Strong Correlations and High Temperature Superconductivity: Families of Materials and Theoretical Trends.

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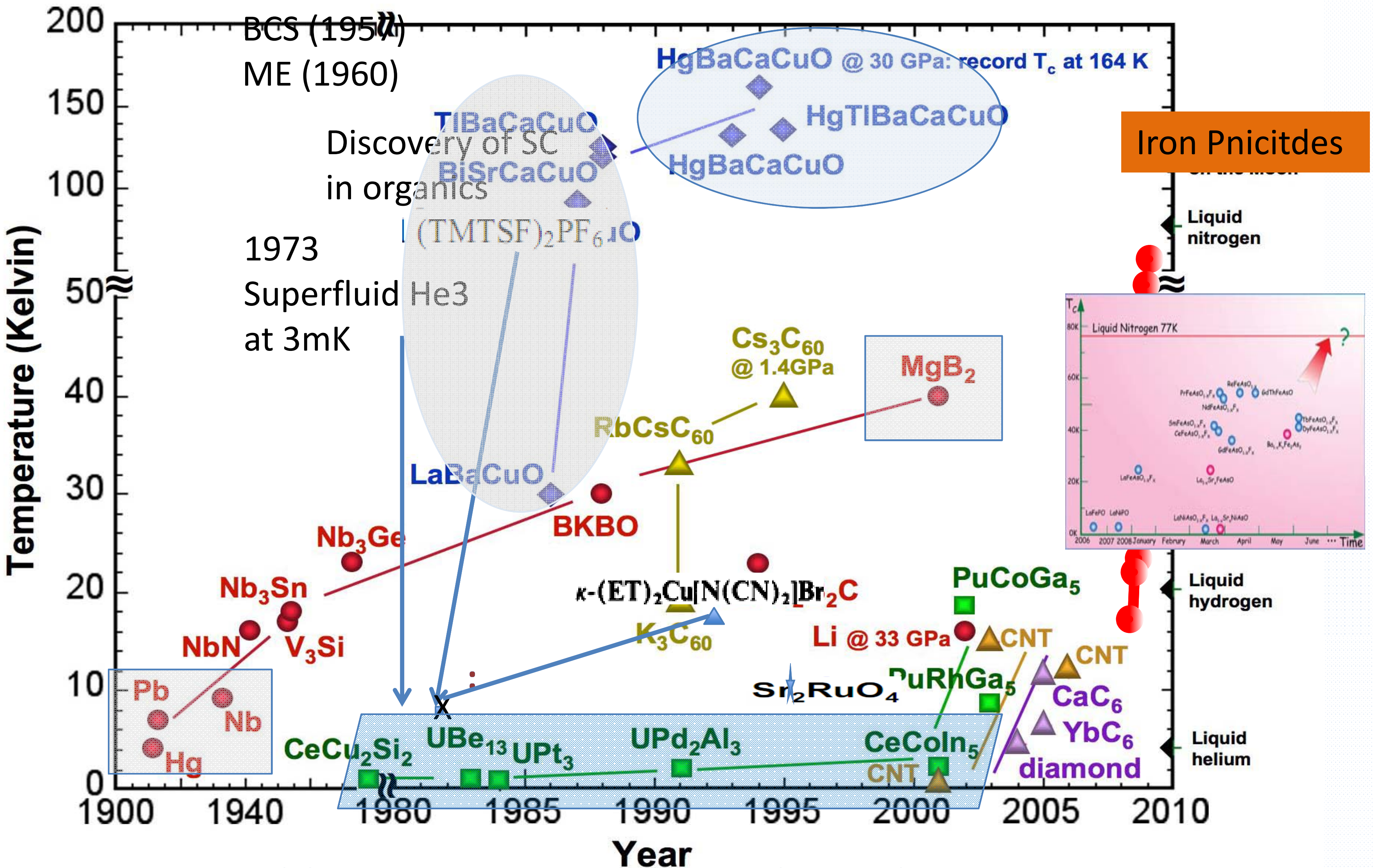
“T_c vs. Time”

http://science.energy.gov/~/media/bes/pdf/reports/files/sc_rpt.pdf



BCS (1957)
ME (1960)

Discovery of SC
in organics

1973
Superfluid He3
at 3mK

Iron Pnicitdes

http://www.sc.doe.gov/bes/reports.lists.html

Heavy Fermion Superconductivity

1979: Frank Steglich discovers superconductivity in CeCu2Si2 a **heavy fermion material. Superconductivity occurs with an enormous heat capacity jump.**

- People did not believe superconductivity was possible in systems with magnetic moments.
- Superconductivity had been detected and dismissed in UBe13 (as a U filamentary effect) in 1975, and CeCu2Si2 in 1978 (but only in a footnote, and the authors did not recognize it as a genuine effect, since it was not believed it was possible).

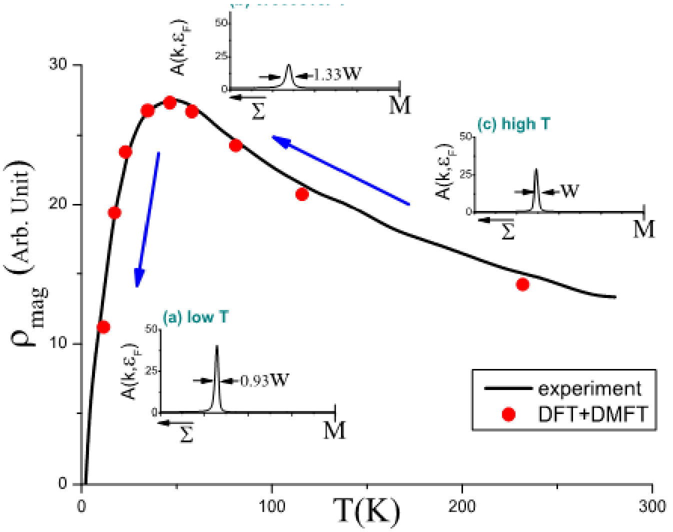
Curiosities, until … CeCoIn5 115 (2d analog of a cubic system CeIn5) PuCoGa5 "115" is a 20 K superconductor in the heavy fermion family.

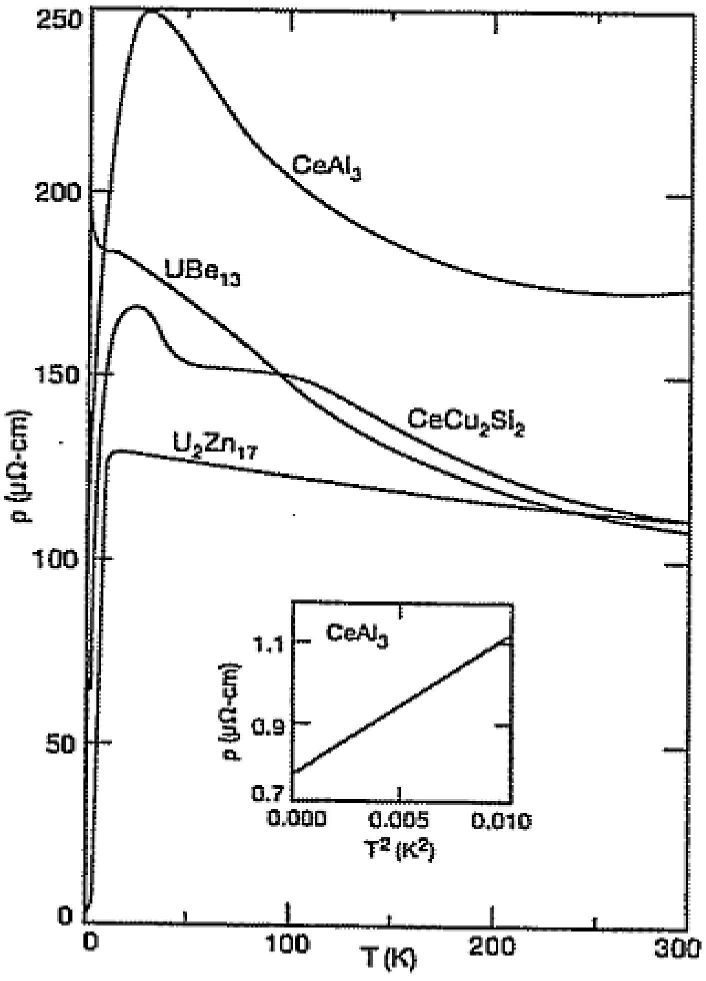
Does Superconductivity Emerge from a Fermi Liquid State ?

