Magnetism and Superconductivity

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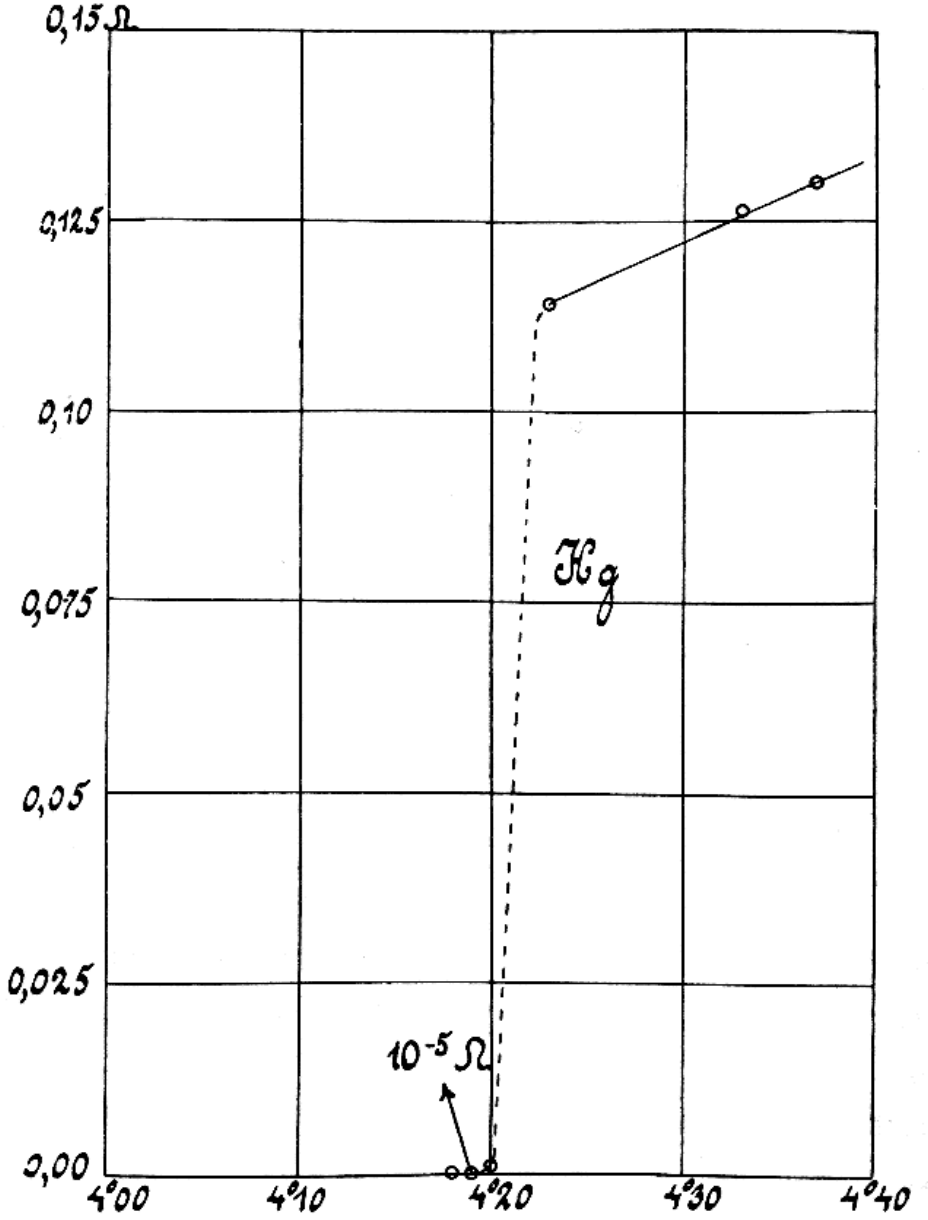
"Oh, East is East, and West is West, and never the twain shall meet" (Rudyard Kippling)

Main co-worker: Igor I. Mazin

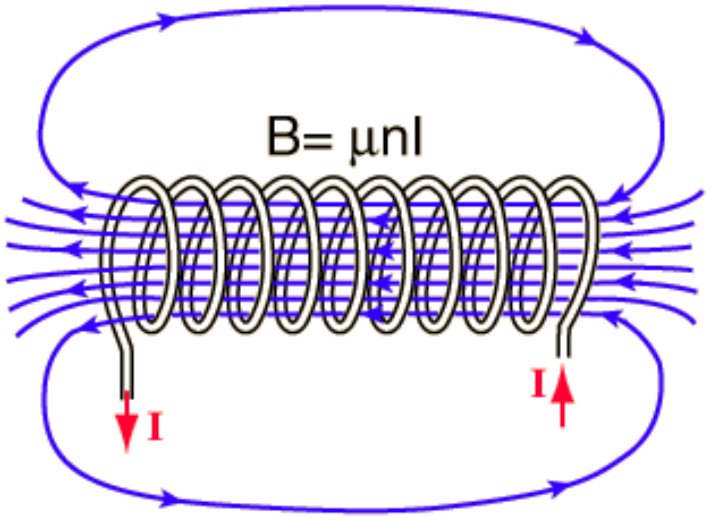
Supported by DOE, BES, Materials Sciences and Engineering and the S3TEC EFRC.

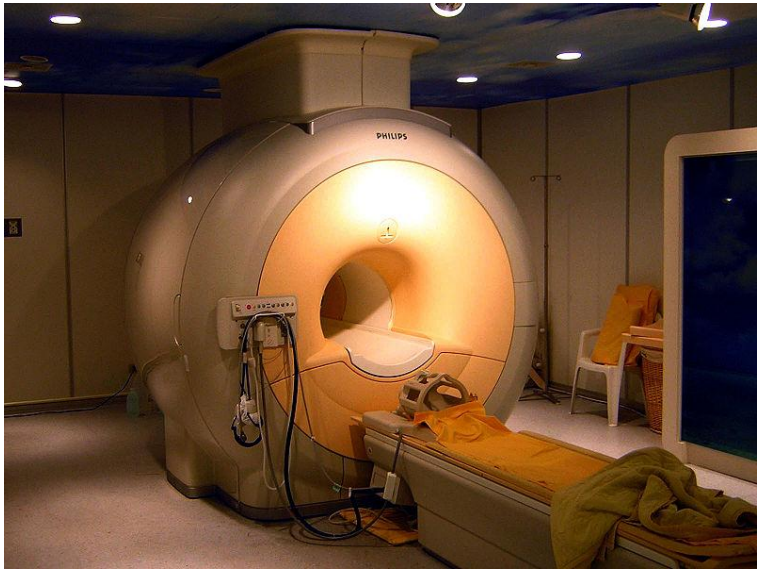
Superconductivity - 1911

H. Kamerlingh Onnes



Uses

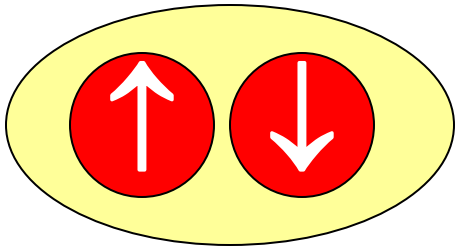


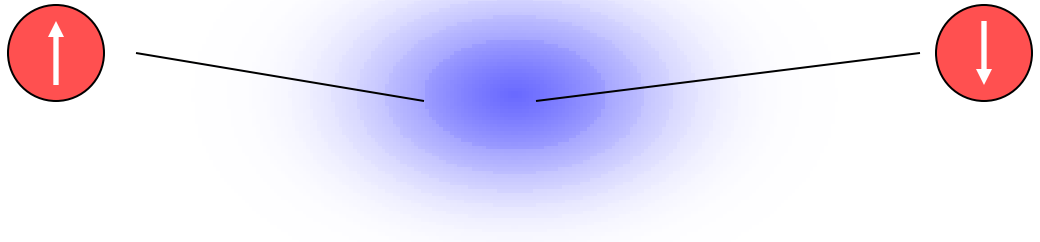


Limited by critical field, critical current, critical temperature

Bardeen Cooper Schrieffer - 1957

Singlet (*s*,*d*)



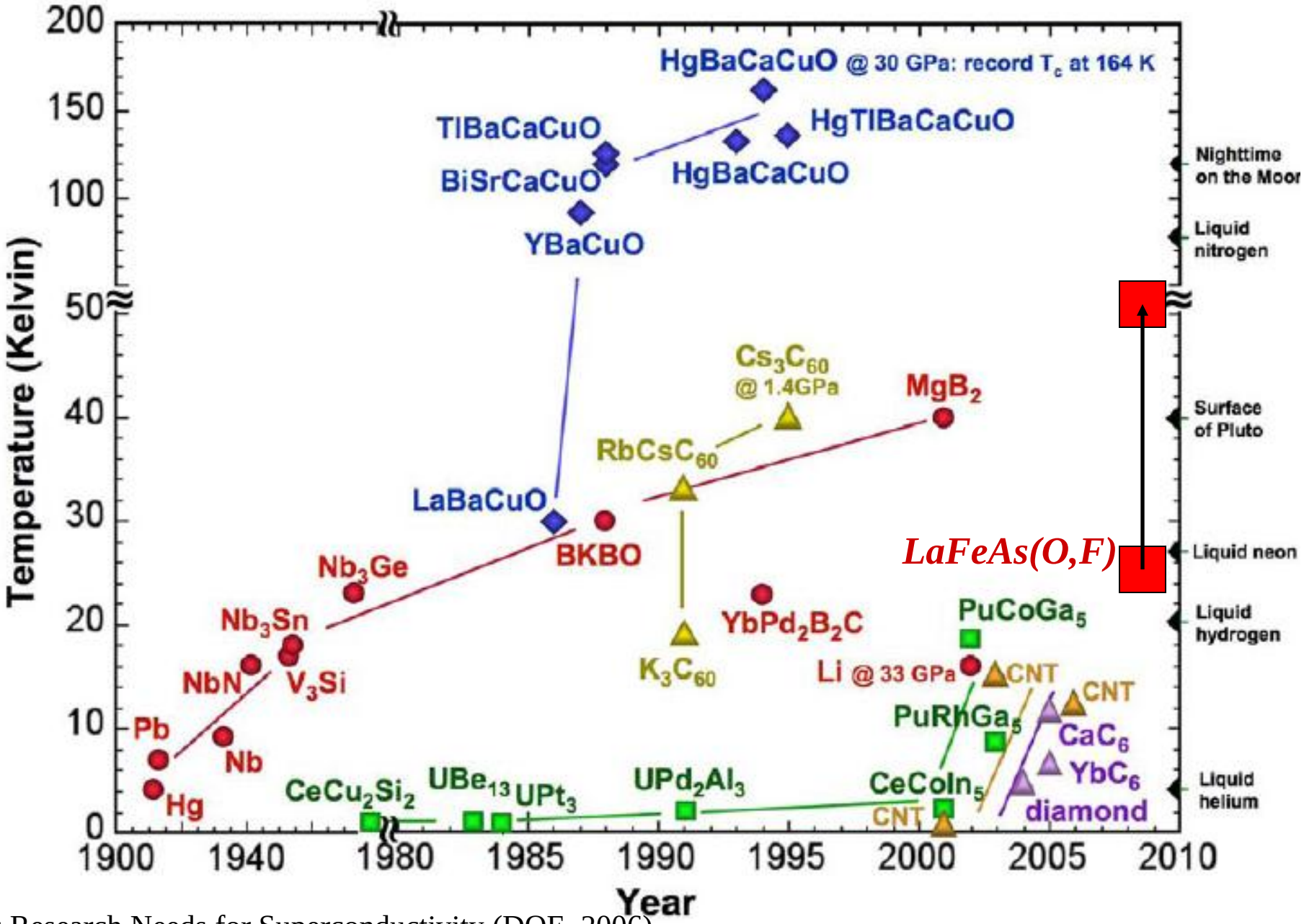


Hg, Pb, Cuprates

Singlet Channel:
Charge fluctuations (phonons) are attractive.
Ferromagnetic fluctuations are pair breaking
Spin fluctuations in general are repulsive.

Since electron phonon is always attractive the *s*-wave channel is most favored by it.

Materials



Basic Research Needs for Superconductivity (DOE, 2006)

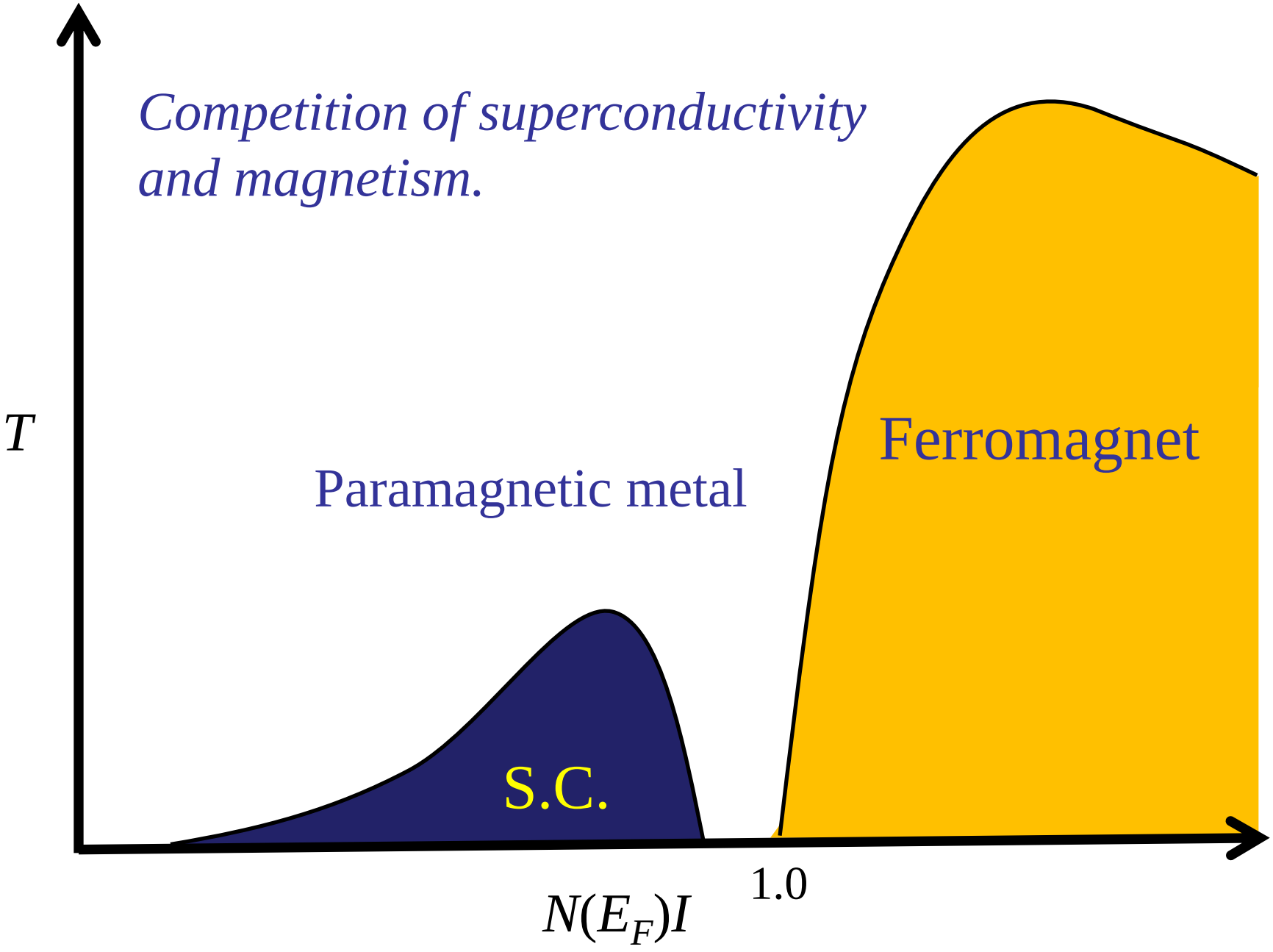
[4]P. W. Anderson and A. H. Dayem, Phys. Rev. Letters 13, 195 (1964). See also J. Lambe, A H. Silver, J. E. Mercereau, and R. C. Jaklevic, Phys. Letters 11, 16 (1964).
[5]A. H. Dayem and C. C. Grimes, Appl. Phys. Letters 9, 47 (1966).
[6]P. L. Richards, J. Opt. Soc. Am. 54, 1474 (1964).
[7]E. Riedel, Z. Naturforsch. 19a, 1634 (1964).
[8]N. R. Werthamer, Phys. Rev. 147, 255 (1966).
[9]I. K. Yanson, V. M. Svistunov, and I. M. Dmitrenko, Zh. Eksperim. i Teor. Fiz. 48, 976 (1965) [translation: Soviet Phys.—JETP 21, 650 (1965)]; D. N. Langenberg, D. J. Scalapino, B. N. Taylor, and R. E. Eck, Phys. Rev. Letters 15, 294, 842(E) (1965); D. N. Langenberg, D. J. Scalapino, and B. N. Taylor, Proc. IEEE 54, 560 (1966).

EFFECT OF FERROMAGNETIC SPIN CORRELATIONS ON SUPERCONDUCTIVITY*

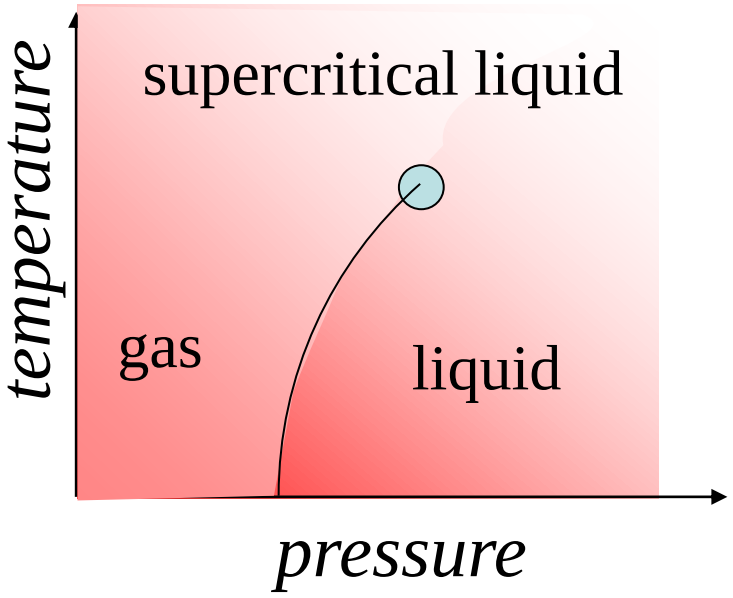
N. F. Berk and J. R. Schrieffer
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania
(Received 24 June 1966)

Pd is not a superconductor because of nearness to ferromagnetism.

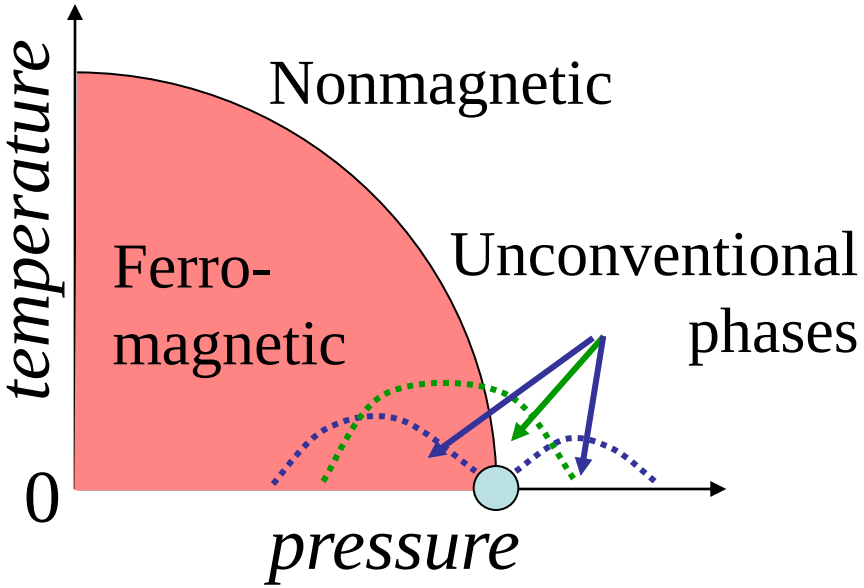
Inferred Phase Diagram



Metals Near Quantum Critical Points



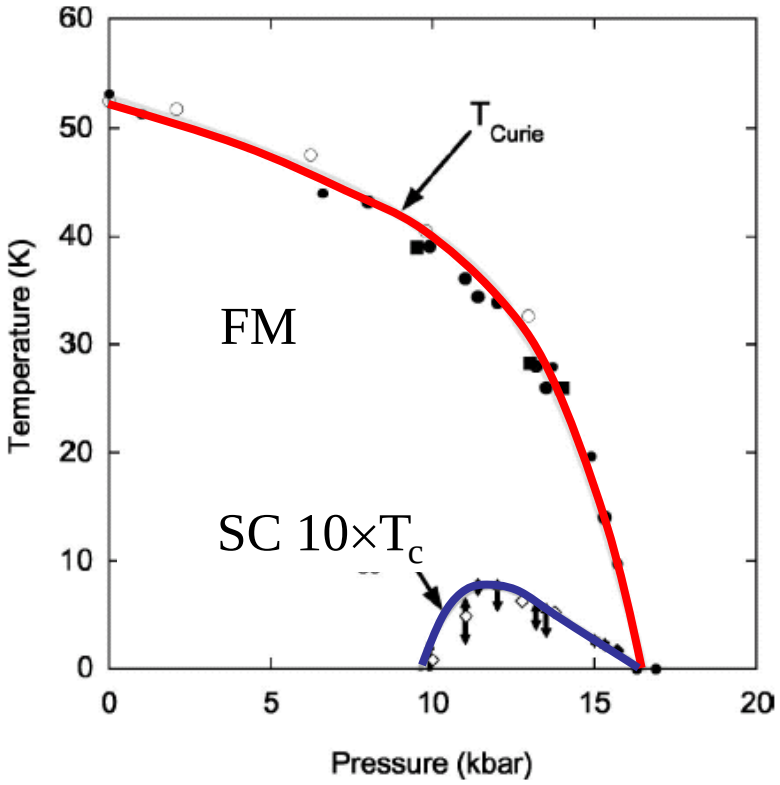
Classical criticality: Thermal density fluctuations grow indefinitely close to the Critical Point (CP).



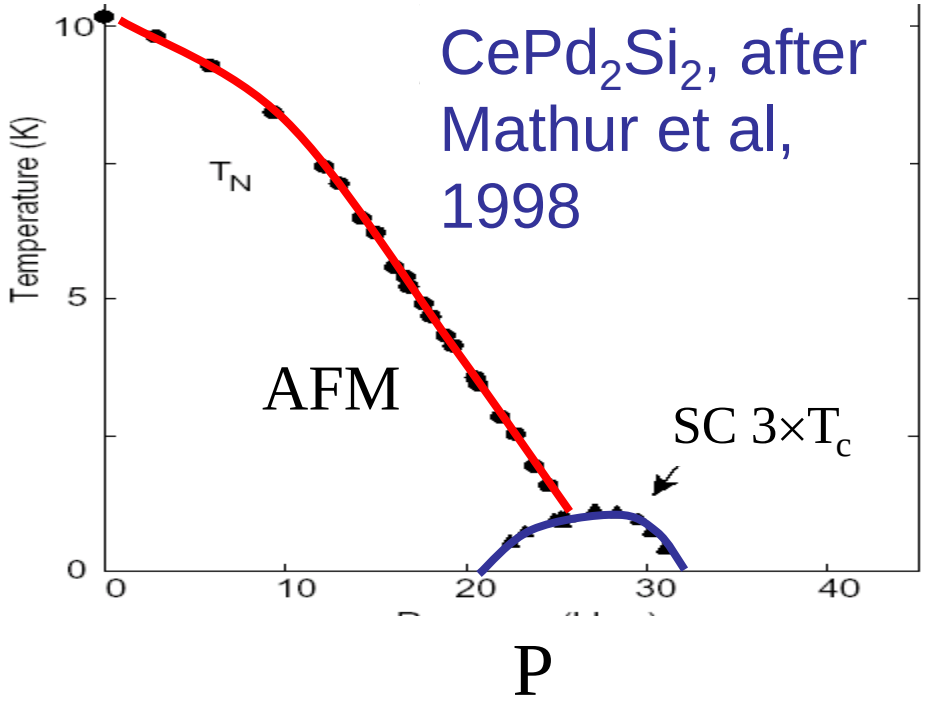
Quantum criticality: Quantum density fluctuations grow indefinitely close to the Quantum Critical Point (QCP).

Interesting things happen near critical points: In this region fluctuations are important and DFT does badly.

Something Different?



