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1957-18

Miniworkshop on Strong Correlations in Materials and Atom Traps

4 - 15 August 2008

Theory and experimental overview of the Iron Based Pnictides

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Iron based high temperature superconductors

K Haule, Rutgers University

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Technologically relevant

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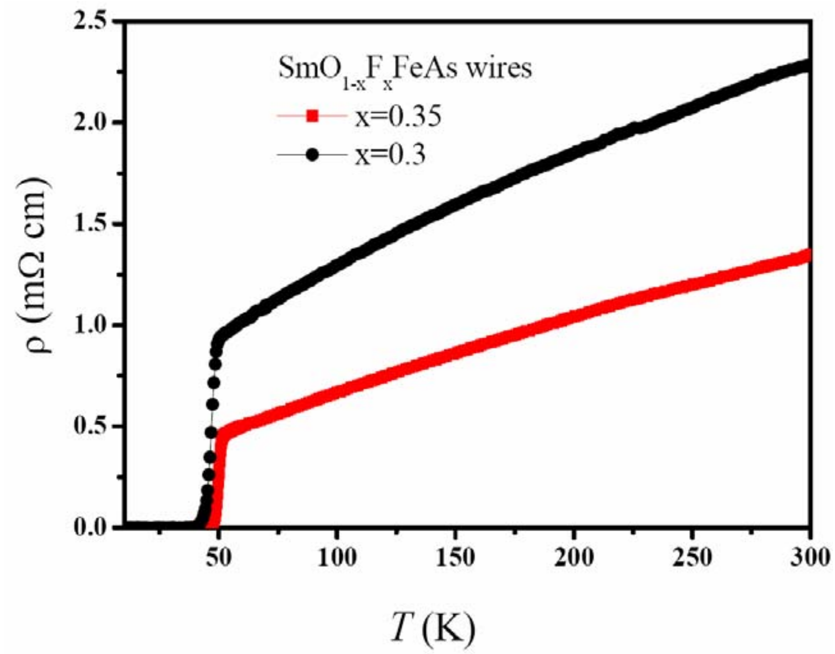
Wires fabricated by the powder-in-tube (PIT) method:



Zhaoshun Gao, et.al., arXiv 0806.2451

Jc up to 2×105 A/cm^2

(Hc_2) up to 120 T

More three-dimensional than cuprates

How it all started….

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J|A|C|S COMMUNICATIONS

Published on Web 02/23/2008

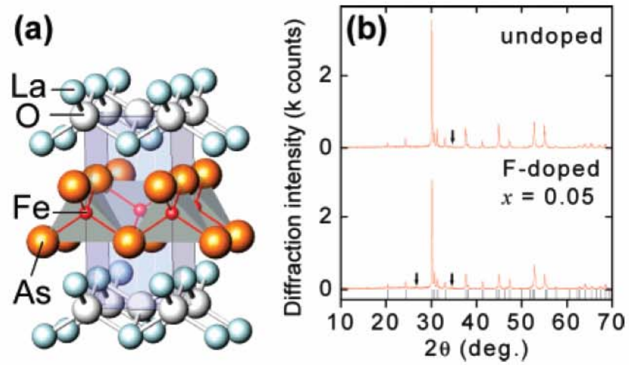
Iron-Based Layered Superconductor $La[O_{1-x}F_x]FeAs$ ($x = 0.05-0.12$) with $T_c = 26$ K

Yoichi Kamihara,*,† Takumi Watanabe,‡ Masahiro Hirano,†,§ and Hideo Hosono†,‡,§

ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan

Received January 9, 2008; E-mail: hosono@msl.titech.ac.jp

Discovery of the copper-based superconductor $La_{2-x}Ba_xCuO_4$[1] with a high transition temperature (T_c) triggered extensive research with the intention of developing new transition-metal-based superconductors.[2,3] Currently, high T_c superconductors are limited to layered perovskites that contain CuO_2 structural units as the conduction layers. However, the T_c of the non-Cu-based superconductors in this category has remained low, although spin triplet superconductivity has been found in UPt_3 ($T_c \sim 0.54$ K)[4] and Sr_2RuO_4 ($T_c \sim 1.4$ K).[5,6] Here, we report a layered iron-based compound, LaOFeAs, which undergoes superconducting transition under doping with F^- ions at the O^{2-} site. Its T_c exhibits a



Published in Chemical journal (Journal of American Chemical Society)
Received January 2008, published online Feb 2008

And exploded....

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Department of Physics and Astronomy

more than 23 cond-mat's in March 2008

arXiv:0803.0128v2

Superconducting properties of Fe-based layered superconductor $LaO_{0.9}F_{0.1-}$ FeAs

G. F. Chen,[1] Z. Li,[1] G. Li,[1] J. Zhou,[1] D. Wu,[1] J. Dong,[1] W. Z. Hu,[1] P. Zheng,[1] Z. J. Chen,[1] H. Q. Yuan,[2,3] J. Singleton,[2] J. L. Luo,[1] and N. L. Wang[1]

[1]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
[2]National High Magnetic Field Laboratory, MS-E536, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA
[3]Department of Physics, Zhejiang University, Hangzhou 310027, China

We have employed a new route to synthesize single phase F-doped LaOFeAs compound and confirmed the superconductivity above 20 K in this Fe-based system. We show that t[...] conductor has a rather high upper critical field of over 50 T. A clear signature of su[...] gap opening below T_c was observed in the far-infrared reflectance spectra, with 2 [...] Furthermore, we show that the new superconductor has electron-type conducting c[...] rather low carrier density.

arXiv:0803.0928v2

Nodal Gap in Fe-Based Layered Superconductor $LaO_{0.9}F_{0.1-\delta}$FeAs Probed by Specific Heat Measurements

Gang Mu, Xiyu Zhu, Lei Fang, Lei Shan, Cong Ren and Hai-Hu Wen*

National Laboratory for Superconductivity, Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, People's Republic of China

We report the specific heat measurements on the newly discovered Fe-based layered superconductor $LaO_{0.9}F_{0.1-\delta}$FeAs with the onset transition temperature $T_c \approx 28$ K. A nonlinear magnetic field dependence of the electronic specific heat coefficient $\gamma(H)$ has been found in the low temperature limit, which is consistent [...]tion for a nodal superconductor. The maximum gap value $\Delta_0 \approx 3.4\pm0.5$ meV was derived by [...] based on the d-wave model. We also detected the electronic specific heat difference between 9 [...]de temperature region, a specific heat anomaly can be clearly observed near T_c. The Debye tem- [...] sample was determined to be about 315.7 K. Our results suggest an unconventional mechanism [...]perconductor.

[...]74.20.Rp, 74.25.Bt, 65.40.Ba, 74.70.Dd

arXiv:0803.0429v2

$LaFeAsO_{1-x}F_x$: A low carrier density superconductor near itinerant magnetism

D.J. Singh and M.-H. Du

Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114

(Dated: July 9, 2008)

Density functional studies of 26K superconducting LaFeAs(O,F) are reported. We find a low carrier density, high density of states, $N(E_F)$ and modest phon[...] frequencies relative to T_c. The high $N(E_F)$ leads to proximity to itinerant magnetism, with com[...] magnetic fluctuations and the balance between these controlled b[...] is in a unique class of high T_c superconductors: high $N(E_F)$ ioni[...]

arXiv:0803.1279v1

Correlated electronic structure of $LaO_{1-x}F_x$FeAs

K. Haule, J. H. Shim, and G. Kotliar

Department of Physics, Rutgers University, Piscataway, NJ 08854, USA

(Dated: July 11, 2008)

We compute the electronic structure, momentum resolved spectral function and optical conductivity of the new superconductor $LaO_{1-x}F_x$FeAs within the combination of the Density functional theory and the Dynamical Mean Field Theory. We find that the compound in the normal state is a strongly correlated metal and the parent compound is a bad metal at the verge of the metal insulator transition. We argue that the superconductivity is not phonon mediated.

>260 preprints at the end of July

mostly from China!

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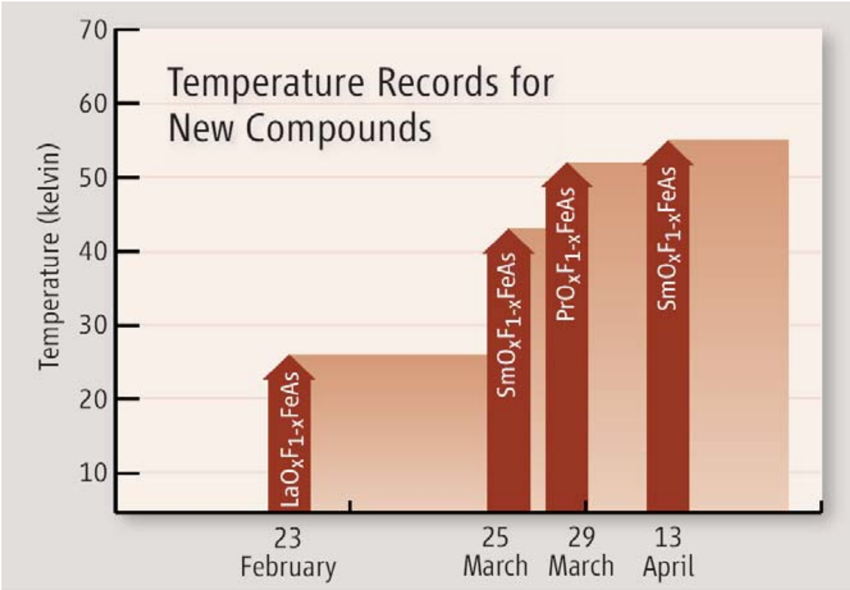
First family of SC



Smaller c ↑

$SmF_xO_{1-x}FeAs$ $x\sim0.2$ d)	Tc=55K, cm/0803.3603 a=3.933A, c=8.4287A
$PrF_xO_{1-x}FeAs$ c)	Tc=52K, cm/0803.4283 a=3.985A, c=8.595A
$CeF_xO_{1-x}FeAs$ b)	Tc=41 K, cm/0803.3790 a=3.996A, c=8.648A
$LaF_xO_{1-x}FeAs$ a)	Tc=26 K, JACS-2008 a=4.036A, c=8.739 A
$La_{1-x}Sr_xOFeAs$	Tc=25K, cm/0803.3021, a=4.035A, c = 8.771A

a) Y. Kamihara et.al., Tokyo, JACS
b) X.H. Chen, et.al., Beijing,arXiv: 0803.3790
c) Zhi-An Ren, Beijing, arXiv: 0803.4283
d) Zhi-An Ren, Beijing, arXiv: 0804.2053.