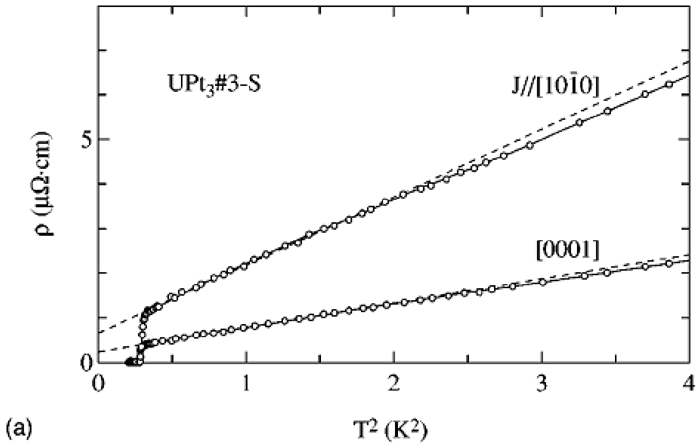
Tc/TF , does it have meaning ?

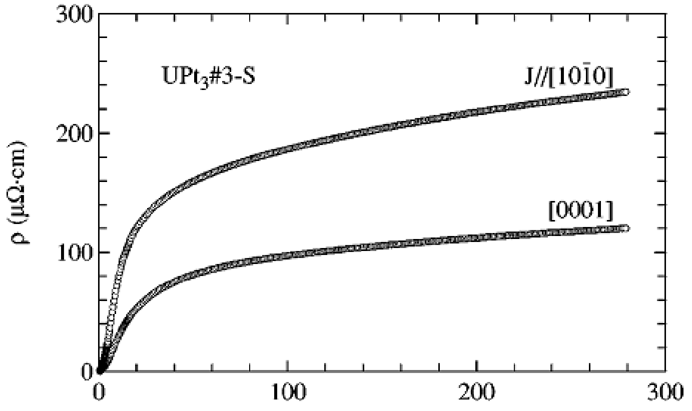
In ME theory coupling is multiplied by Z, is emergence of SC from an incoherent state different ?

Local Approximation works well for normal state.





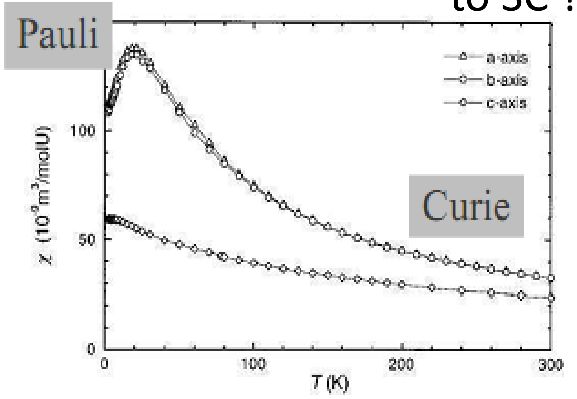




The integral of gamma (T) gives the entropy contained in the superconducting state at Tc. The integrals of the entropies give the condensation energy.

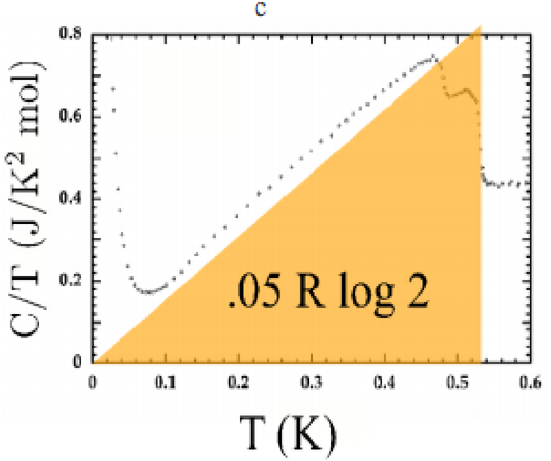
UPt_3

From FL to SC ?



Pauli paramagnetic by 30K

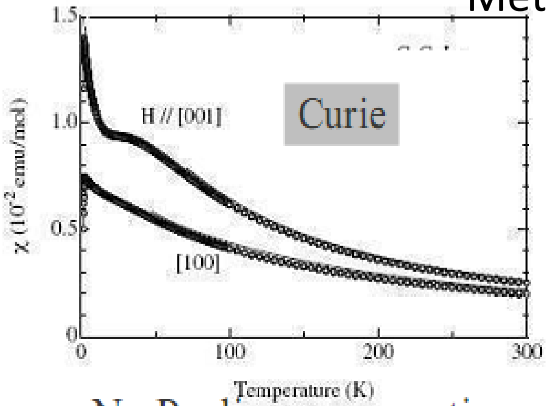
$T_c = 0.5$K



Frings *et al.* J. Magn. Magn. Mater. **31**, 240(1983)
Brison *et al.* J. Low Temp. Phys. **95**, 145(1994)

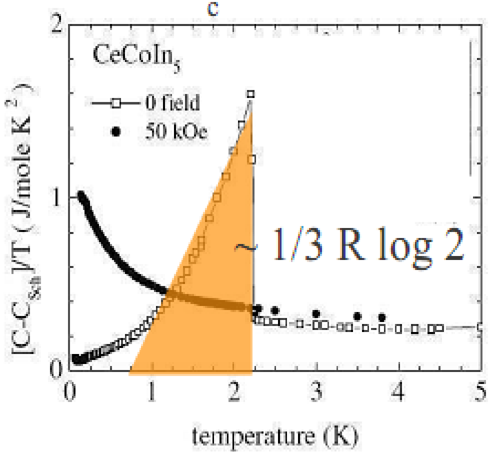
$CeCoIn_5$

From Incoherent Metal to SC



No Pauli paramagnetism

$T_c = 2.3$K



Shishido *et al.* JPSJ **71**, 162 (2002)
Petrovic *et al.* J.Phys Condens. Matter **13** 337 (2001)

$$S = \int_0^T \frac{C(T')}{T'} dT'$$

$$E_n(T) - E(T) = \int_T^\infty [C_n(T') - C_{sc}(T')] dT'$$

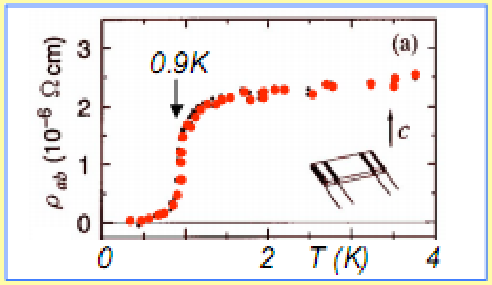
$$F_n(T) - F(T) = \int_T^\infty [S_n(T') - S(T')] dT'$$

