

J.H. Tapp et al., PRB 78, 060505 (2008)

α-FeSe

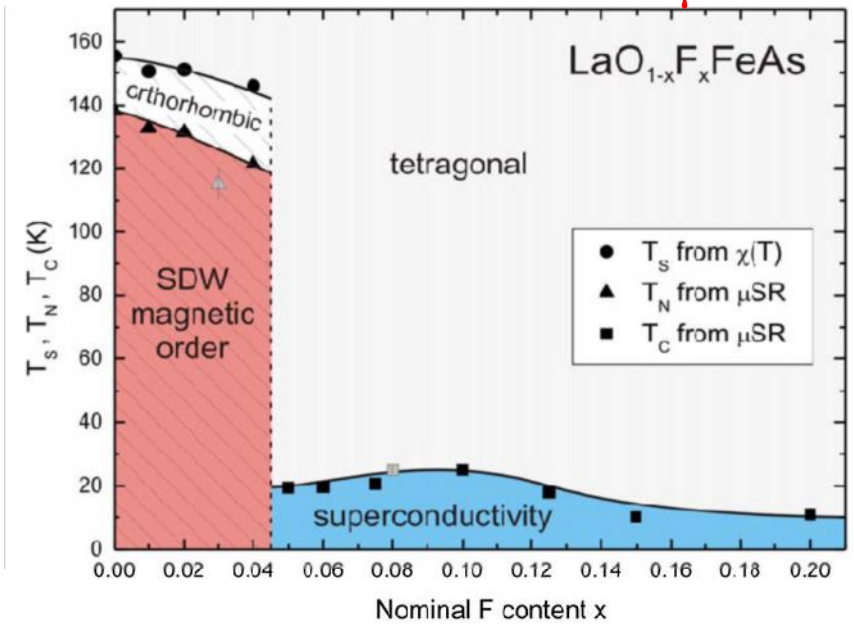
- PbO-type structure
- *P4/nmm*, *a*=3.77 Å, *c*=5.48 Å
- Fe (0,0,0) As(0, ½, z_{As})
- *d*(Fe-As)=2.38 Å,
- As-Fe-As=104.5°; 111.8°; 112.2°