UGe_2, after Huxley et al, 2001 and Saxena et al, 2000



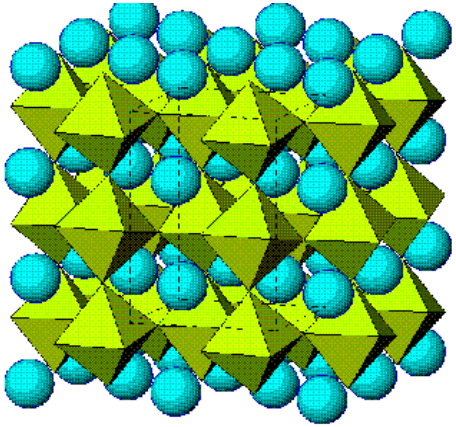
$CePd_2Si_2$, after Mathur et al, 1998

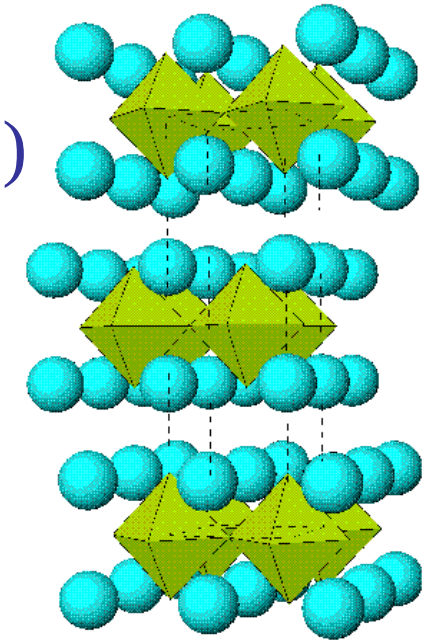
Interesting things may happen near critical points: In this region fluctuations are important and DFT does badly.

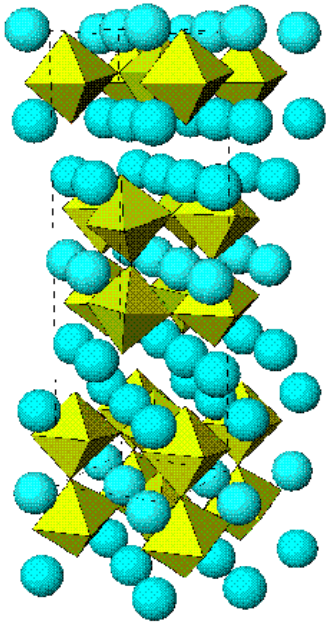
“Strontium Ruthenate”

$Sr_{n+1}Ru_nO_{3n+1}$

Ru^{4+} (4 d-electrons)







$n = \infty$

Ferromagnet

$n = 1$

Triplet superconductor

$n = 2$

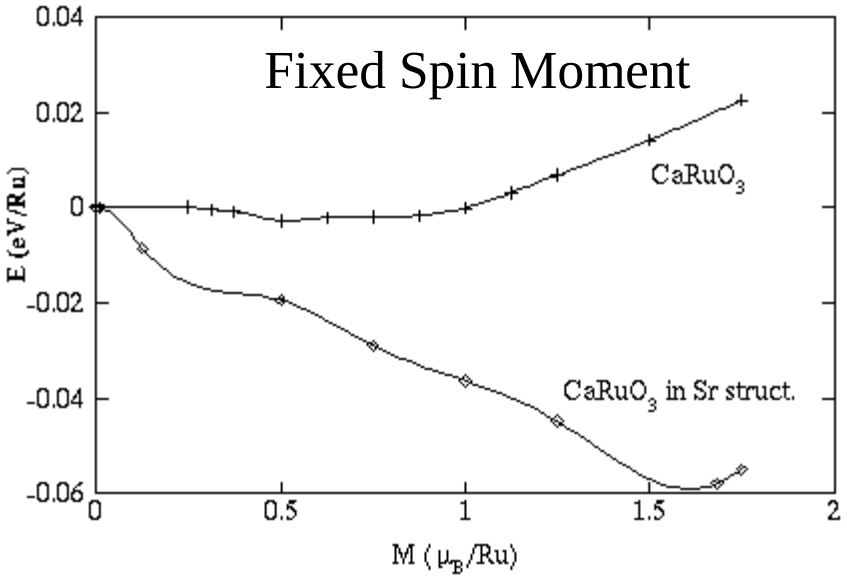
Metamagnetic quantum critical point

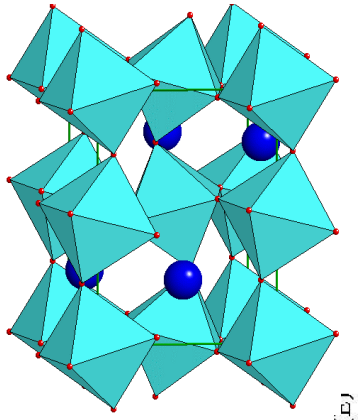
Magnetic Order in $Sr_{1-x}Ca_xRuO_3$

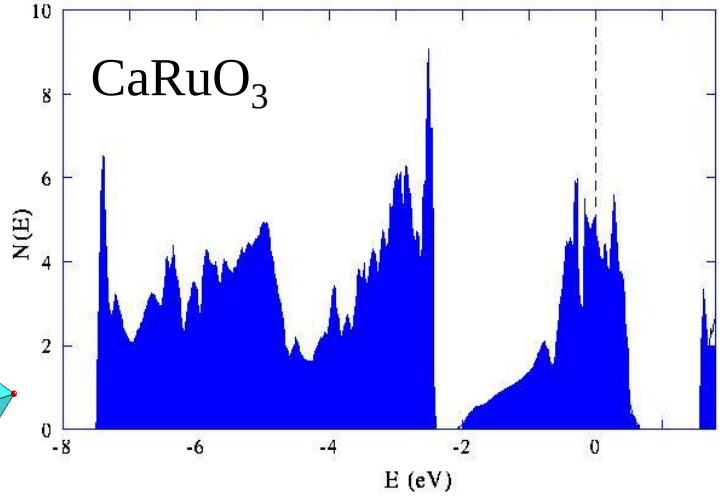
Experiment:

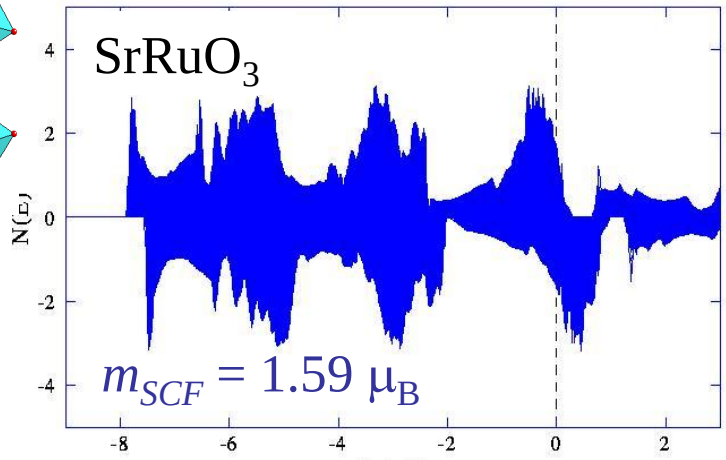
- $SrRuO_3$ is FM T_C~165K.
- T_C fall smoothly with x, reaching 0 near x=1.
- $CaRuO_3$ was reported AFM, but now thought PM.

LSDA: Octahedral Tilt Broadens DOS.









Itinerant Stoner Explanation

STONER PICTURE

$\Delta E = \frac{1}{2} \int_0^m [m' \, dm' / N(m')] - I_{TOT} m^2/4$ with $I_{TOT} = \sum_\alpha I_\alpha \nu_\alpha^2$

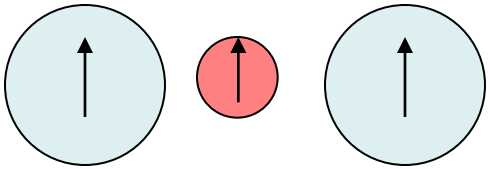
$\Delta E = -I_{TOT} m^2/4 = -\sum_\alpha I_\alpha m_\alpha^2 /4$ and $N = \sum_\alpha N_\alpha \nu_\alpha$

For $SrRuO_3$

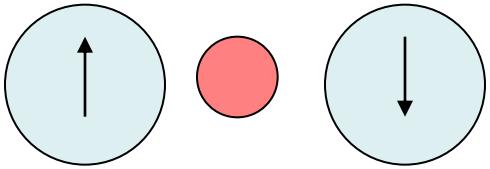
- I_{TOT} = 0.41eV
- I_{Ru} = 0.35eV

➔ Significant on-site O contribution

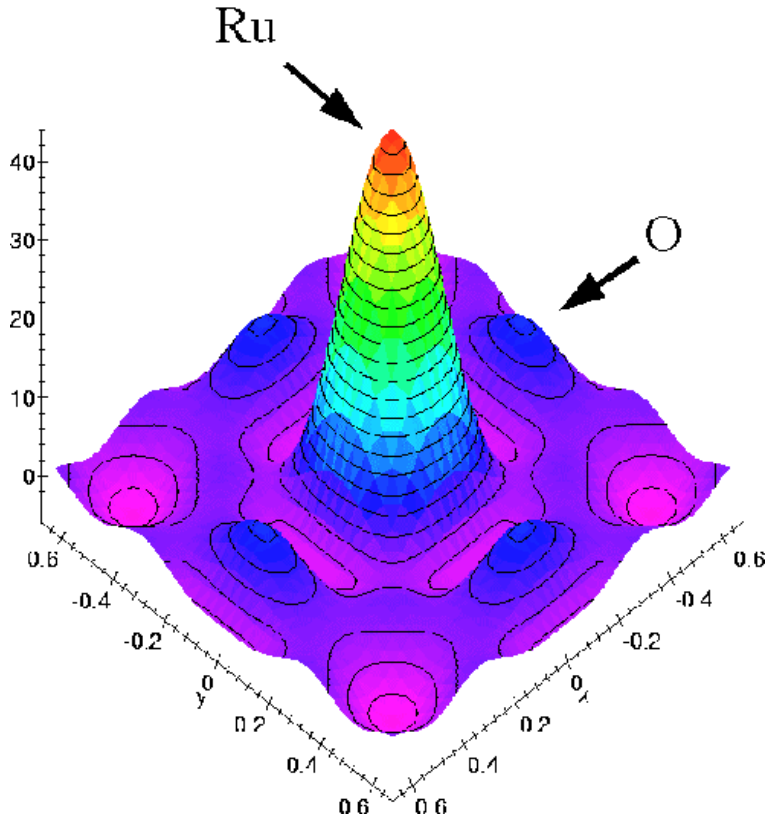
- Favors Ferromagnetism.



- Over Antiferromagnetism.



Also band KE.



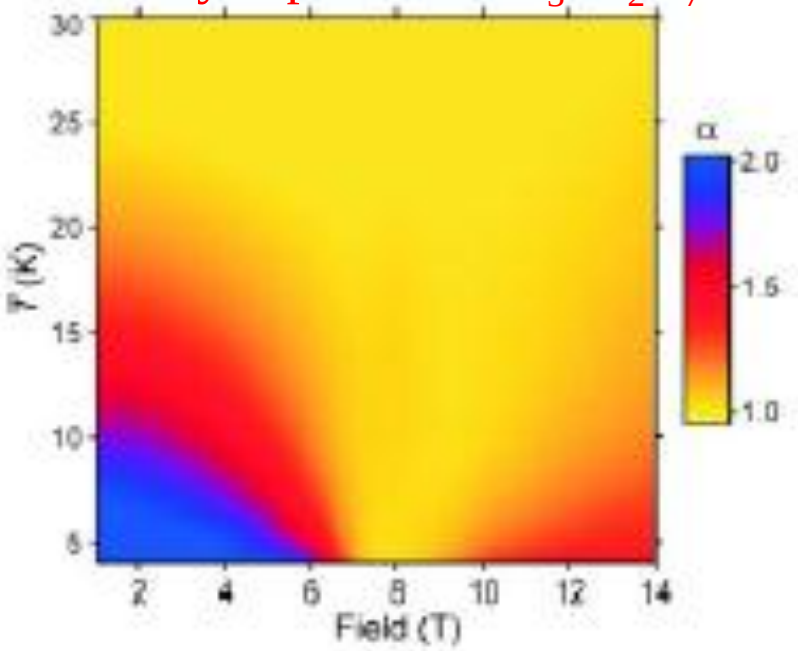
Nagler and Chakoumakos, ORNL

Quantum Critical Points and the LDA

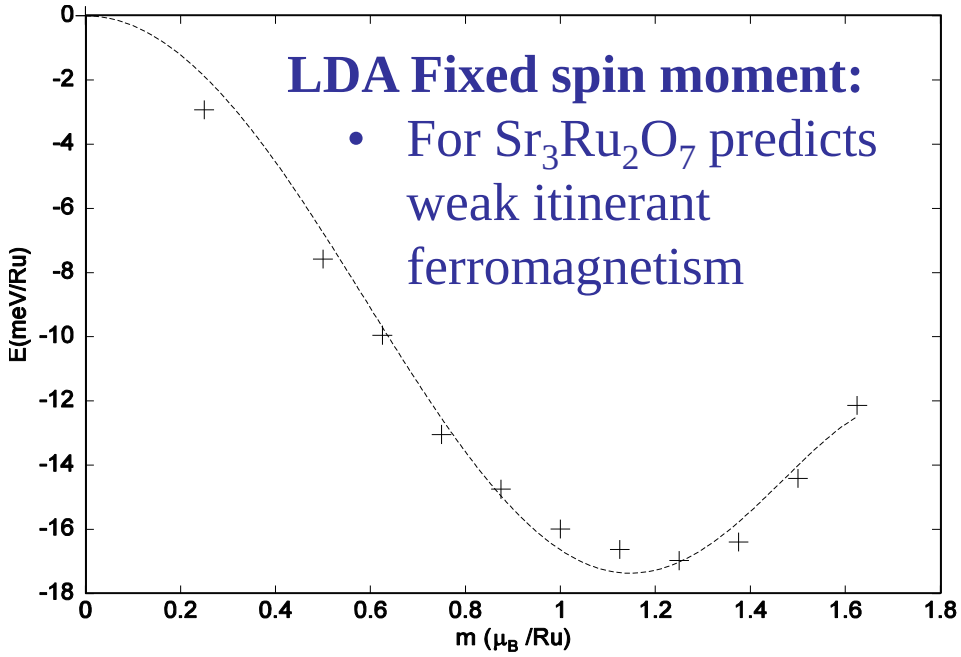
Density Functional Theory: LDA & GGA are widely used for first principles calculations but have problems:

- Mott-Hubbard: Well known poor treatment of on-site Coulomb correlations.
- Based on uniform electron gas. Give mean field treatment of magnetism: Fluctuations missing (generally small, but important near quantum critical points)

Resistivity exponent in $Sr_3Ru_2O_7$



Grigera *et al.*, Science (2001).



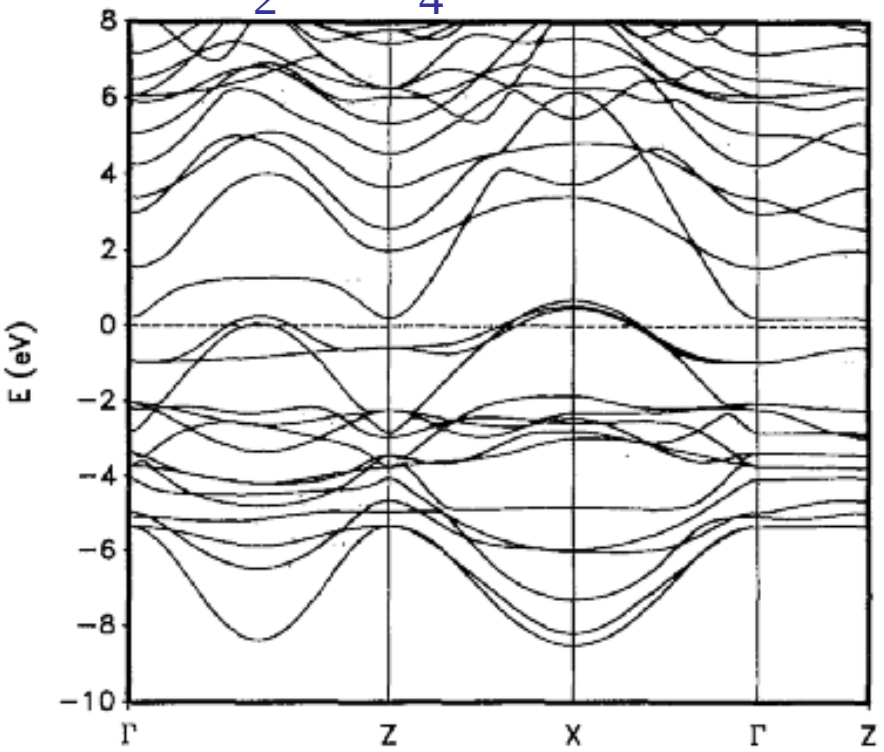
LDA Fixed spin moment:

- For $Sr_3Ru_2O_7$ predicts weak itinerant ferromagnetism

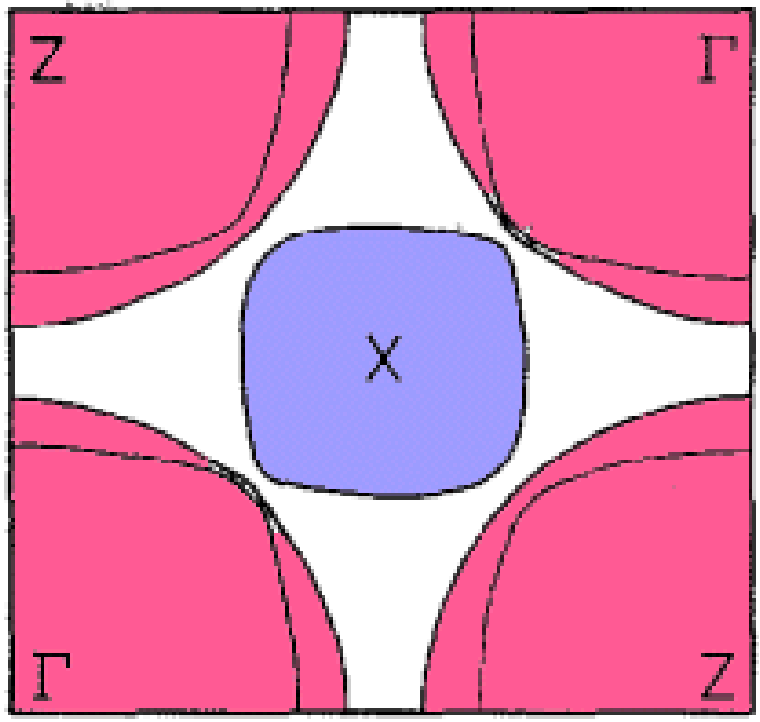
LDA overestimate of ferromagnetic tendency is a signature of quantum critical fluctuations – neglected fluctuations suppress magnetism

Electronic Structure of Sr_2RuO_4

Sr_2RuO_4 - I4/*mmm*



•3 t_{2g} derived bands at E_F: d_{xy}, d_{xz}, d_{yz}.



•Highly 2D electronic structure.
•FS agrees in detail with dHvA.
•Mass renormalizations ~ 4

What are the pairing interactions on the FS? Unconventional symmetry ➔ not electron-phonon.

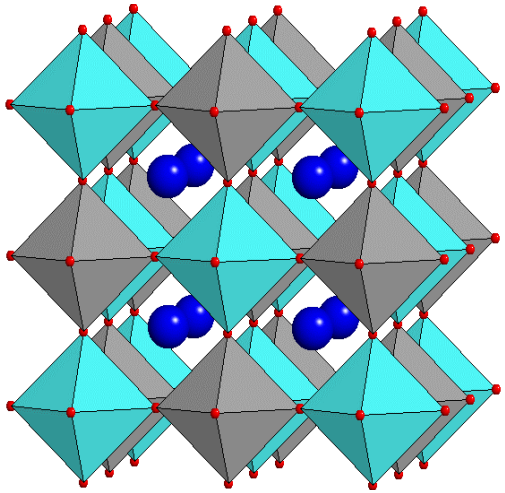
➔ Spin-fluctuations?

SPIN-FLUCTUATIONS

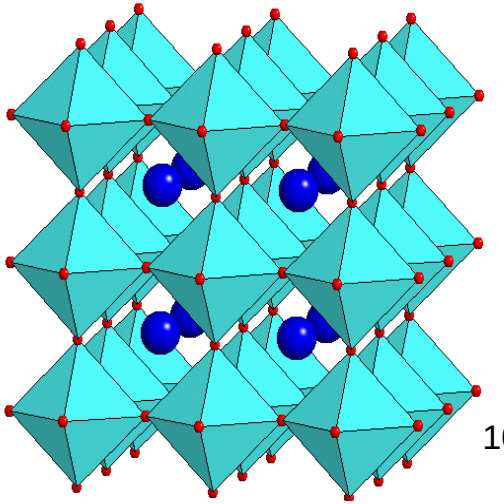
Ingredients:

1. On-Site Stoner (O) - Ru-O hybridization

Sr_2YRuO_6 - no shared O
➔AFM



$SrRuO_3$ - shared O
➔FM

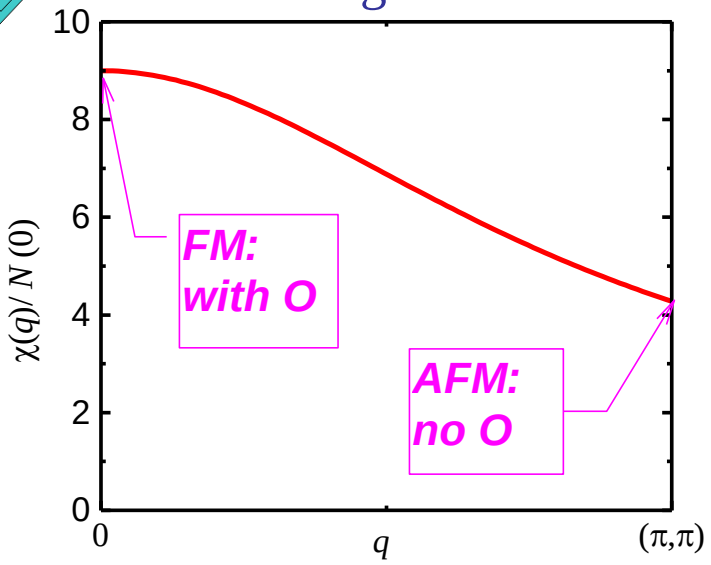


Sr_2RuO_4 - shared O
➔FM flucts.

- Shared O in RuO_2 planes will favor FM fluctuations.

- Can model by smooth background using calculations of
  - I_{Ru} and I_O.
  - Projections of $N(E_F)$.
  - Taking full O contribution at **k**=(0,0) and no O contribution at **k**=(½,½).

Ferromagnetic Part



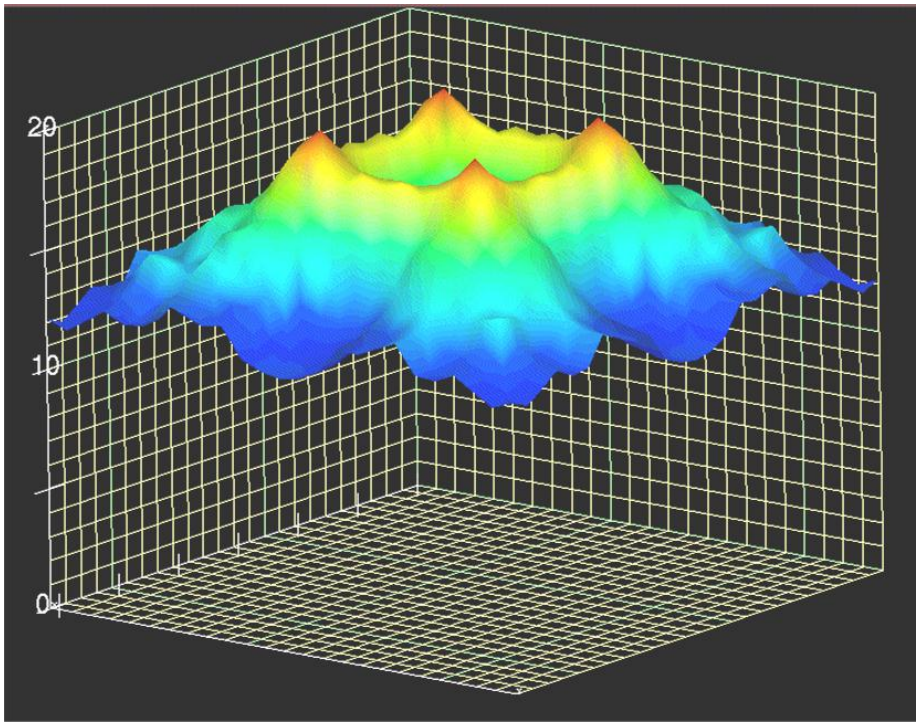
SPIN-FLUCTUATIONS (CON'T)

2. Nesting:

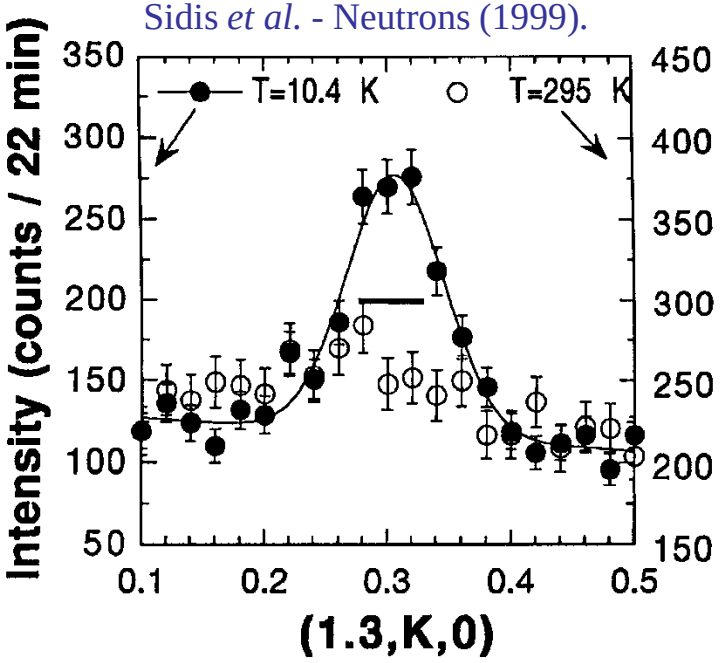
$$\chi(\mathbf{q}) = \frac{\chi_0(\mathbf{q})}{1 - I(\mathbf{q})\chi_0(\mathbf{q})}$$

Previous slide had $I(q)$ from Stoner but no **q** dependence in χ_0

Fermi Surfaces: Simple and 2-dimensional ➔ strong nesting.