Rare earth's:

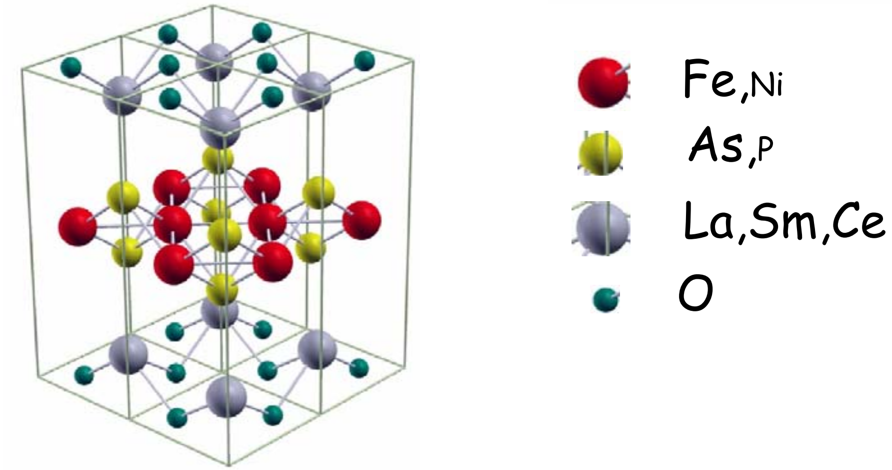
57 La 138.90	58 Ce 140.11	59 Pr 140.90	60 Nd 144.24	61 Pm (145)	62 Sm 150.36	63 Eu 151.96

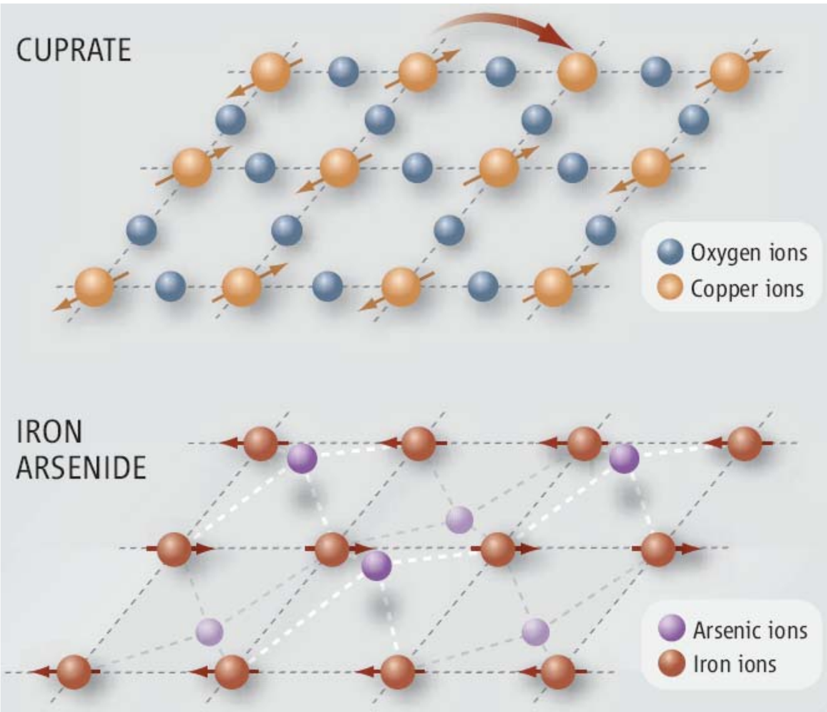
Crystal Structure: Tetragonal I4/mmm

R $O_{1-x}F_x$ FeAs
R O_{1-x} FeAs

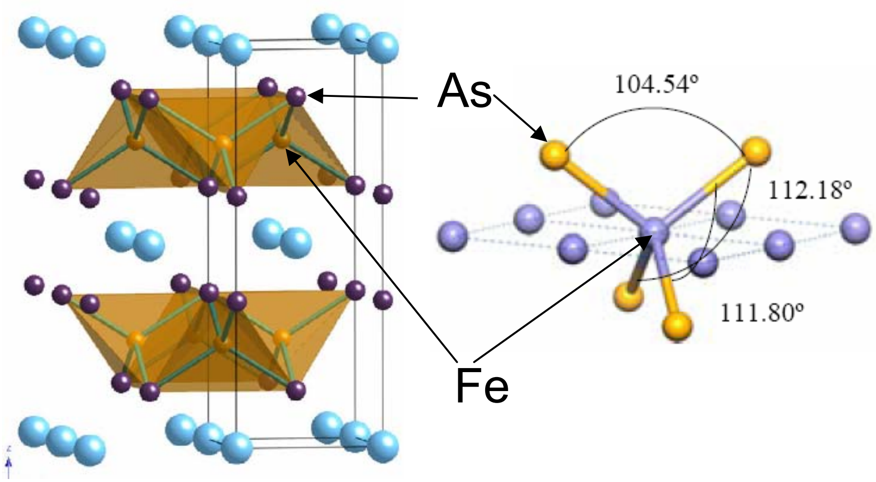
F not important, vacancy fine

- 2D square lattice of Fe
- Fe - magnetic moment
- As-similar then O in cuprates





But As not in plane!



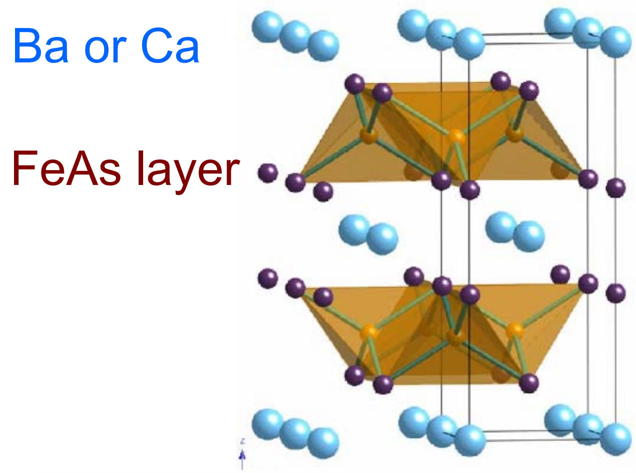
Perfect tetrahedra 109.47°

Variety of materials

R $O_{1-x}F_x$ FeAs electron doped

$(Ba_{1-x}K_x)Fe_2As_2$ (Tc=38K, x~0.4), hole doped (not electron doped)

Marianne Rotter et.al., arXiv:0805.4630



$CaFe_2As_2$, (Tc=12K @ 5.5GPa),

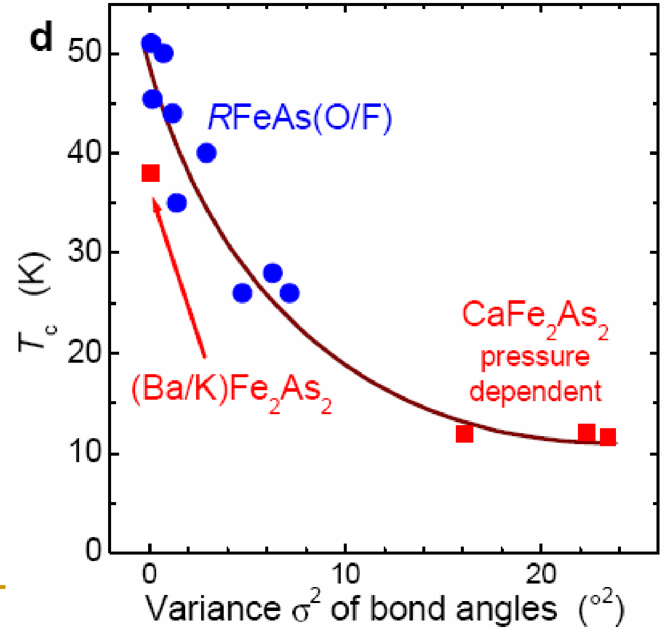
Milton S. Torikachvili, arXiv:0807.0616v2

Li_{1-x}FeAs, (Tc=18K),

X.C.Wang et.al., arXiv:0806.4688

$FeSe_{1-0.08}$, (Tc=27K @ 1.48GPa), **No arsenic ☺!**

Yoshikazu Mizuguchi et.al., arXiv: 0807.4315



A. Kreyssig, arXiv:0807.3032

Bond angle seems to matter most.

Perfect tetrahedra (109.47°) -> higher Tc

What is the glue?