S. Margadonna et al., Chem. Commun.78, 5607 (2008)

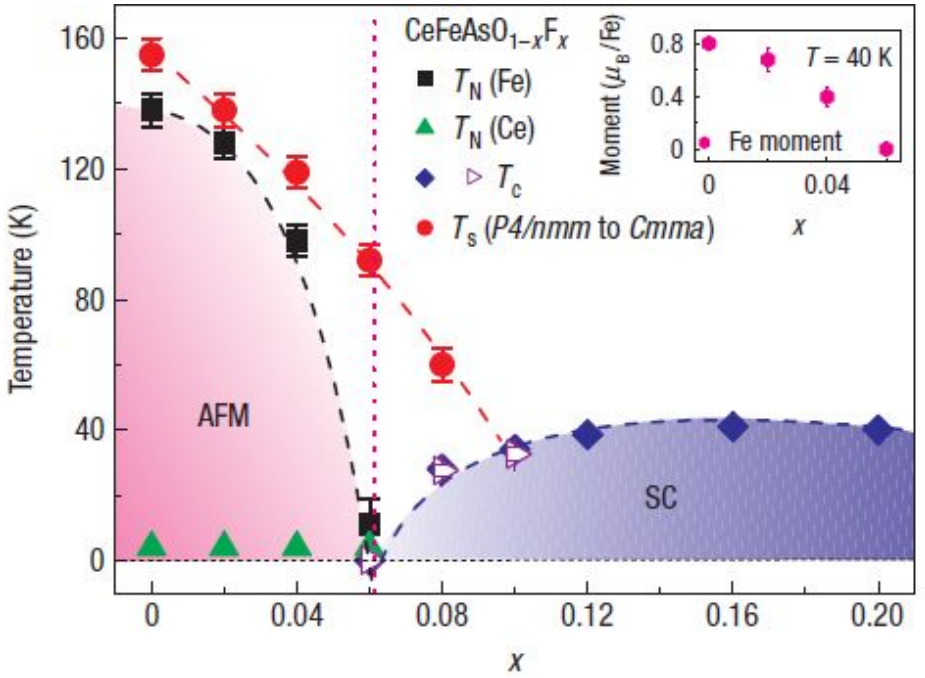
F.C. Hsu et al., arXiv:0807.2369

ReOFeAs: phase diagram

H. Luetkens et al., arXiv:0806.3533 **μSR**

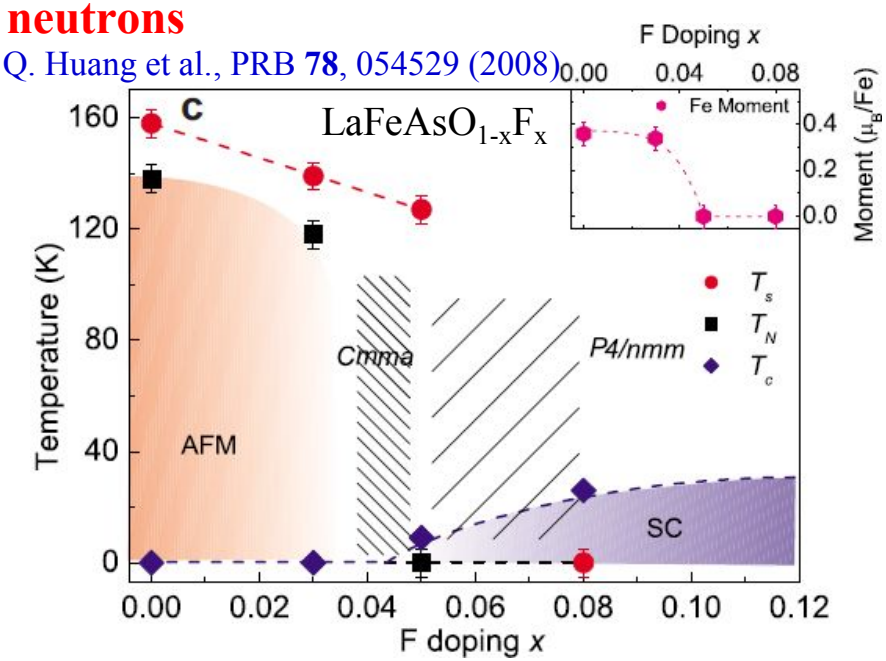


J. Zhao et al., Nature Materials **7**, 953-959 (2008). **neutrons**



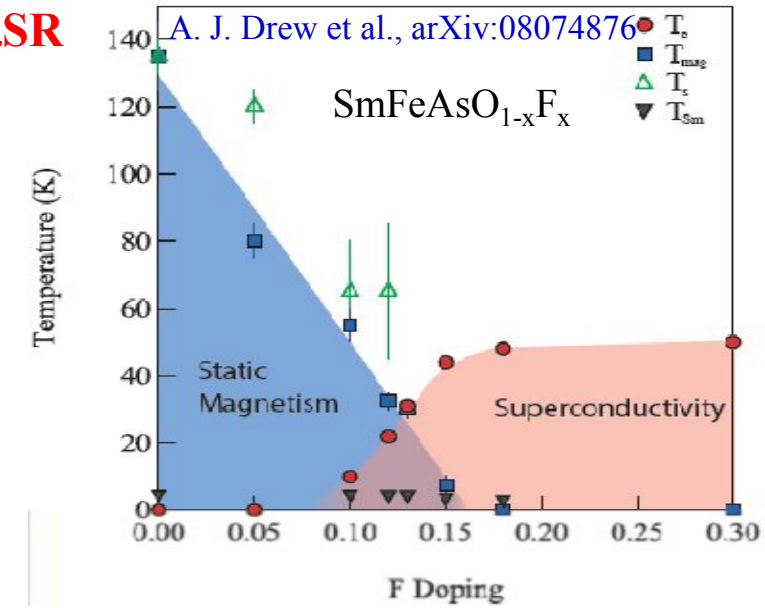
neutrons

Q. Huang et al., PRB **78**, 054529 (2008)



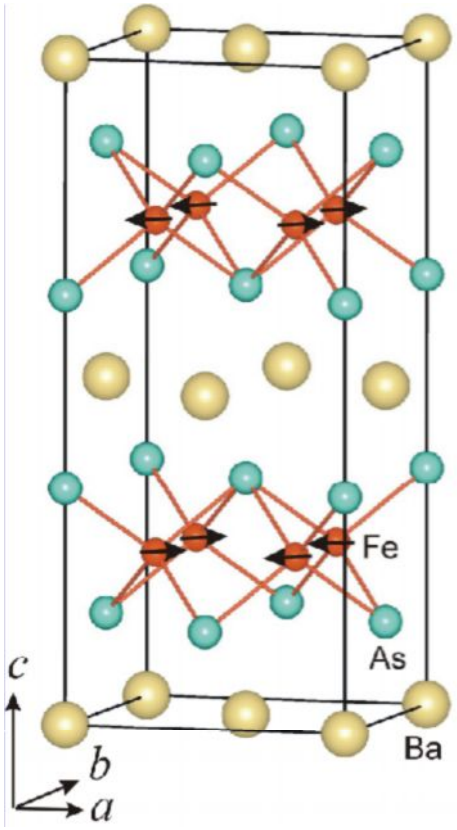
μSR

A. J. Drew et al., arXiv:08074876

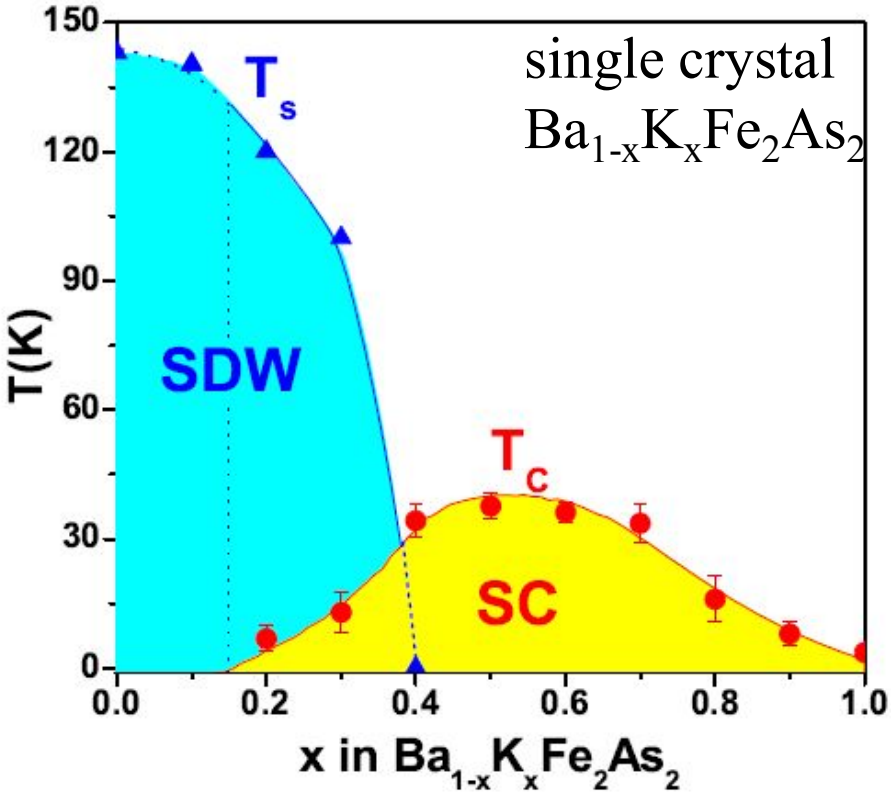


Magnetic properties of 122

Neutron scattering



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

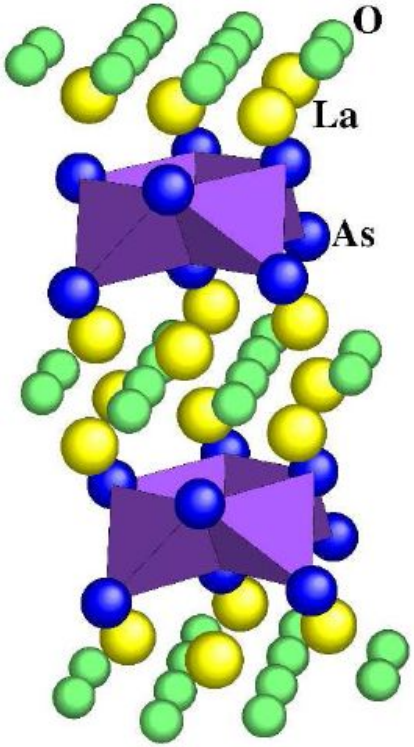


H. Chen et al., arXiv:0807.3950 (2008)

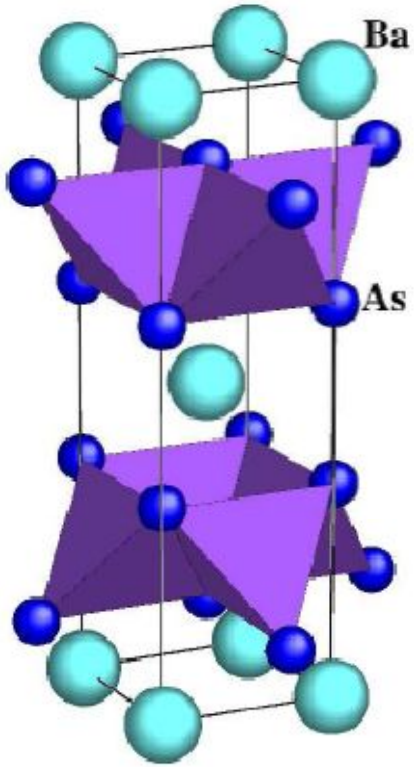
- 142K [220K][1] – T(*I4/mmm*)→O(*Fmmm*)
- 142K [220K][1] – AFM order of Fe with $\sqrt{2}a\times\sqrt{2}b\times 2c$ cell, stripes along b [a][1]
- m_{Fe}=0.87 μ_B at 5K for $BaFe_2As_2$
- m_{Fe}=0.94 μ_B at 10K for $SrFe_2As_2$

[1] for $SrFe_2As_2$, J. Zhao et al., PRB **78**, 140504 (2008)

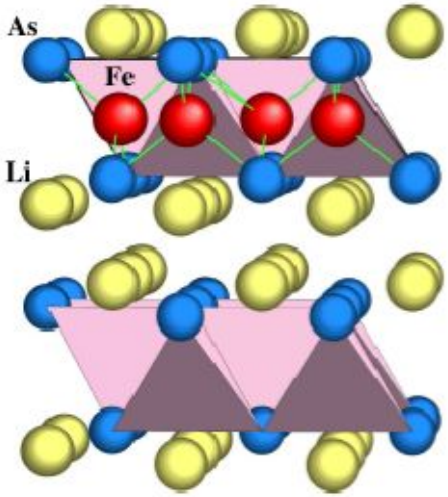
Summary: essentially physics of FeAs layers!



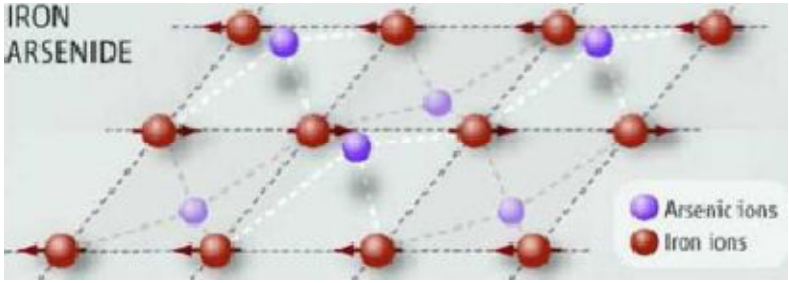
LaOFeAs



$BaFe_2As_2$



LiFeAs



FeAs tetrahedra form two-dimensional layers surrounded by LaO, Ba or Li.
Fe ions inside tetrahedra form a square lattice.

Magnetic (AFM) fluctuations possible?

LDA calculations for FeAs superconductors

LaOFeP S. Lebègue, PRB **75**, 035110 (2007)

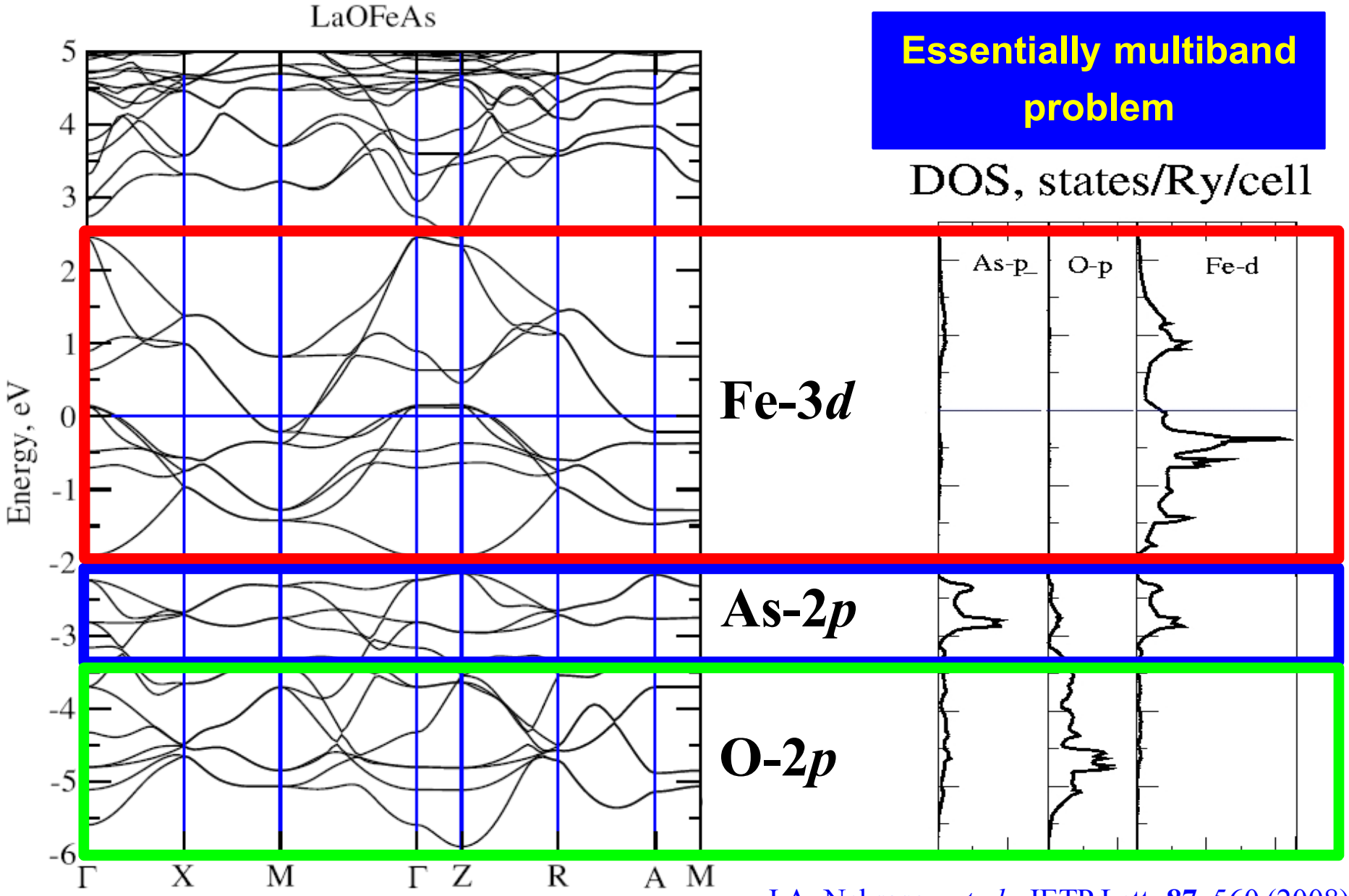
LaOFeAs D.J. Singh and M.H. Du, PRL **100**, 237003 (2008)
L. Boeri et al., PRL **101**, 026403 (2008)
I.I. Mazin et al., PRL **101**, 057003 (2008)
G. Xu et al., Europhys. Lett. **82**, 67002 (2008)
I.A. Nekrasov *et al.*, JETP Lett. **87**, 560 (2008)

122 I.A. Nekrasov *et al.*, JETP Lett. **88**, 144, 543, 679 (2008)
I.R. Shein and A.L. Ivanovskii, JETP Lett. **88**, 115 (2008)
D.J. Singh, PRB 78, 094511 (2008)
F. Ma et al., arXiv:0806.3526 (2008)

α-FeSe A. Subedi et al., Phys. Rev. B **78**, 134514 (2008)

and many others…

LDA band structure of tetragonal LaOFeAs



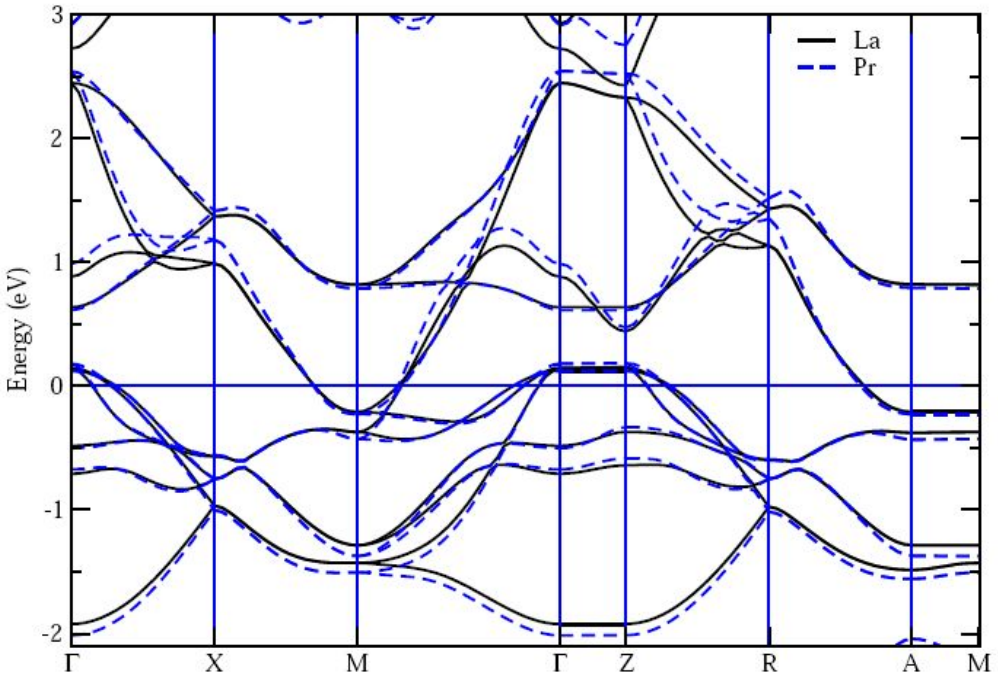
Essentially multiband problem

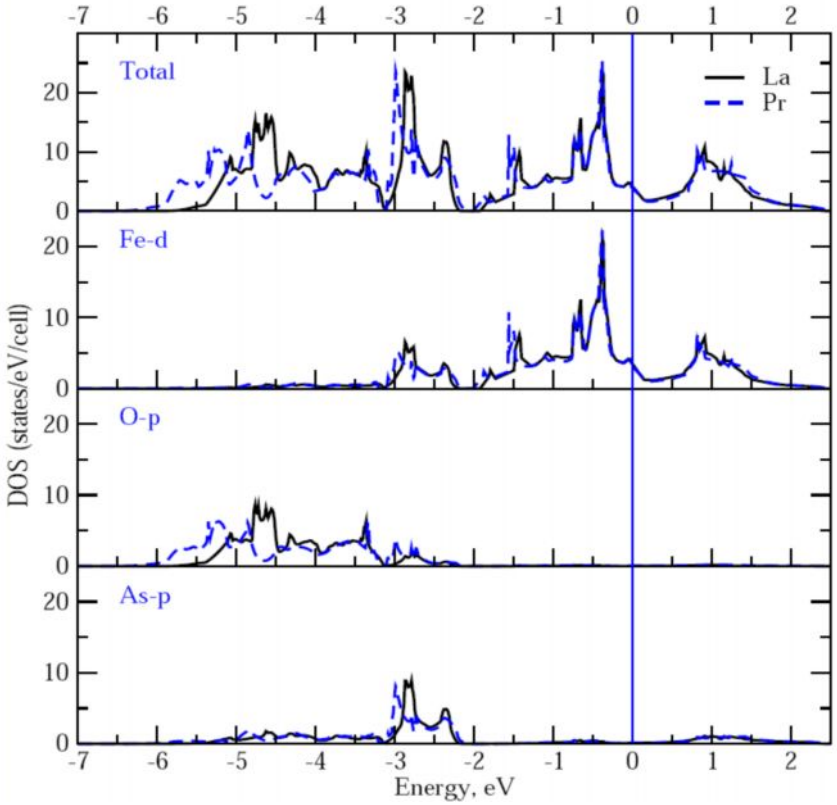
I.A. Nekrasov *et al.*, JETP Lett. **87**, 560 (2008)

REOFeAs:

Rare-Earth Puzzle

ReOFeAs	La	Ce	Pr	Nd
T_c, K	26	41	52	51.9





No significant changes by RE substitution!