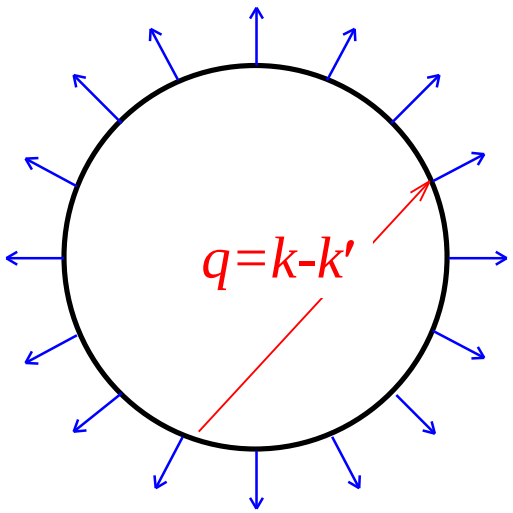


Sidis *et al.* - Neutrons (1999).



SUPERCONDUCTIVITY

e.g.



Triplet works in BCS gap equation provided that the pairing at small **q** is dominant (s.f. are attractive for triplet).

- Non-*s* depends on q dependence in $V(q)$.
- Generally higher ℓ needs more structure in $V(q)$.
- The details of the Fermi surface and $V(q)$ are crucial.

Singlet:

$$V(\mathbf{q}) = - \frac{I^2(q)\chi_0(\mathbf{q})}{1 - I^2(\mathbf{q})\chi_0(\mathbf{q})}$$

Triplet:

$$V(\mathbf{q}) = \frac{I^2(q)\chi_0(\mathbf{q})}{1 - I^2(\mathbf{q})\chi_0(\mathbf{q})}$$

Note signs

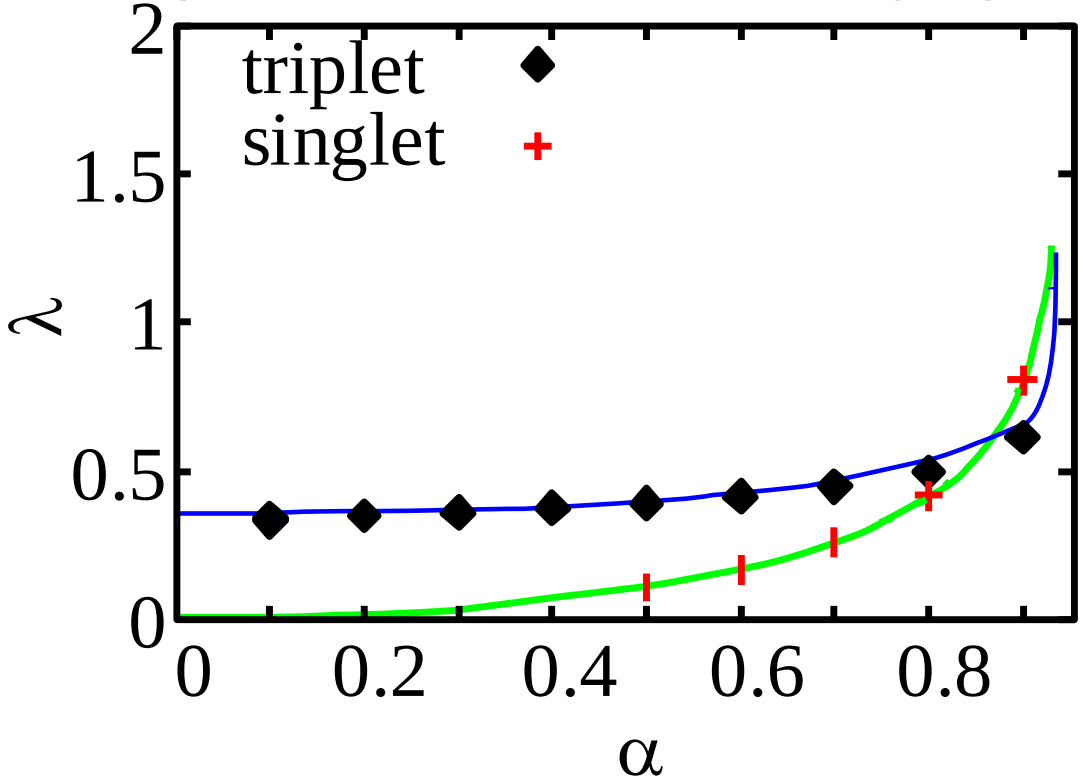
SUPERCONDUCTIVITY (Con't)

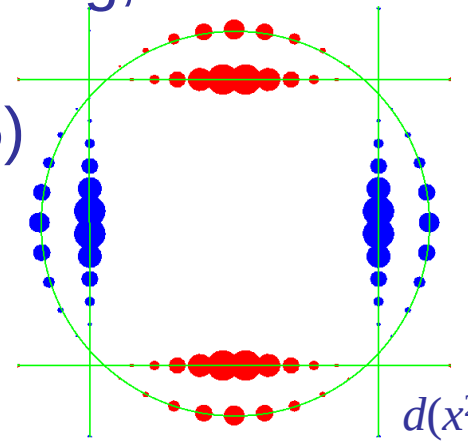
What we did:

- Calculate matrix elements $V_{\mathbf{k},\mathbf{k}'}$ for a set of **k**,**k**' on the FS.
- Set-up gap equation -- diagonalize V.
- Use $\chi_0(q) = N(0) + \alpha\chi_{nesting}(\mathbf{q})$. -- *i.e.* FM Stoner + adjustable strength nesting -- α = 0 means no nesting; α = 0.98 is AFM.

Result:

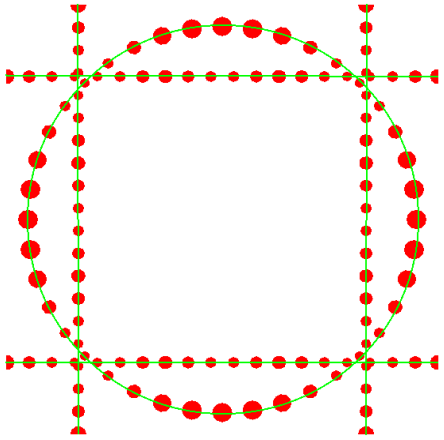
- Triplet wins over a wide range (α < .85)





$d(x^2\text{-}y^2)$

Note lack of pairing on α sheet.



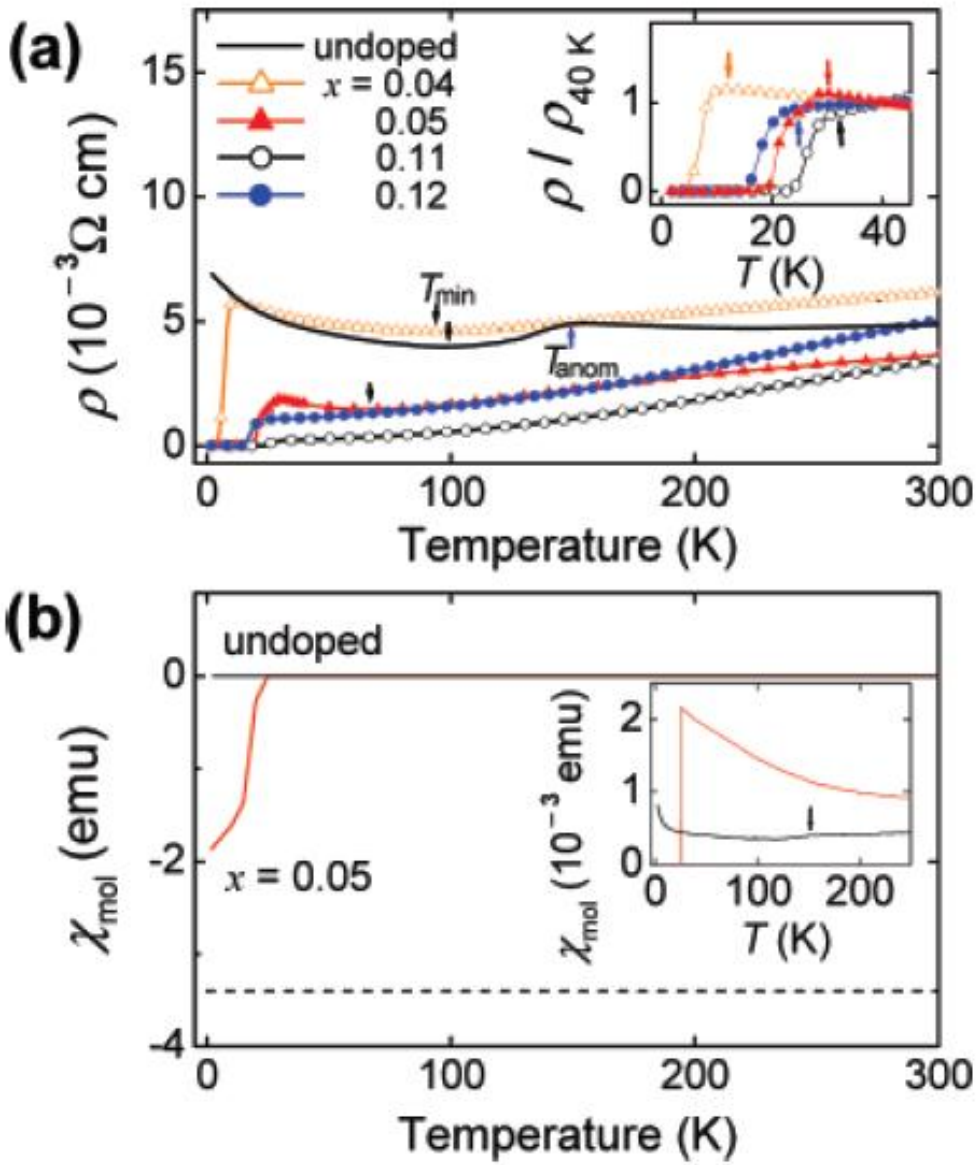
Discovery of Superconductivity in Fe-As Compounds

Kamihara *et al.*, JACS, 2006

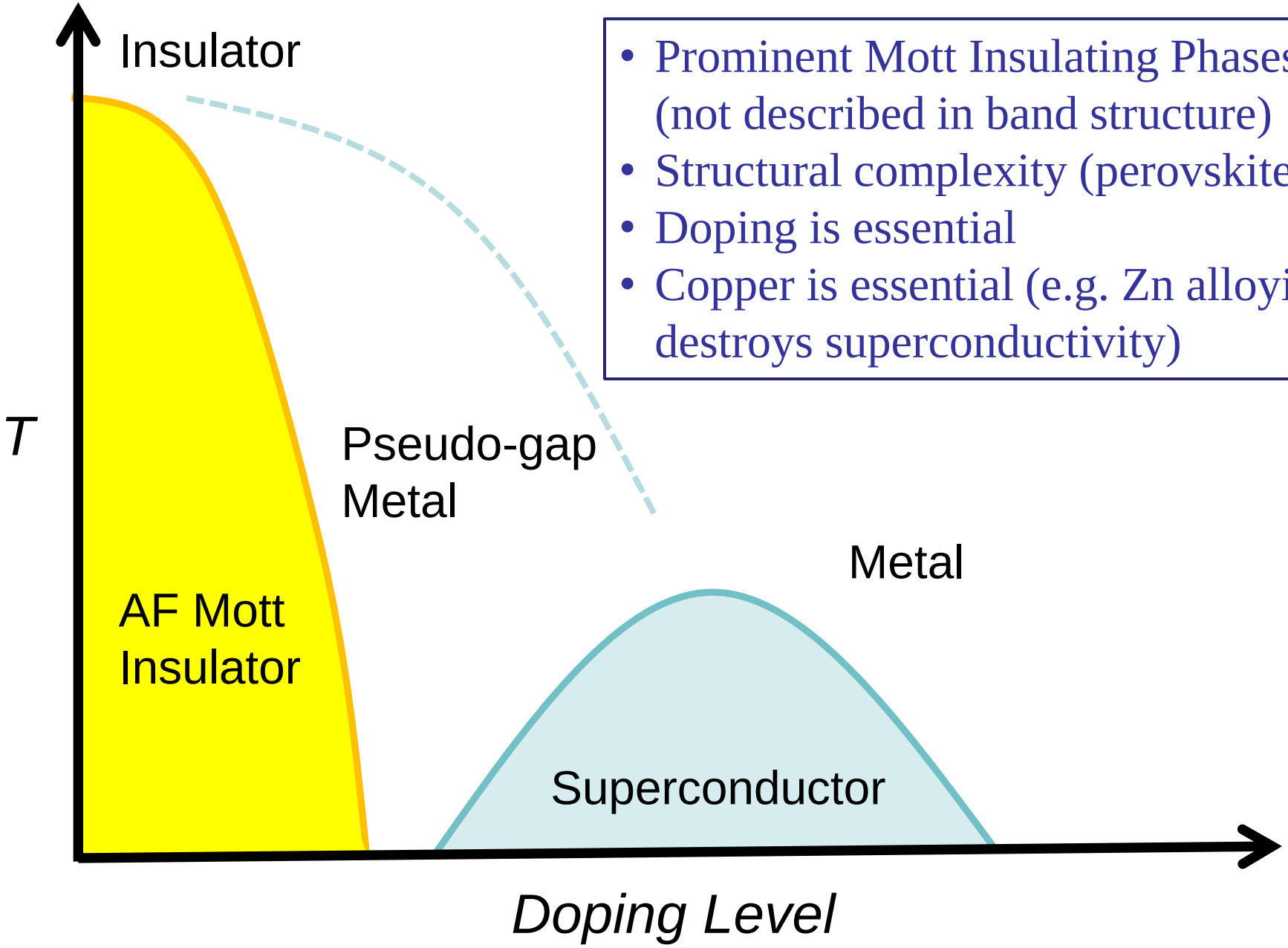
LaFePO, $T_c \sim 4K$

Kamihara, Watanabe and Hosono, JACS, Feb. 2008

$LaFeAsO_{1-x}F_x$ T_c=26K

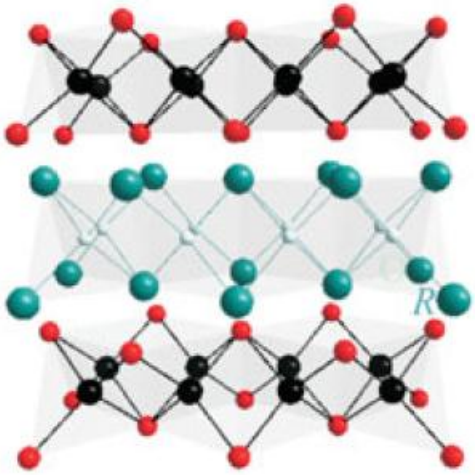


A Brief Introduction to Cuprates



- Prominent Mott Insulating Phases (not described in band structure)
- Structural complexity (perovskite)
- Doping is essential
- Copper is essential (e.g. Zn alloying destroys superconductivity)

A Big Family of High T_c Superconductors



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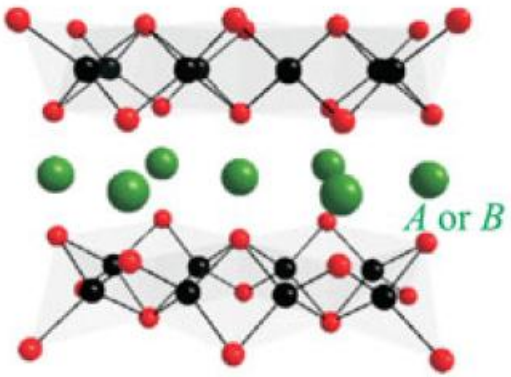

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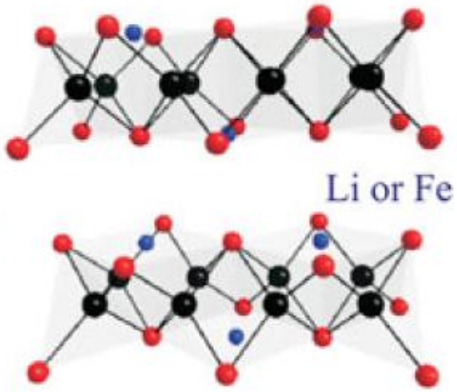

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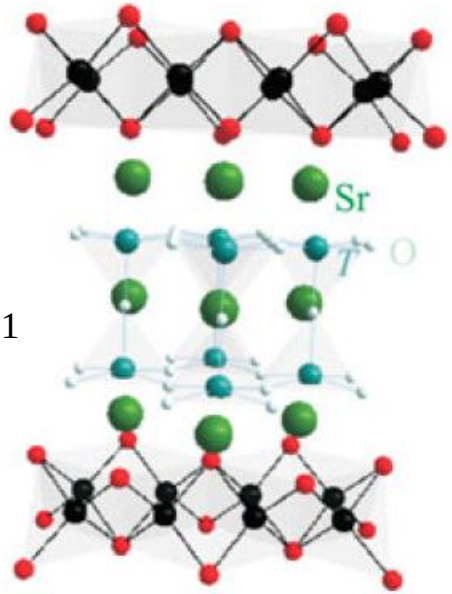

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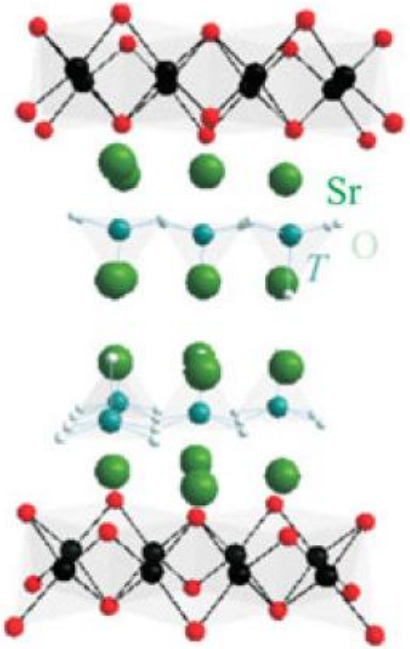

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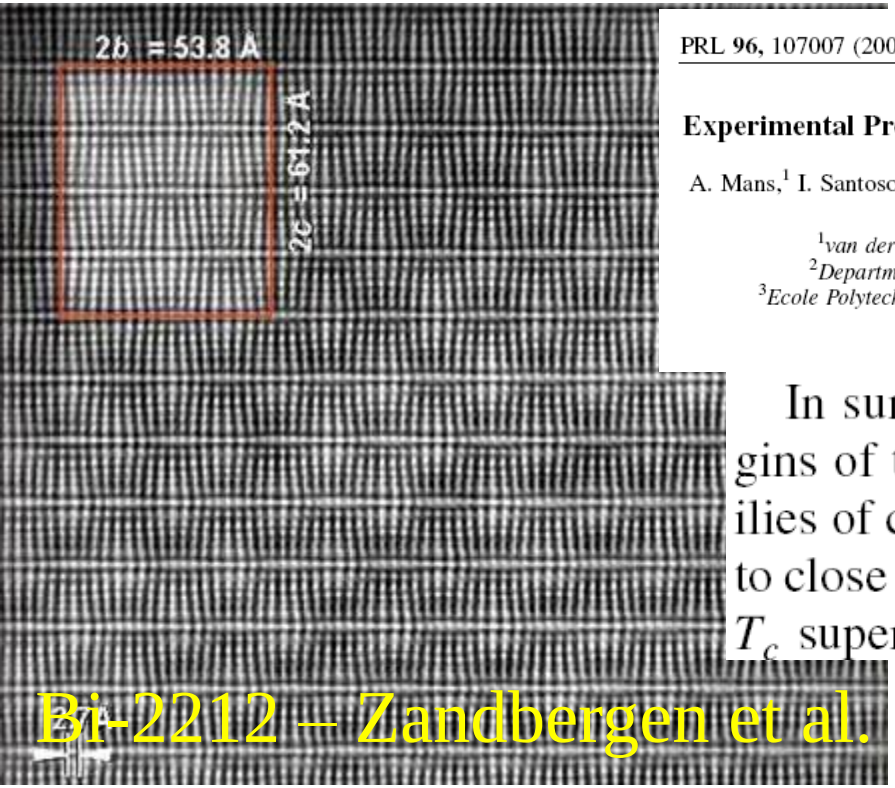
Sefat *et al.*, MRS Bull. **36**, 216 2011

Common Features:

- High T_c.
- Near magnetism.
- Fe square lattice.
- Near divalent Fe.
- Tetrahedral coordination.

A Word About Structure

- Large size of As^{3-},Se^{2-} relative to Fe^{2+} leads to tetrahedral structures with anion contact (edge shared tetrahedra). Tendency to high symmetry, small unit cells without structural distortion.
- Cuprates, etc. are based on corner shared units, with resulting tendency to complex structure distortions. The interplay with properties greatly complicates the physics.



Bi-2212 – Zandbergen et al.