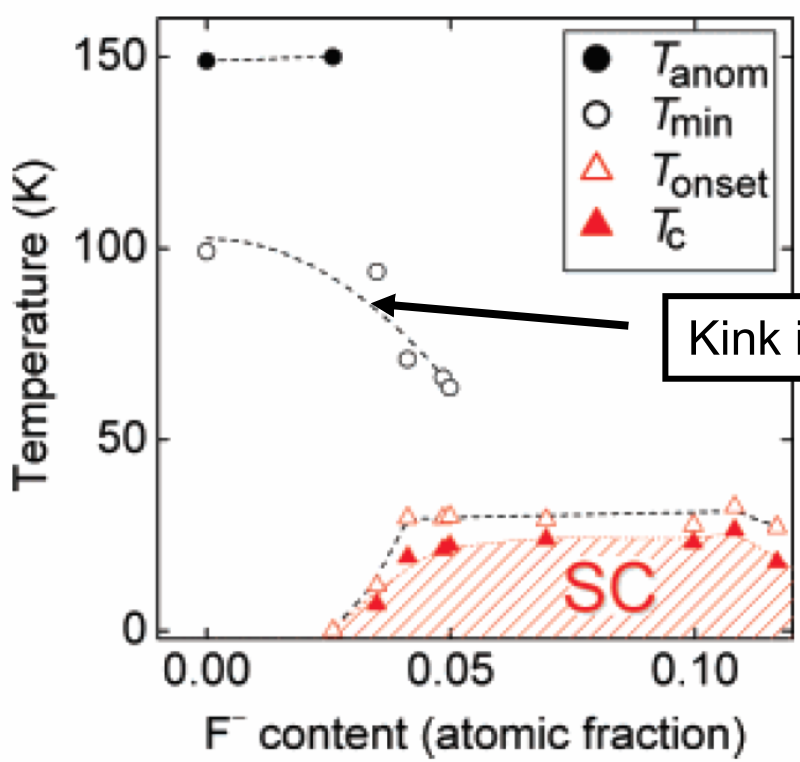
KH, J.H. Shim, G. Kotliar, cond/mat 0803.1279 (PRL. 100, 226402 (2008)):

Phonons give Tc<1K

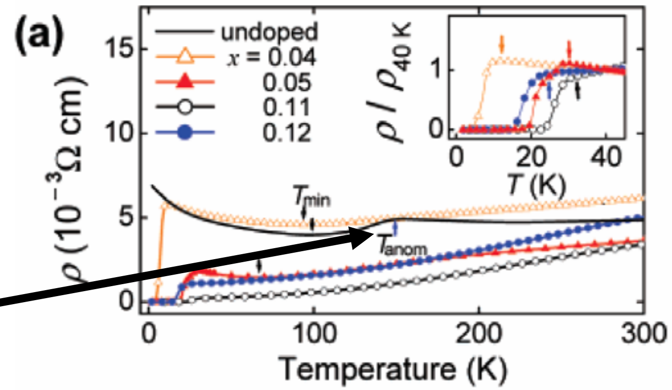
L. Boeri, O. V. Dolgov, A. A. Golubov arXiv:0803.2703 (PRL, 101, 026403 (2008)):

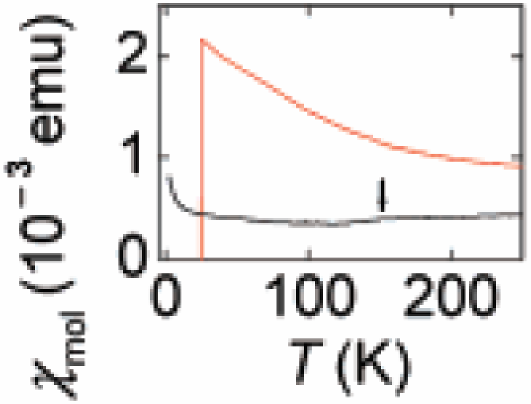
λ<0.21, Tc<0.8K

Not conventional superconductors!



Kink in resistivity





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

Huge spin susceptibility (50 x Pauli)

Phase diagrams SmFeAsO

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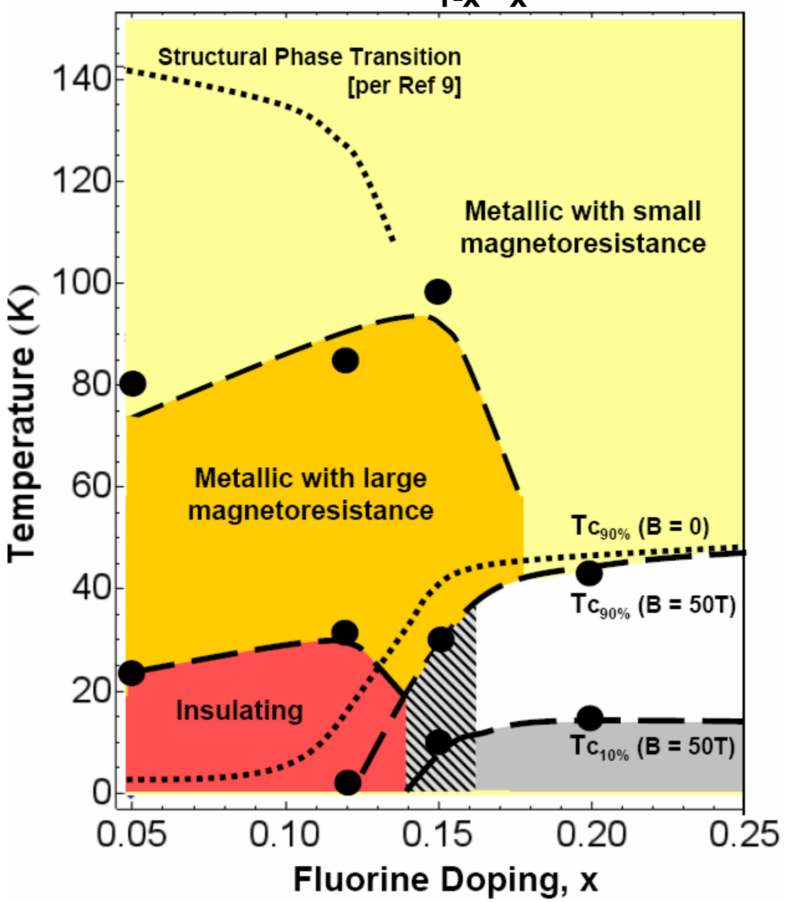
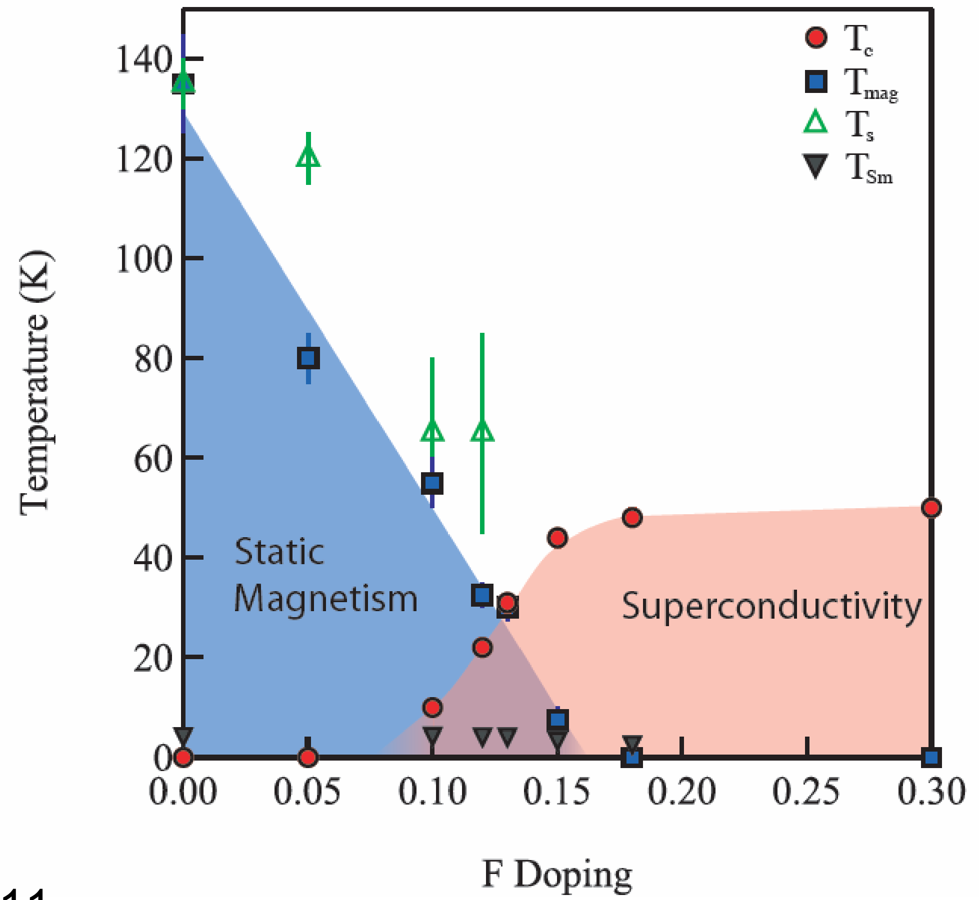
magneto-transport experiments

$SmFeAsO_{1-x}F_x$



S.C. Riggs et.al., arXiv: 0806.4011

muon spin rotation

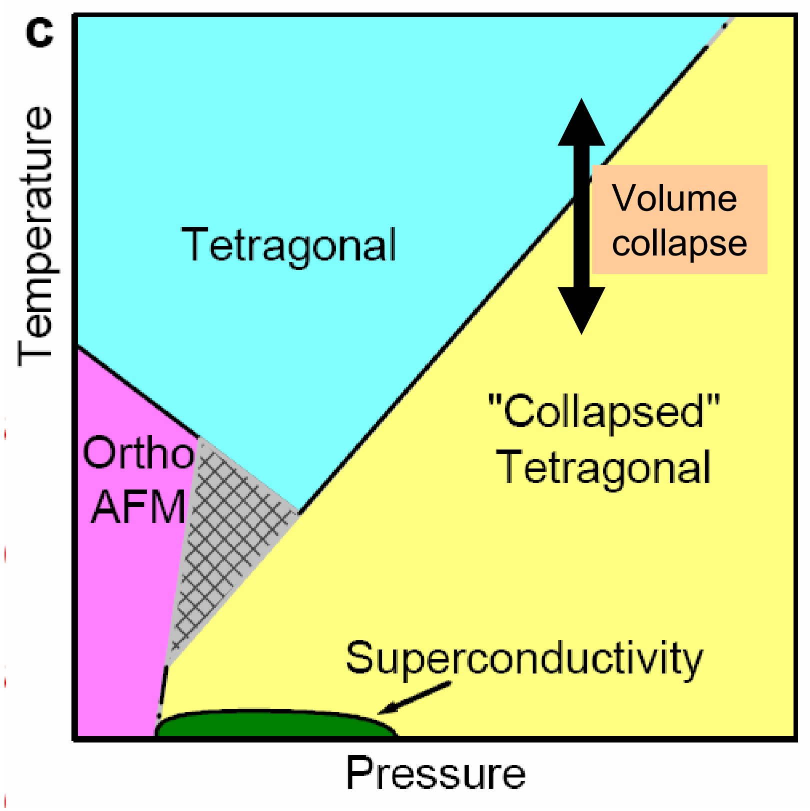


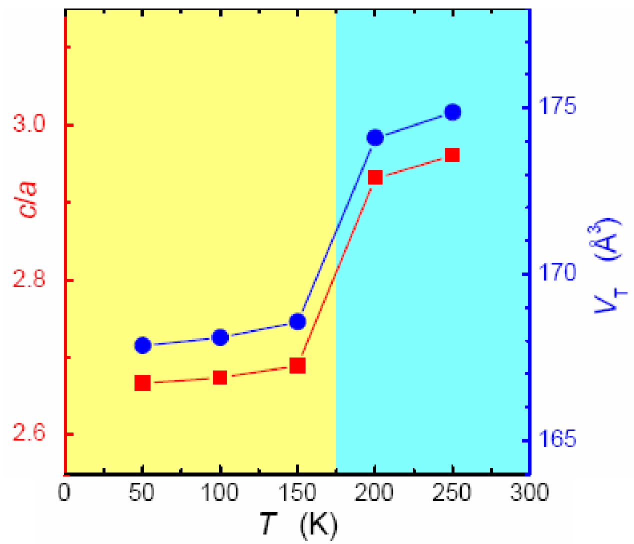
A. J. Drew et.al., arXiv:0807.4876.