REOFeAs:

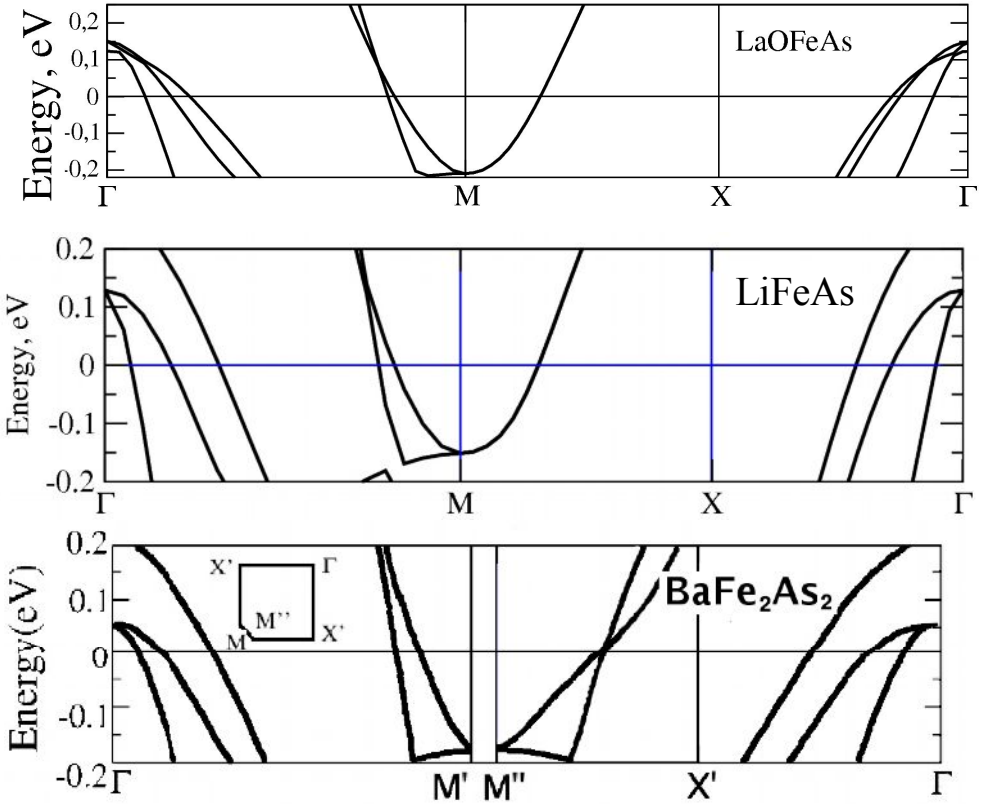
Rare-Earth Puzzle

ReOFeAs	La	Ce	Pr	Nd
T_c, K	26	41	52	51.9

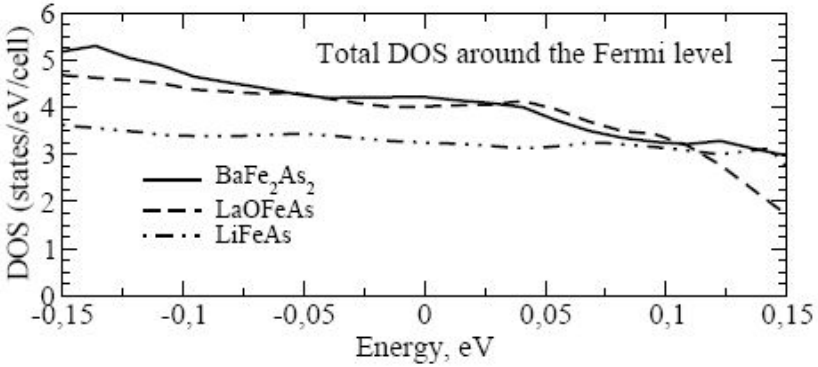
- Different samples quality (effects of disorder)
- HP synthesis of $LaO_{1-x}Fe_xAs$ with T_c=41K
  (W. Lu *et al.* Solid State Comm. **148,** 168 (2008))

$YFeAsO_{1-x}F_x$ **T_c=10 K** (S.V. Chong *et al.*, arXiv: 0808.0288)
$Gd_{1-x}Y_xFeAsO_{0.8}F_{0.2}$ **T_c=10 K** (K. Kadowaki *et al.*, arXiv: 0808.0289)
$YFeAsO_{1-\delta}$ **T_c=46.5 K** (J. Yang *et al.*, arXiv: 0809.3582)

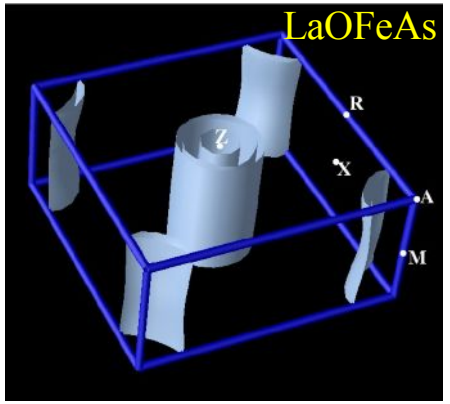
LDA bands and Fermi surface: 1111, 122, 111

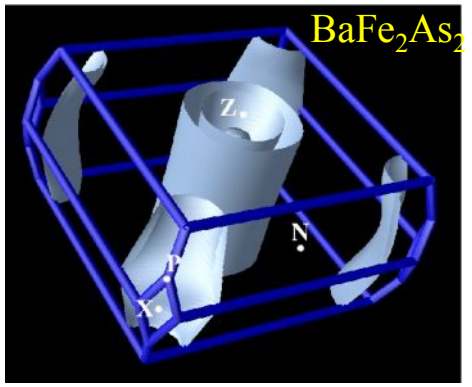


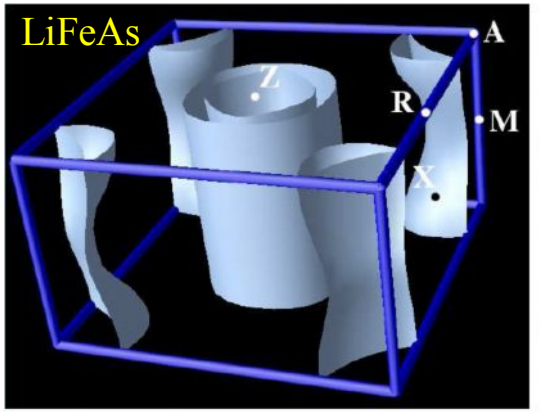
I.A. Nekrasov *et al.*, JETP Lett. **88**, 144, 543, 679 (2008)



Multiple bands (close to and at the Fermi level) spectrum formed (practically) only by *d*-states of Fe. Fermi surface consists of several hole-like and electron-like cylinders, with its "own" superconducting gap at each cylinder.



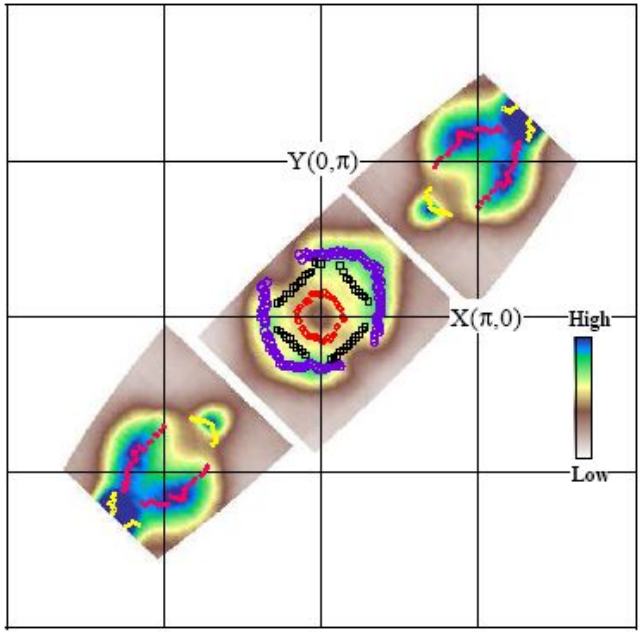




Fermi Surface and Band Renormalization in (Sr,K)Fe_2As_2 Superconductor from Angle-Resolved Photoemission Spectroscopy

Haiyun Liu[1], Wentao Zhang[1], Lin Zhao[1], Xiaowen Jia[1], Jianqiao Meng[1], Guodong Liu[1], Xiaoli Dong[1], G. F. Chen[2], J. L. Luo[2], N. L. Wang[2], Wei Lu[1], Guiling Wang[3], Yong Zhou[3], Yong Zhu[4], Xiaoyang Wang[4], Zhongxian Zhao[1], Zuyan Xu[3], Chuangtian Chen[4], X. J. Zhou[1,*]

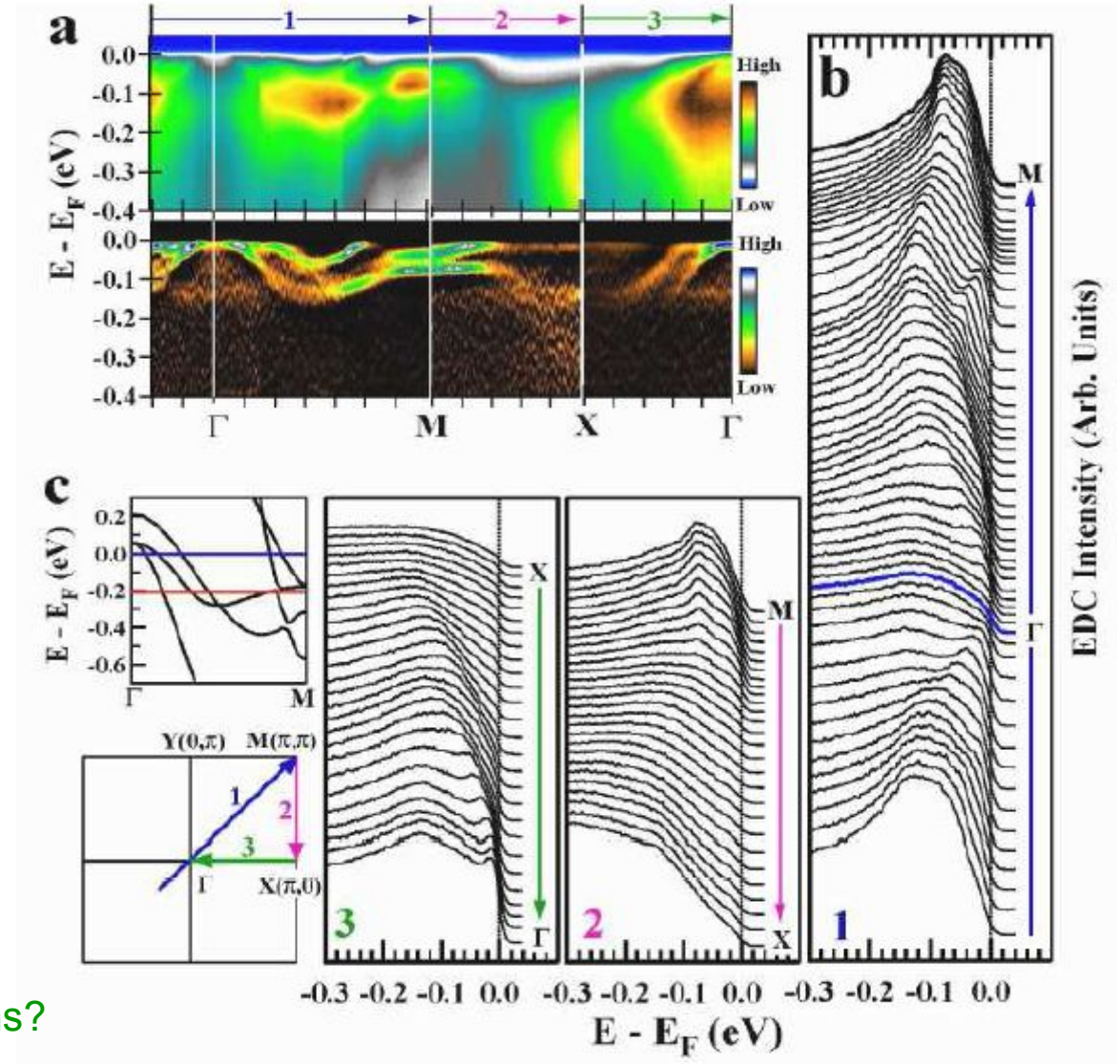
arXiv: 0806.4806



Three hole cylinders!