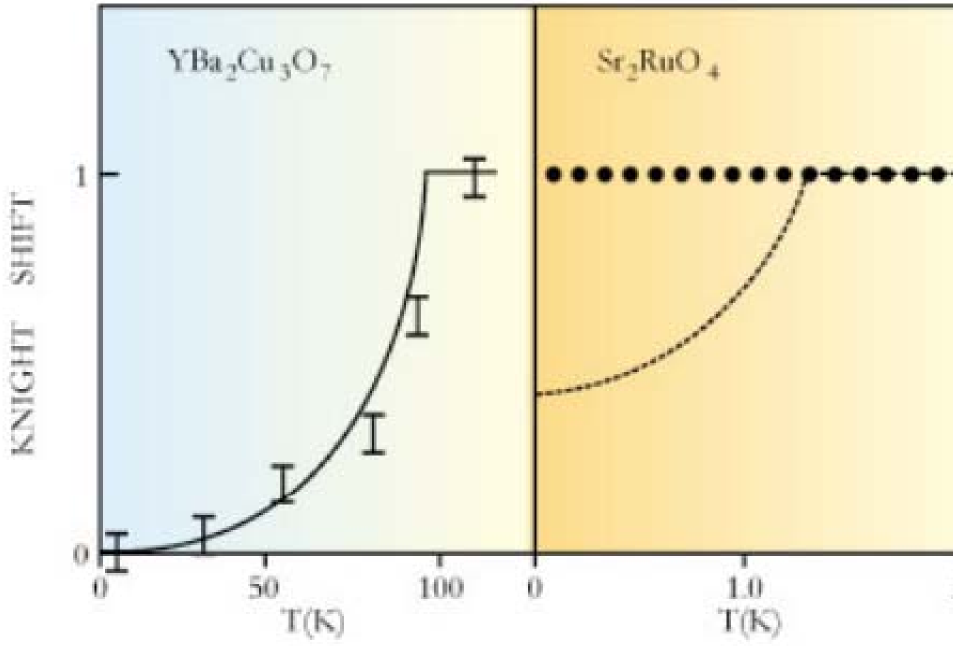
Sn(T)-S(T)=0 at Tc and at T=0

Superconductivity

$T_{c,\,max} = 1.5\ K$

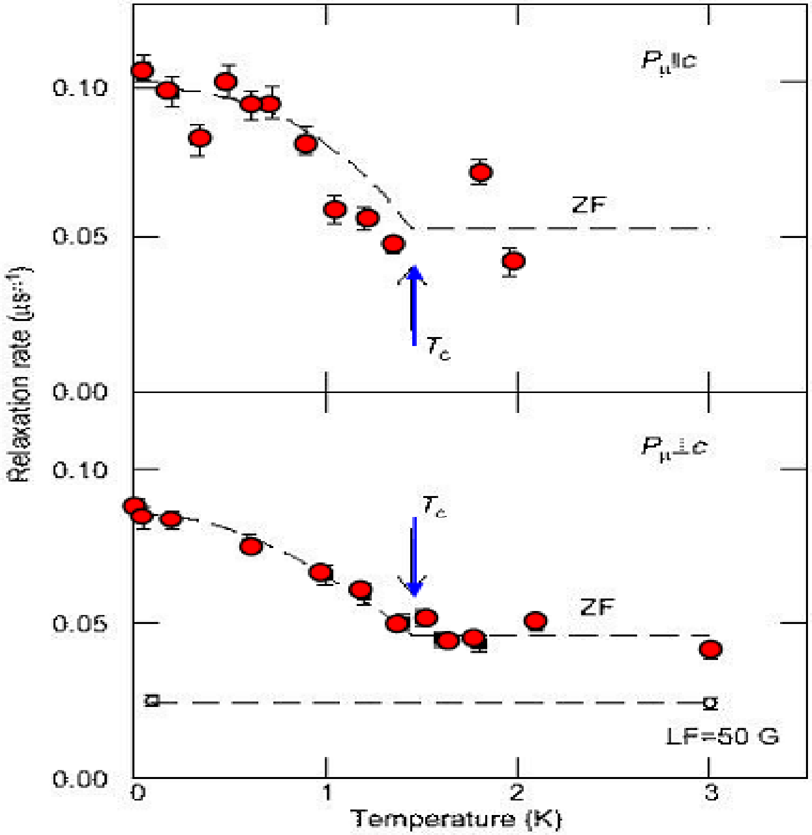
Maeno, Bednorz et al, (1994)





Ishida et. al. Nature 396, 658 (1998)

$$\vec{d} = \hat{z}(k_x \pm i k_y)$$

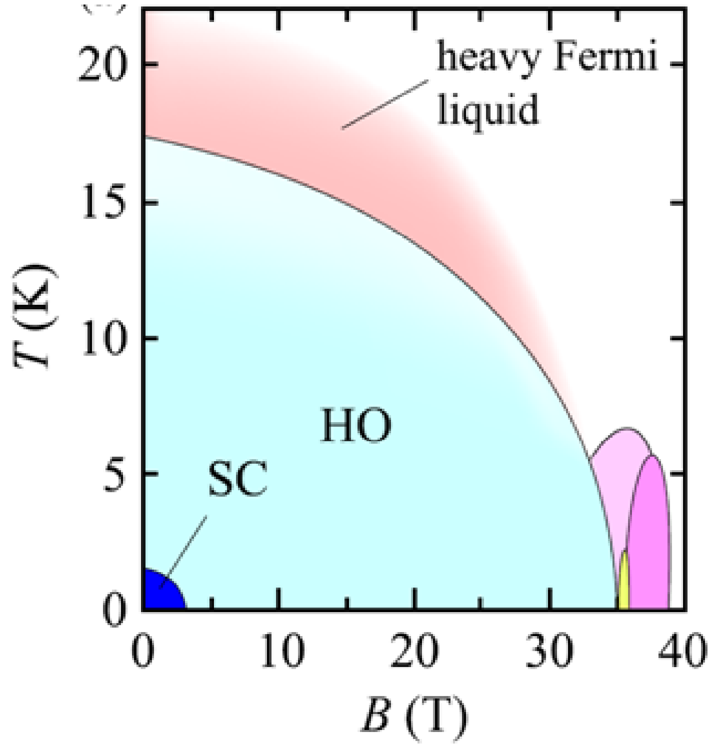


Luke, Uemura et al. (1998)

T.M. Rice & M. Sigrist, J. Phys. Cond. Mat. **7**, L43 (1995)

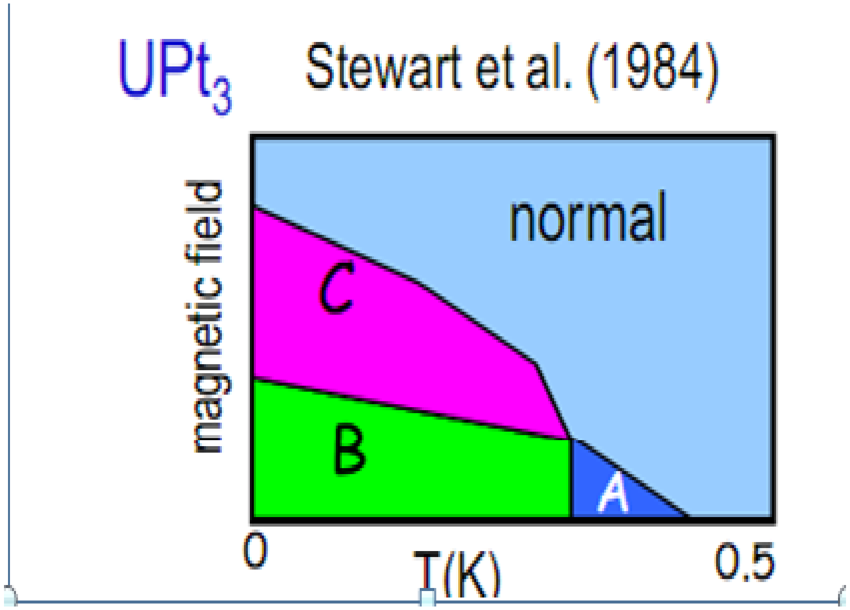
See however later Knight shift expts.

Common Features of Many Heavy Fermion Systems :
Interplay with (parasitic ?)magnetism.



$$\Delta = \Delta_0 \sin\frac{k_z}{2}c\left(\sin\frac{k_x+k_y}{2}a \pm i\sin\frac{k_x-k_y}{2}a\right)$$

“Singlet “: even parity



Two dimensional representation. Odd parity. Several basis functions possible.

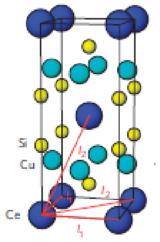
$$\mathrm{Re}[f_+(\vec{k})^2]f_z(\vec{k})\hat{z},\ \mathrm{Im}[f_+(\vec{k})^2]f_z(\vec{k})\hat{z}$$

$$f_x(\vec{k}) \equiv \sin(k_x a) + \sin(k_x a/2)\cos(\sqrt{3}k_y a/2)$$

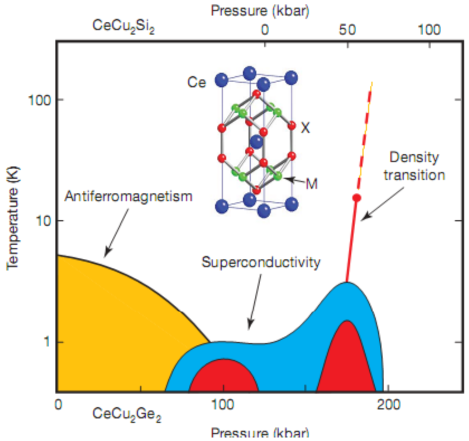
$$E_{2u}\ (\Gamma_6^-) \qquad f_y(\vec{k}) \equiv \pm\sqrt{3}\cos(k_x a/2)\sin(\sqrt{3}k_y a/2)$$