- Very similar to cuprates, log(T) insulator due to impurities

Phase diagrams

$CaFe_2As_2$ under pressure Stoichiometric compound





A. Kreyssig et.al, arXiv: 0807.3032

Common features of the parent compound

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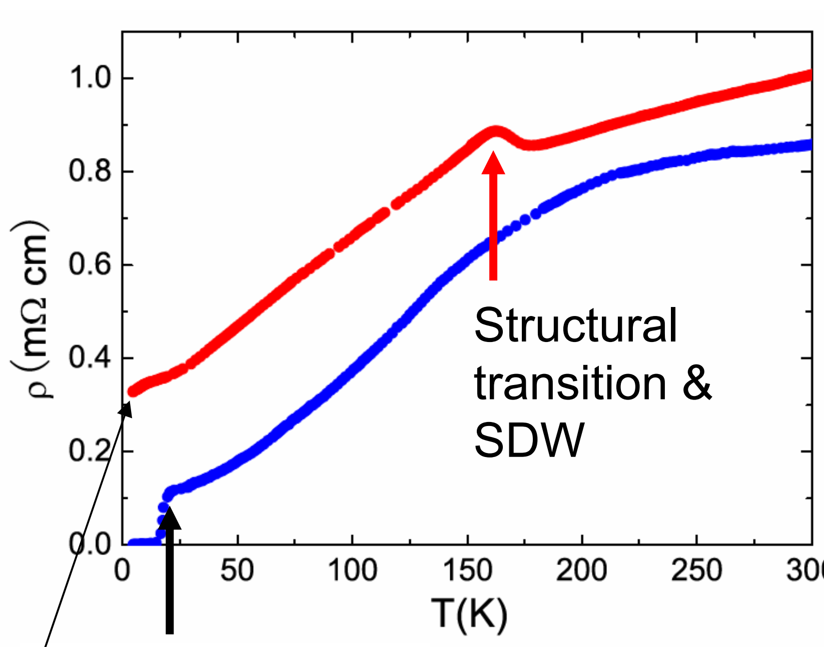
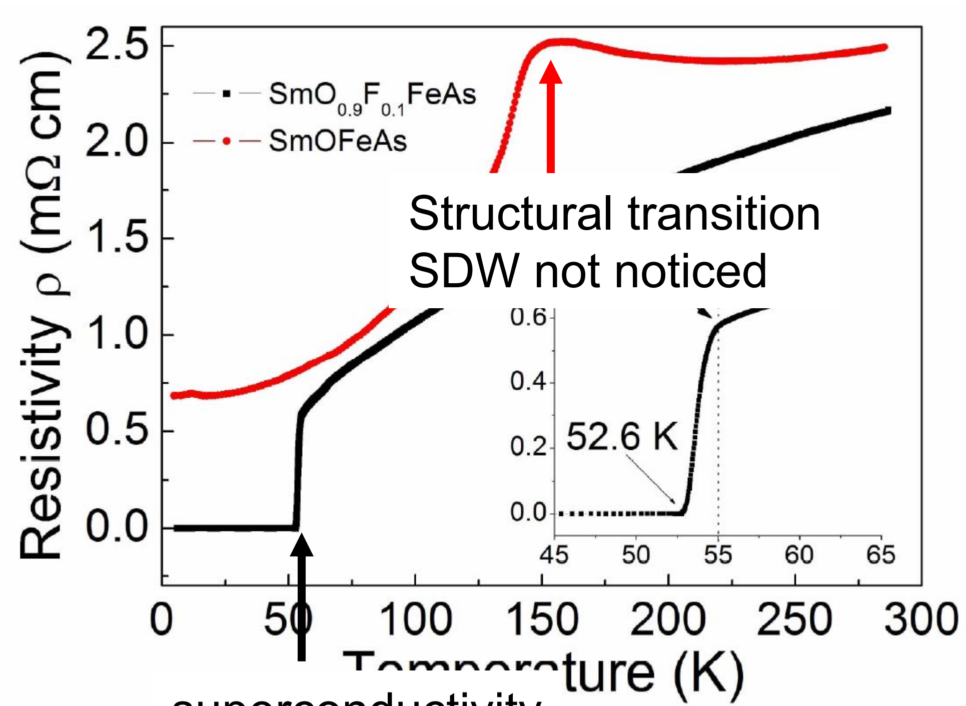
$CaFe_2As_2$ and $Ca_{0.5}Na_{0.5}Fe_2As_2$



superconductivity

Very unusual

SmOFeAs



superconductivity

Enormous normal state resistivities!

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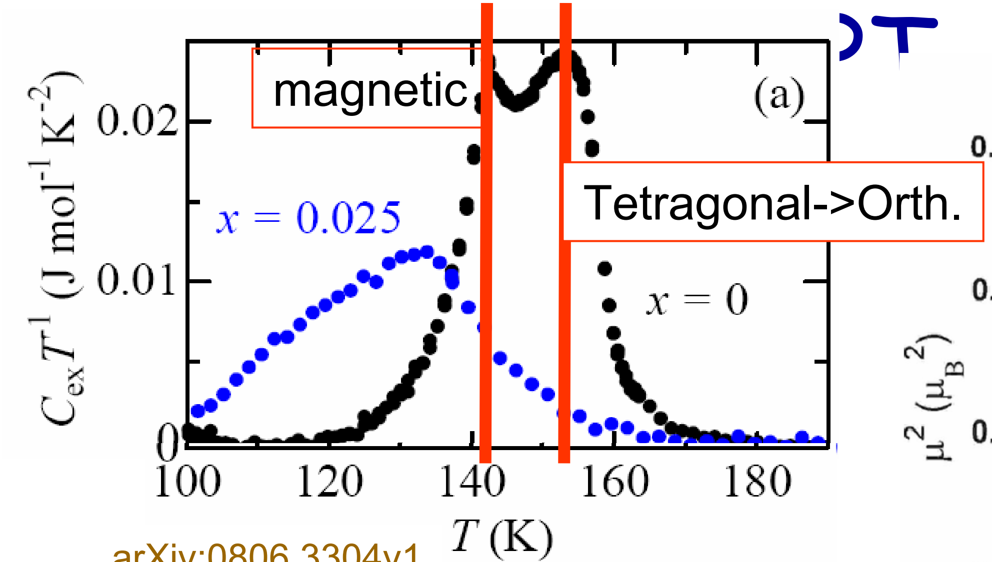
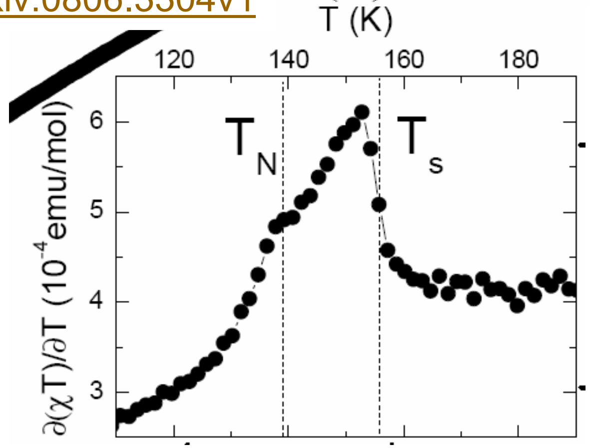
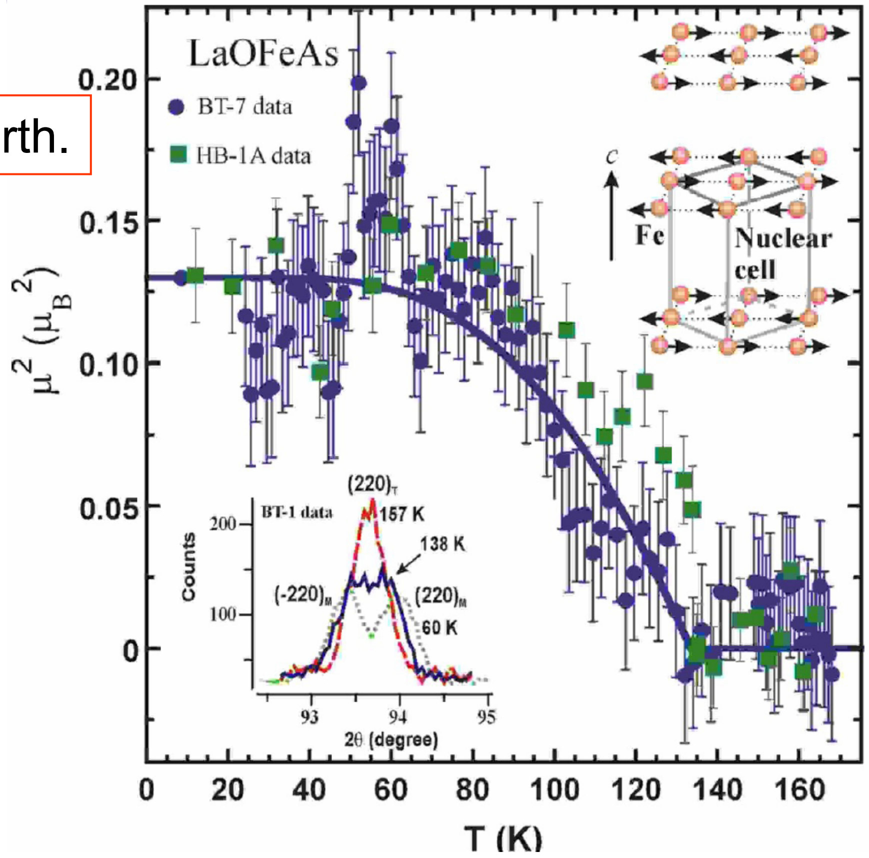
Magnetic and structural



arXiv:0806.3304v1



R. Klingeler et.al., arXiv:0808.0708v1



Clarina de la Cruz, Nature 453, 899 (2008).