T_c=21 K

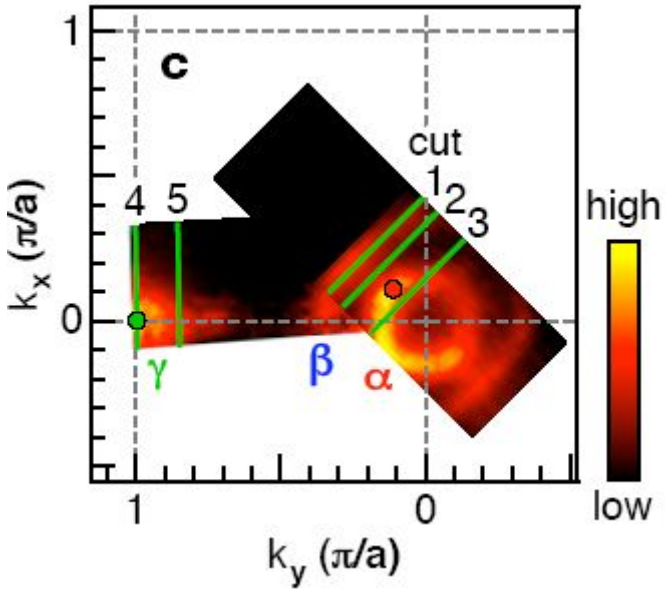
Band narrowing due to correlations?

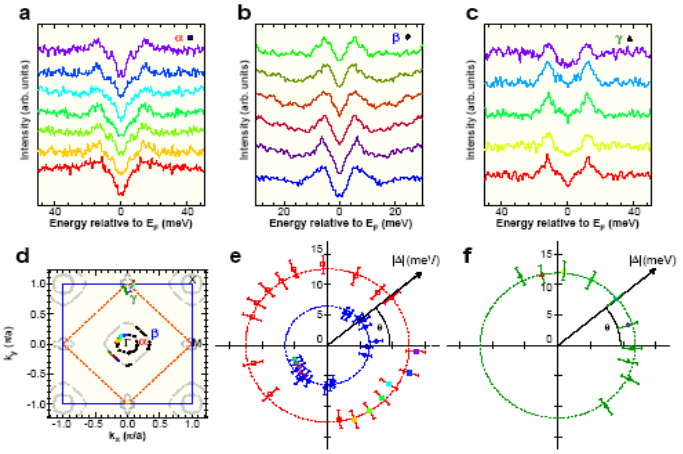


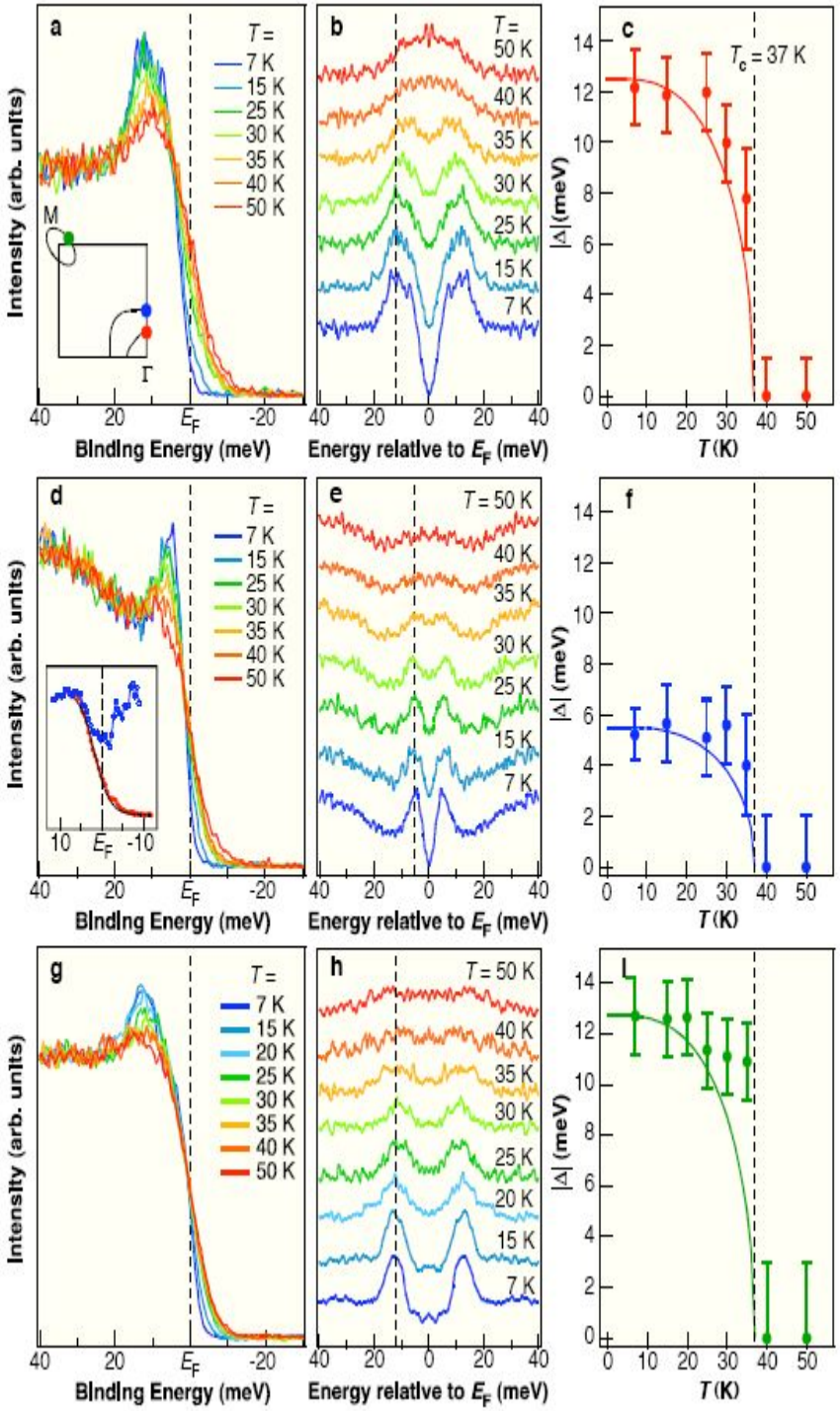
Observation of Fermi-surface-dependent nodeless superconducting gaps in $Ba_{0.6}K_{0.4}Fe_2As_2$

H. Ding[1], P. Richard[2], K. Nakayama[3], T. Sugawara[3], T. Arakane[3], Y. Sekiba[3], A. Takayama[3], S. Souma[2], T. Sato[3], T. Takahashi[2,3], Z. Wang[4], X. Dai[1], Z. Fang[1], G. F. Chen[1], J. L. Luo[1], and N. L. Wang[1]