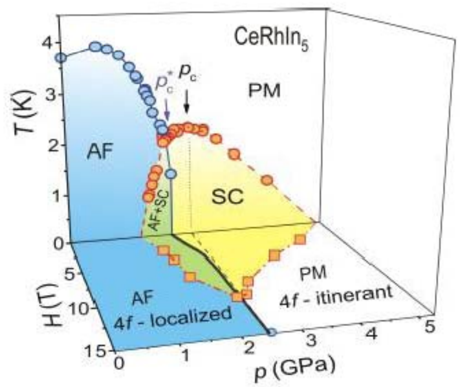
$$f_z(\vec{k}) \equiv \sin(k_z c).$$

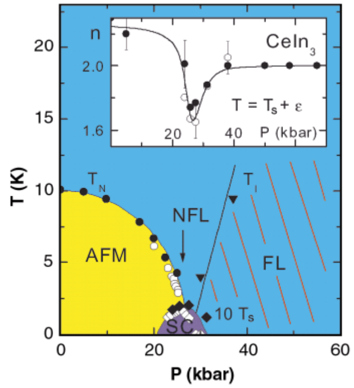
Unconventional Superconductivity Loves Company
the company of a competing phase



heavy fermions

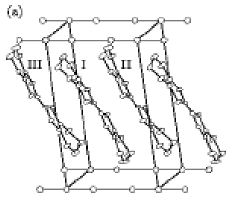




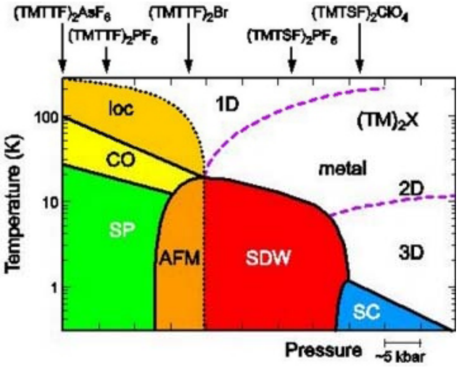


Cuprates

Cubic QCP



organics



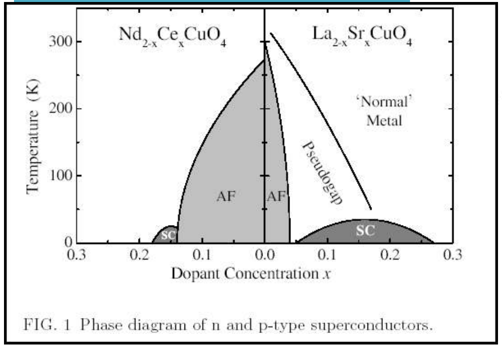


FIG. 1 Phase diagram of n and p-type superconductors.

"GENERIC "

Superconductivity is "close " to and AF phase. SF mediation of high Tc?

Spin Fluctuation Viewpoint

- Theory of nearly ferromagnetic transition metals. Spin fluctuations contribute to thermodynamics and are pair breakers. RPA (mid sixties)
- They played an important role in mediating p –type superconductivity in Helium3 (seventies)
- Collective modes in itinerant systems, giving rise to important thermodynamical contributions near a QCP (seventies).Treatments beyond RPA.
- Theories. Effective theory: QP interacting with bosons. Microscopic theories such as Hubbard model.
- Heavy Fermion superconductivity (Beel Monod Bourbonnais Emery, Miyake Schmidt Rink, Varma, Scalapino, Hirsch, Loh) motivated the extensions to d singlet pairing. Also organics(Emery).

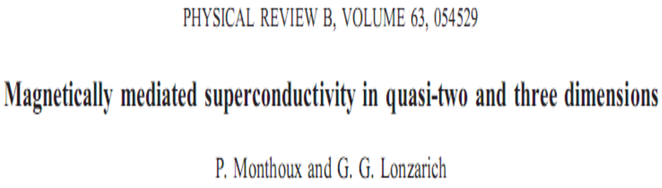
- Intensive studies of this mechanism for the cuprates (Scalapino, Pines, Montoux, Ueda, Moriya, Lonzarich, Tremblay, ……)

Correlated Superconductivity Point of View

- The ideas emerged in response to the discovery of high Tc (P.W Anderson's 1987 Science article). Connection between superconductivity and proximity to a Mott insulator spin liquid.
- (1987-1988)Mathematical formulation with slave boson mean field theory on a plaquette, and variational Gutzwiller RVB wave functions, predicted the d wave superconductivity. Slave boson MFT predicted a pseudogap at finite temperatures.
- The approach to the Mott insulator renormalizes the kinetic energy , pairing of spins gets stronger as the insulator is approached, Trvb increases. Singlets formation M* finite Z proportional to doping.

  Repulsion does not matter for pairing.
- The proximity to the Mott insulator reduce the local charge stiffness. Superconductivity requires formation of quasiparticles. T_{BE} goes to zero
- Superconducting dome. Proximity to localization/delocalization transition matters for finding optimal Tc.
- Pseudogap has same symmetry as superconducting state.
- Significantly improved formulation with DMFT. (single site and cluster, over the past decade, continues today).

Paramagnons and Phonons: the main Differences


PHYSICAL REVIEW B, VOLUME 63, 054529

Magnetically mediated superconductivity in quasi-two and three dimensions

P. Monthoux and G. G. Lonzarich

$$S_{\text{eff}}=\sum_{\mathbf{p},\alpha}\int_0^\beta d\tau\,\psi^\dagger_{\mathbf{p},\alpha}(\tau)(\partial_\tau+\epsilon_{\mathbf{p}}-\mu)\psi_{\mathbf{p},\alpha}(\tau)$$

$$-\frac{g^2}{6}\sum_{\mathbf{q}}\int_0^\beta d\tau\int_0^\beta d\tau'\,\chi(\mathbf{q},\tau-\tau')\mathbf{s}(\mathbf{q},\tau)\cdot\mathbf{s}(-\mathbf{q},\tau').$$

- Phonons are fundamental degrees of freedom, spin fluctuations are emergent degrees of freedom, much harder to evaluate their parameters.
- Phonons propagate, spin fluctuations are damped. No precise analogy between Debye energy and T0.
- Spin fluctuations are important ONLY when they are close to an instability, so the analogy is with ANHARMONIC phonons (difficult problem).
- Weak coupling approximations capture the key ideas. [RPA, 2PSCS….] . Infrared singularities in 2d, not fully sorted out.
- Strong k dependence of the coupling, solve full k and omega dependent Dyson equations .
- Self consistency vs non self consistency at one particle level. [TPSC uses bare greens functions to be able to reach stronger couplings, mix self consistency inside the SC state?]

In the absence of a completely accepted theory, one can look at the phase diagrams and the issues surrounding superconductivity in a given class of materials keeping both the spin fluctuation theory (or soft mode exchange for other competing phases) and the correlated superconductivity theory as alternative complementary points of view.

At each stop one needs to ascertain, key variables for determining the occurrence superconductivity transition ?

- Degree of two dimensionality ?
- Degree of coherence incoherence ?
- Proximity to the localization transition ?
- Pairing Mechansims
- Factors limiting the Tc
- Proximity or connection to other phases.
- …………

Previous Lecture. Derived ME for multiband case, can be adapted to anisotropic SC

$$i\omega Z(i\omega)_j = i\omega + \pi T \sum_{\varpi<\Theta} \lambda(i\omega - i\varpi)_{jj'} \frac{i\varpi Z_{j'}(i\varpi)}{[\phi(i\varpi)_{j'}{}^2 + \varpi^2 Z_{j'}(i\varpi)^2]^{1/2}}$$