PRL 96, 107007 (2006) PHYSICAL REVIEW LETTERS week ending 17 MARCH 2006

Experimental Proof of a Structural Origin for the Shadow Fermi Surface of $Bi_2Sr_2CaCu_2O_{8+\delta}$

A. Mans,[1] I. Santoso,[1] Y. Huang,[1] W. K. Siu,[1] S. Tavaddod,[1] V. Arpiainen,[2] M. Lindroos,[2] H. Berger,[3] V. N. Strocov,[4] M. Shi,[4] L. Patthey,[4] and M. S. Golden[1]

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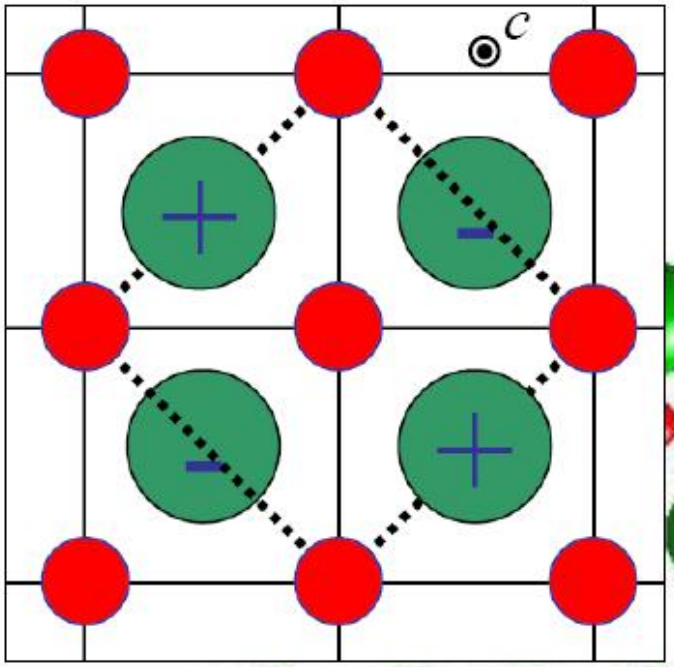
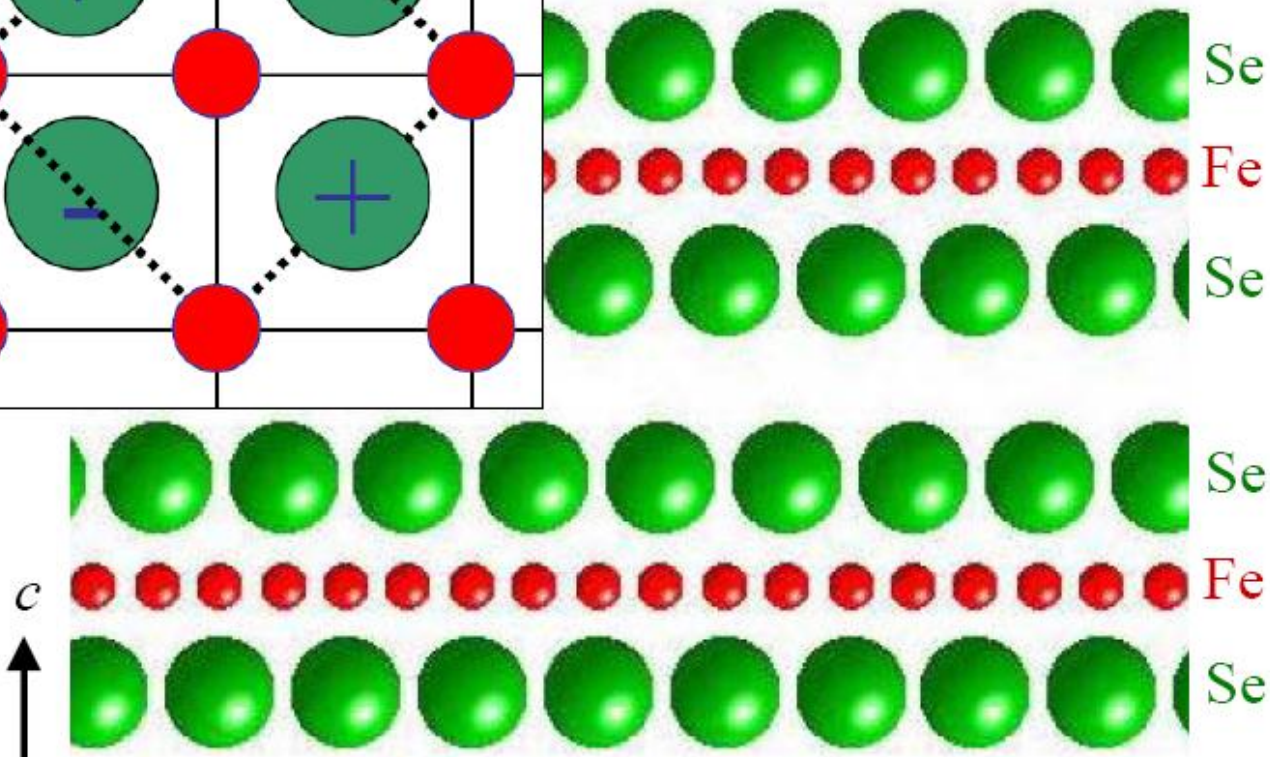
(Received 3 August 2005; published 16 March 2006)

In summary, by proving the microscopic structural origins of the shadow bands in the Bi2212 and Bi2201 families of cuprate superconductors, we have finally been able to close this chapter in the rich and complex tale of the high T_c superconductors.

FeSe - The "Simplest" Fe-Superconductor

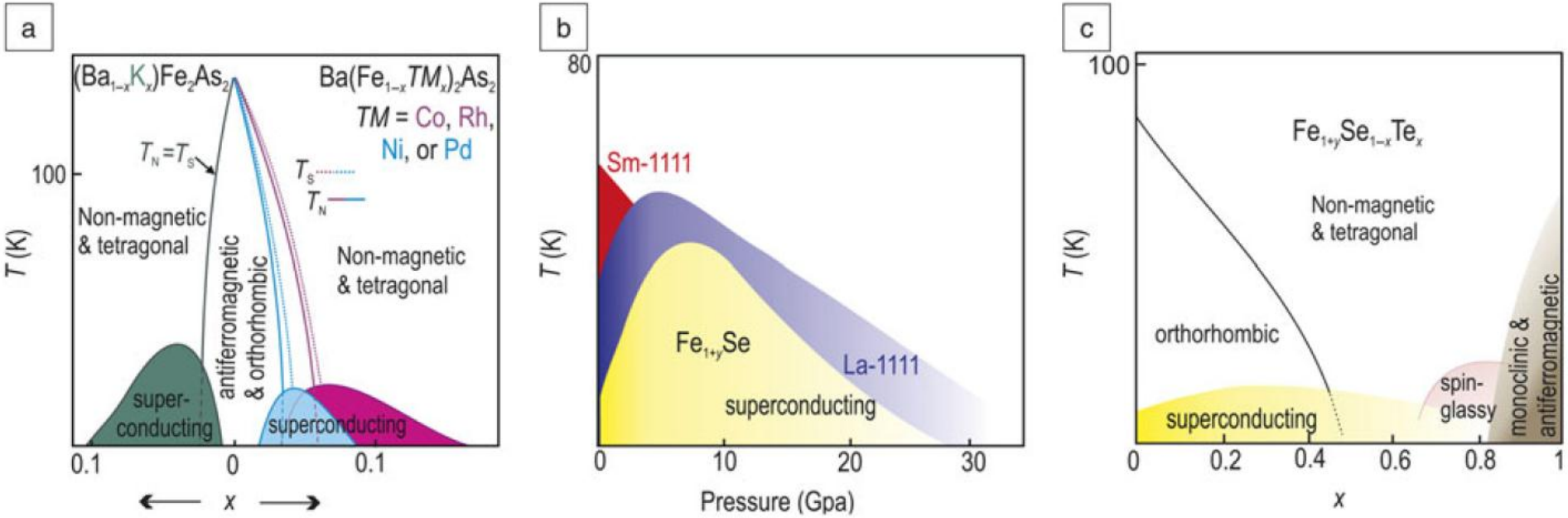
- Simple tetragonal structure, four atoms per unit cell (Hagg and Kindstrom, Z. Phys. Chem. (1933).
  - Actual material is $Fe_{1+x}Se$, with extra Fe in holes of Se lattice.
  - LiFeAs is similar, but extra sites are filled with Li.





$d_{Fe\text{-}Fe}$= 2.66 Å

Some Phase Diagrams



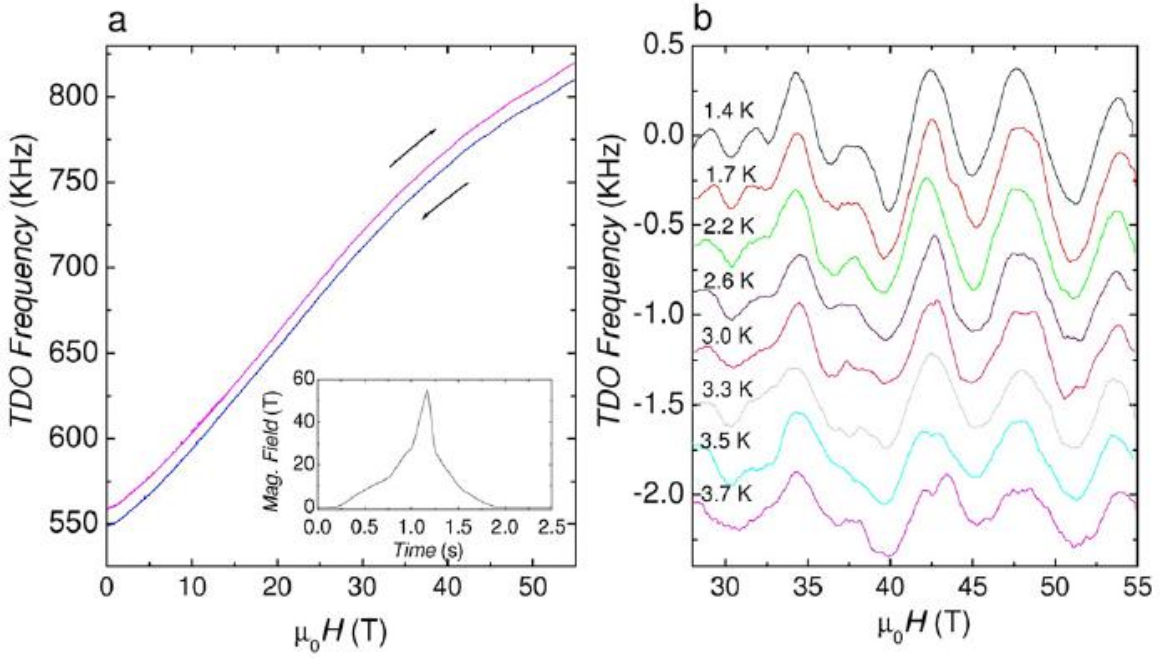
Sefat *et al.*, MRS Bull. **36**, 216 (2011)

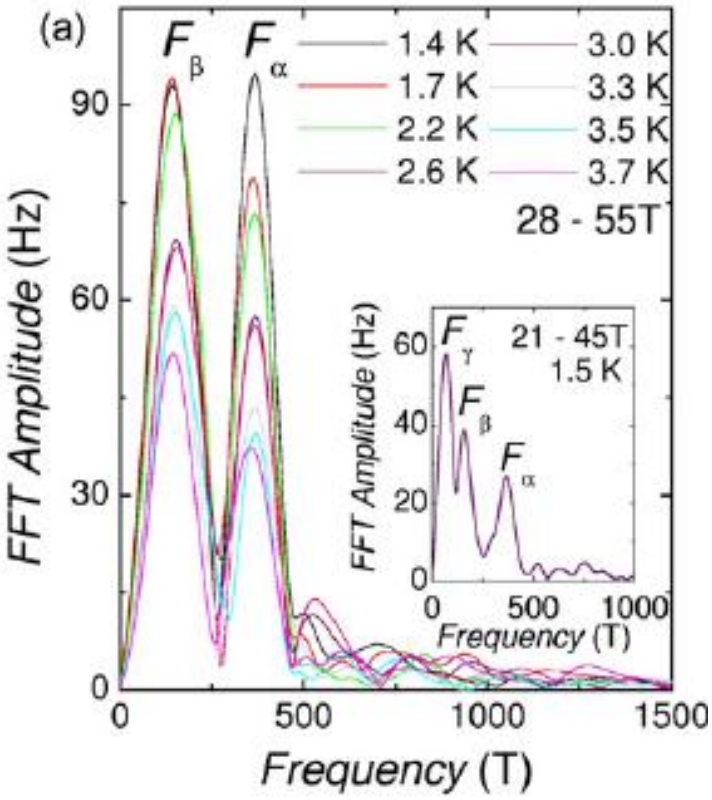
Not List:

- Doping is not essential.
- Not in proximity to Mott phases.
- Magnetic order & superconductivity not incompatible (compete).
- Orthorhombicity occurs without magnetic order, but not always, and highest T_c is tetragonal (but large orthorhombic regions).
- Maximum T_c in different families is not so different (factor of ~2).

Metallic Antiferromagnetic State

$SrFe_2As_2$ (Sebastian *et al.*)



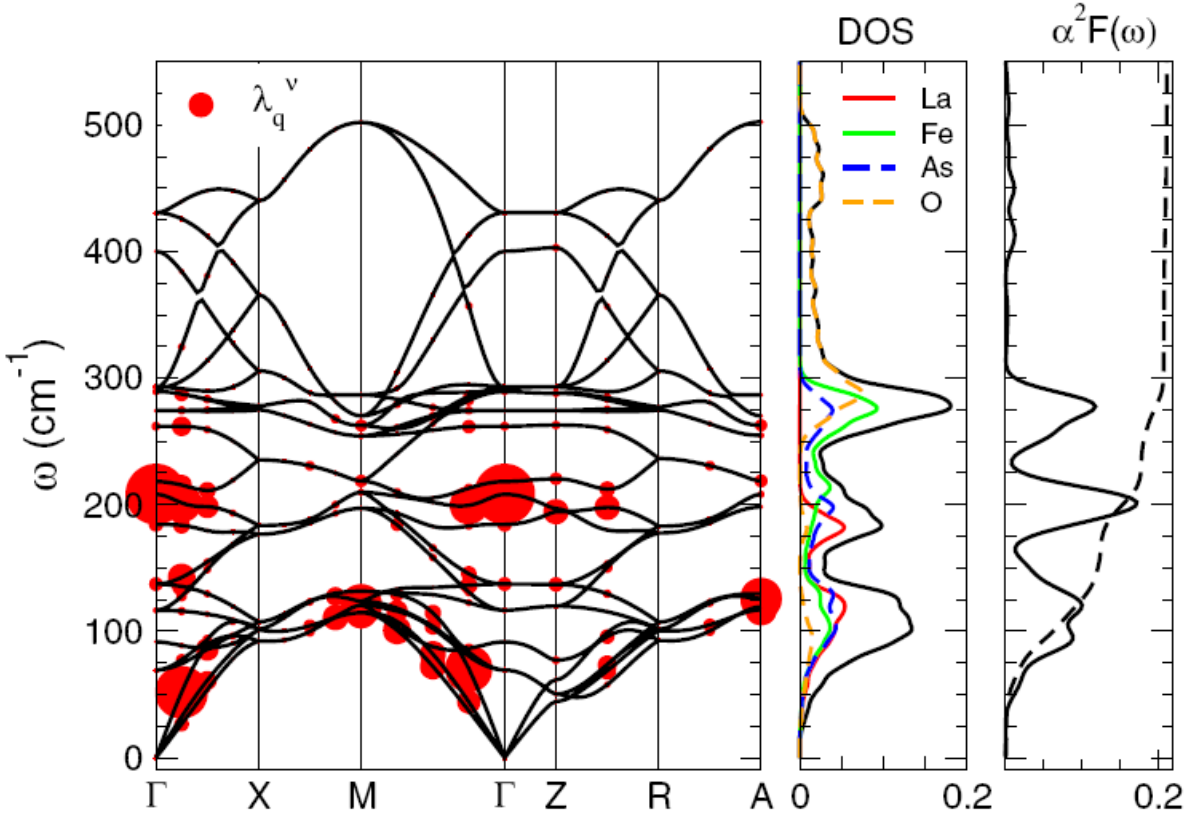


Shubnikov – de Hass measured by tunnel diode method.

SDW state has quantum oscillations reflecting a Fermi surface and is therefore a metal.

Phonons and Electron-Phonon Interaction

- First principles calculations allow direct calculation of pairing interaction, and almost first principles calculation of T_c.
- Calculations show weak coupling, no superconductivity (λ_{ep}~0.2).



- Fe/As phonons are below 300 cm^{-1}.
- Corresponding Ni compounds, LaNiPO, LaNiAsO, $BaNi_2As_2$ ... are electron-phonon superconductors!
- Fe compounds are not electron-phonon superconductors.

Boeri, et al., PRL (2008); also Mazin, et al., PRL (2008).

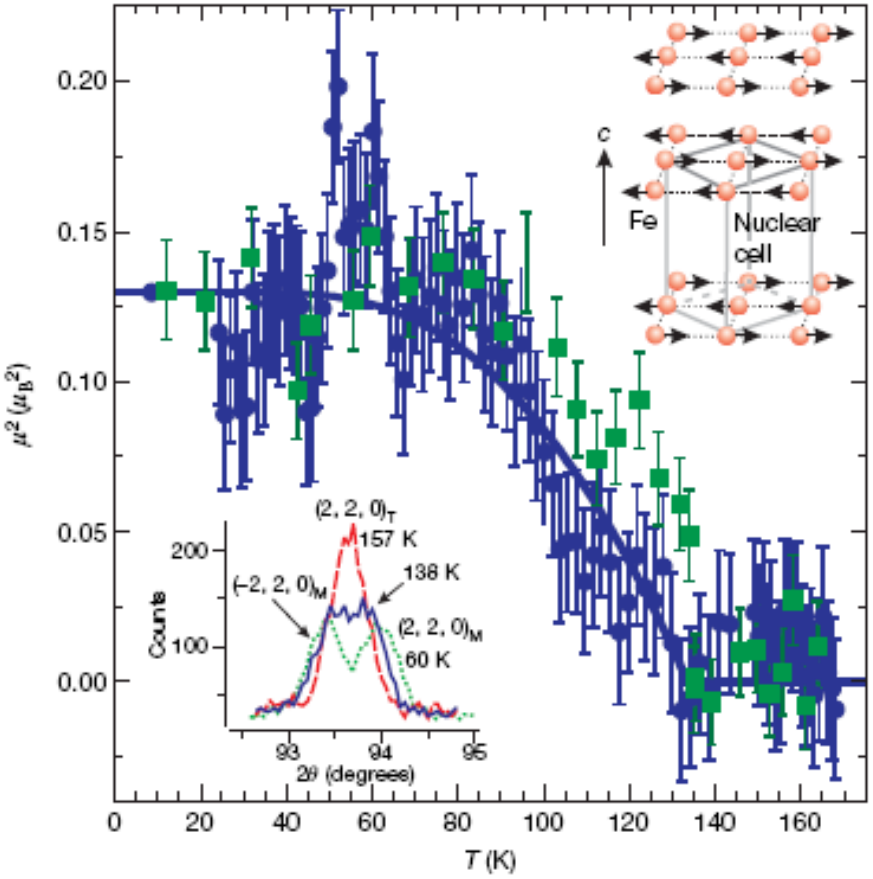
Neutron Scattering – Magnetism & Structure

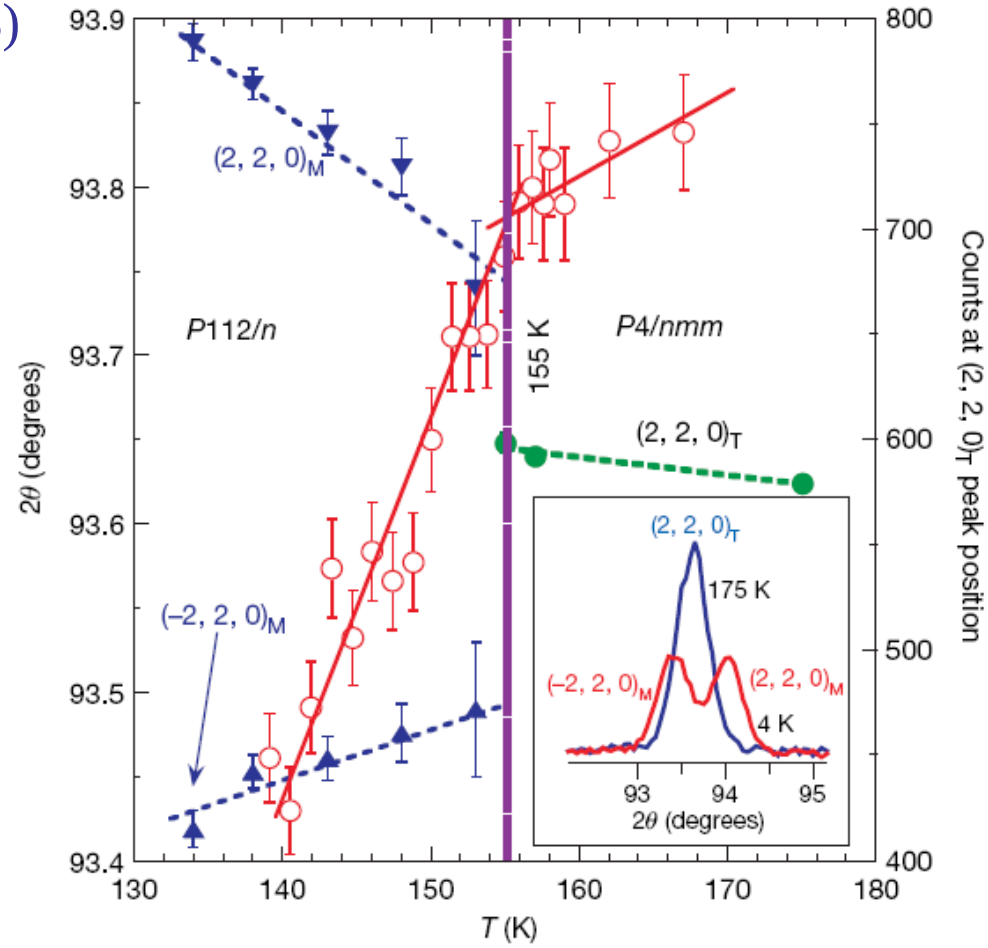
LaFeAsO:

Ordered m(Fe) = 0.36 μ_B

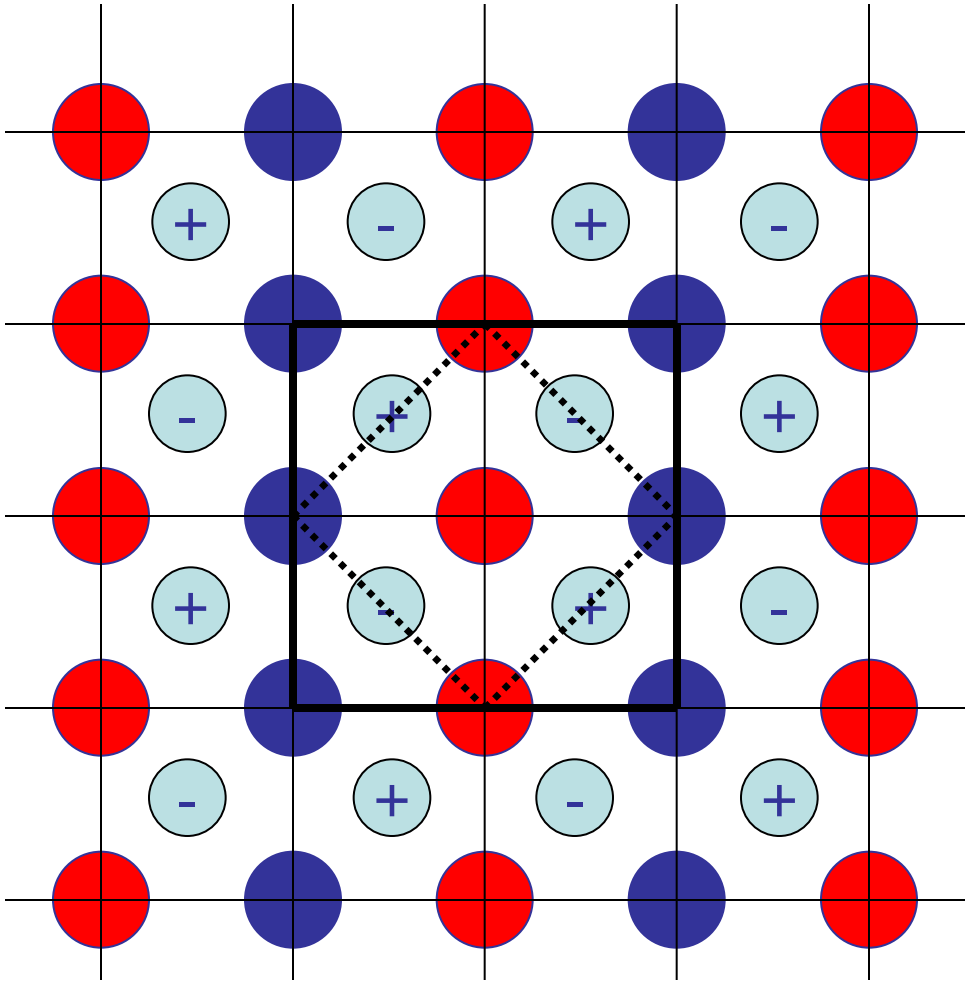
(other compounds so far are between 0.3 and 1 μ_B)

C. de la Cruz et al., Nature **453**, 899 (2008)





In-plane SDW structure



1 D Chains of parallel spin Fe atoms.

Hund's Coupling

- Hund's coupling in 3d ions is strong (Stoner I~0.8 eV)
- Spin-fluctuations are then expected to couple to electronic states in the *d*-band going up to high energy (i.e. the *d*-band width) – may be observable in spectroscopy. Drude weight seems reduced in optics.