arXiv: 0807.0419

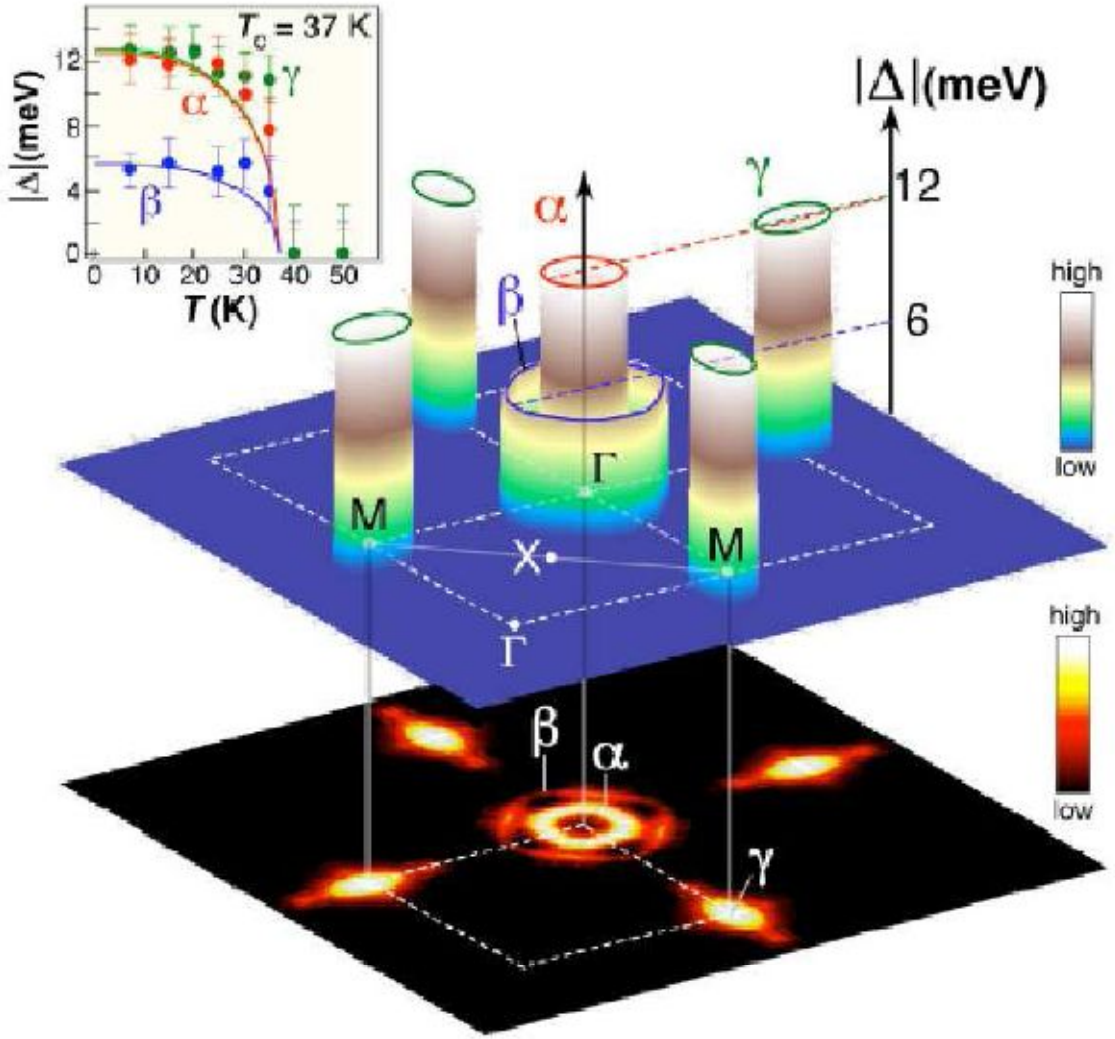






Superconducting gap – ARPES data

arXiv: 0807.0419

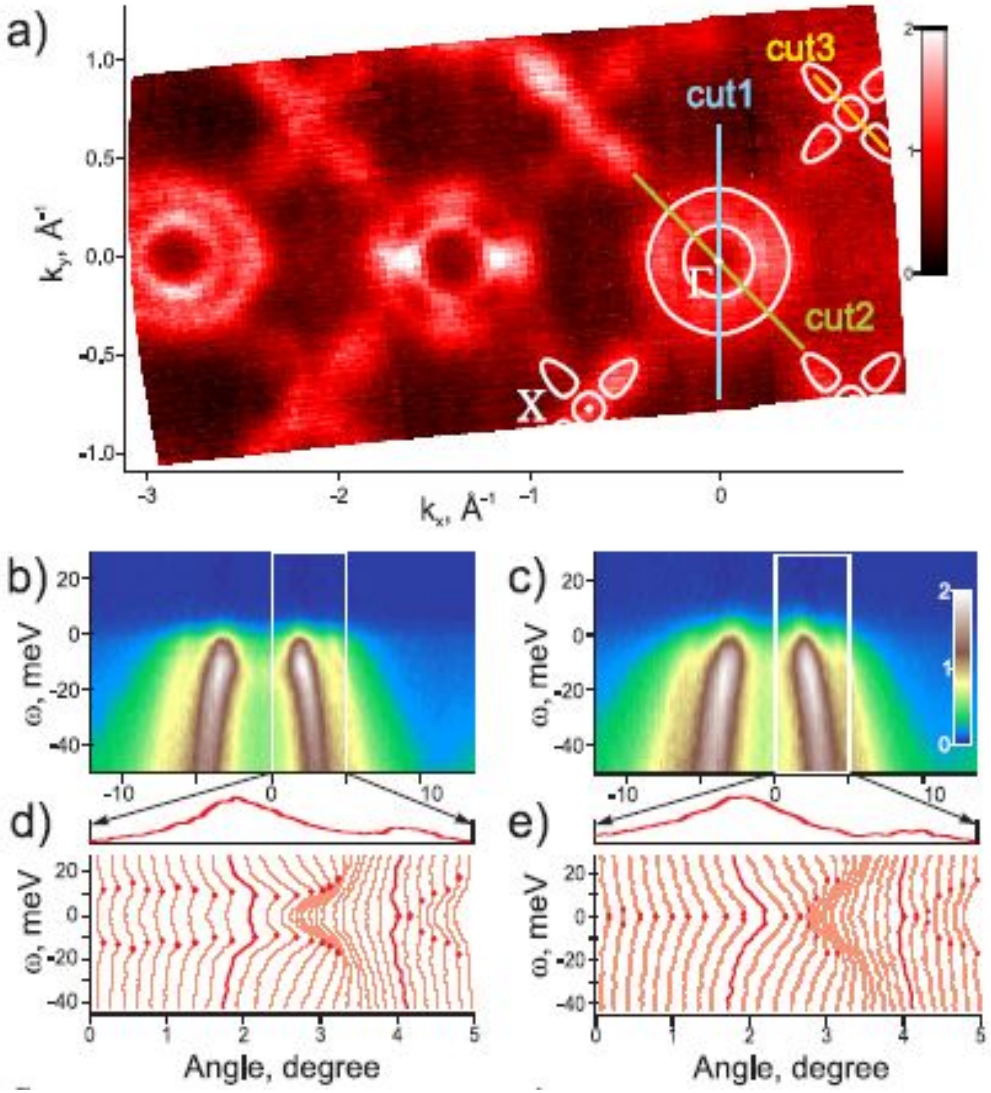


Schematic picture of superconducting gaps in $Ba_{0.6}K_{0.4}Fe_2As_2$. Lower picture represents Fermi surfaces (ARPES intensity), upper insert – temperature dependence of gaps at different sheets of the Fermi surface.

arXiv: 0809.4455

Momentum dependence of the superconducting gap in $Ba_{1-x}K_xFe_2As_2$

D. V. Evtushinsky,[1] D. S. Inosov,[1,2] V. B. Zabolotnyy,[1] A. Koitzsch,[1] M. Knupfer,[1] B. Büchner,[1] G. L. Sun,[2] V. Hinkov,[2] A. V. Boris,[2] C. T. Lin,[2] B. Keimer,[2] A. Varykhalov,[3] A. A. Kordyuk,[1,4] and S. V. Borisenko[1]



Ref. num.	2	3	4	5	6	This paper
T_c	53 K	37 K	35 K	53 K	37 K	32 K
Inner Γ-barrel	20	12.5	12	15	12	9.2 ± 1
Outer Γ-barrel	—	5.5	8	—	6	<4
X-pocket	—	12.5	10	—	11	9 ± 2
Blades	—	—	(11)	—	—	~9
Gap anisotropy	—	<3	2	<5	<3	<1.5

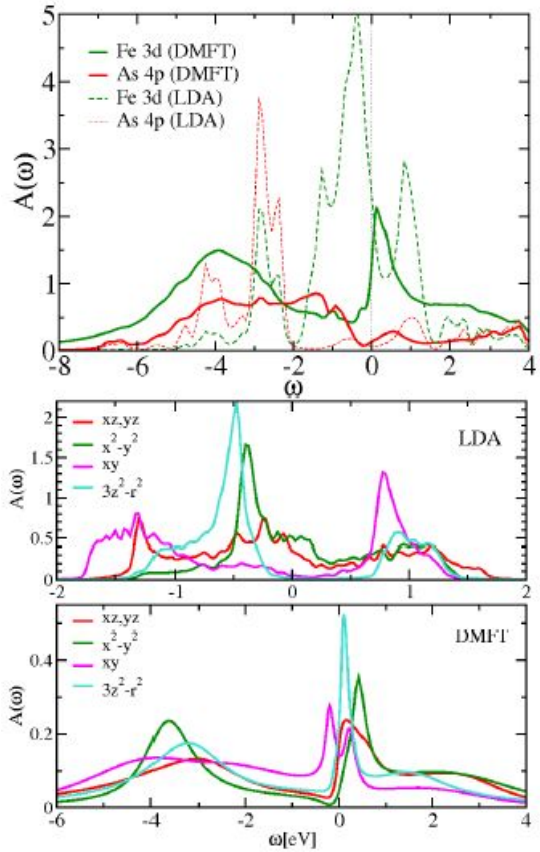
Table I: Momentum dependence of the superconducting gap in iron-arsenic superconductors, as revealed by ARPES studies from five independent groups, sorted by the time of appearance on the arXiv.org. Values of the gap and estimates of the gap anisotropy on the inner Γ-barrel are given in millielectron-volts.

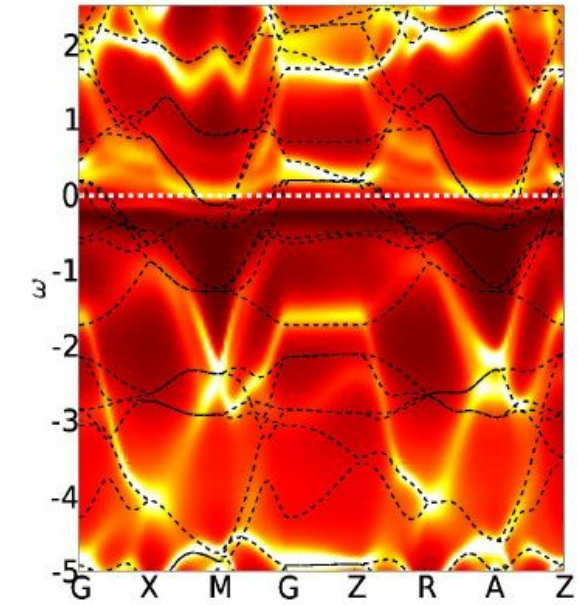
Ref. num.	2	3	4	5	6	7	8	9	This paper
Large gap	9	8.1	8.2	6.8	7.5	3.7	9.6	4	6.8
Small gap	—	3.6	5.5	—	3.9	—	3.4	—	<3

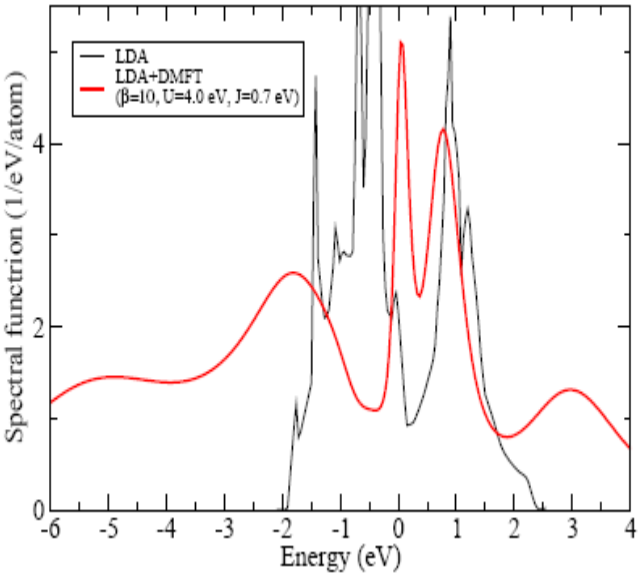
Table II: Coupling strength, $2\Delta/k_BT_c$, in iron-arsenic superconductors, as revealed by different experimental techniques — compare to the BSC universal value 3.53. Most of the available studies reveal two superconducting gaps of different magnitudes, which are represented in the table as "large" and "small". Refs. 2, 3, 4, 5, 6 are ARPES studies, Refs. 7, 8 are Andreev spectroscopy studies, Ref. 9 is a specific heat study.

LDA+DMFT: strong or intermediate correlations?

K.Haule et al. Phys. Rev. Lett. 100, 226402 (2008), arXiv: 0803.1279

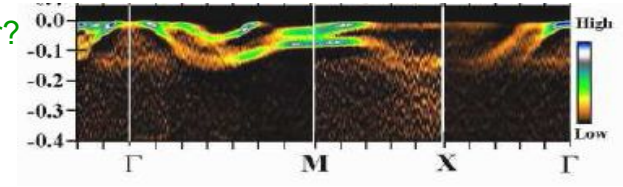






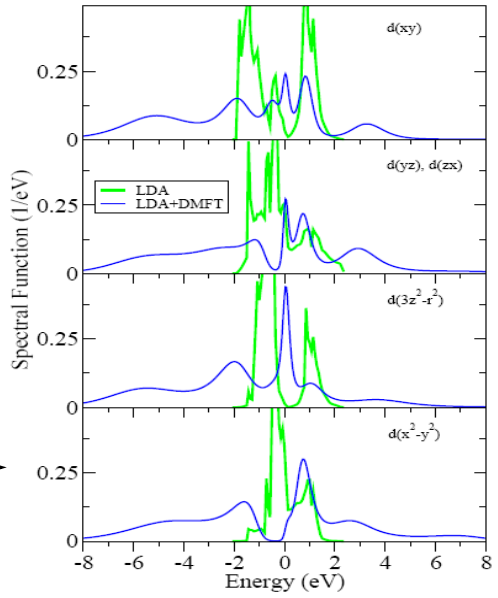
U=4.5eV makes system Mott insulator?

arXiv: 0806.4806



A.O.Shorikov et al. arXiv: 0804.3283

Parameters the same: U=4eV, J=0.7eV,
but results quite different?!



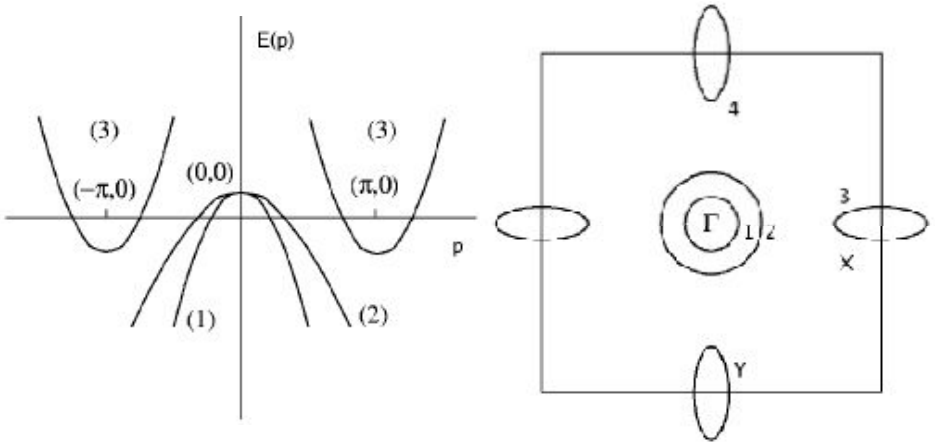
Simple model of multiple – band superconductivity

V. Barzykin, L.P. Gorkov. Pis'ma ZhETF 88, 142 (2008); arXiv: 0806.1993

$$\Delta_i(p) = T\sum_{j;\omega_n}\int V^{i,j}(p-p')dp' F_j(\omega_n,p')$$

Δ_i, ν_i - a superconducting gap and DOS on the i-th sheet of the Fermi surface

$$V = \begin{pmatrix} u & w & t & t \\ w & u' & t & t \\ t & t & \lambda & \mu \\ t & t & \mu & \lambda \end{pmatrix}$$



Schematic electronic spectrum and Fermi surfaces of FeAs superconductor in the extended band picture.