In single crystals of 122 seems T_M and T_S close or the same

Fe magnetism ?

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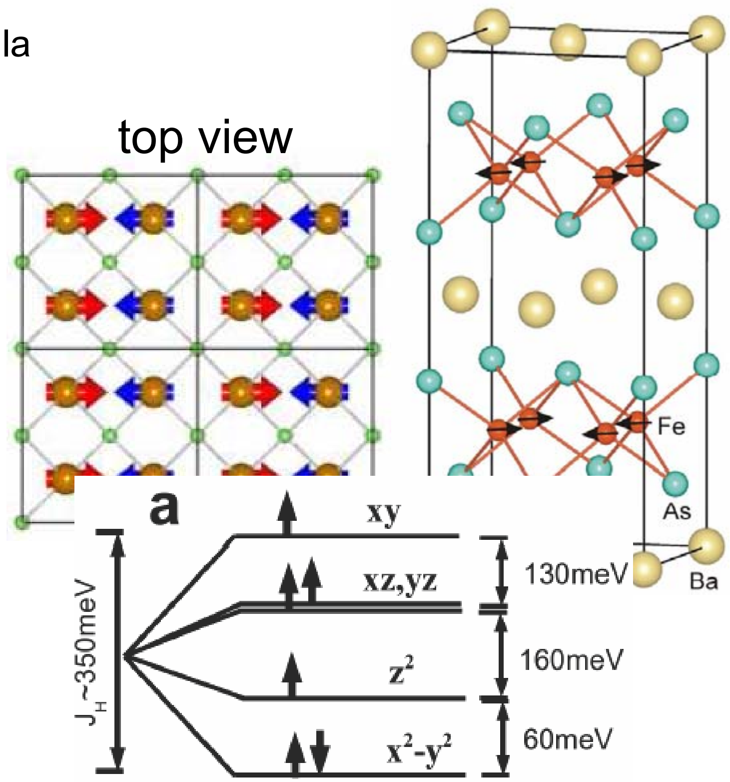
Weak structural distortion ~150 K: from tetragonal to orthorombic

SDW (stripe AFM) at lower T

Neutrons by: Clarina de la Cruz et.al, Nature 453, 899 (2008).

side view

top view



SDW temperature and magnetic moment vary strongly between compounds:

LaFeAsO: T_{SDW}~140K μ~0.3-0.4μB (a)

NdFeAsO: T_{SDW}~1.96K μ~0.9μB/Fe (b)

$BaFe_2As_2$: T_0~T_{SDW}~100K μ~0.9μB/Fe (c)

$SrFe_2As_2$: T_0~T_{SDW}~205K μ~1.01μB/Fe (d)

(a) Clarina de la Cruz et.al, Nature 453, 899 (2008).

(b) Jan-Willem G. Bo, et.al., arXiv:0806.1450

(c) Huang, Q. *et al.,* arXiv:0806.2776

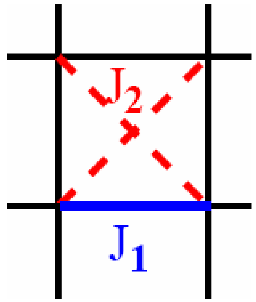
(d) K. Kaneko et.al., arXiv: 0807.2608

But Iron Fe^{2+} has 6 electrons, **[Ar] 3d6 4s0** and spin S=2.

Why is not μ larger?
Why it varies so much?

Itinerancy & Frustration

The undoped compound is metal (although very bad one ~1mΩcm), hence moment is partially screened



Magnetic exchange interaction is very frustrated (Qimiao Si, Elihu Abrahams, arXiv:0804.2480)

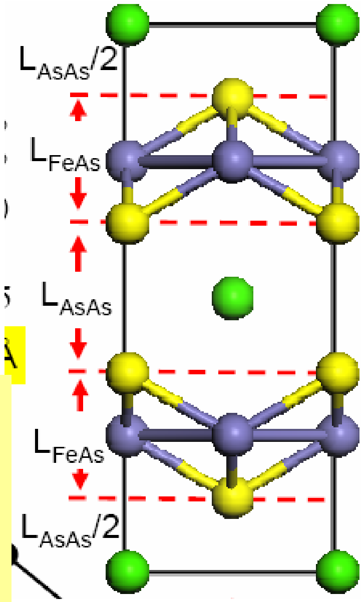
Exchange interactions are such that J2~J1/2, very strong frustration, (KH, G. Kotliar, arXiv: 0805.0722)

For the doped compound, LDA structural optimization fails for non-magnetic state!
(It is very good if magnetism is assumed)

For non-magnetic state, LDA predicts 1.34Å shorter FeAs distance (10.39 instead of 11.73).
One of the largest failures of LDA.