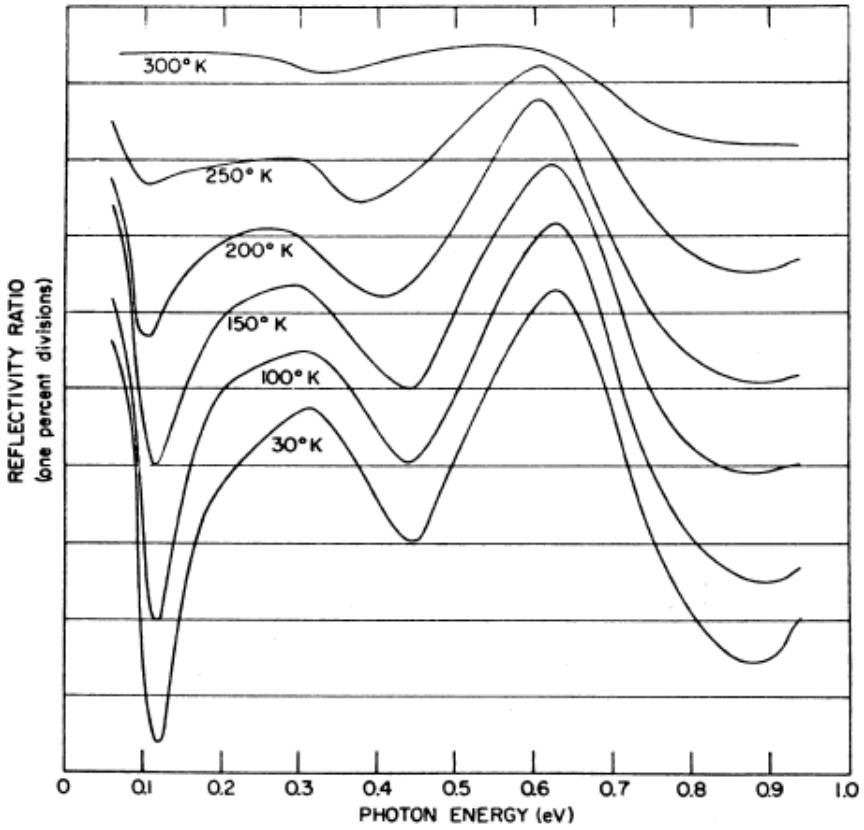
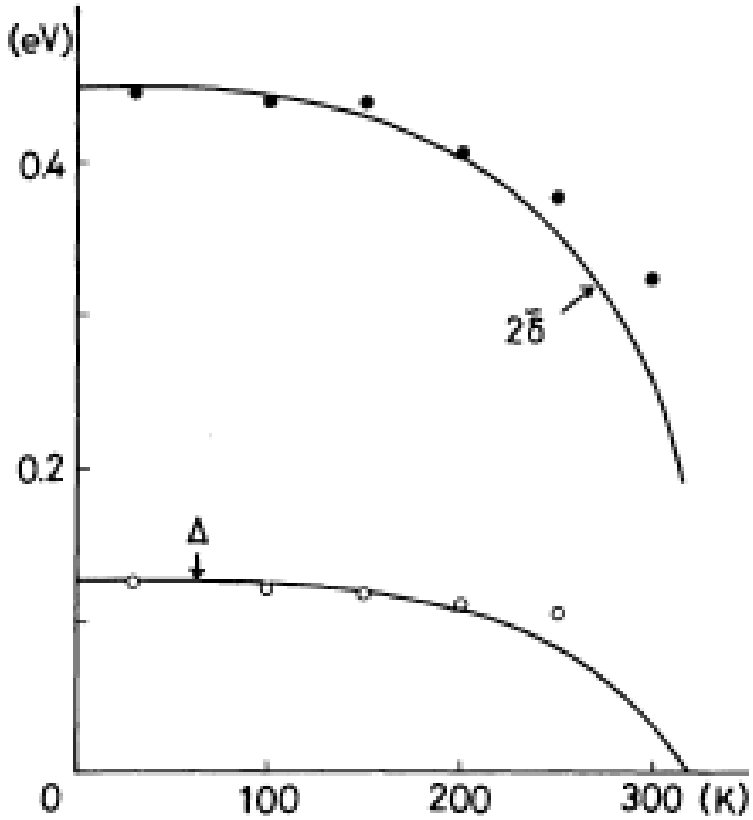


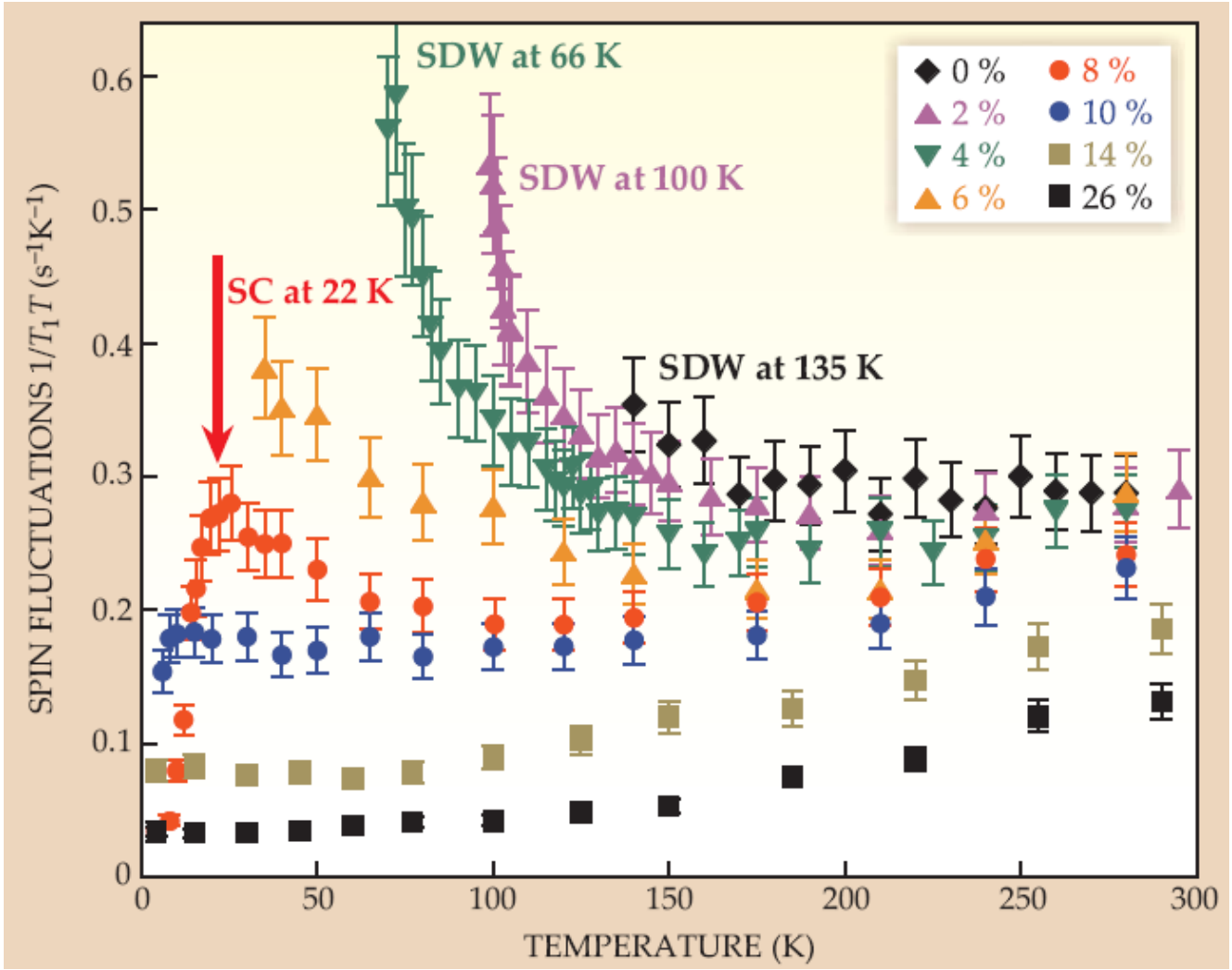
Fig. 3. The temperature dependent reflectivity of chromium normalized to $T=400$ K.

Cr metal: Machida et al., JPSJ (1984).



NMR: Connection of SDW and SC States

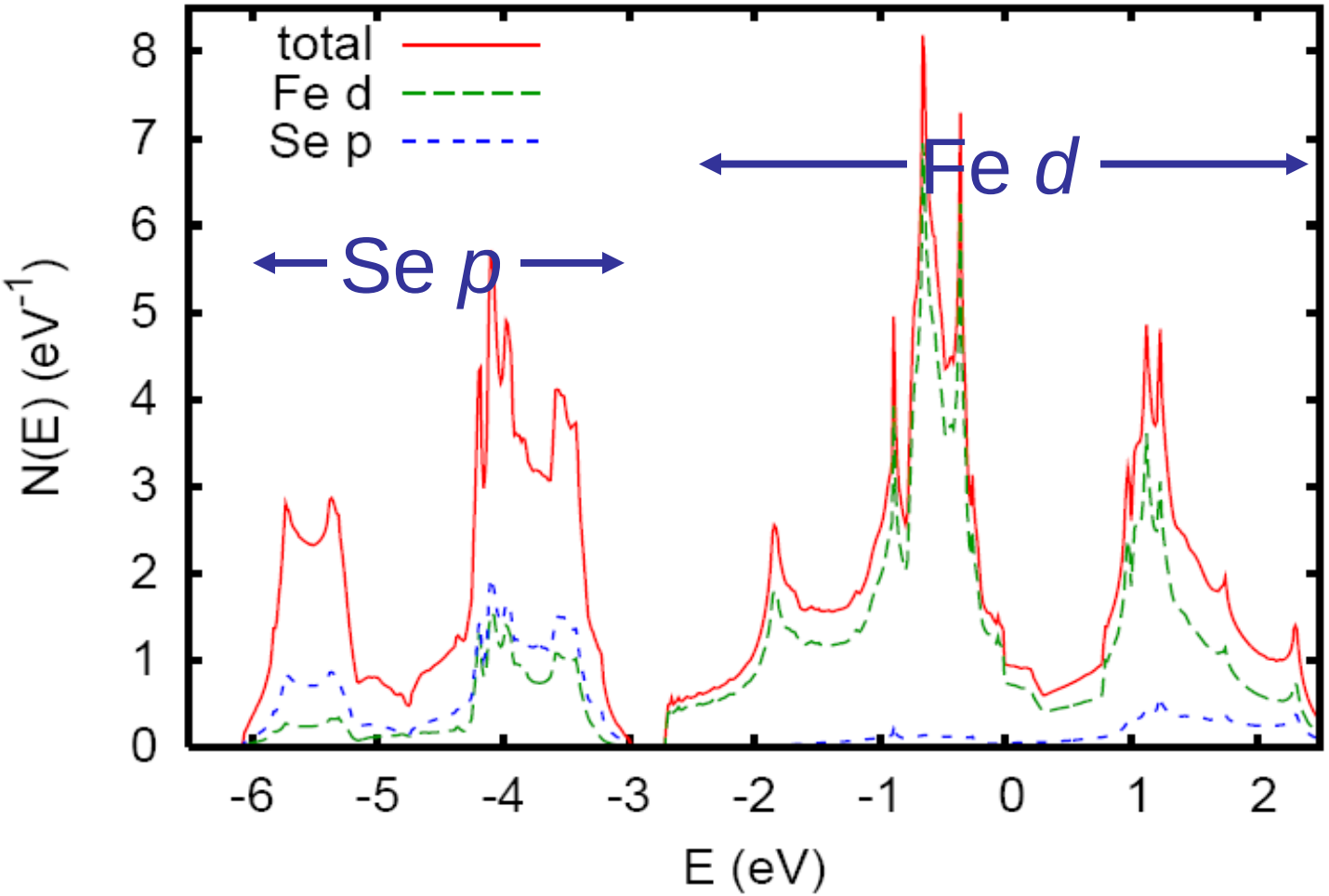
$1/T_1T$ shows strong spin fluctuations (constant for ordinary F.L.)



Ning, et al., JPSJ **78**, 013711 (2009).

LDA Electronic Structure of FeSe

- A rather ionic material – Fe^{2+} and Se^{2-} with some hybridization, as in an oxide ➔ metallic sheets of Fe^{2+} modified by interaction of anions.
- Pauling electronegativities: Fe = 1.83; Se = 2.55; As = 2.18.



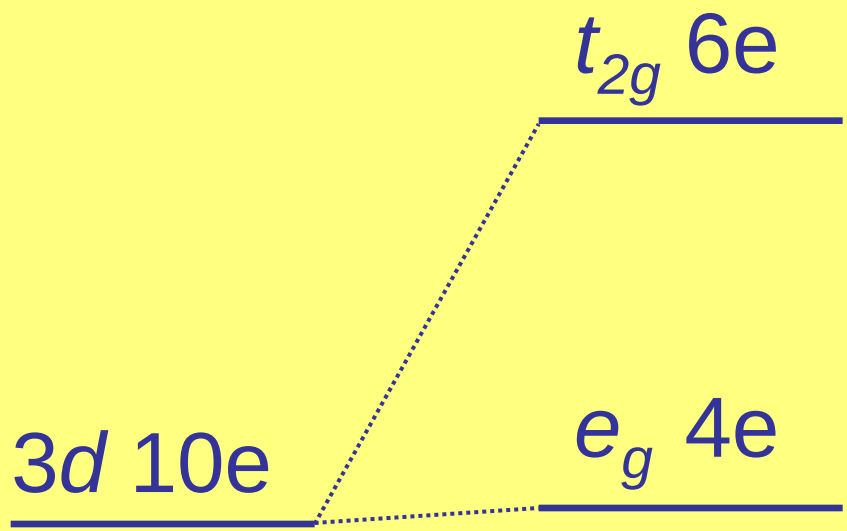
Fe^{2+} ➔ d^6

$N(E_F)$ is at bottom of pseudogap.

Formation of Band Structure

- Bands from -2 eV to +2 eV are derived from Fe^{2+} *d*-states.
- Fe^{2+} has 6 *d*-electrons.

Tetrahedral Crystal Field Scheme:

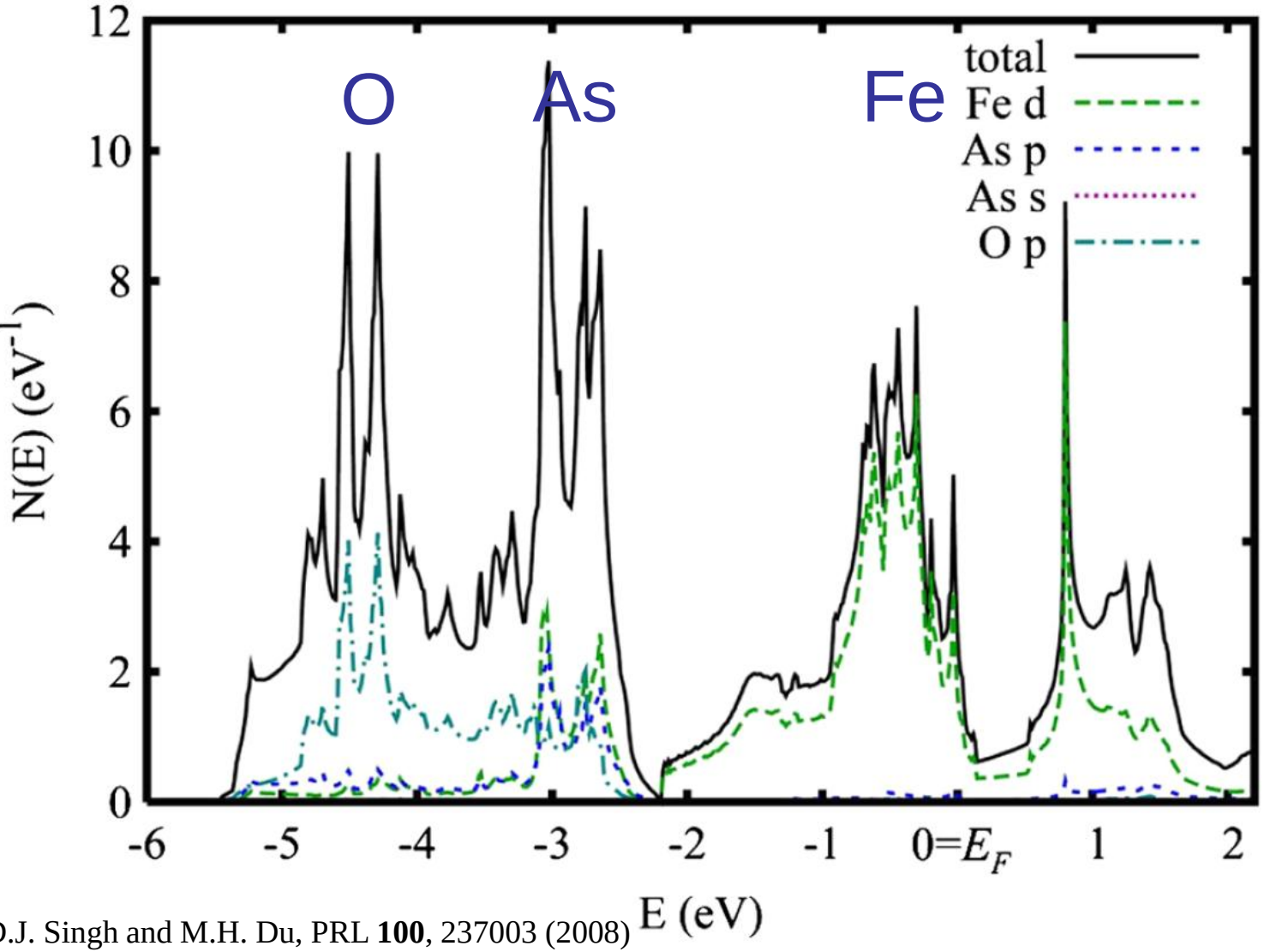


Does not correspond to the calculated electronic structure.

Key is the short Fe-Fe bond length → direct Fe-Fe interactions.

Arsenide Electronic Structure: LaFeAsO

- LaFeAsO: Rather ionic electronic structure: O^{2-}, As^{3-}, La^{3+}
- Bands near E_F are derived from Fe with little As admixture



Metallic sheets of Fe^{2+}

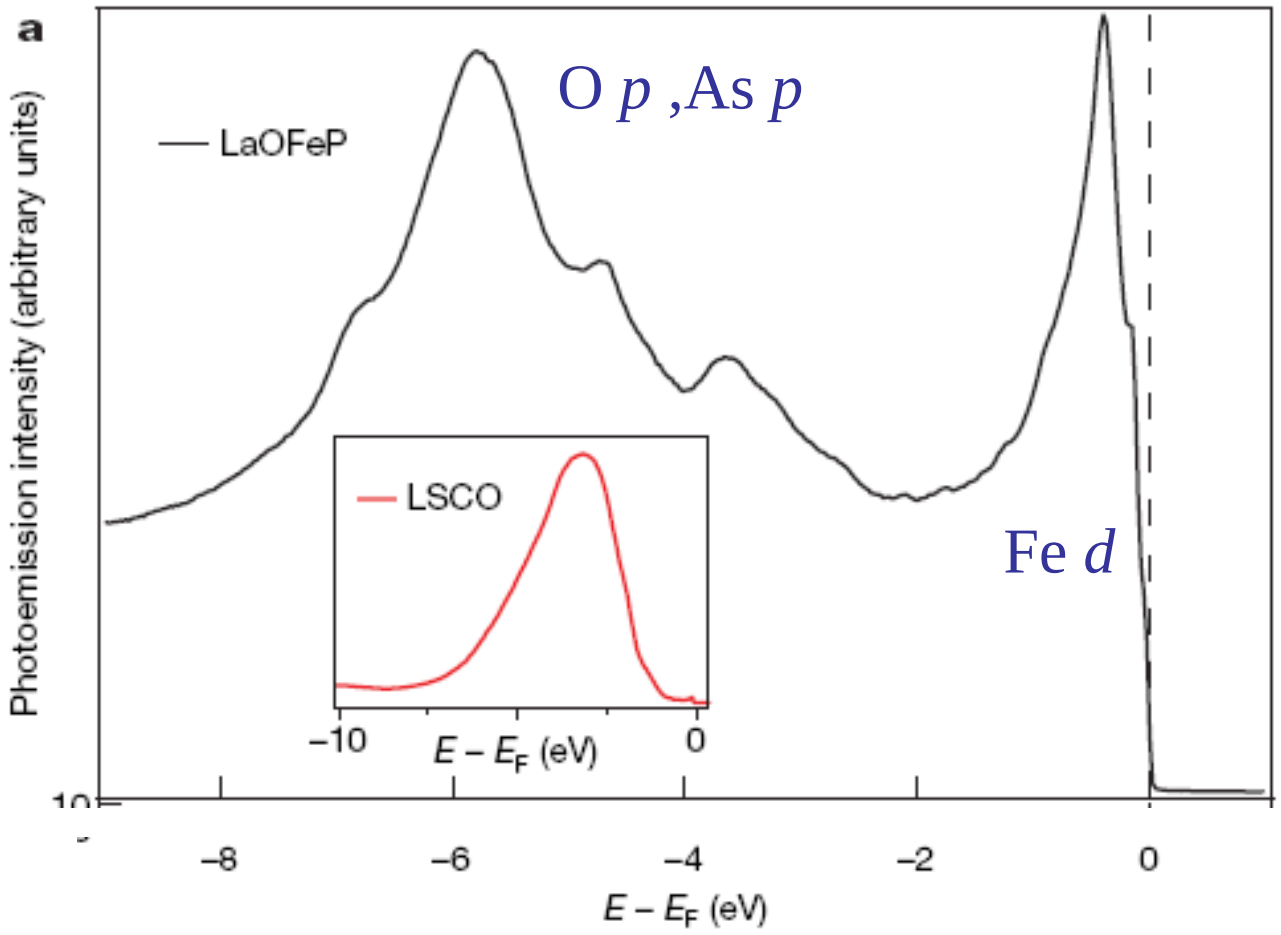
E_F is at the bottom edge of a pseudogap

High $N(E_F)$ ➔ near magnetism

D.J. Singh and M.H. Du, PRL **100**, 237003 (2008)

Metallic Character

Photoemission: LaFePO (D.H. Lu et al.)

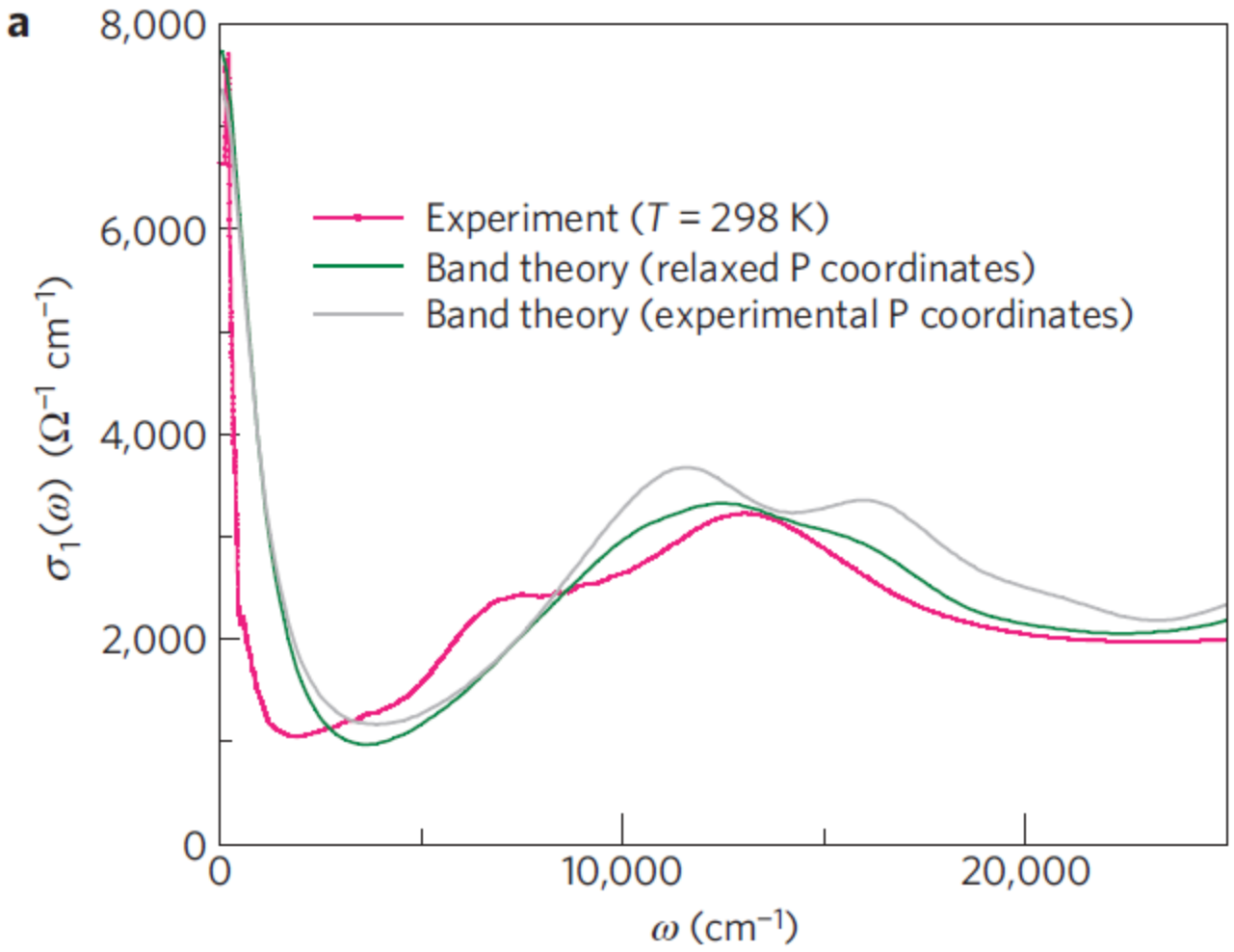


Very prominent Fermi edge (not like cuprates).

Fe d bands are narrower (by ~2) compared to LDA.