$V^{i,j}$ - intraband and interband pairing coupling constants matrix.

$\lambda = V^{eX,eX} = V^{eY,eY}$ - pairing interactions on the same electronic pockets at point X or Y,

$\mu = V^{eX,eY}$ - connects electrons of different electronic pockets,

$u = V^{h1,h1}$, $u' = V^{h2,h2}$, $w = V^{h1,h2}$ - BCS interactions within two hole-like pockets,

$t = V^{h,eX} = V^{h,eY}$ - couple electrons at points X and Γ.

$$\Delta_i = -\sum_j V^{i,j}\nu_j\Delta_j \ln\frac{2\gamma\omega_c}{\pi T_c}$$

$$T_c = \frac{2\gamma\omega_c}{\pi} e^{-1/g_{eff}}$$

$1/g_{eff}$

! H.Suhl, B.Matthias, L.Walker Phys.Rev.Lett. 3, 552 (1959) V.Moskalenko FMM 4, 503 (1959)

$$g_{eff}\Delta_i = \sum_j g_{ij}\Delta_j$$

E. Z. Kuchinskii[1], *M. V. Sadovskii*[1]

Pis'ma v ZhETF, vol. 89, iss. 3, pp. 176 – 180

arXiv: 0901.0164

$$g_{ij} \equiv -V^{i,j}\nu_j$$

Matrix of dimensionless coupling constants

$$Det(g_{ij} - g_{eff}\delta_{ij}) = 0$$

Secular equation, physical solution corresponds to a maximal positive value of g_{eff}, which determines the highest value of T_c

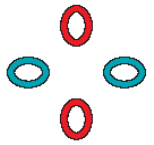
Tecnicalities:

Symmetry

$\nu_3=\nu_4$ ⟶

1) $d_{x^2-y^2}$ pairing $\quad \Delta_1 = \Delta_2 = 0, \quad \Delta_3 = -\Delta_4 = \Delta$

$$g_{eff} = (\mu - \lambda)\nu_3$$



2) $s^{\pm}$ pairing $\quad \Delta_3 = \Delta_4$

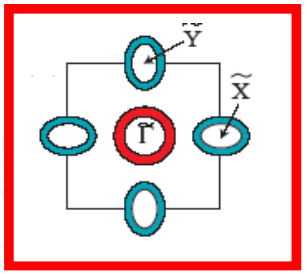
t<0 (repulsive) → $\Delta_3/\Delta_{1,2}>0$

t>0 (attraction) → $\Lambda_3/\Delta_{1,2}<0$

$$g_{eff}\Delta_1 = -u\nu_1\Delta_1 - w\nu_2\Delta_2 - t\nu_3(\Delta_3+\Delta_4)$$
$$g_{eff}\Delta_2 = -w\nu_1\Delta_1 - u'\nu_2\Delta_2 - t\nu_3(\Delta_3+\Delta_4)$$
$$g_{eff}(\Delta_3+\Delta_4)/2 = -t\nu_1\Delta_1 - t\nu_2\Delta_2 - (\lambda+\mu)\nu_3(\Delta_3+\Delta_4)/2$$
$$(g_{eff} - (\mu-\lambda)\nu_3)(\Delta_3 - \Delta_4) = 0$$

$$-\hat{g} = \begin{pmatrix} u\nu_1 & w\nu_2 & 2t\nu_3 \\ w\nu_1 & u'\nu_2 & 2t\nu_3 \\ t\nu_1 & t\nu_2 & 2\bar{\lambda}\nu_3 \end{pmatrix}$$

where $\bar{\lambda} = \frac{\lambda+\mu}{2}$



T<T_c $\quad \Delta_i = \sum_j g_{ij}\Delta_j \int_0^{\omega_c} d\xi \frac{th\frac{\sqrt{\xi^2+\Delta_j^2}}{2T}}{\sqrt{\xi^2+\Delta_j^2}}$

T→0 $\quad \Delta_i = \sum_j g_{ij}\Delta_j F\left(\frac{\Delta_j}{\omega_c}\right) \qquad F(x) = ln\left(\frac{1+\sqrt{1+x^2}}{|x|}\right)$

Tecnicalities:

- V. Barzykin, L.P. Gorkov. Pis'ma ZhETF 88, 142 (2008); arXiv: 0806.1993

$V(p\text{-}p') \to V(0) \longrightarrow u = u' = w\ (= \lambda\ ?)$

$$\Delta_1 = \Delta_2 = \kappa\Delta, \quad \Delta_3 = \Delta_4 = \Delta \qquad \kappa^{-1} = -(g_{eff} + u(\nu_1 + \nu_2))/(t\nu_3)$$

$$2g_{\text{eff}} = -u(\nu_1 + \nu_2) - 2\bar{\lambda}\nu_3 + \sqrt{(u(\nu_1 + \nu_2) - 2\bar{\lambda}\nu_3)^2 + 8t^2\nu_3(\nu_1 + \nu_2)}$$

- O.V.Dolgov, I.I.Mazin, D.Parker, A.A.Golubov, arXiv: 0810.1476
  two-band model, interband coupling only

$$-g_{ij} = \begin{pmatrix} 0 & w\nu_2 \\ w\nu_1 & 0 \end{pmatrix} \qquad \frac{\Delta_2}{\Delta_1} = \sqrt{\frac{\nu_1}{\nu_2}}$$

$BaFe_2As_2$ $\quad \nu_2/\nu_1 \approx 1.26 \longrightarrow \Delta_1/\Delta_2 \approx 1.12 < 2$!

Model parameters

$g=g_{11}=-u\nu_1=0.2$

$\frac{\nu_2}{\nu_1} \approx 1.18, \quad \frac{\nu_3}{\nu_1} \approx 0.64$ for ReOFeAs(1111)

$\frac{\nu_2}{\nu_1} \approx 1.26, \quad \frac{\nu_3}{\nu_1} \approx 0.34$ for $BaFe_2As_2$(122)

Pairing interactions on hole – like cylinders and between them, as well as on electron – like cylinders and between them, are most probably determined by electron - phonon interaction (u, u', w, λ, μ < 0 - attraction),
interband pairing interaction between hole - like and electron - like cylinders is probably due to antiferromagnetic fluctuations and is repulsive (t > 0).

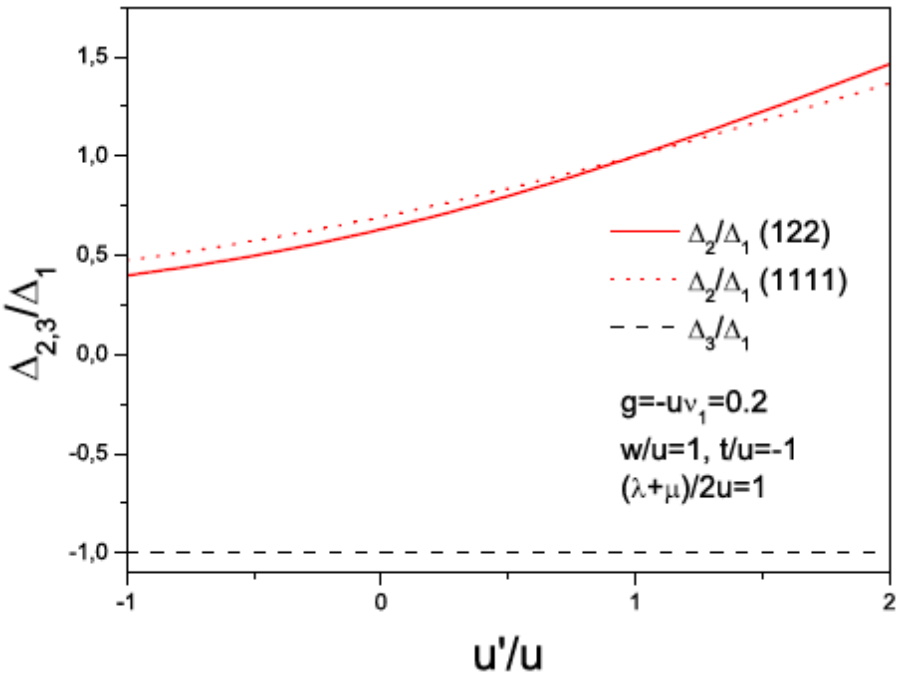
Parameter t from coupling constants matrix enters in secular equation, determining g_{eff}, only via t^2, i.e. independent of sign. Thus its sign does not change the value of an effective pairing coupling constant and that of T_c. Repulsion between quasiparticles on hole - like and electron - like cylinders does not suppress, but actually enhances superconductivity leading to the increase of g_{eff}. Also the sign change of t does not change the absolute values of gaps on different cylinders.

$w/u = 1, \; t/u = -1, \; \lambda/u = 1,$

which guarantees us the ratio $|\Delta_3/\Delta_1|= 1$ for any values of u' and arbitrary ratios of partial densities of states at different cylinders.

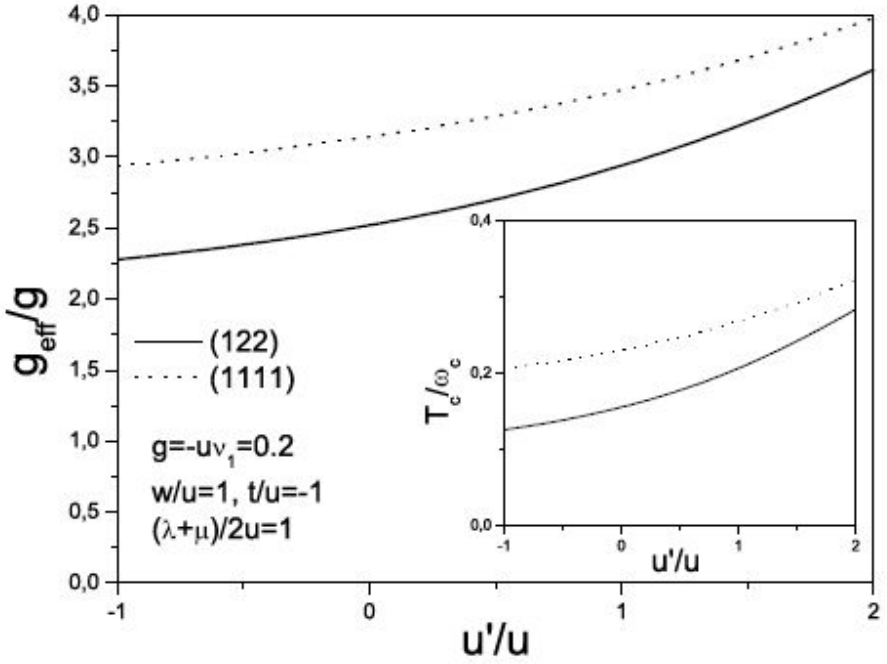
Gap ratios for for different u'/u:

$T \to 0$



Despite rather large number of free parameters of the model it is not easy to obtain the observable in ARPES experiments values of the ratios $|\Delta_2/\Delta_1| \approx 0.5$ and $|\Delta_3/\Delta_1| \approx 1$. In fact it requires small enough attraction (or even repulsion, $u' > 0$) on the "large" hole - like cylinder.

Effective coupling – from weak to strong?



1. No interband pairing

$$\hat{g} = \begin{pmatrix} g_1 & 0 & 0 & 0 \\ 0 & g_2 & 0 & 0 \\ 0 & 0 & g_3 & 0 \\ 0 & 0 & 0 & g_4 \end{pmatrix} \longrightarrow g_{eff} = max(g_i)$$

! **Effective coupling constant g_{eff} is significantly larger than the pairing constant g on the small hole - like cylinder**. It can be said that coupling constants from different cylinders effectively produce "additive" effect. In fact this can lead to high enough values of T_c even for relatively small values of intraband and interband pairing constants.