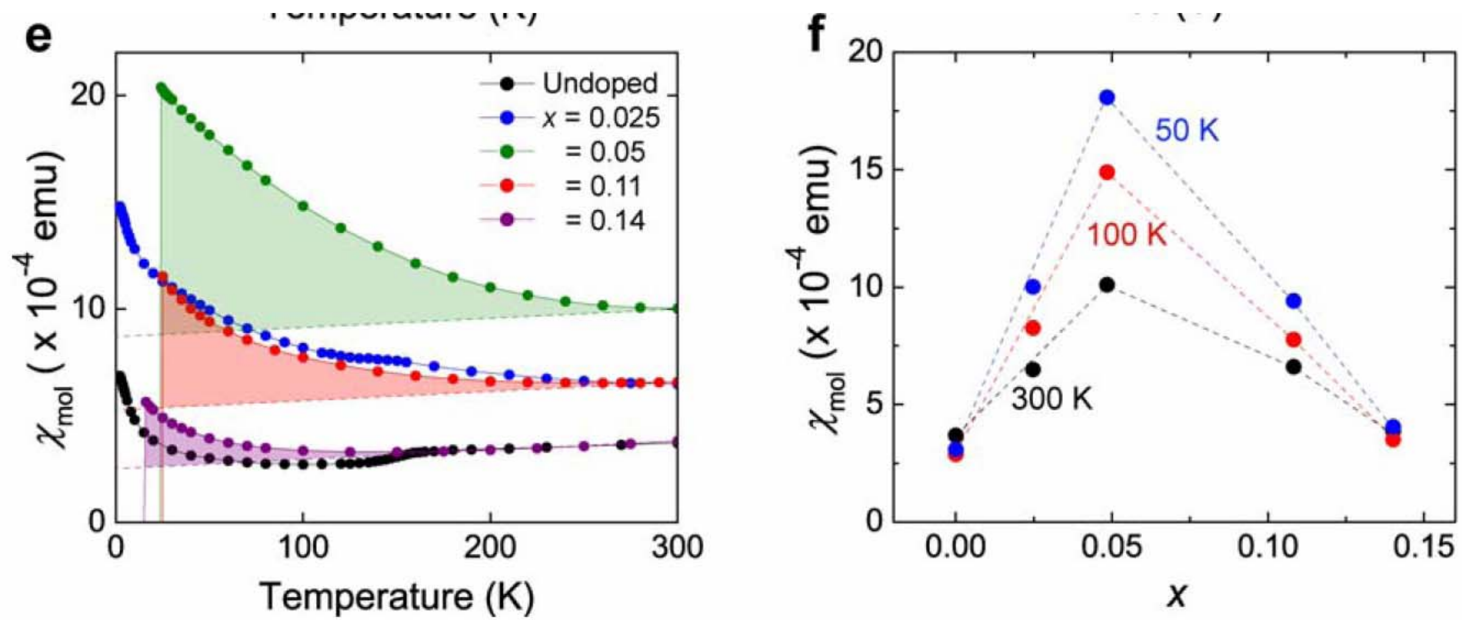
T. Yildirim, arXiv: 0807.3936

Paramagnetic state must have (fluctuating) magnetic moments not captured in LDA



Signatures of moments

Doped LaOFeAs

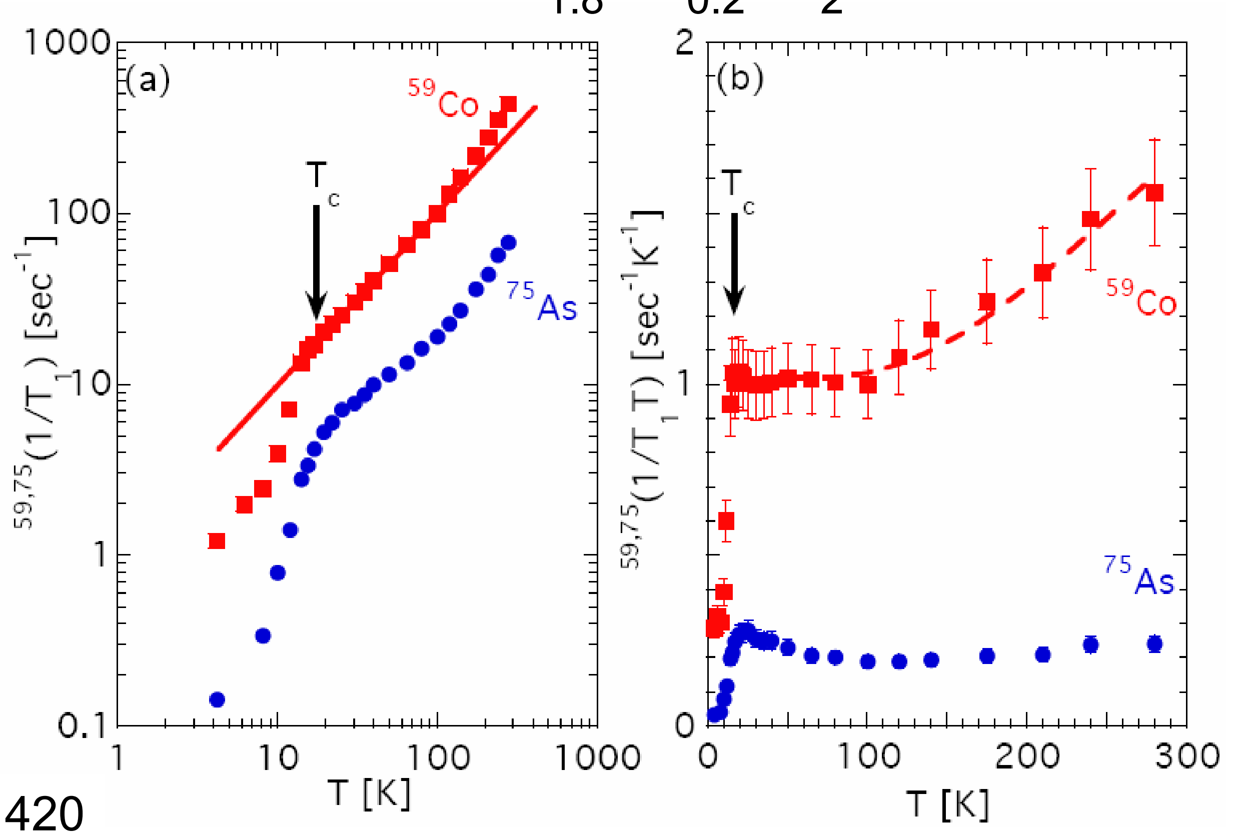


Susceptibility 50xlarger than Pauli LDA
T. Nomura et.al., 0804.3569

Nonmagnetic impurities not detrimental to SC

•Fe replaced by Co
•Impurities do not destroy SC (like Zn doping in cuprates)
•No signature of Curie-Weiss susc.

$BaFe_{1.8}Co_{0.2}As_2$: Tc~22K



F.L. Ning et.al, arXiv:0808.1420

Band structure of LaOFeAs

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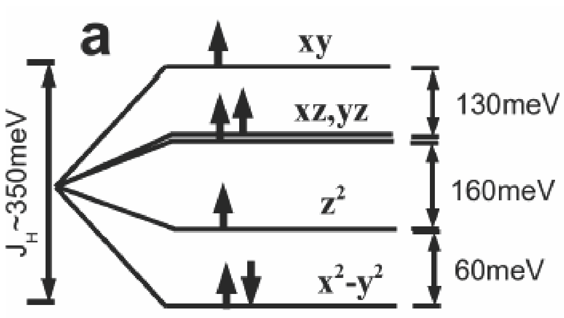
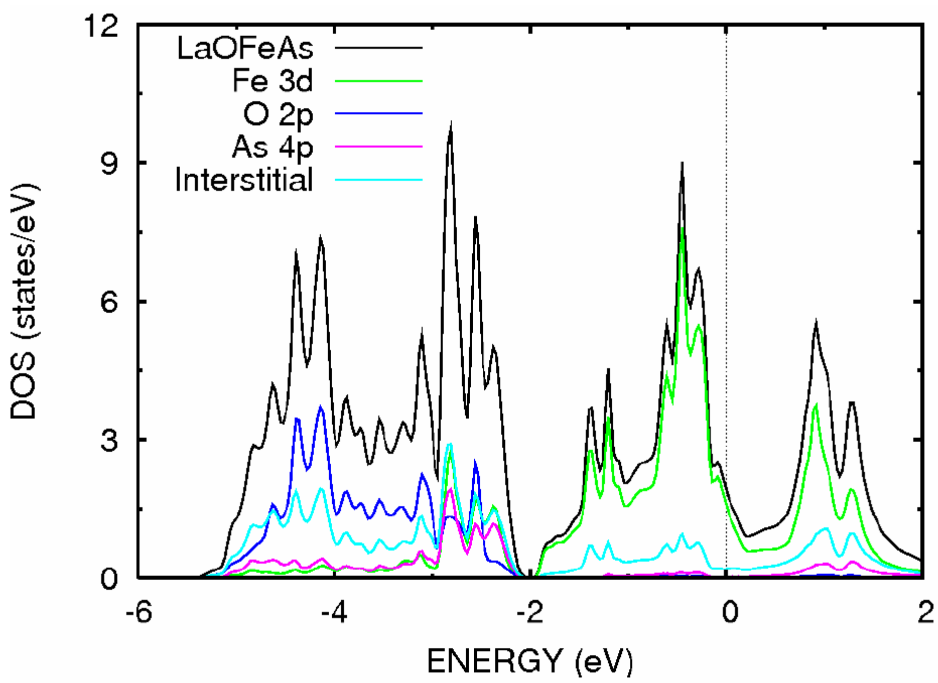
LDA: Mostly iron bands at EF
(correlations important)

6 electrons in 5 Fe bands:
Filling 6/10 -> large spin



The 5-band Hubbard-type model
As(p)-Fe(d) hybridization weak

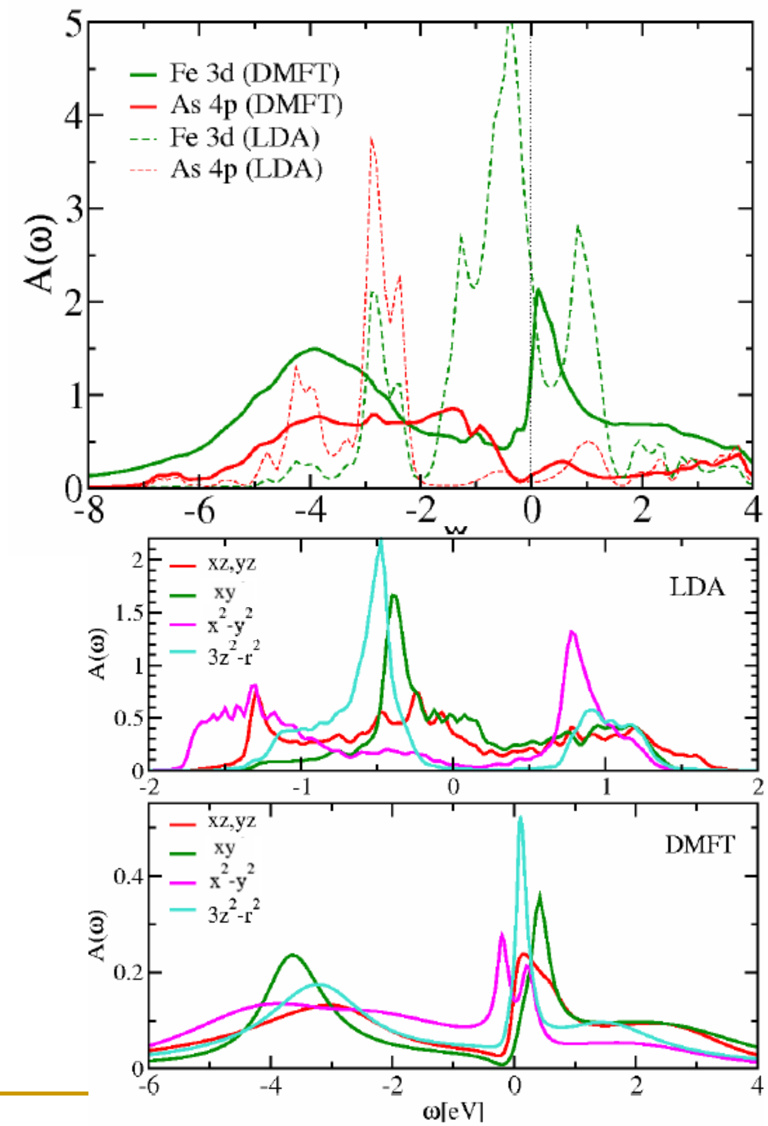
LDA DOS



KH, J.H. Shim, G. Kotliar, cond/mat 0803.1279
(PRL. 100, 226402 (2008)):

DMFT for $LaF_xO_{1-x}FeAs$

LDA+DMFT: LaOFeAs is at the verge
of the metal-insulator transition
(for realistic U=4eV, J=0.7eV)
For a larger (U=4.5, J=0.7eV) semiconducing
insulator



Not a one band model: all 5 bands important
(for J>0.3)

Need to create a singlet out of spin and orbit

Importance of Hund's coupling

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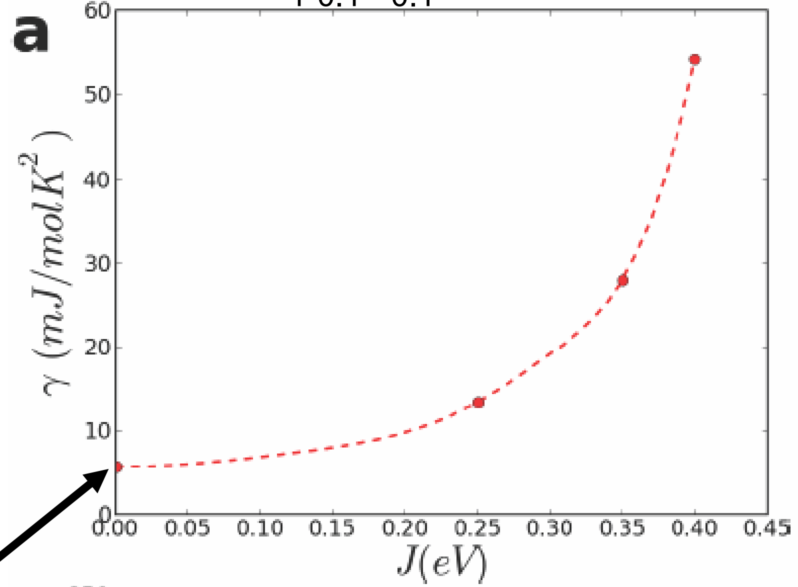
Hubbard U is not the "relevant" parameter.