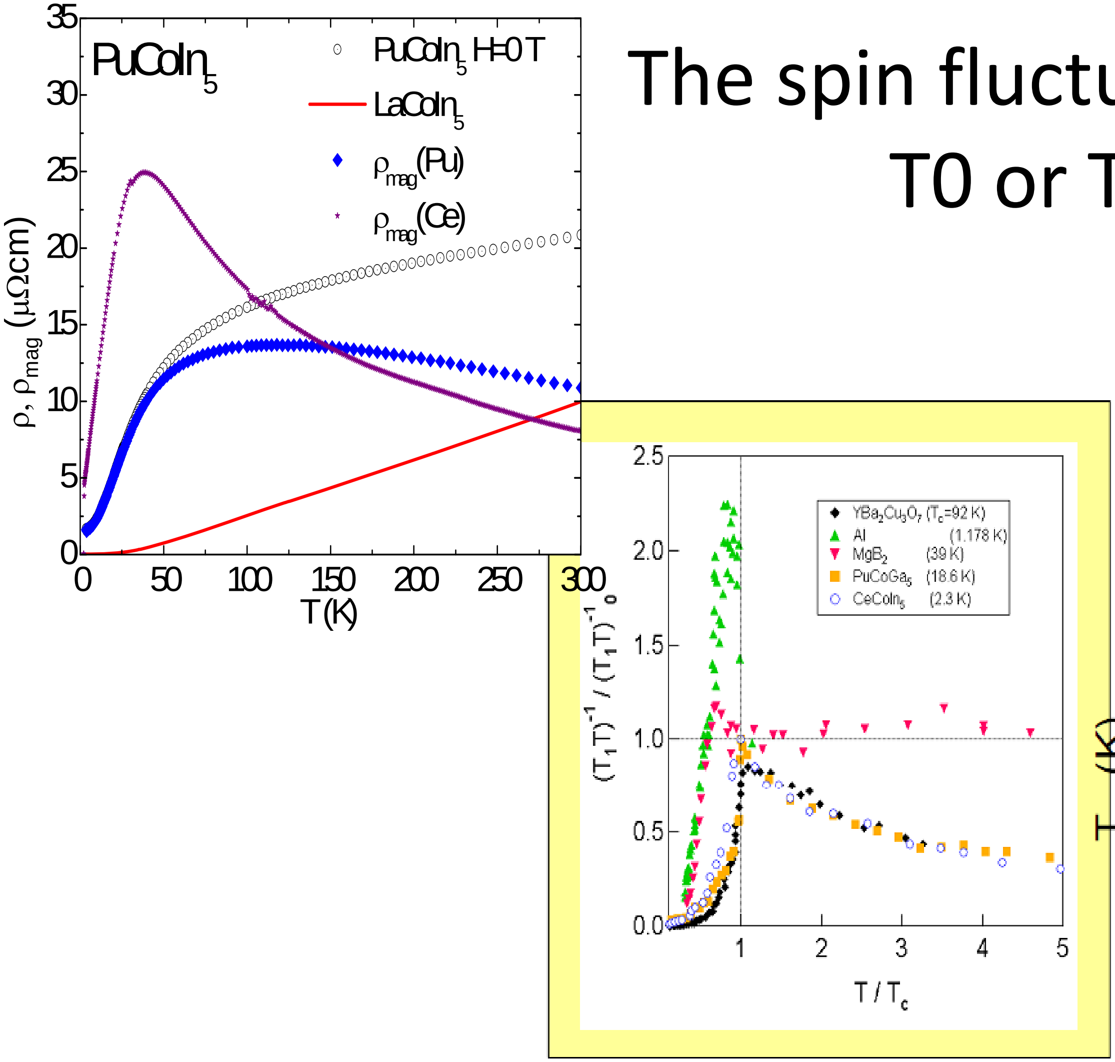
$$\phi(i\omega)_j = \pi T \sum_{\varpi<\Theta} \lambda(i\omega - i\varpi)_{j,j'} \frac{\phi_{j'}(i\varpi)}{[\phi_{j'}(i\varpi)^2 + \varpi^2 Z_{j'}(i\varpi)^2]^{1/2}}$$

Interpret j now as an angular momentum index on the fermi surface, j=1 A1g, j=2 B2g

$T_c = \langle\omega\rangle \exp[-(1+\lambda_1)/\lambda_2]$

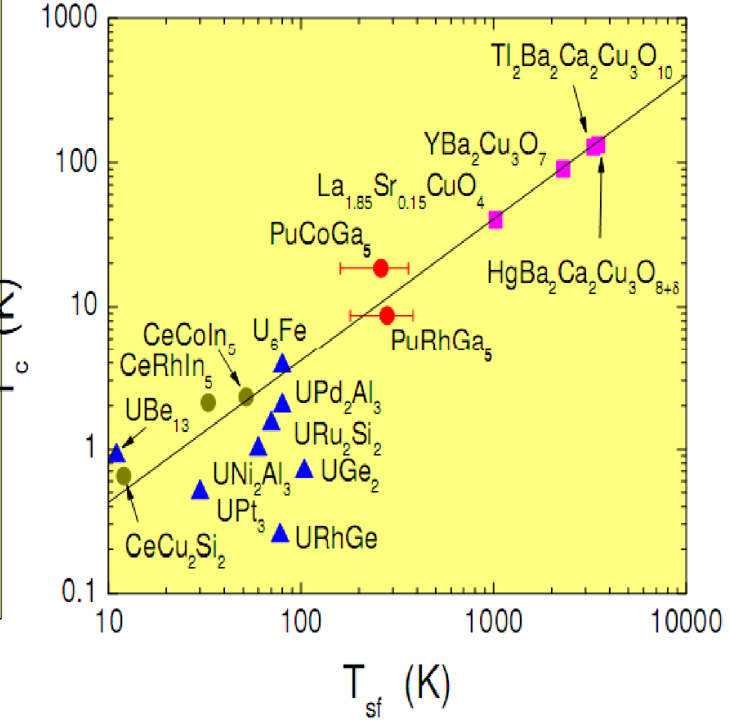
In the spin fluctuation model the lambdas are taken to be quite large and <w>= Tsf. See Lonzarich and Montoux (PRB) who solve the equations in the Full BZ.

The spin fluctuation damping scale T0 or Tsf controls Tc



N. J. Curro et al., Nature **434**, 622 (2005).

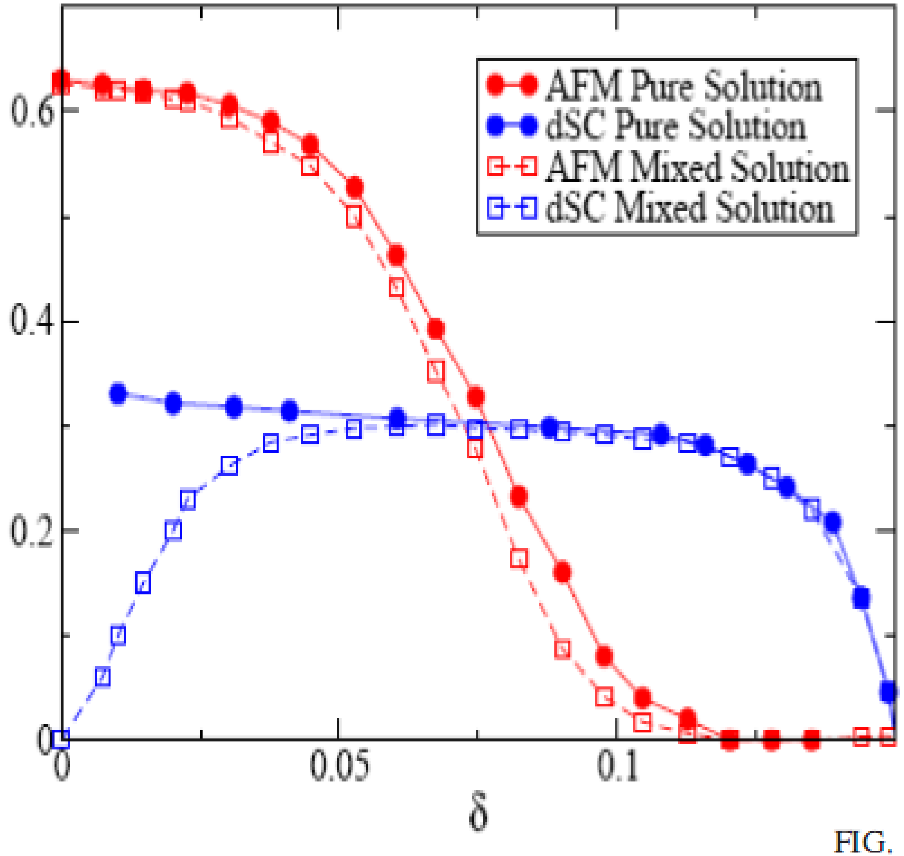
after T. Moriya and K. Ueda, Rep. Prog. Phys. **66**, 1299 (2003)



Is this a predictive tool that allows to “guess” Tc from two normal state properties ????

What determines if magnetism and d wave superconductivity coexists microscopically or not ?