- g_{eff}, T_c ($d_{x^2-y^2}$ pairing) < g_{eff}, T_c ($s^{\pm}$ pairing)
- $T_c(122)/T_c(1111) = 0.67 \leftrightarrow 38\text{K}/55\text{K} \approx 0.69$ for u'/u=0 (!)

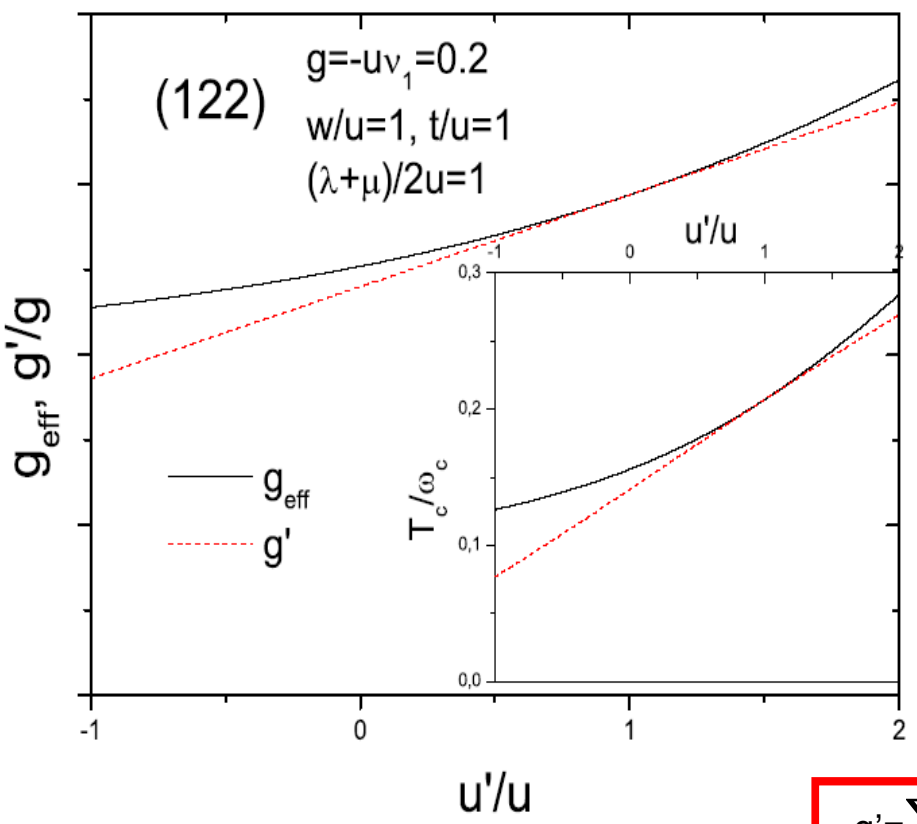
Value of T_c in multiple bands systems is determined by the **relations between partial densities of states** (and pairing constants) on different sheets of the Fermi surface, **not only by the total density of states** at the Fermi level.

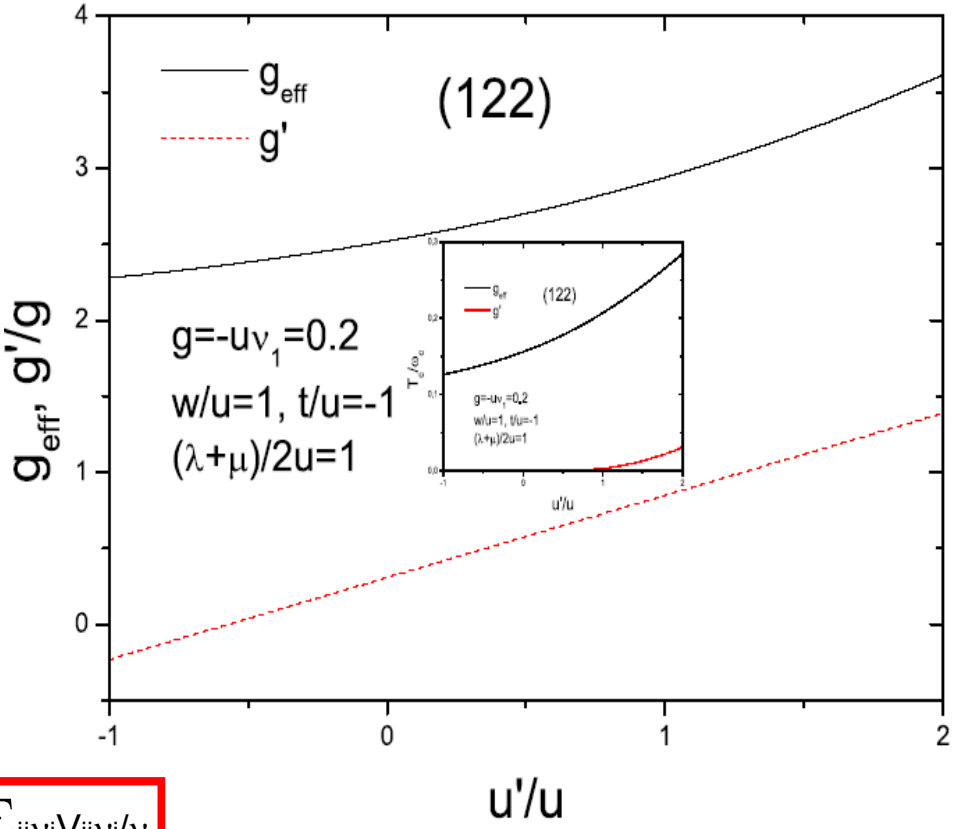
2. All pairing interactions (both intraband and interband) are just the same - u, and all partial densities of states on all four Fermi surface pockets are also the same - ν_1.

$$\hat{g} = -u\nu_1 \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \longrightarrow g_{eff} = 4g = -4u\nu_1$$

Is there a nontrivial "optimal" band structure (number of bands etc.)?

Relation to “Eliashberg” coupling constant





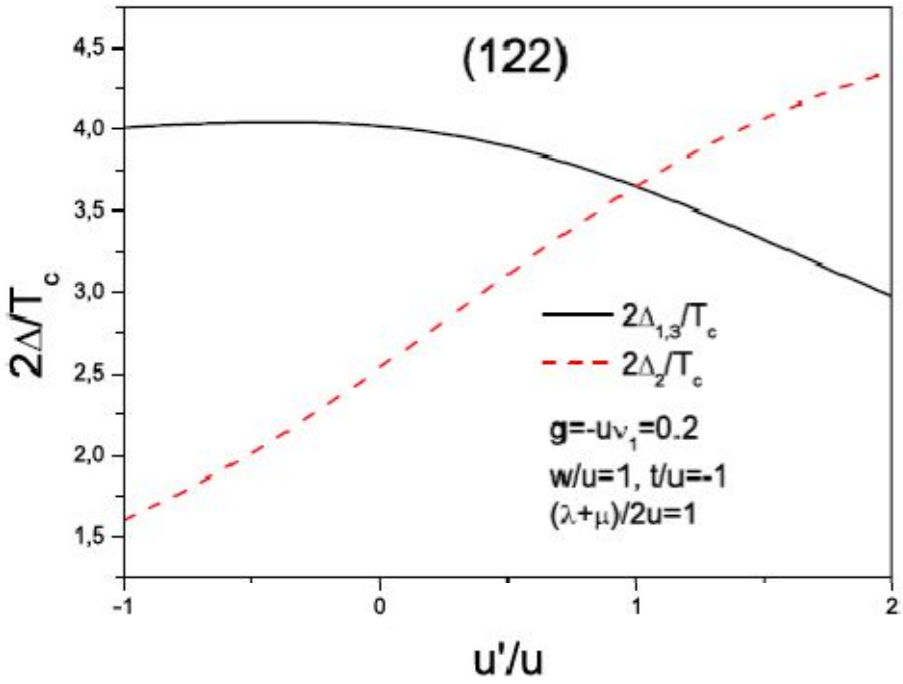
$-g' = \sum_{ij} \nu_i V_{ij} \nu_j / \nu$

Determines specific heat renormalization!

In general $g' < g_{eff}$!

Difference between g’ (“Eliashberg”) and g_{eff} in case of interband repulsion is rather dramatic!

Gap/Tc ratios:



Characteristic ratio $2\Delta/T_c$ can be significantly different from the standard BCS value $2\Delta/T_c = 3.5$. However, the findings values are much lower than the ratios observed in ARPES experiments, where the typical values are $2\Delta_{1,3}/T_c \approx 7.5$ and $2\Delta_2/T_c \approx 3.7$, which is apparently due to the strong coupling effects important in real systems.

Multiple Gaps and Superfluid Density from Interband Pairing in Iron Oxypnictides

L. Benfatto[1,2], M. Capone[2,3], S. Caprara[2], C. Castellani[2], and C. Di Castro[2]

arXiv: 0807.4408

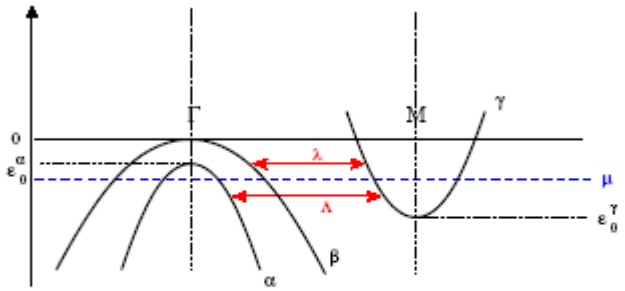


FIG. 1: (Color Online) Schematic of the multiband model used in this work. The two hole bands α, β are centered around the Γ point, the electron bands around the M point.

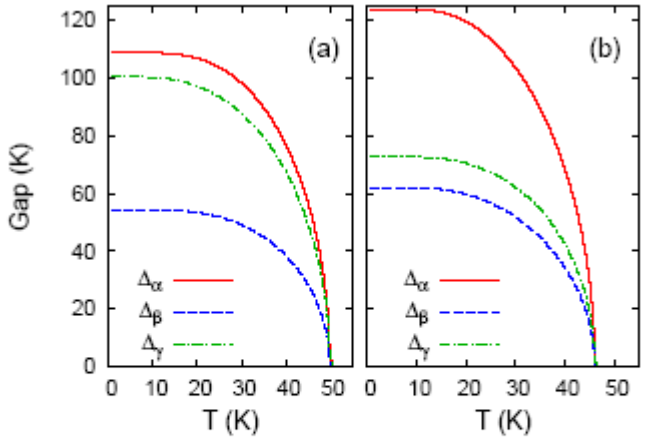
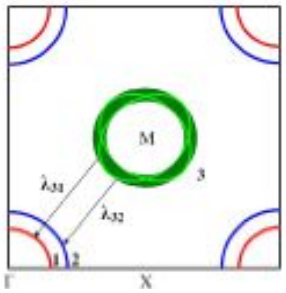


FIG. 2: (Color Online) (a): Temperature dependence of the SC gaps in the hole and electron bands. The parameter values are optimized to obtain the same gap value in the α and γ bands (values in eV). Moreover, we used $\lambda = \Lambda/2$ to have $\Delta_\beta = \Delta_\alpha/2$. (b): SC gaps for the hopping parameters estimated from ARPES measurements of Ref.[7] at half-filling.