Optics

LaFePO (M.M. Qazilbash et al.)



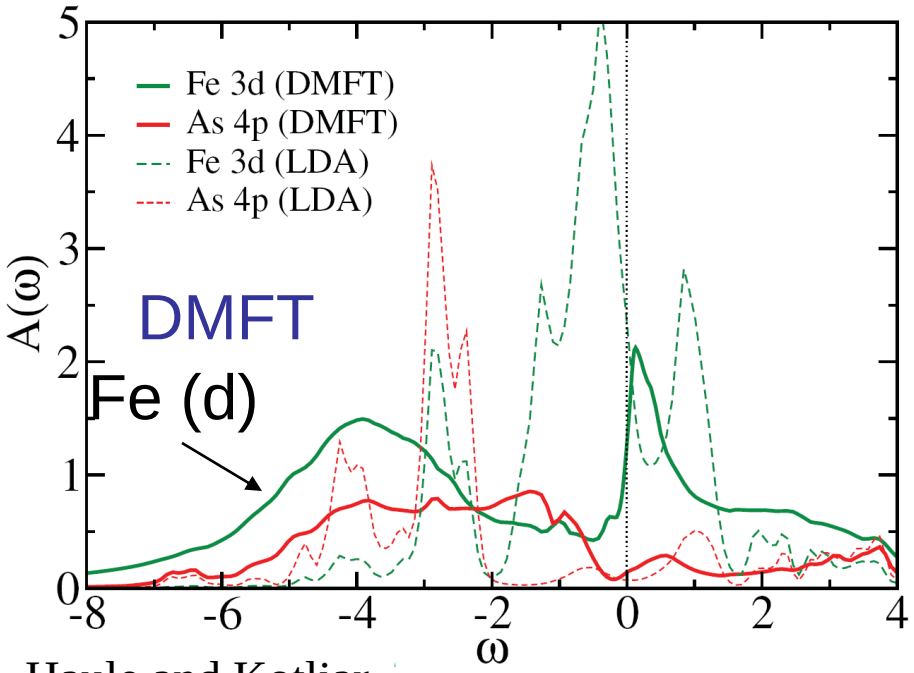
Drude has lower weight than in band calculation.

Re-distrubution of spectral weigh in d-bands.

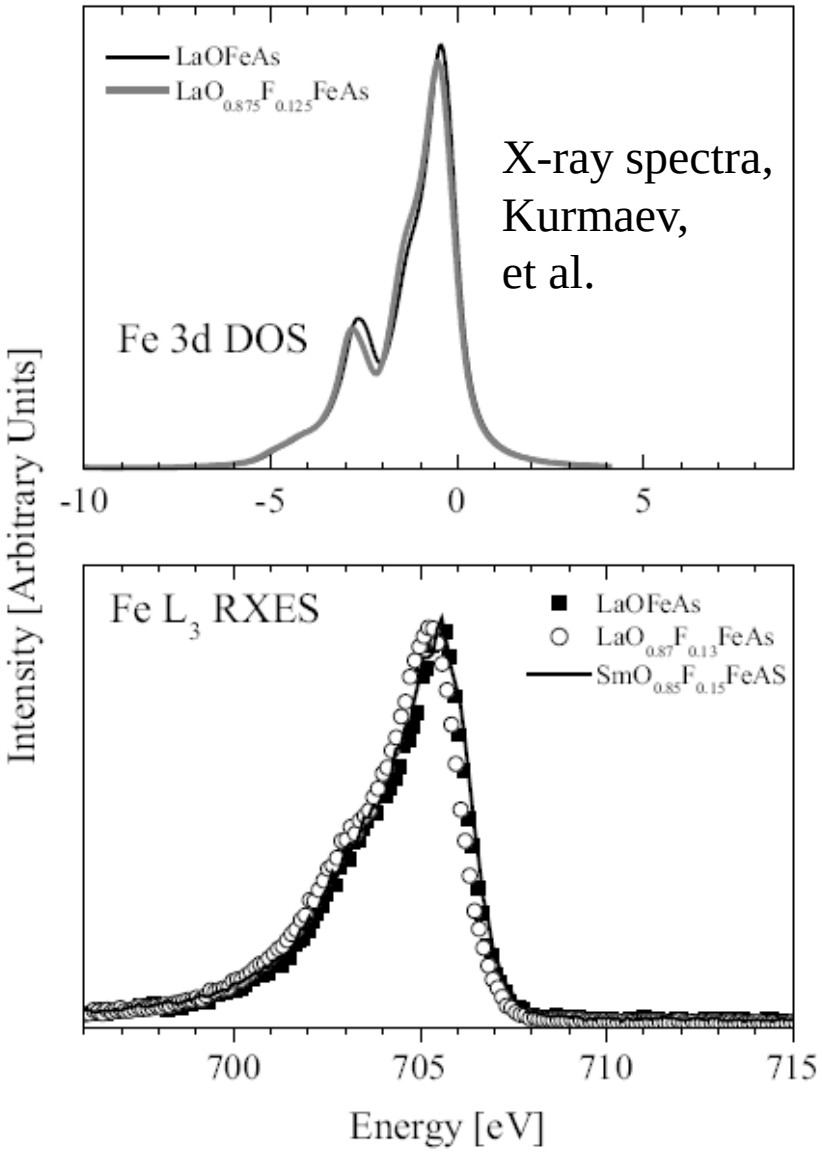
No Hubbard bands.

Coulomb Correlations

- LDA and correlated approaches give different predictions.
- So far Hubbard bands are not seen; strong Fe d character is seen at Fermi edge.
- There is however a renormalization of ~2 in band width c.f. LDA.



Haule and Kotliar



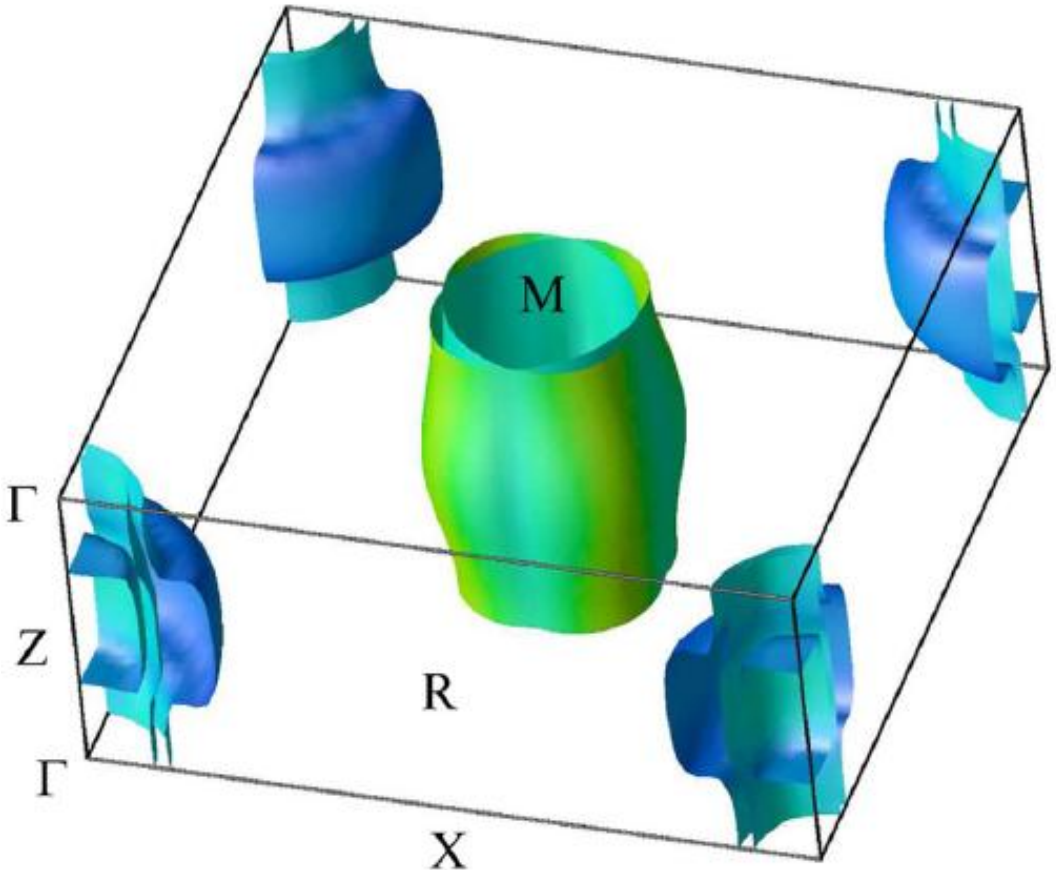
PRL 100, 237003 (2008) PHYSICAL REVIEW LETTERS week ending 13 JUNE 2008

Density Functional Study of $LaFeAsO_{1-x}F_x$: 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, USA

(Received 4 March 2008; published 12 June 2008)



Fermi Surface of LaFeAsO

(not spin polarized)

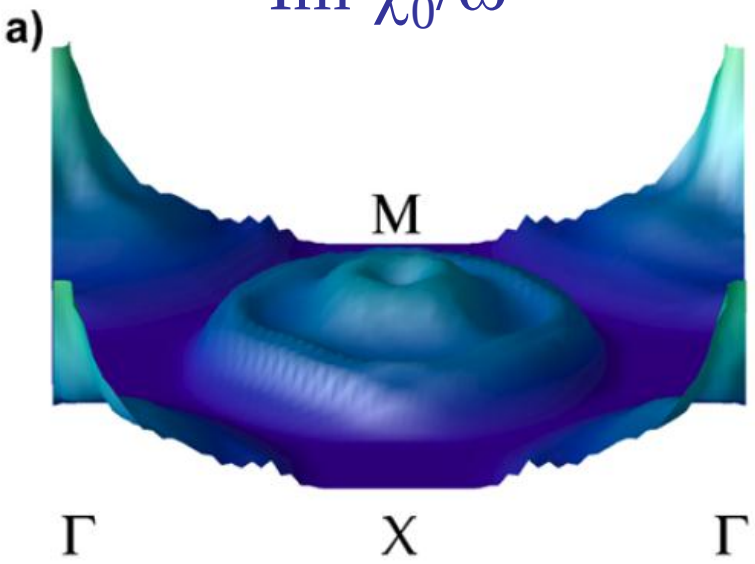
Low carrier density:
$n_e = n_h = 0.13$ / Fe

Band anisotropy: $\langle v_x^2 \rangle / \langle v_z^2 \rangle \sim 15$ ➔
a modest value that is favorable for applications.

Lindhard Function (Metal Physics)

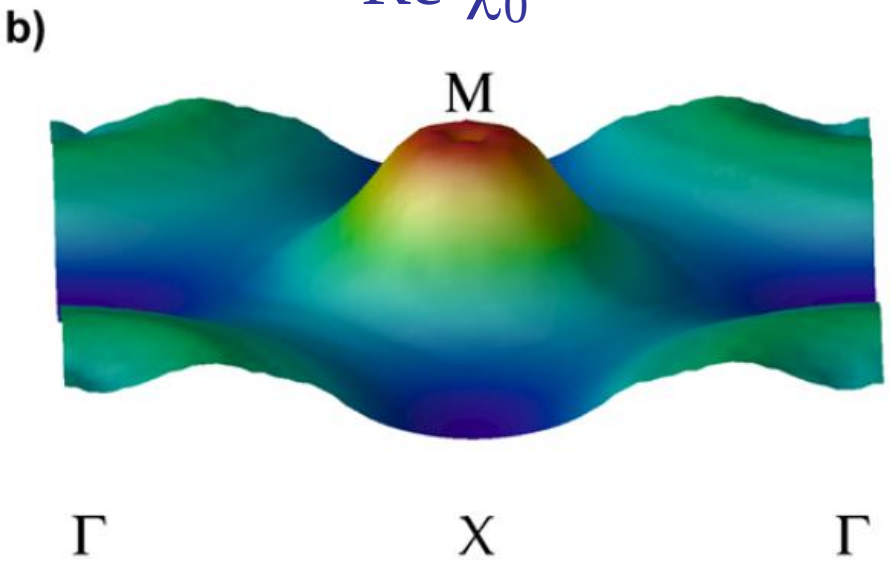
- LaFeAs(O,F) neglecting matrix elements:

Im χ_0/ω



Scattering, Transport

Re χ_0



Magnetism, Superconductivity

Note the pronounced peak at the zone corner.

I.I. Mazin, D.J. Singh, M.D. Johannes and M.H. Du, PRL **101**, 057003 (2008)

Spin Fluctuations and Superconductivity

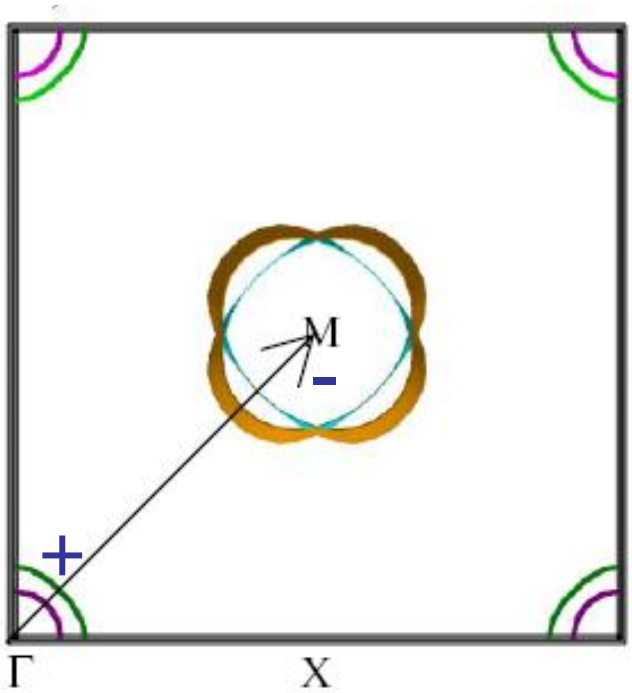
One way to proceed (weak coupling):

- Calculate matrix elements $V_{\mathbf{k},\mathbf{k}'}$, for a set of $\mathbf{k},\mathbf{k}'$ on the FS.
- Set-up gap equation -- diagonalize V.

Berk-Schrieffer-Fay-Appel weak coupling theory, 1966-1980:

Singlet:

$$V(\mathbf{q}) = - \frac{I^2(q)\chi_0(\mathbf{q})}{1 - I^2(\mathbf{q})\chi_0^2(\mathbf{q})}$$



Electron doped LaFeAsO

In a singlet channel there is a minus sign for spin fluctuations (repulsive), which then favors opposite order parameters on the electron and hole sheets ➔ s +/- state.

Note prior work, Aronov & Sonin (1972); Kuroki and Arita (2001)

Does not have an obvious strongly q-dependent interaction for nodes in a FS.

I.I. Mazin, D.J. Singh, M.D. Johannes and M.H. Du, PRL **101**, 057003 (2008)

nature Vol 456|18/25 December 2008|doi:10.1038/nature07625

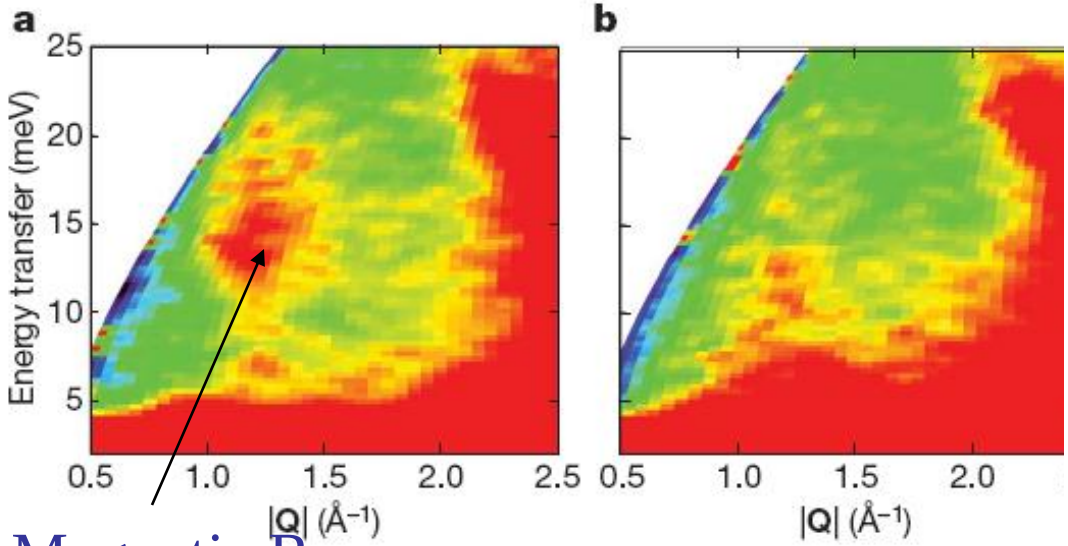
LETTERS

Unconventional superconductivity in $Ba_{0.6}K_{0.4}Fe_2As_2$ from inelastic neutron scattering

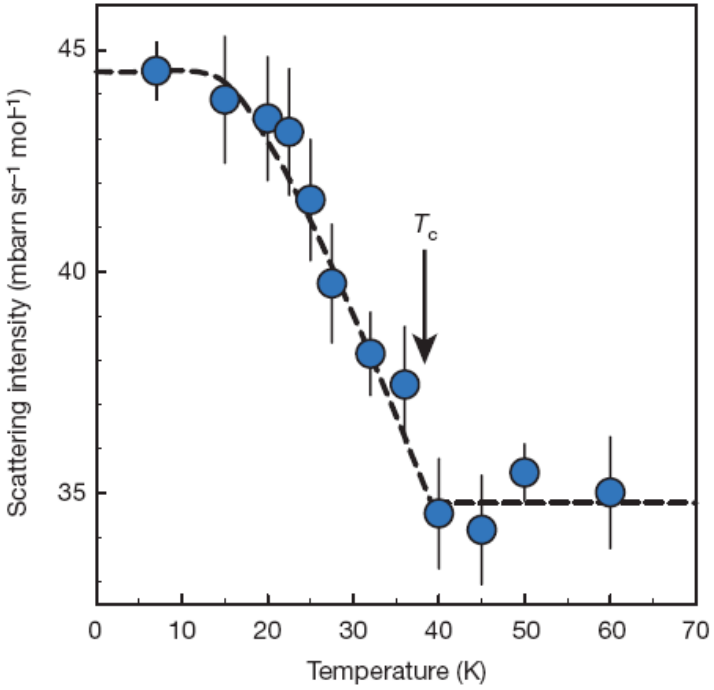
A. D. Christianson[1], E. A. Goremychkin[2,3], R. Osborn[2], S. Rosenkranz[2], M. D. Lumsden[1], C. D. Malliakas[2,4], I. S. Todorov[2], H. Claus[2], D. Y. Chung[2], M. G. Kanatzidis[2,4], R. I. Bewley[3] & T. Guidi[3]

T=7K

T=50K



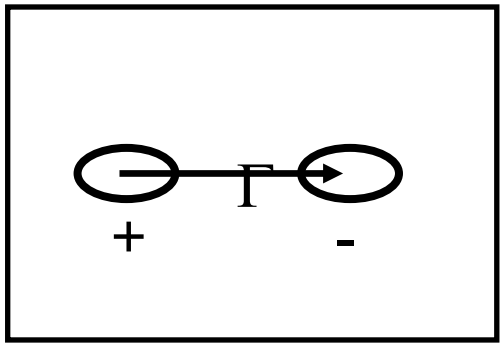
Magnetic Resonance



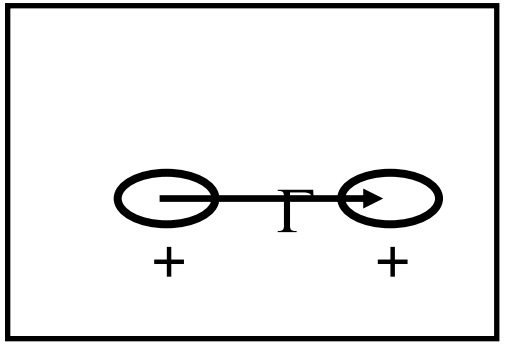
Sign changing gap with q corresponding to (π,π)

Small Fermi Surfaces in General

- Does superconductivity arise in general if one has small Fermi surfaces with nesting driven spin fluctuations? – Answer seems to be no.



p-wave state (triplet): spin-fluctuation pairing interaction has + sign ➔ Pair breaking for the state shown.



s-wave state (singlet): spin-fluctuation pairing interaction has – sign ➔Pair breaking for the state shown.

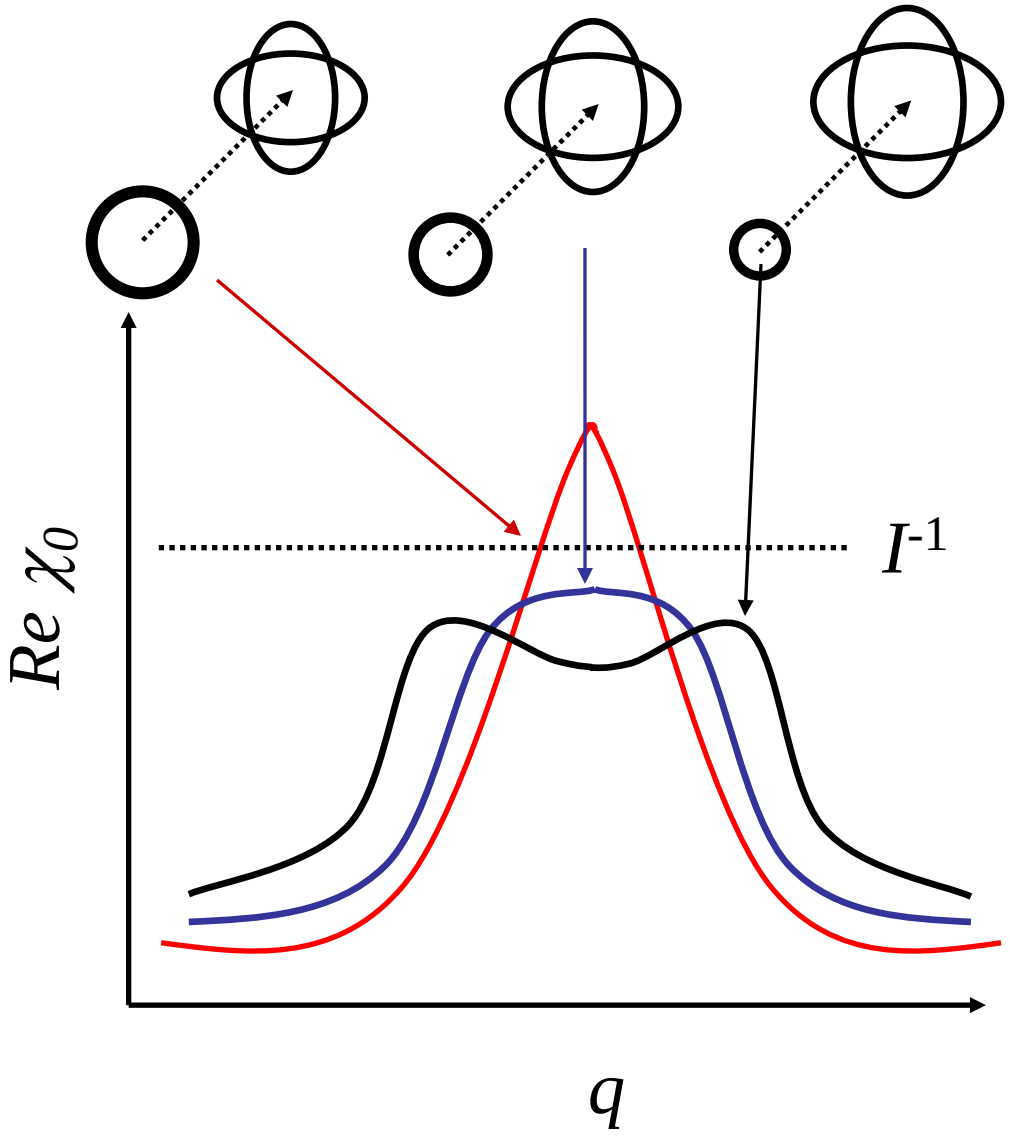
e.g. small pockets on Na_xCoO_2 (Johannes et al., 2004).