The **Hund's coupling** brings correlations!

Specific heat within LDA+DMFT
for $LaO_{1-0.1}F_{0.1}FeAs$ at U=4eV

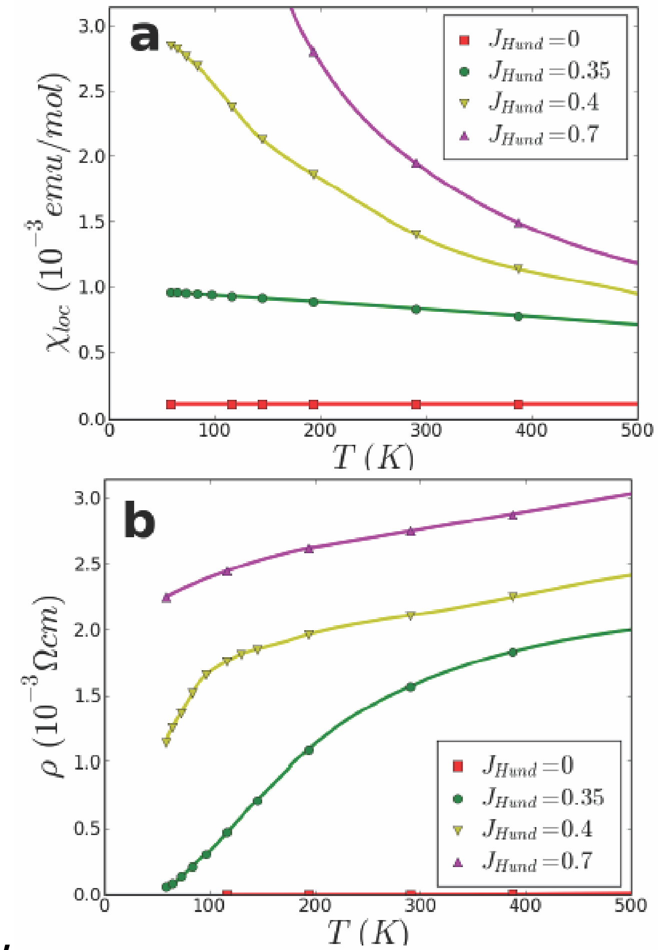


LDA value

For J=0 there is negligible mass enhancement at U~W!

The coupling between the Fe magnetic moment and the mean-field medium (As-p,neighbors Fe-d) becomes ferromagnetic for large Hund's coupling!

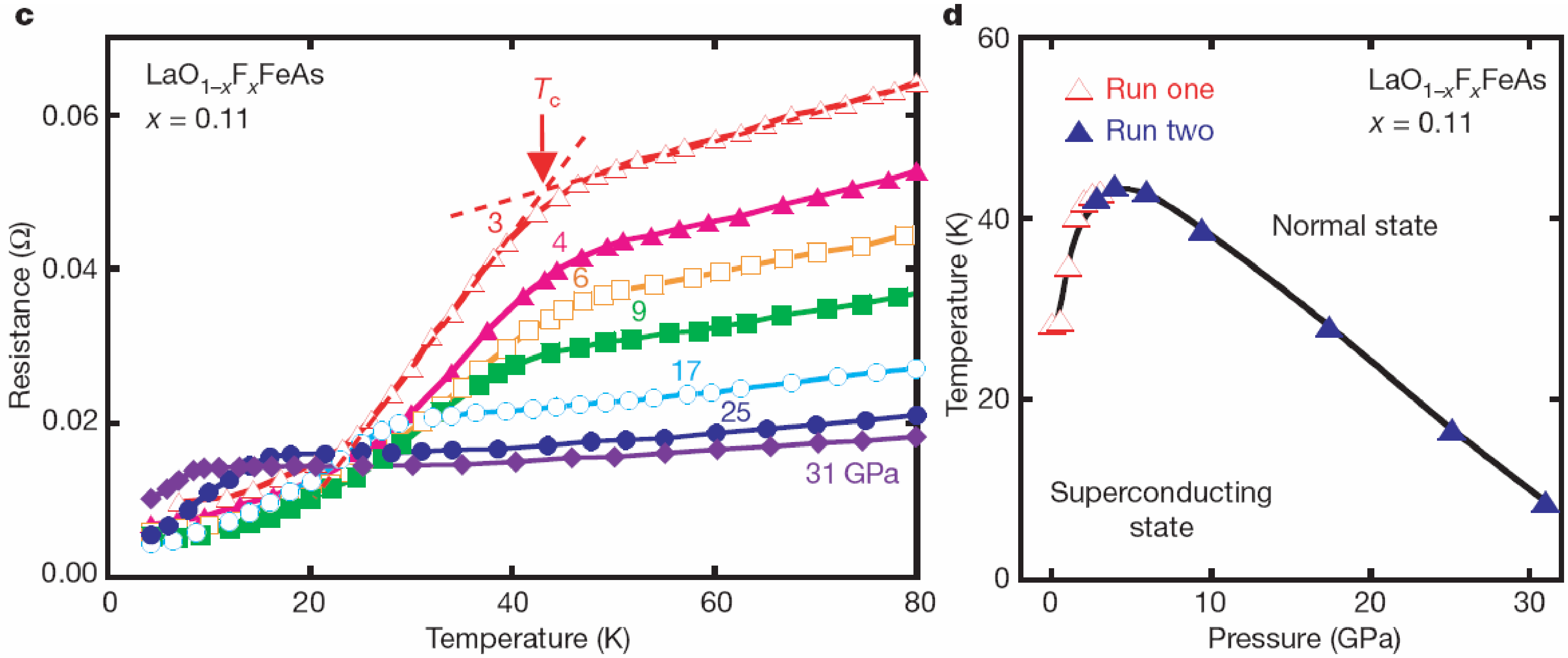
$LaO_{1-0.1}F_{0.1}FeAs$



J~0.35 gives correct order of Magnitude for both χ and ρ.

KH, G. Kotliar, cond/mat 0803.1279

LaOFeAs under pressure Tc~43K



Hiroki Takahashi et.al., *Nature* **453**, 376-378 (2008)

Very incoherent in normal state (large resistivity) → High Tc

ARPES on $Ba_{0.6}K_{0.4}Fe_2As_2$

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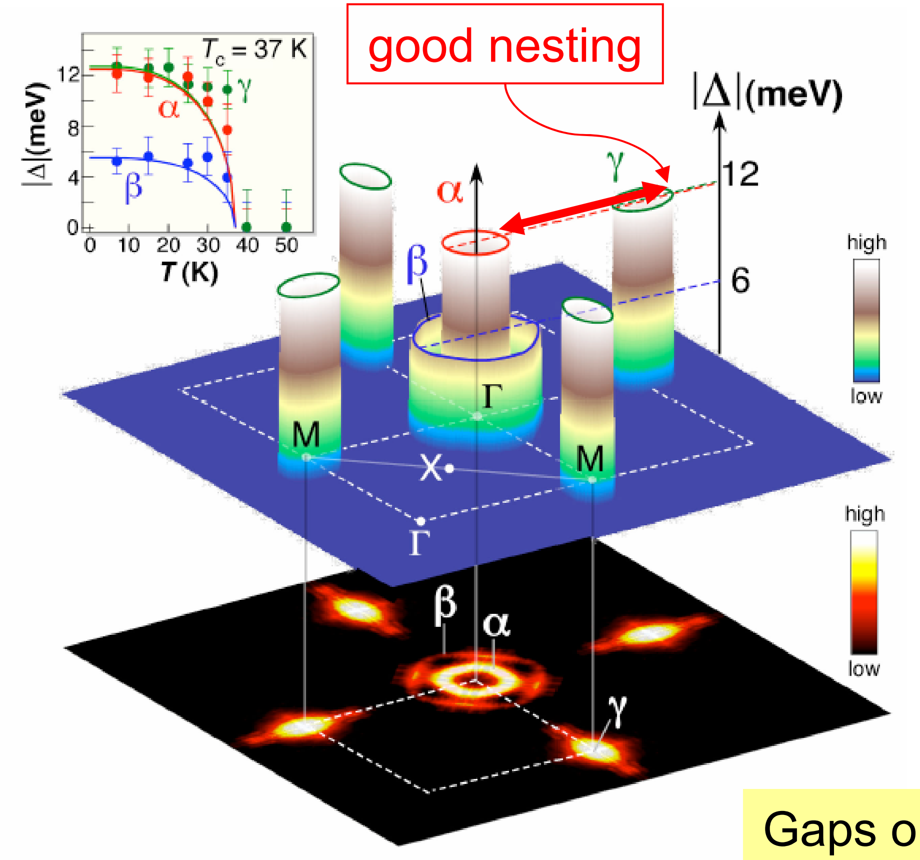
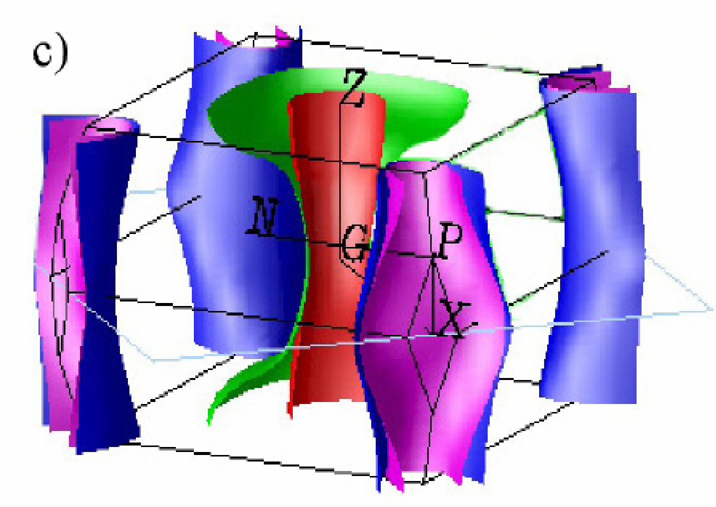