Possible answer from CDMFT, it is the correlation strength



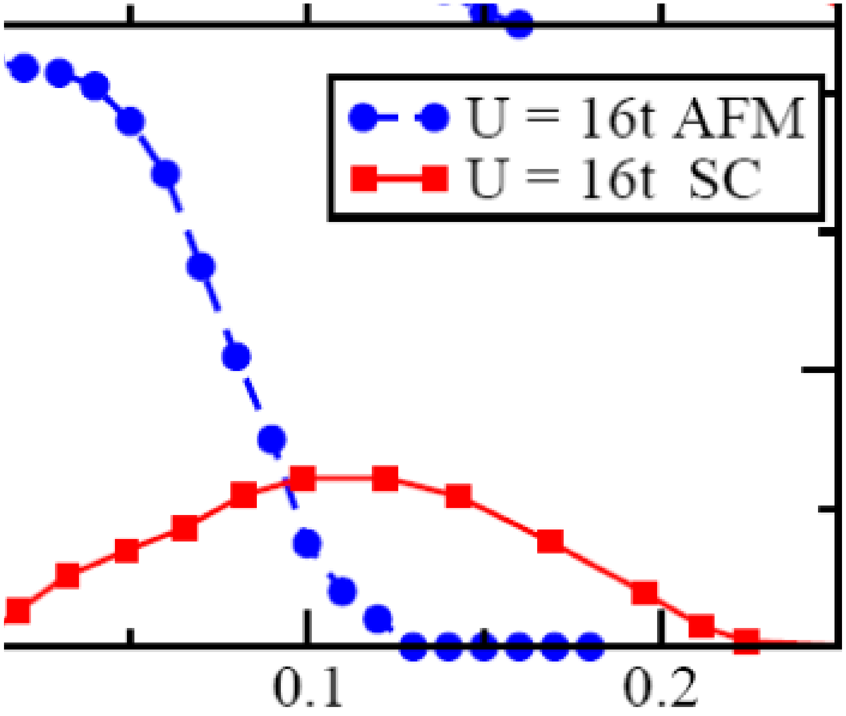


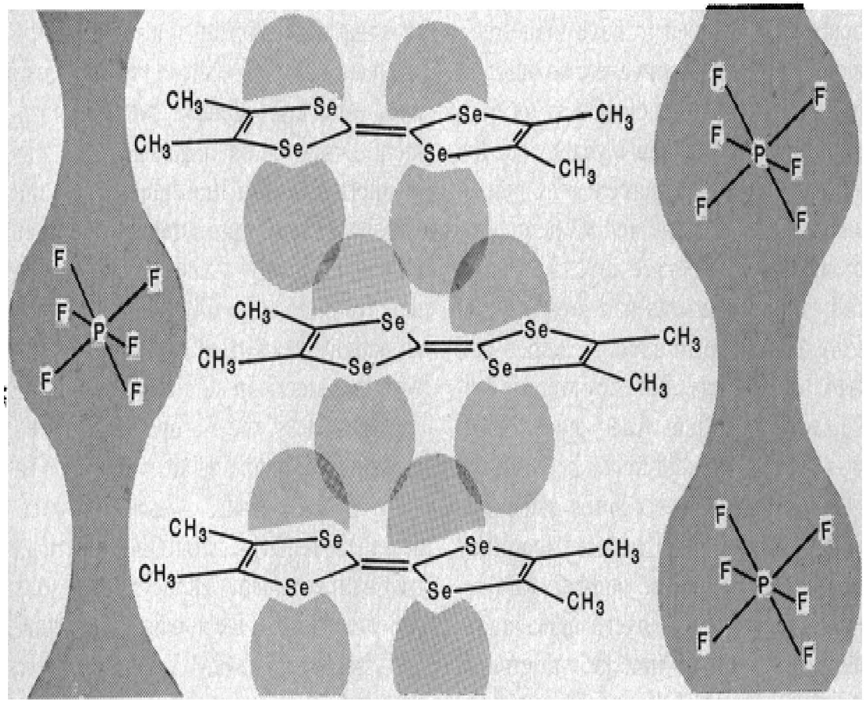
FIG. 2. (Color online) AFM and *d*SC order parameters as a function of doping for four $U/t=4$. We compare the values of the order parameters in the pure solutions (full line and closed circles) with the values in the mixed solution (dashed line and open squares). The *d*SC order parameter was multiplied by a factor of 10 for graphical purposes.

M. Capone and G. Kotliar
Phys. Rev. B **74**, 054513 (2006)

Organic salts are charged layers . The salts are inert and negatively charged. The organic molecules form stacks which are positively charged.

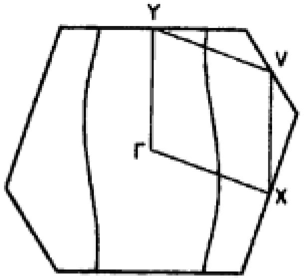
Number of Organic Superconductors Grows

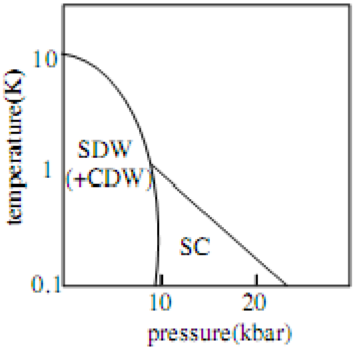
New discoveries suggest that the superconductivity of certain organic salts is a general phenomena



"Zig-zag" stacks

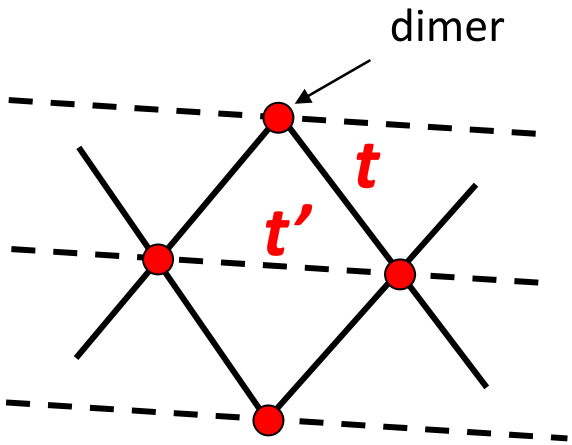
In Bechgaard salts such as $(TMTSF)_2PF_6$*, the planar organic molecules are stacked like pancakes with every other molecule slightly offset. This provides niches in which the inorganic salts sit. The shaded areas represent regions of charge density.*





Common theme in many high Tc, charged layers. Bechgaard salts, Cuprates, MgB2 , Kappa Organics