Three-band s± Eliashberg theory and the superconducting gaps of iron pnictides

G.A. Ummarino,* M. Tortello, D. Daghero, and R.S. Gonnelli

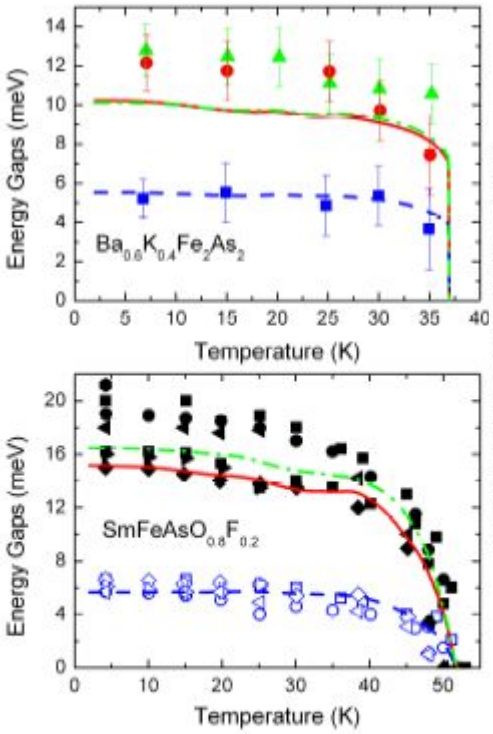
arXiv: 0904.1808



Under these approximations, the electron-boson coupling-constant matrix is then [8]:

$$\begin{pmatrix} 0 & 0 & \lambda_{31}\nu_1 \\ 0 & 0 & \lambda_{32}\nu_2 \\ \lambda_{31} & \lambda_{32} & 0 \end{pmatrix}$$

where $\nu_1 = N_1(0)/N_3(0)$, $\nu_2 = N_2(0)/N_3(0)$ and $N_i(0)$ is the normal density of states at the Fermi level for the i-band ($i = 1, 2, 3$ according to Fig.1).



Another important result of the model is the temperature dependence of the gaps. Figure 3 shows this dependence for the experimental gaps (symbols) together with the theoretical $\Delta_i(T)$ curves obtained by the three-band Eliashberg model (lines) for $Ba_{0.6}K_{0.4}Fe_2As_2$ (upper panel) and $SmFeAsO_{0.8}F_{0.2}$ (lower panel). The parameters used for the 122 compound are $\Omega_0 = 10$ meV, $\lambda_{31} = 4.267$ and $\lambda_{32} = 0.569$; for the 1111 compound we used $\Omega_0 = 10$ mev, $\lambda_{31} = 14.520$ and $\lambda_{32} = 1.708$. The experimental temperature dependence of the gaps shown in the upper panel is rather unusual with the gaps slightly decreasing with increasing temperature until they suddenly drop close to T_c. The theory reproduces very well this behavior, which is possible only in a very strong coupling regime [16]. The different temperature dependence observed in the lower panel of Fig. 3 results from a complex non-linear dependence of Δ_i vs. T curves on λ_{31}.

Very strong (!) coupling

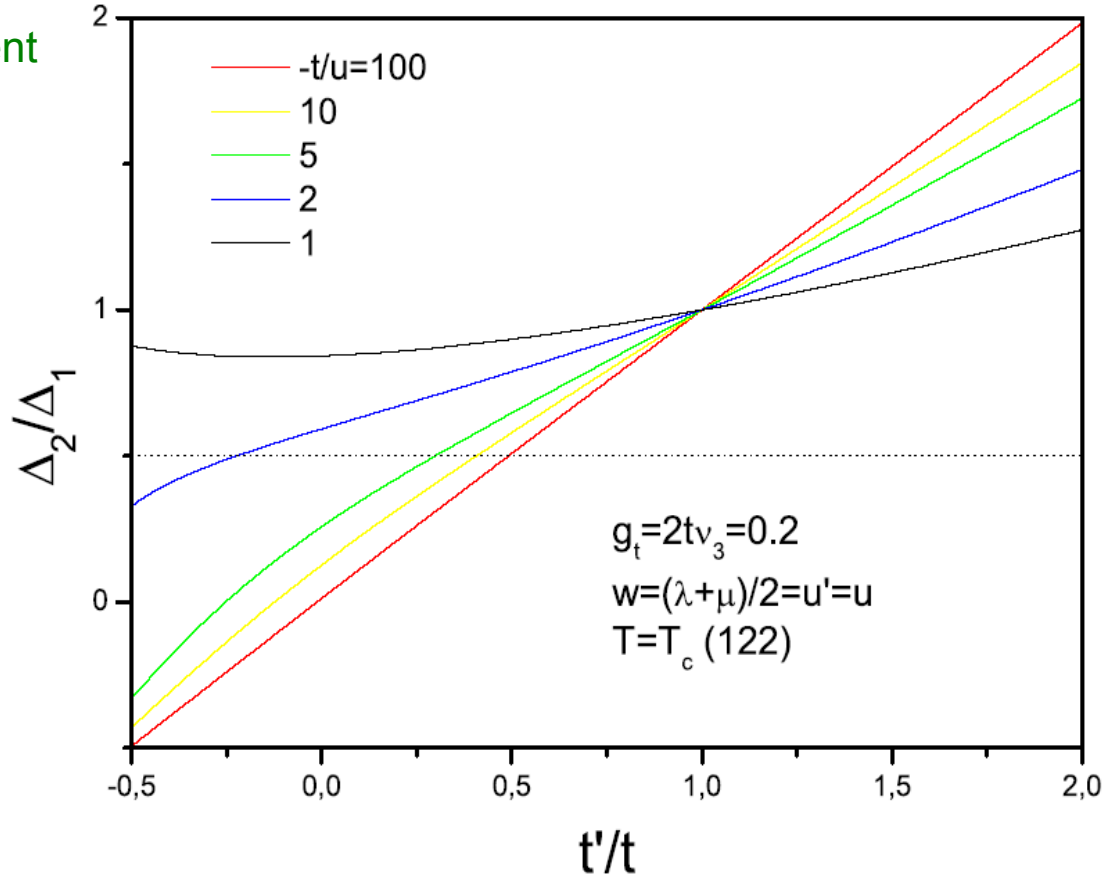
and $\lambda_{31} >> \lambda_{32}$?

FIG. 3: Calculated temperature dependence of the gaps for $Ba_{0.6}K_{0.4}Fe_2As_2$ ($T_c = 37$ K, upper panel) and for $SmFeAsO_{0.8}F_{0.2}$ ($T_c = 52$ K, lower panel): $\Delta_1(T)$ (red solid line), $\Delta_2(T)$ (blue dashed line) and $\Delta_3(T)$ (green dash-dot line). Symbols are experimental data from ref. [12] (upper panel) and ref. [13] (lower panel).

Gap ratios for different t'/t:

More general case, different interband couplings:

$$V = \begin{pmatrix} u & w & t & t \\ w & u' & t' & t' \\ t & t' & \lambda & \mu \\ t & t' & \mu & \lambda \end{pmatrix}$$



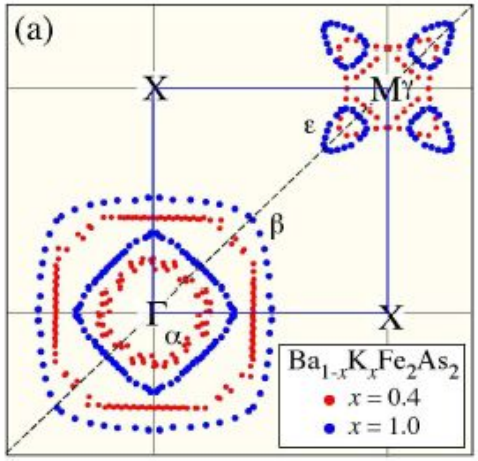
Again it is not easy to obtain the observable in ARPES experiments values of the ratios $|\Delta_2/\Delta_1| \approx 0.5$ and $|\Delta_3/\Delta_1| \approx 1$ for reasonable relations, between interband couplings – intraband processes actually complicate this task!.

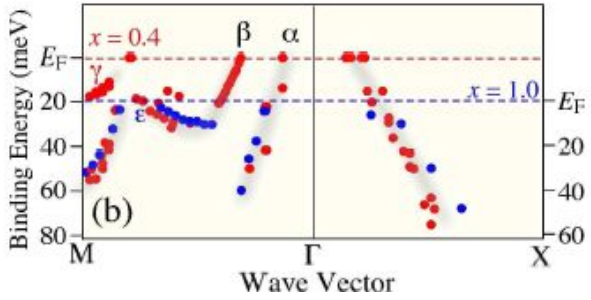
Band Structure and Fermi Surface of an Extremely Overdoped Iron-Based Superconductor KFe_2As_2

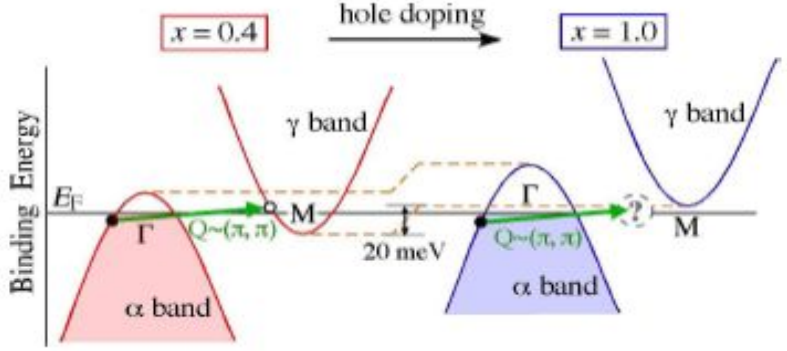
T. Sato,[1,2] K. Nakayama,[1] Y. Sekiba,[1] P. Richard,[3] Y.-M. Xu,[4] S. Souma,[3] T. Takahashi,[1,3] G. F. Chen,[5] J. L. Luo,[5] N. L. Wang,[5] and H. Ding[5]

arXiv:0810.3047

$T_c = 3$ K





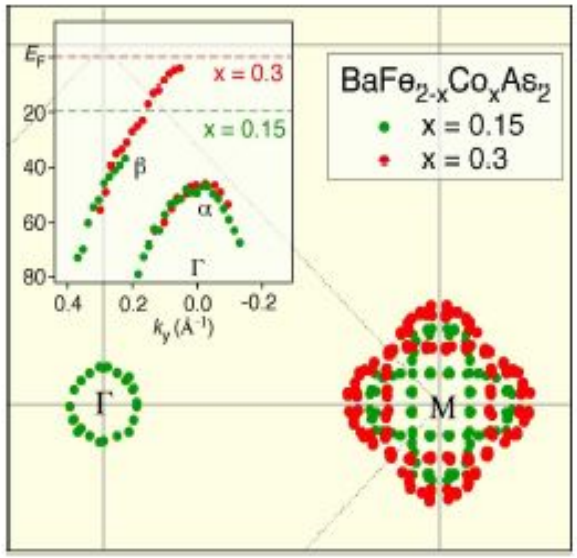


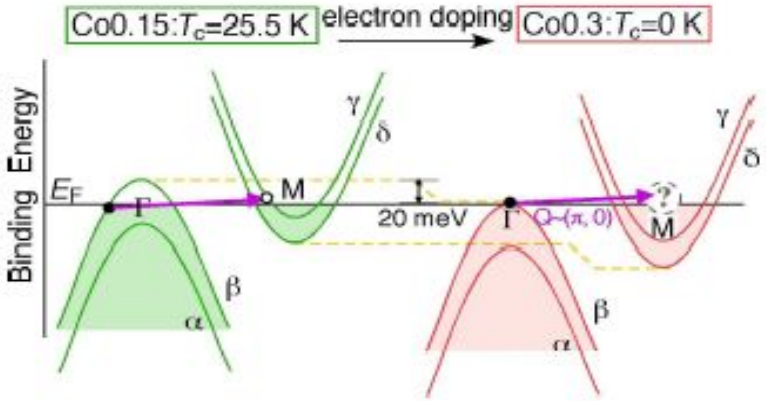
Electronic structure of heavily electron-doped $BaFe_{1.7}Co_{0.3}As_2$ studied by angle-resolved photoemission

Y. Sekiba[1], T. Sato[1,2], K. Nakayama[1], K. Terashima[3], P. Richard[4], J. H. Bowen[5], H. Ding[5], Y.-M. Xu[6], L. J. Li[7], G. H. Cao[7], Z.-A. Xu[7], and T. Takahashi[1,4]

arXiv:0810.3047

$T_c = 0$ K





Conclusions and problems that remain to be solved

- Gap ratios in FeAs superconductors can be reasonably explained, but are coupling constants realistic?
- Effective pairing coupling increases due to multiple bands. A reason for high Tc in FeAs layers?
- Total DOS at the Fermi level is not crucial for Tc?
- Average (“Eliashberg”) coupling constant is irrelevant for Tc calculations in case of interband repulsion.
- Phonons are insufficient to obtain high Tc, interband repulsive interactions are important?
- Multiple bands – a direct way to increase Tc but is there an “optimal” band structure?