H. Ding et.al., arXiv:0807.0419

LDA(LAPW) calculation



C. Liu, et.al., arXiv: 0806.3453

Gaps on the two FS around Γ are very different

Large gap in the inner Γ and M

Small gap in the outer Γ pocket

Anisotropy of the gap

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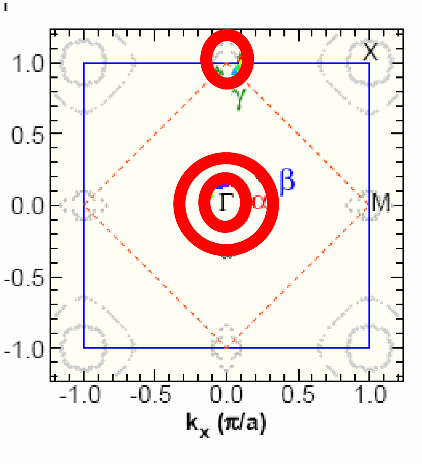
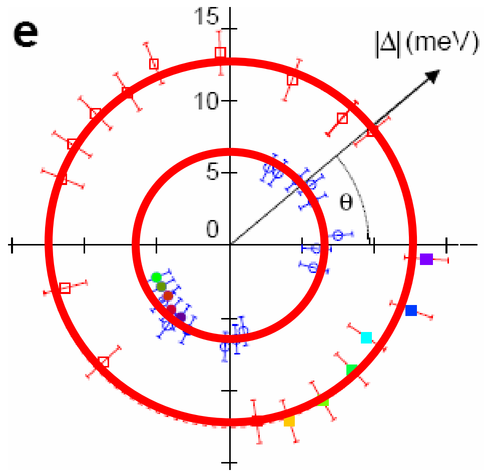
Department of Physics and Astronomy

Fermi surface

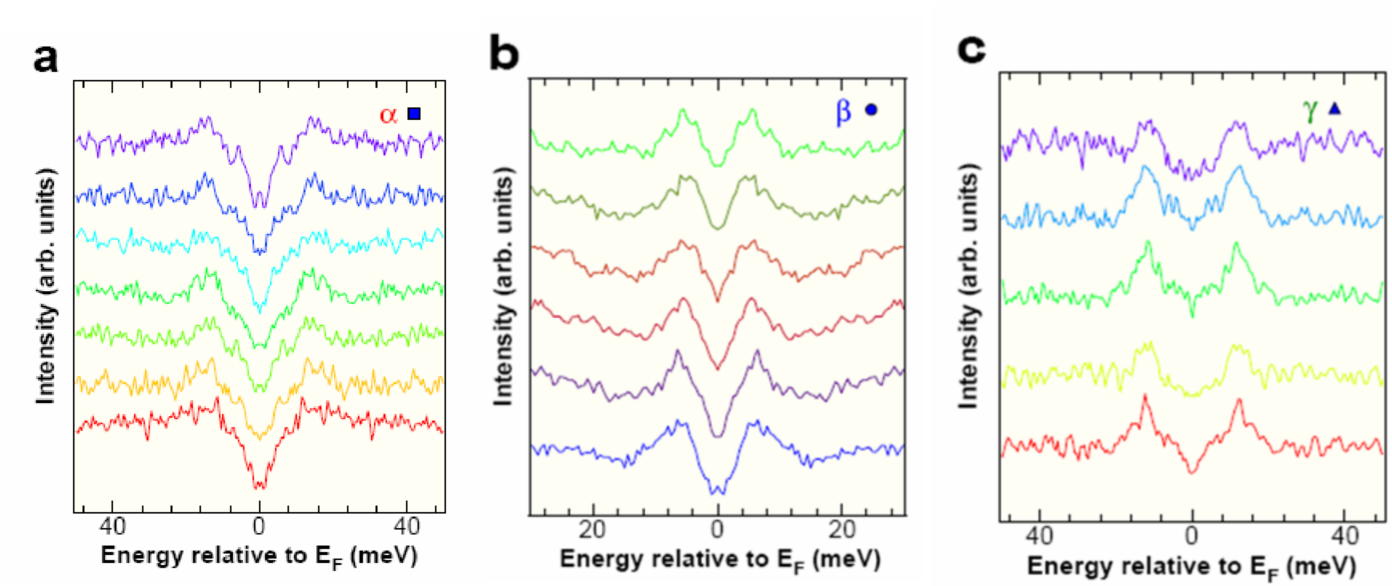


Gap size



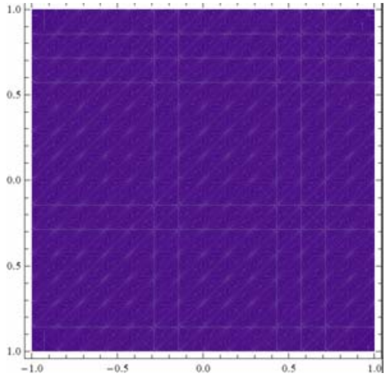
H. Ding et.al., arXiv:0807.0419

Negligible anisotropy.
D-wave gap excluded!



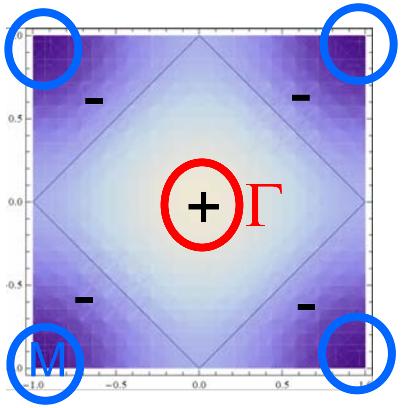
Other common possibilities

s-constant



maybe

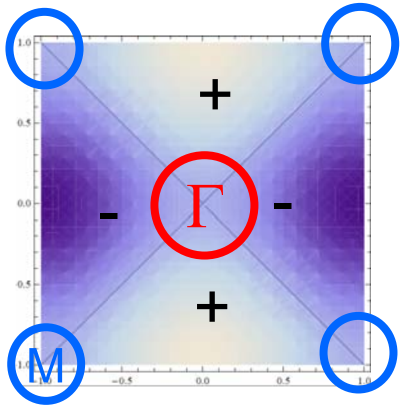
ex-s ~ cos(kx)+cos(ky)



No nodes,
but gap different sign
on Γ and M

maybe

d ~ cos(kx)-cos(ky)



~~Nodes in the gap~~

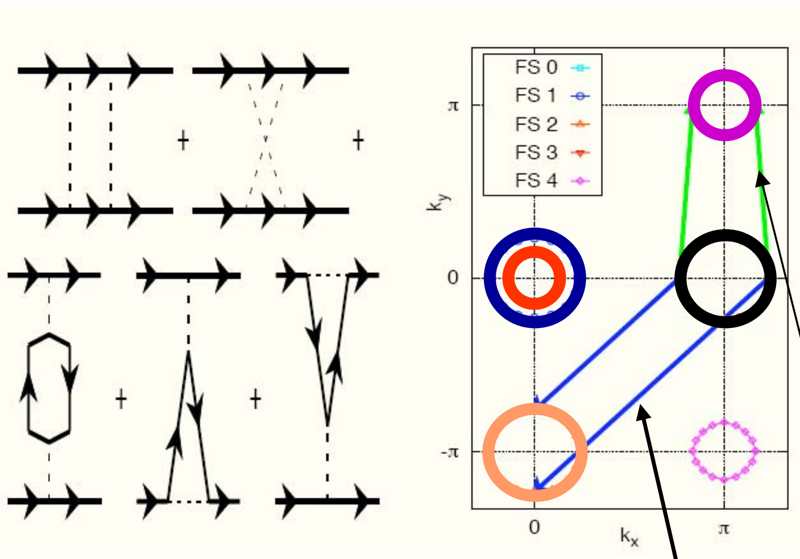
no

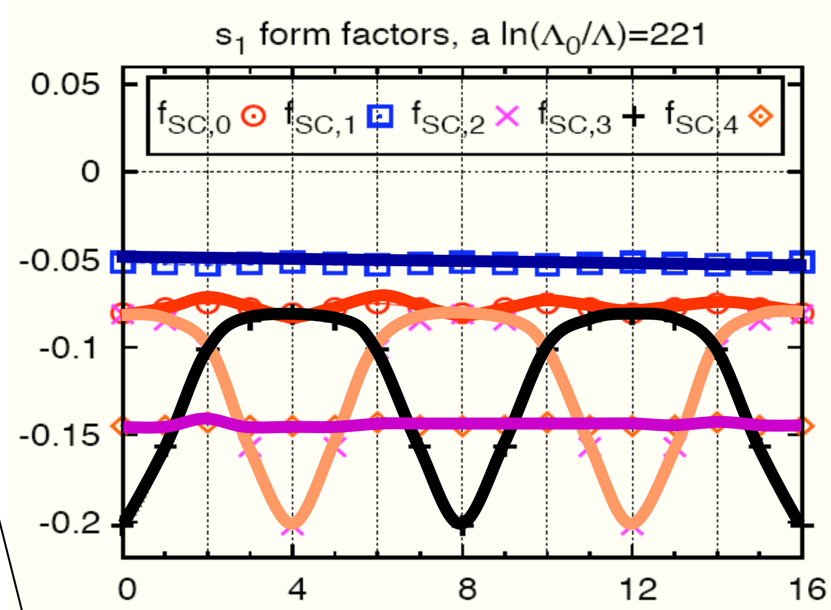
…and many other possibilities

One more possibility

Fa Wang et.al., arXiv: 0807.0498

Numerical Renormalization Group ~ “advanced” way of summing LOD





inter-pocket Josephson tunneling

The gap has the same sign on all FS pockets.

Conclusions

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- Variety of materials with common SDW feature and SC
  - 1111: LaOFeAs, CeOFeAs,…SmOFeAs
  - 122: BaFe2As2, CaFe2As2
  - LiFeAs
  - FeSe, FeTe
- Highest Tc~55K achieved in $SmF_xO_{1-x}FeAs$
- Some similarities with cuprates, but also differences (Co doping)
- Correlations weaker than in cuprates (not doped Mott insulators)
- ARPES shows almost uniform gap on FS sheets (s-wave, extended s-wave,….)
- Other probes of gap symmetry are still controversial ($1/T_1 \sim T^3$, $1/\lambda^2$~exp/powerlaw, Cv~exp/powerlaw)