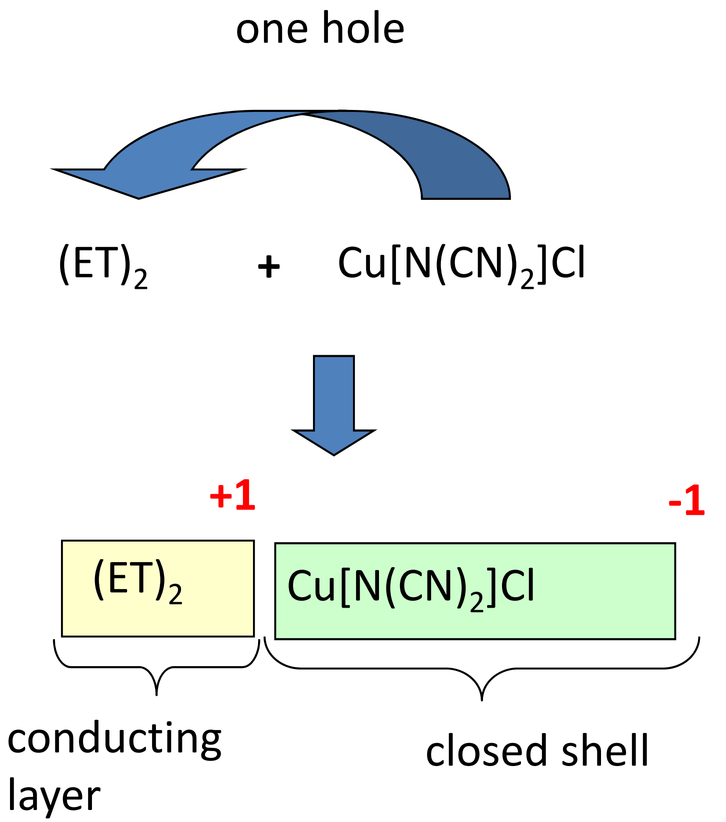
conducting layer



equivalent model

top view

one hole/one or two dimer



one hole

$(ET)_2$ + $Cu[N(CN)_2]Cl$

+1 -1

$(ET)_2$ $Cu[N(CN)_2]Cl$

conducting layer

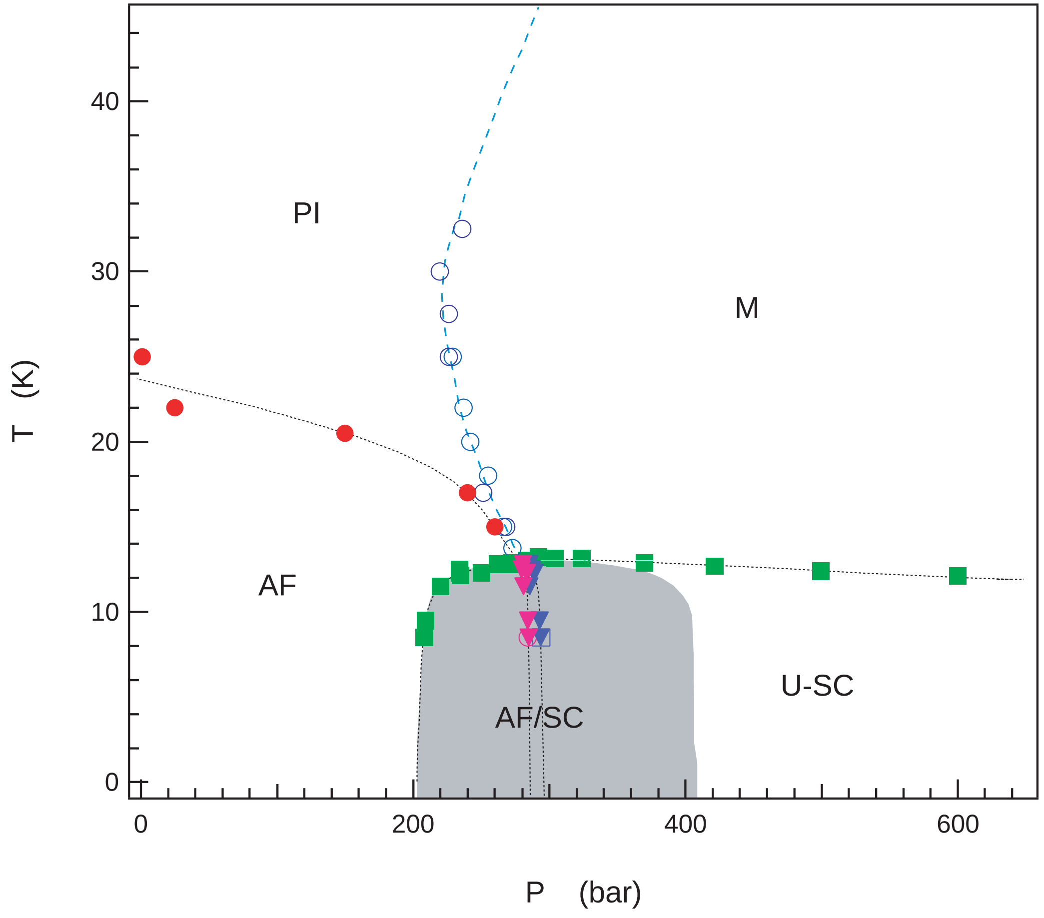
closed shell

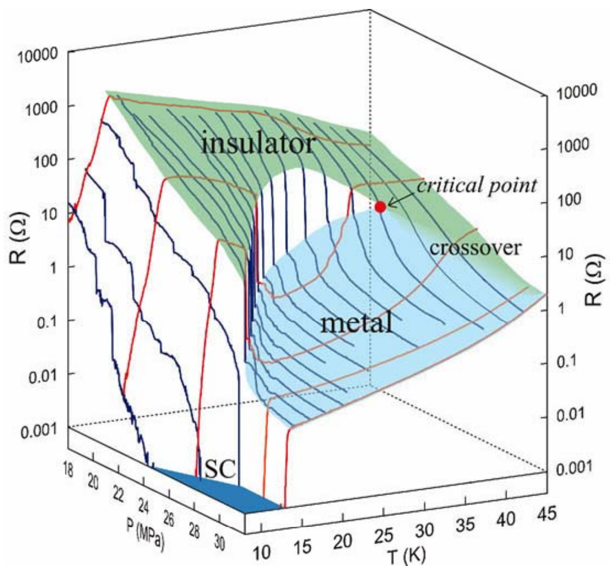
(insulating layer)

Half Filling or Quarter Filling

H. Kino and H. Fukuyama, JPSJ **65**, 2158 (1996)

In Kappa Organics one can identify the Mott transition point.





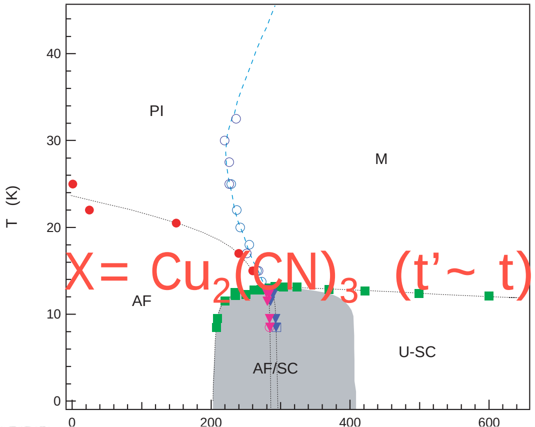
F. Kagawa, K. Miyagawa, + K. Kanoda

PRB **69** (2004) +Nature **436** (2005)

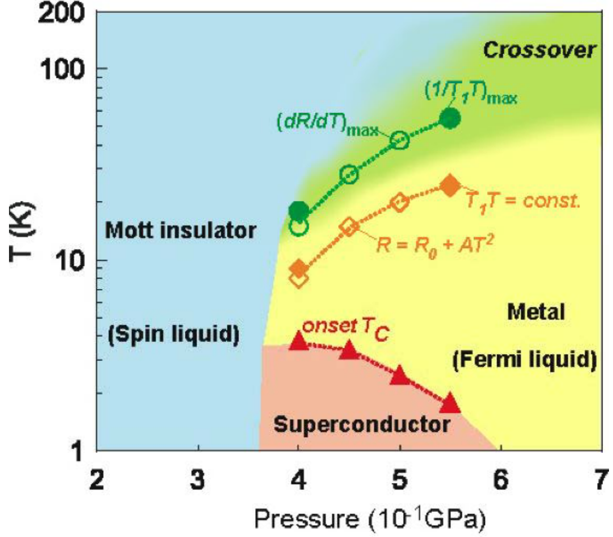
Phase diagram of (X=$Cu[N(CN)_2]Cl$)