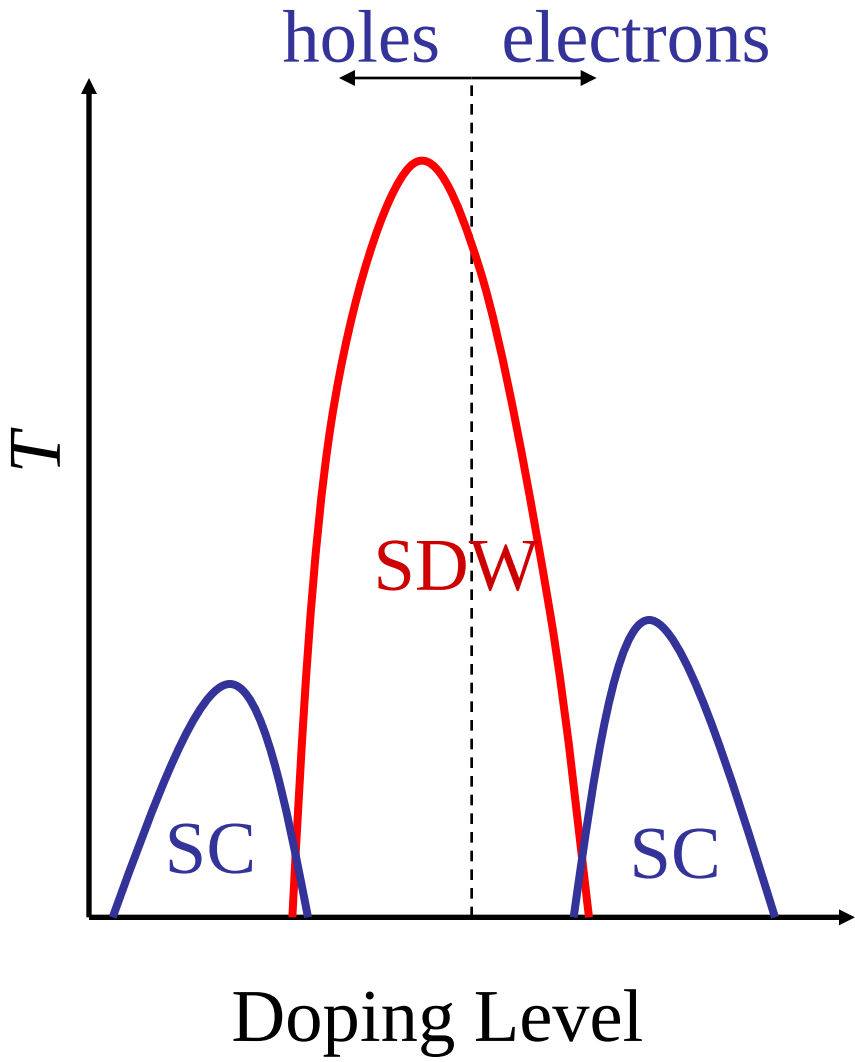
In such cases, look for chemistry with strong electron phonon and low Stoner parameter, to obtain Kohn anomaly and e-p superconductivity or maybe strange states, e.g. odd frequency.

Normal Metallic State

- Low carrier density semi-metal (dis-connected small Fermi surfaces).
- Less anisotropic than cuprates, even $YBa_2Cu_3O_7$.
- High $N(E_F)$.
  - Near itinerant magnetism in general.
  - Expect short coherence length relative to T_c.
  - Expect high superfluid density.
- Electron-Phonon interaction is weak ($\lambda \sim 0.2$, $T_c = 0$)

Nesting, Doping and the Lindhard Function





Disorder affects both magnetism and superconductivity

Neutron Scattering – Structure Details

LaFeAsO (Tetragonal → Orth/Mono):

Table 2 | Properties of LaOFeAs at 4 K

a, Refined structure parameters

Atom	Site	x	y	z	B (Å²)
La	2e	¼	¼	0.1426(3)	0.54(6)
Fe	2f	¾	¼	0.5006(12)	0.16(4)
As	2e	¼	¼	0.6499(4)	0.23(7)
O	2f	¾	¼	−0.0057(17)	0.69(7)

z_{As}(4K) = 1.308 Å

z_{As}(175K)=1.317 Å

$LaFeAsO_{0.92}F_{0.08}$ (Tetragonal):

Table 3 | Properties of $LaO_{0.92}F_{0.08}FeAs$ at 10 K (first line), 35 K (second line) and 175 K (third line)

a, Refined structure parameters

Atom	Site	x	y	z	B (Å²)
La	2c	¼	¼	0.1448(3)	0.40(5)
		¼	¼	0.1458(3)	0.50(5)
		¼	¼	0.1446(3)	0.73(5)
Fe	2b	¾	¼	½	0.32(4)
		¾	¼	½	0.41(4)
		¾	¼	½	0.65(4)
As	2c	¼	¼	0.6521(4)	0.41(7)
		¼	¼	0.6515(4)	0.40(6)
		¼	¼	0.6527(4)	0.69(7)
O/F	2a	¾	¼	0	0.53(6)
		¾	¼	0	0.62(6)
		¾	¼	0	0.71(6)

z_{As}(10K) = 1.323 Å

z_{As}(175K)=1.331 Å

Non-magnetic LDA calc. (LaFeAsO – Tetragonal)

z_{As}(LDA) = 1.159 Å

A huge difference!

C. de la Cruz et al., Nature **453**, 899 (2008)

Structure and Magnetism

- As height is too low by >0.1 Å in non-magnetic LSDA calculations.
- SDW is too robust in DFT.
- Using GGA and including magnetism one can obtain much better As height. In that case magnetism is extremely robust ($m \sim 2\mu_B$) contrary to experiment.
- Discrepancy in As height persists in the paramagnetic (superconducting) doped phases.

Metals Where the LSDA Overestimates Ferromagnetism

Class 1: Ferromagnets where the LDA overestimates the magnetization.

	m (LDA, μ_B/f.u.)	m (expt., μ_B/f.u.)
$ZrZn_2$	0.72	0.17
Ni_3Al	0.71	0.23
Sc_3In	1.05	0.20

Class 2: Paramagnets where the LDA predicts ferromagnetism

	m (LDA, μ_B/f.u.)	m (expt., μ_B/f.u.)
FeAl	0.80	0.0
Ni_3Ga	0.79	0.0
$Sr_3Ru_2O_7$	1.1	0.0
$Na_{0.7}CoO_2$	0.30	0.0

c.f. "Normal" Materials

	m (DFT, μ_B/f.u.)	m (expt., μ_B/f.u.)
bcc Fe	2.17	2.12
$SrRuO_3$	1.59	1.6

Renormalization and The Fluctuation Dissipation Theorem

Relates fluctuation amplitude to dissipation term, i.e. spin fluctuation spectrum:

$$\xi^2 = \frac{4\hbar}{\Omega}\int d^3q \int \frac{d\omega}{2\pi}\frac{1}{2}\,\mathrm{Im}\,\chi(\mathbf{q},\omega)$$

Landau functional approach (after Moriya, Shimizu, others) is based on the magnetic moment dependence of the total energy *without* fluctuations

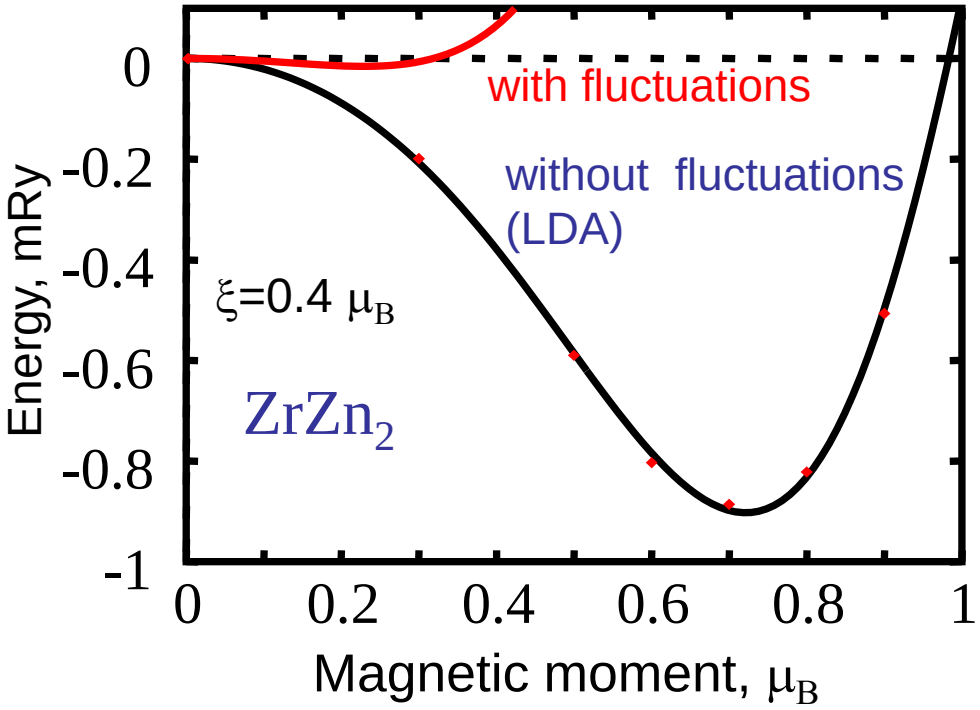
$$\Delta E(M) = aM^2 + bM^4 + cM^6 \qquad a^{-1}/2 = \chi, \text{ susceptibility}$$

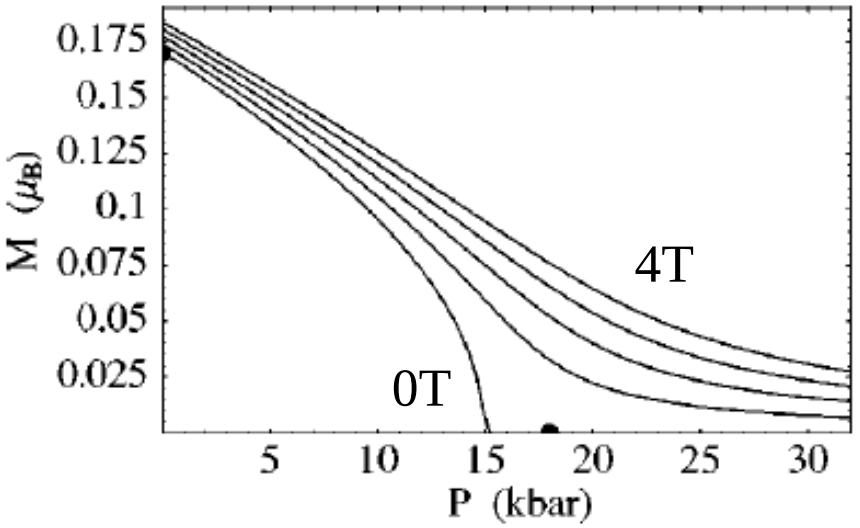
Spin fluctuations renormalize this dependence, i.e. a ➔ α, etc. via integration of the Landau functional with Gaussian of rms width ξ.

1. **Large renormalization ➔ large fluctuation amplitude.**
2. **Large amplitude requires large integral ➔ Im χ large over wide range of q and ω.**

Example: $ZrZn_2$ (Weak Itinerant Ferromagnet)

Bare LDA moment of ~0.7 μ_B to ~0.2 μ_B by fluctuations ξ ~ 0.4 μ_B



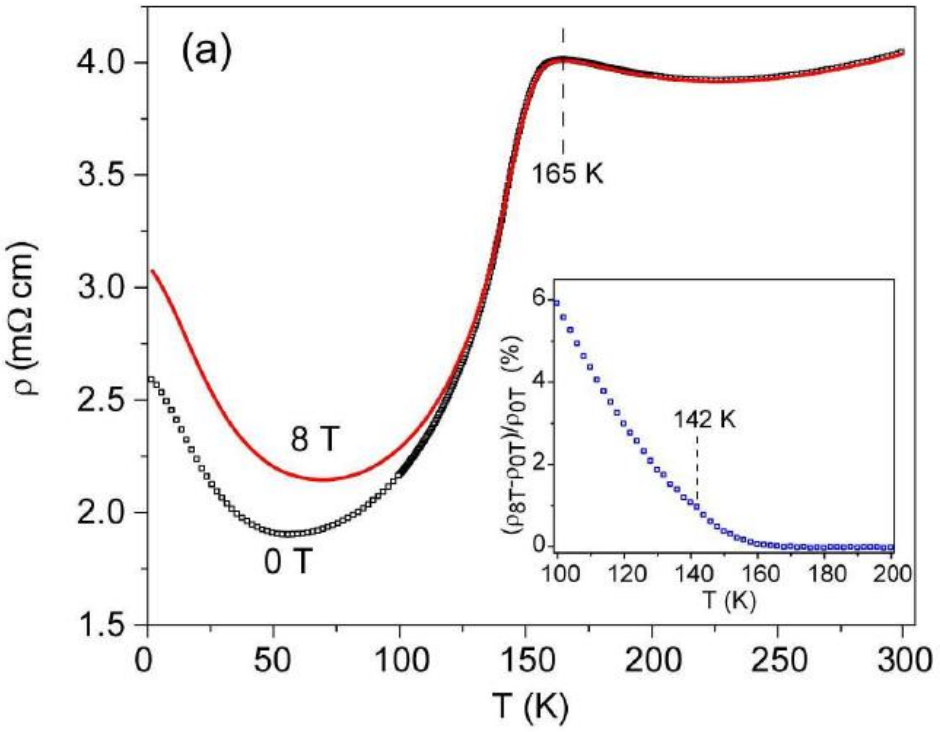


I.I. Mazin and D.J. Singh, Phys. Rev. B **69**, 020402 (2004).

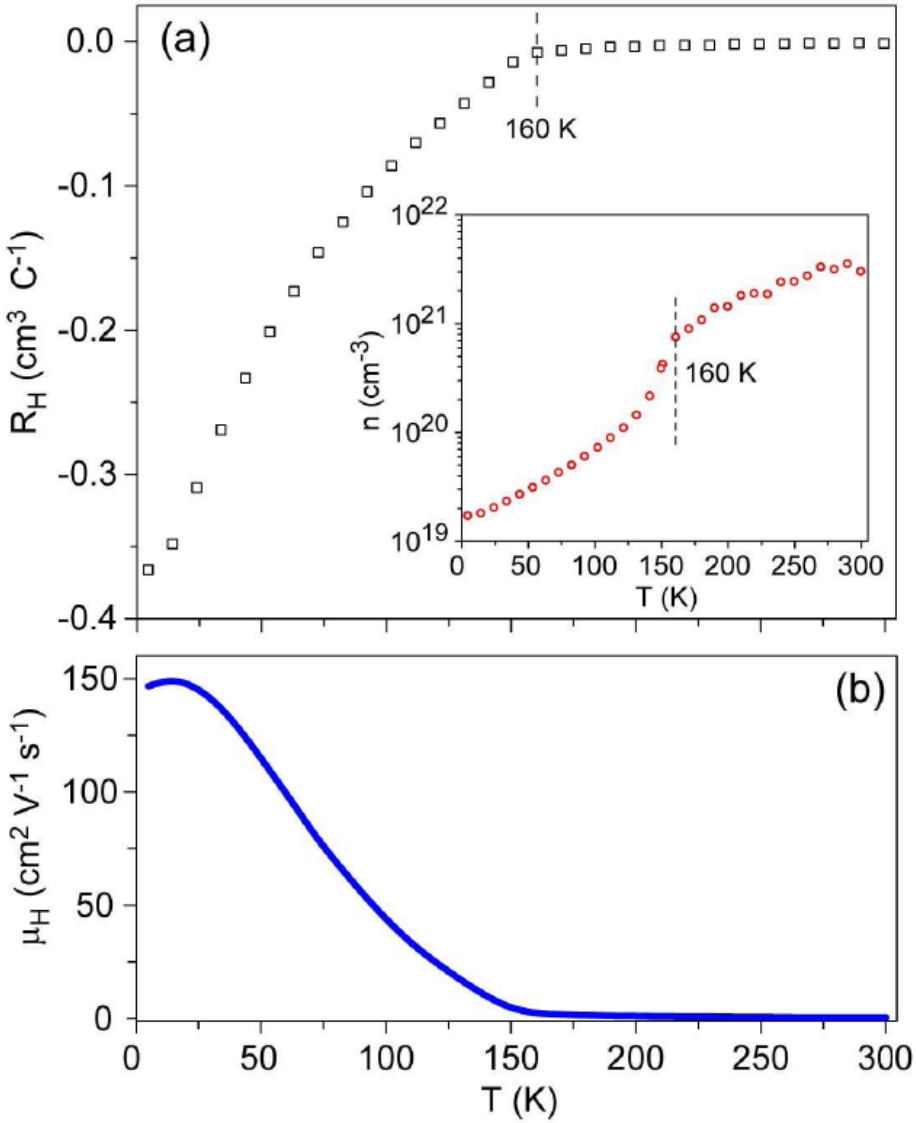
Resistivity in LaFeAsO

McGuire *et al.* (cond-mat):

Resistivity:



Hall:

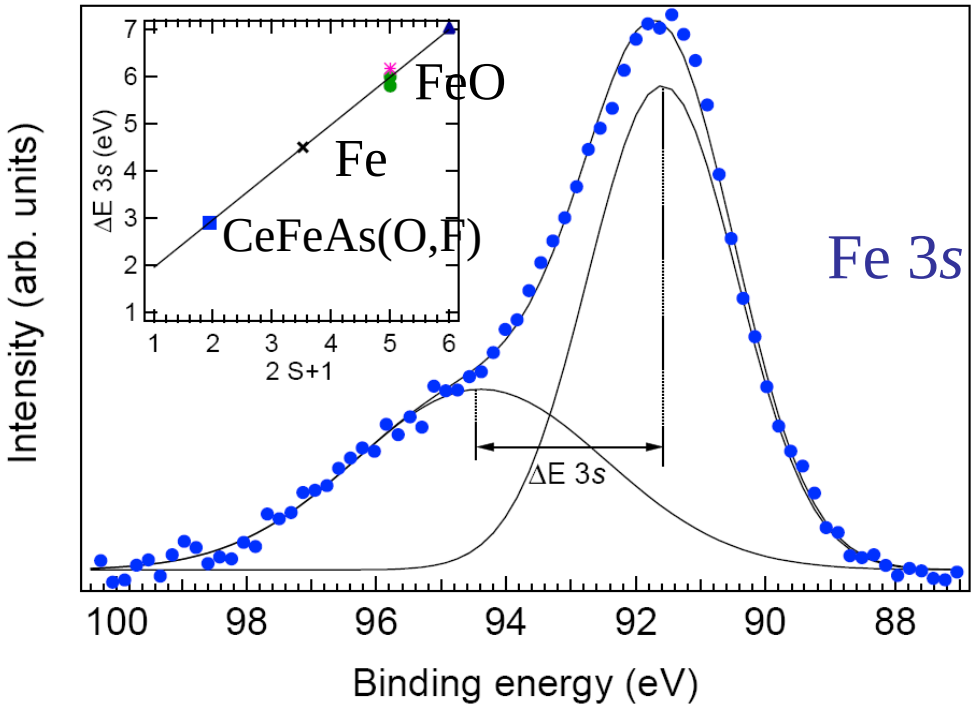


Evidence of strong interplay of magnetic ordering and Fermi surface.

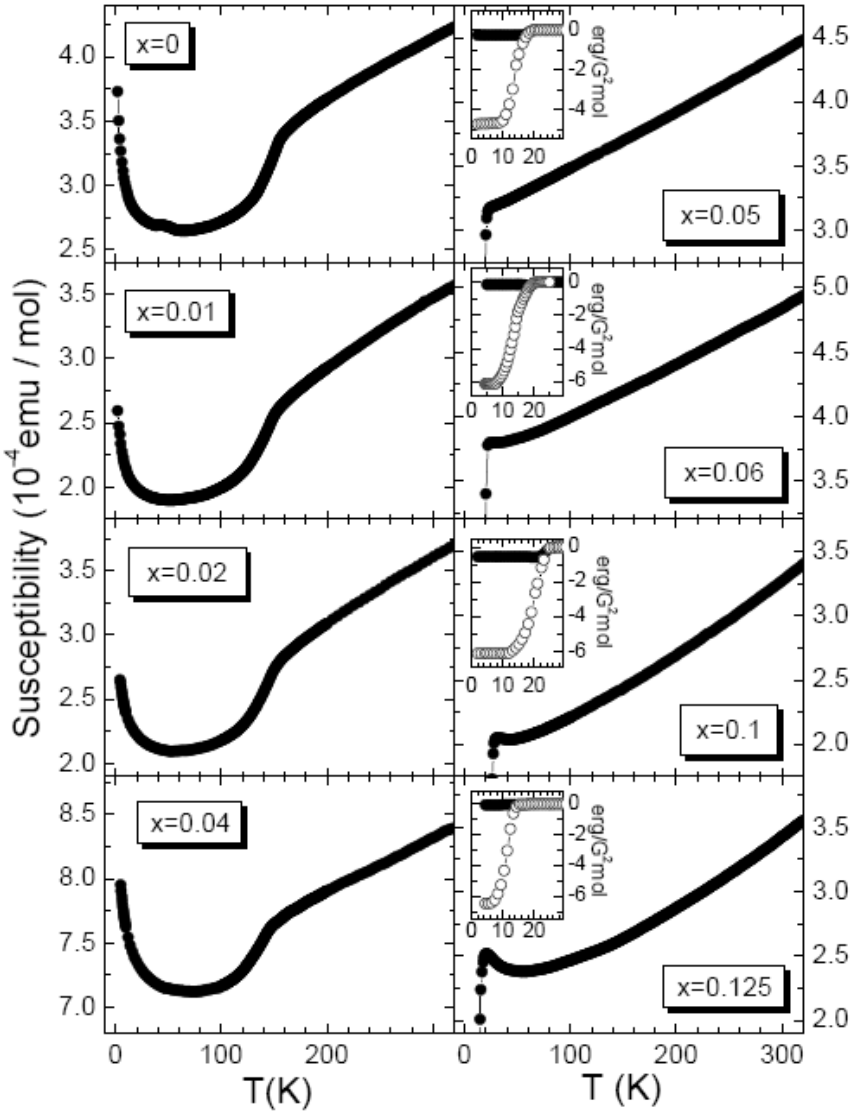
Evidence of spin fluctuations.

Strong Spin Fluctuations in Normal State

- Transport data.
- Susceptibility - $\chi(T)$.
- Spectroscopy.
- Scattering.
- Overly magnetic in LDA.
- Precursor structural transition.



Bondino et al. (2008); c.f. $NbFe_2$

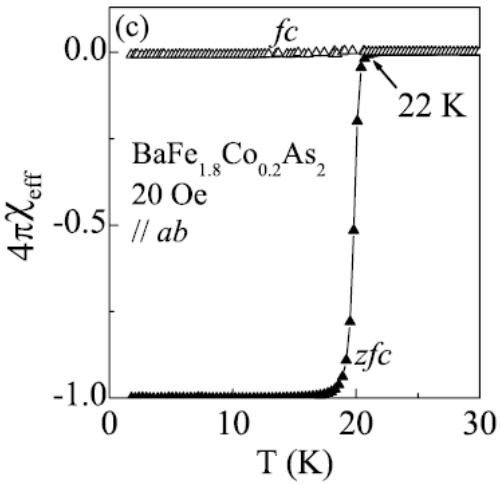


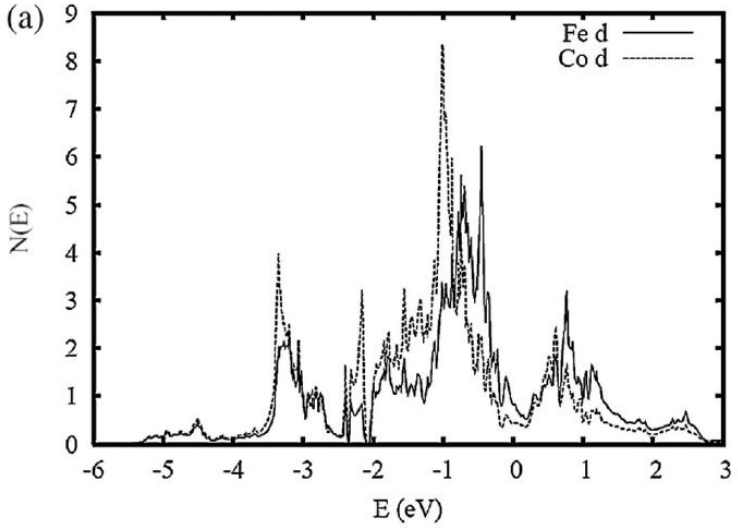
R. Klingeler et al., cond-mat

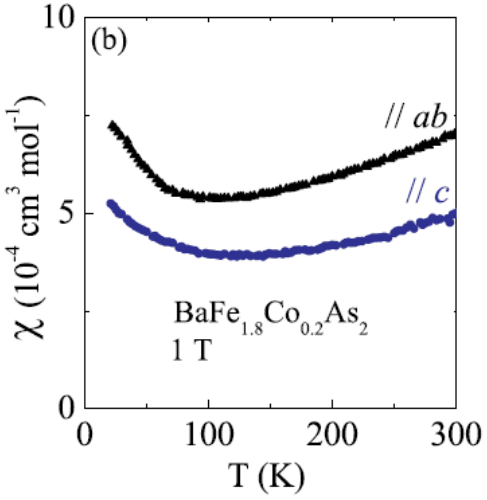
$LaFeAsO_{1-x}F_x$

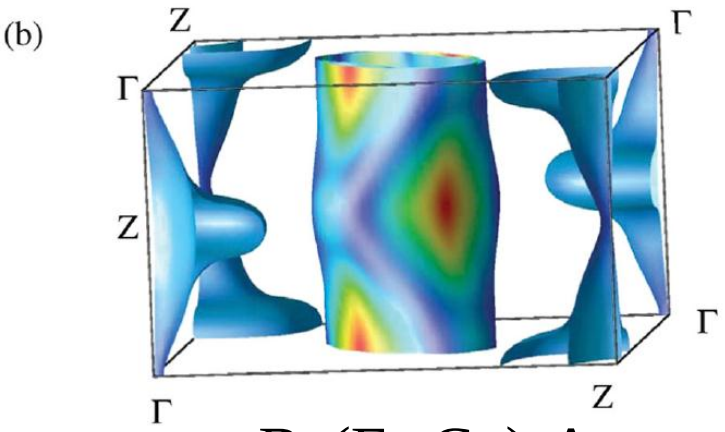
Superconductivity in Metal Doped Materials

- Superconductivity requires destruction of SDW by doping.
- Remarkably, doping with Co or Ni works (*c.f.* cuprates).









$Ba(Fe,Co)_2As_2$

A.S. Sefat, et al., PRL (2008).

Calculations show that alloy behaves very much in a rigid band sense.

Fe-Co-Ni behave very similarly apart from electron count.

Mn and Cr show strong spin dependent hybridization (different).

Is iron essential?

$ThCr_2Si_2$ Structure

JOURNAL OF SOLID STATE CHEMISTRY 56, 278–287 (1985)

The Most Populous of All Crystal Structure Types—the Tetragonal $BaAl_4$ Structure

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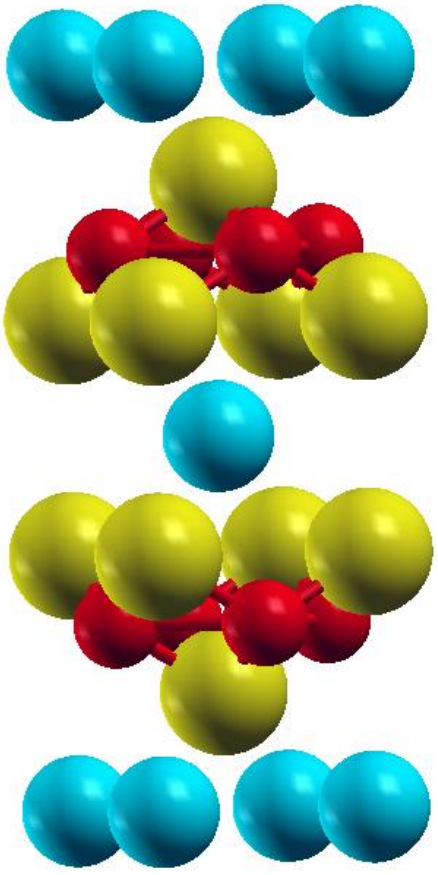
Received April 9, 1984; in revised form August 3, 1984

The $BaAl_4$ ($ThCr_2Si_2$) *tI*10 structure, MN_2X_2, is not only the most populous of all known structure types, being adopted by some 400 phases, but is representative of a new group of metallurgically



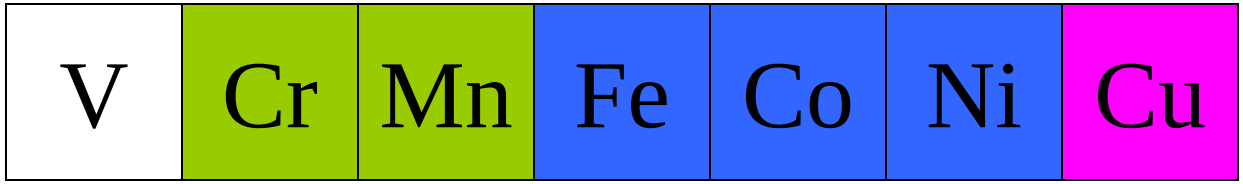
Pearson data-base now has 2,000+ $ThCr_2Si_2$ entries

Can be stabilized with different bonding patterns

➔ extremely wide variety of properties.

Examples: $BaZn_2P_2$, $BaFe_2As_2$, BiN_2Th_2, $CaAl_2Ga_2$, $SrCd_2Ga_2$ …

$ThCr_2Si_2$ Structure DT_2As_2



Strong spin dependent *T*-As hybridization, G-type AF with high T_N.
$BaCr_2As_2$ is itinerant metal. $BaMn_2As_2$ is a semiconductor.

Metallic M^{2+} sheets. As is anionic. *M* can be alloyed.
Fe: SDW and superconductivity.
Co: Near FM
Ni: electron-phonon superconductor.

$BaCu_2As_2$ has Cu d^{10} with As-As and Cu-As sp bonding.

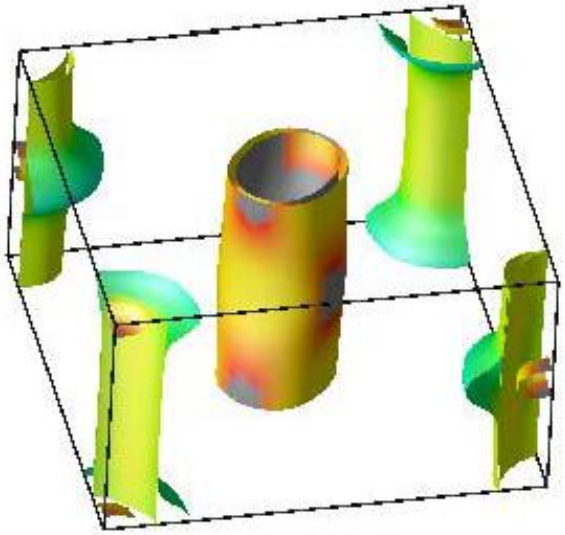
Chemistry of chalcogenides may be expected to differ.

Is Iron Essential for Iron-Based Superconductivity?

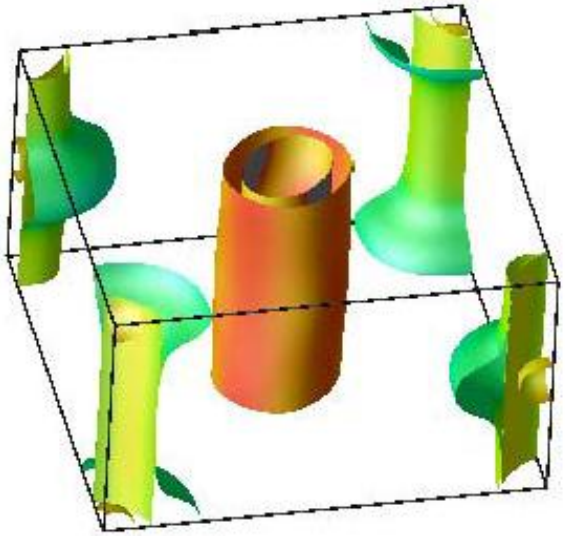
KRu_2As_2; KFe_2As_2; KCo_2As_2: Can we do something with the alloys?

$KFeCoAs_2 \approx BaFe_2As_2$

$KFeCoAs_2$

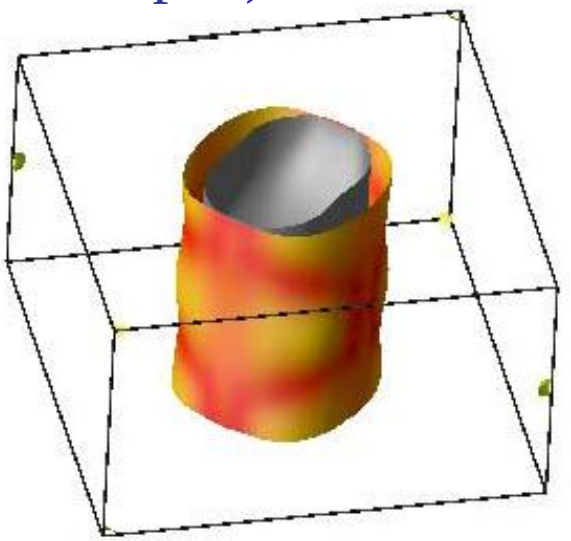


Virtual Crystal



Ordered Cell

$KFe_{0.5}Co_{1.5}As_2$ (overdoped)

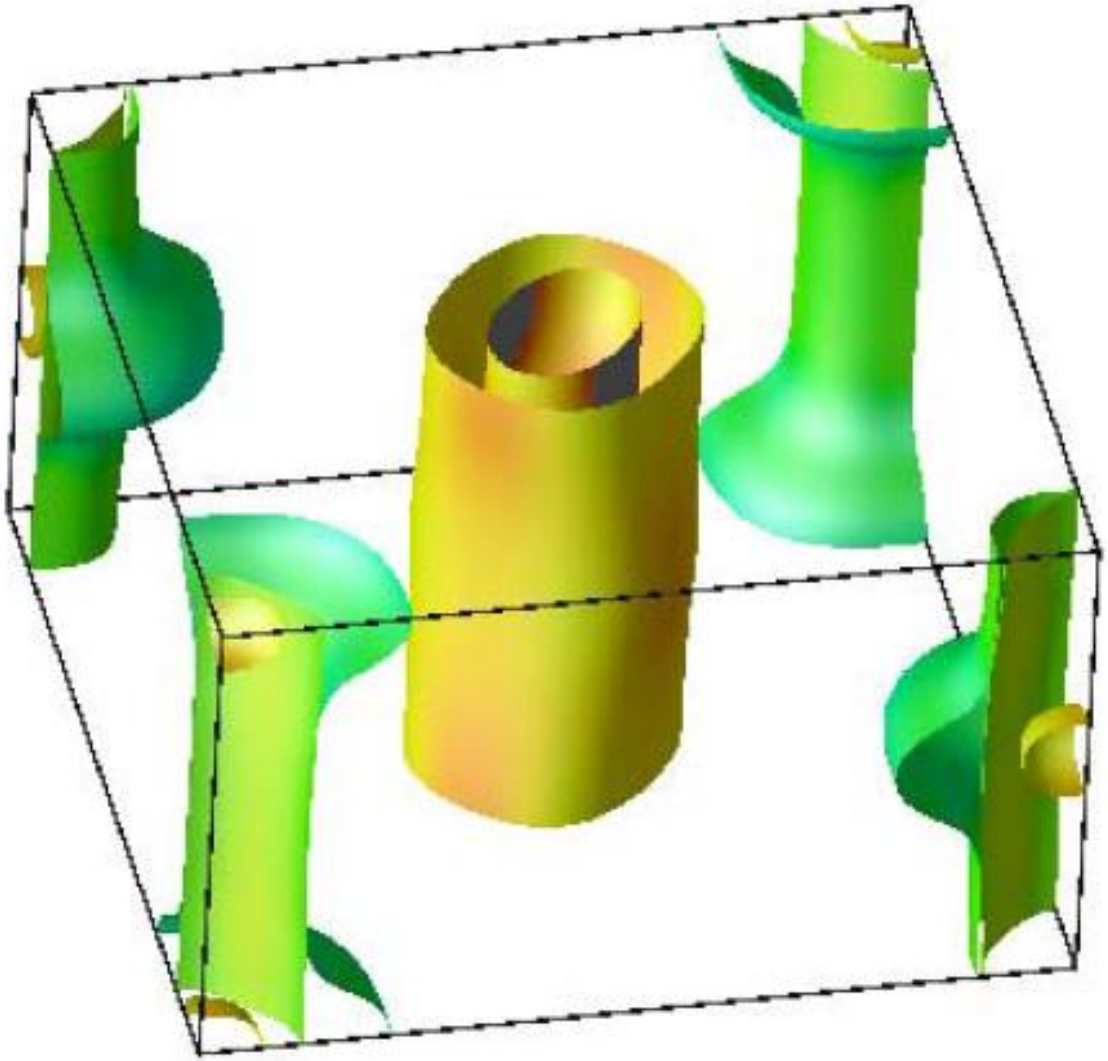


Virtual Crystal

Coherent alloy: Look for superconductivity in $KFe_{1-x}Co_{1+x}As_2$ (Fe-poor)

Also, similar results, but less magnetic for $KRu_{1-x}Co_{1+x}As_2$, but significantly less magnetic (Fe-free).

Fermi Surface of Ordered $KRuCoAs_2$



Do not find SDW magnetic order at this composition.

Will it appear as Ru concentration is reduced.

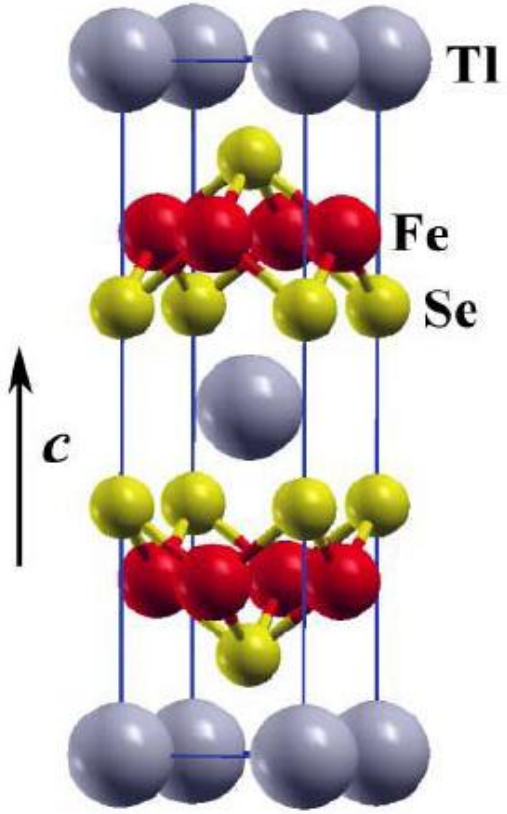
Will superconductivity appear?

$$\chi(\mathbf{q}) = \frac{\chi_0(\mathbf{q})}{1 - \chi_0(\mathbf{q}) I(\mathbf{q})}$$

Ru lowers average Stoner parameter $I(\mathbf{q})$ both because it is $4d$ and because of Ru d – As p hybridization.

Properties of the Over-Doped Side: $TlFe_2Se_2$

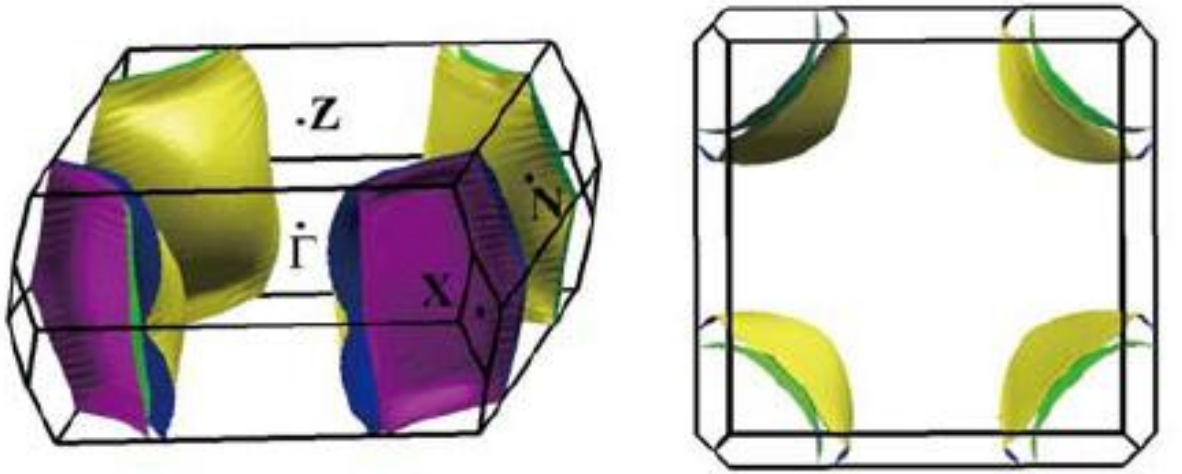
Haggstrom, 1986



Antiferromagnetic with T_N ~ 450 K. Unknown order.

First Principles Results (GGA):

- Electronic structure is very similar to FeSC, but with higher electron count (0.5 e/Fe).
- Strong instability against nearest neighbor AFM (78 meV/Fe) and weaker instability against FM (44 meV/Fe). No instability for SDW type chain order → itinerant n.n. AFM

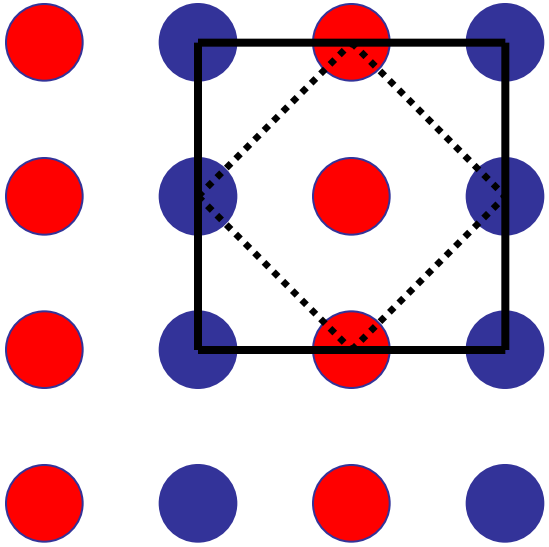


Non spin polarized Fermi surface

Competing Magnetic States

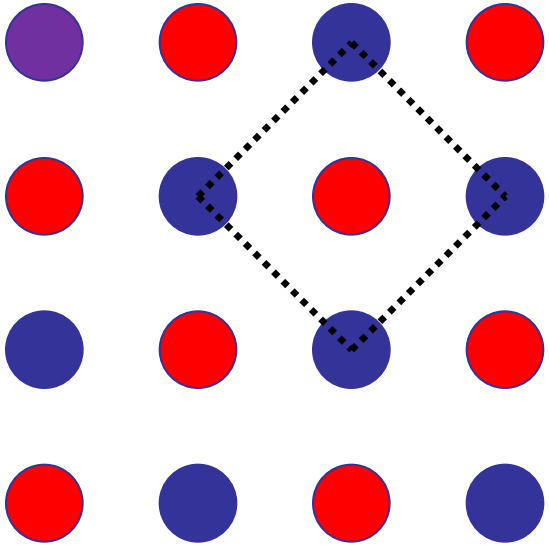
Competition between different magnetic states provides phase space for fluctuations and works against ordering.

SDW - c(2x2)



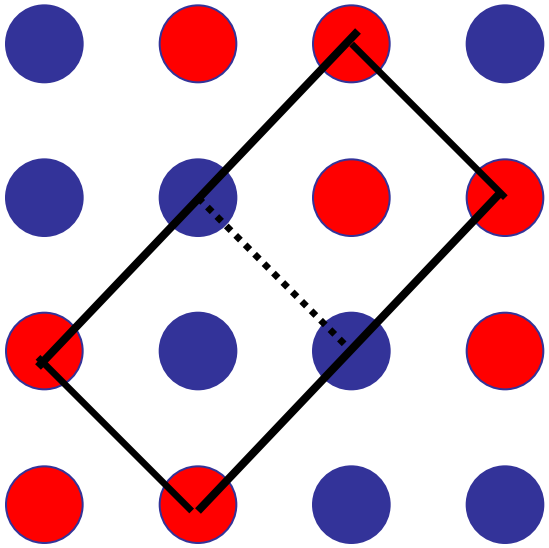
LaFeAsO

N.N (1x1)



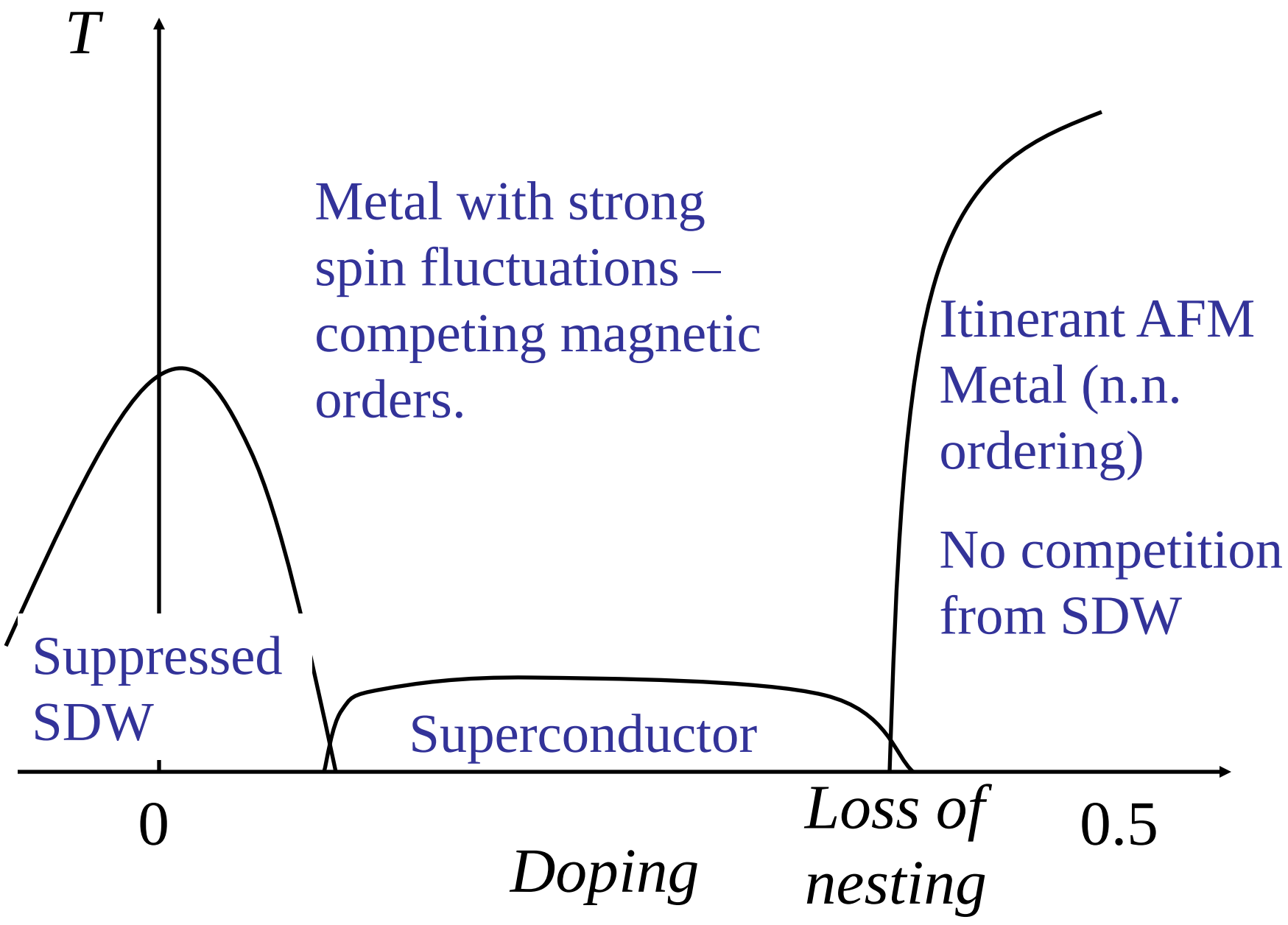
$TlFe_2Se_2$

(2x1)



$Fe_{1+x}Te$

Possible Electron Doped Phase Diagram



Comparison with Cuprates

	Cuprates	Fe-As
Magnetic & superconducting phases	Yes, magnetic phase insulating above & below $T_{N.}$ (Mott insulator)	Yes. Magnetic phase is metallic. Intimate connection of magnetic and superconducting phases
Electronic structure	Moderate $N(E_F)$, large FS at least for optimal doped	High $N(E_F)$, small disconnected FS
Doping	Essential.	Destruction of SDW is enough.
Magnetic character	Local moment	Apparently itinerant with strong renormalization from DFT.
Correlations	Strong. Mott-Hubbard type (e.g. p.e. satellites)	Possibly substantial but different e.g. spin fluctuations. Not Mott-Hubbard type.
Superconductivity	*d*-wave. Nodes. One band. Highly anisotropic	Nodeless (*s* +/- ?). Two band. Less anisotropic (material dependent).
Structure	Oxides, corner shared octahedra -- complex	Simpler – tetragonal / orthorhombic, small unit cells.

Conclusions

- Iron superconductors behave very differently from cuprates – perhaps a rather different mechanism or perhaps we need to look deeper for the connections.
- Strong renormalization of magnetic properties due to strong spin fluctuations – almost certainly necessary for understanding of the normal state and the superconductivity.
- Extended s-wave (+/-) state is a likely scenario.
- Interesting interplay between magnetism and structure.

Questions

- Can we identify materials with “strong” spin fluctuations and quantify “strong”?
- Can we identify competing magnetic states, even those with relatively weak q-dependence?
- Could we connect inelastic scattering with magnetic renormalization (fluctuation-dissipation)?
- Can we connect with transport experiments?
- Can we identify trends in magnetic behavior that would allow us to predict new superconductors, or ways to vary composition to improve superconductivity?
- …