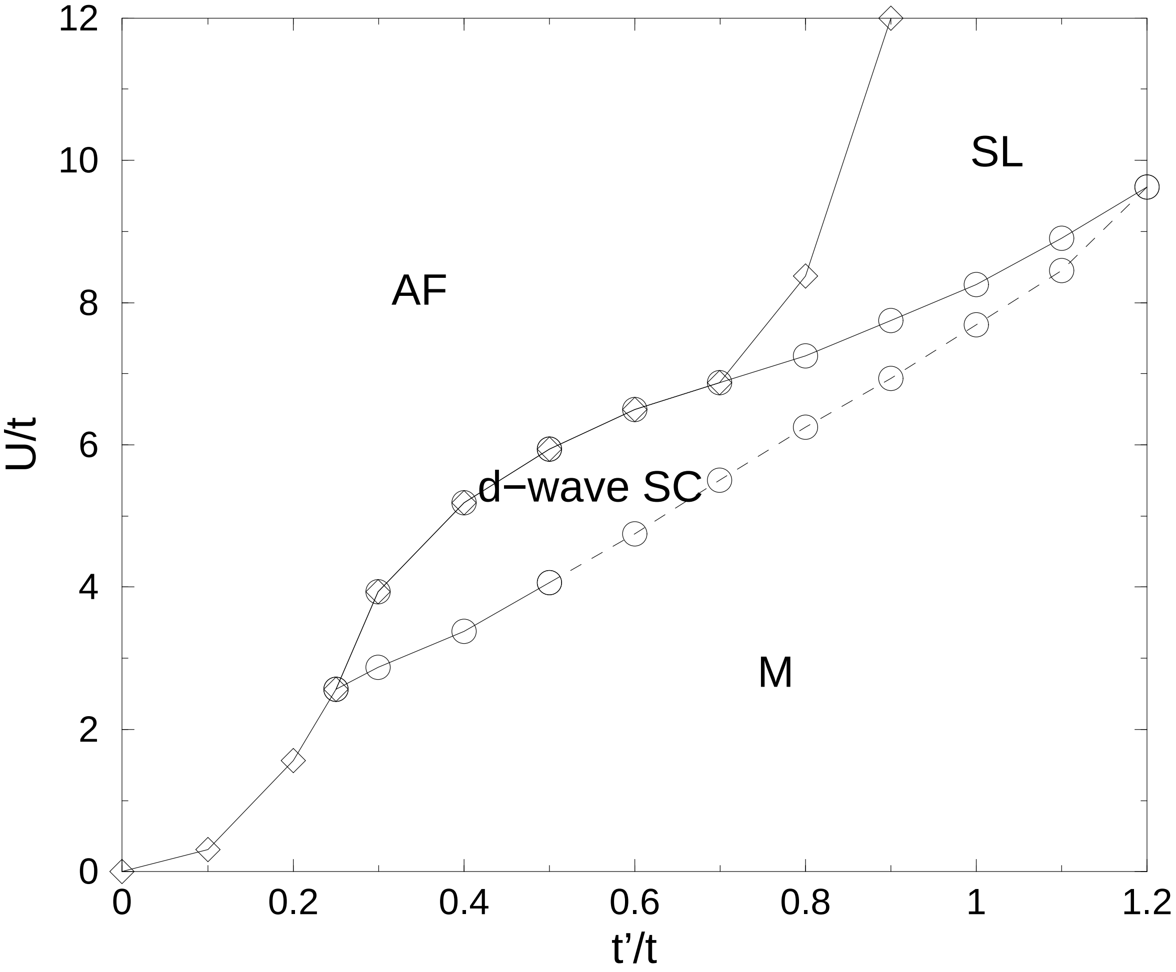
S. Lefebvre et al. PRL **85**, 5420 (2000), P. Limelette, et al. PRL 91 (2003)

Qualitative features of phase diagram are in good agreement with CDMFT.



X= $Cu_2(CN)_3$ (t'~ t)





B Kyung and A M Tremblay PRB (2006)

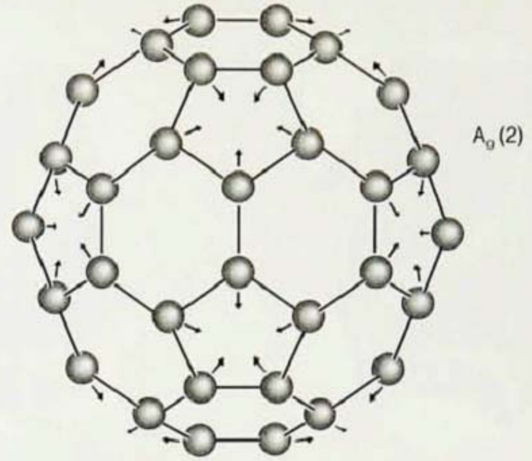
Y. Kurisaki, et al. Phys.
Rev. Lett. **95**, 177001(2005)

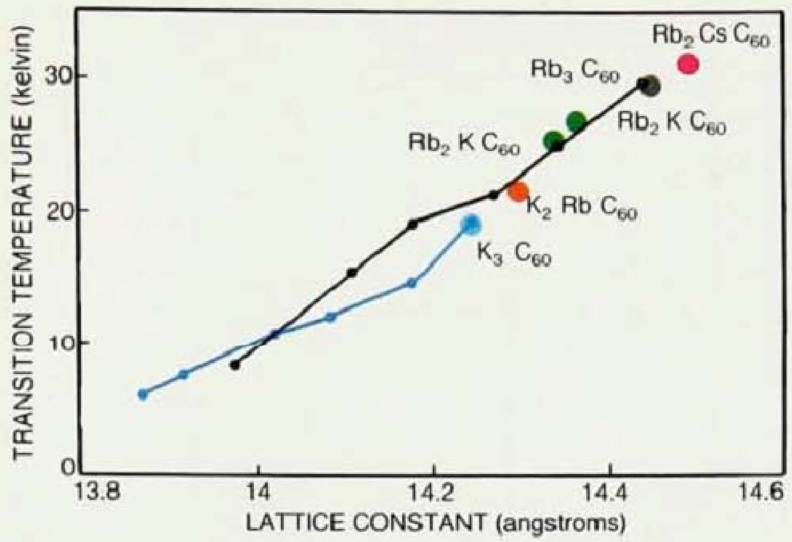
Y. Shimizu, et al. Phys. Rev. Lett. **91**, (2003)

SUPERCONDUCTIVITY IN DOPED FULLERENES

While there is not complete agreement on the microscopic mechanism of superconductivity in alkali-metal-doped C_{60}, further research may well lead to the production of analogous materials that lose resistance at even higher temperatures.

Arthur F. Hebard





PHYSICS TODAY NOVEMBER 1992

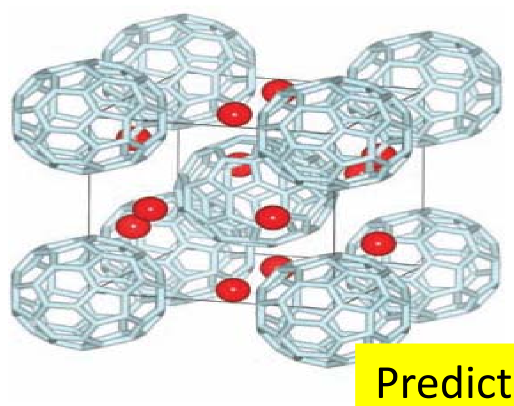
Transition temperature T_c of bulk powder samples of $A_{3-x}A'_xC_{60}$, where A and A' represent K, Rb or Cs, has a nearly linear dependence on lattice constant a. Alkali atoms with larger ionic radii produce a greater effective negative pressure and a larger lattice constant. The lattice constants refer to fcc unit cells. Application of pressure causes a lattice contraction and corresponding decrease in T_c. Results determined for potassium- and rubidium-doped C_{60} (blue and black lines, respectively) overlap with the zero-pressure data. (Adapted from refs. 12 and 13.) **Figure 4**

Expected from BCS

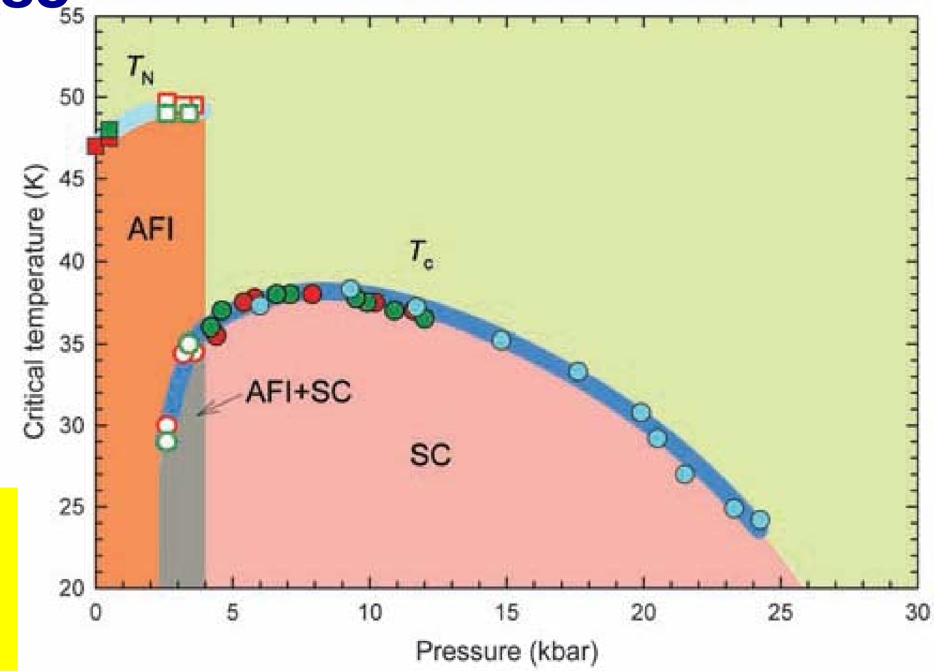
No complete agreement within different ME calculations with different methods. Narro bands. Mu*

Magnetism emerges upon expansion

Science 323 **20 March 2009: 1585**



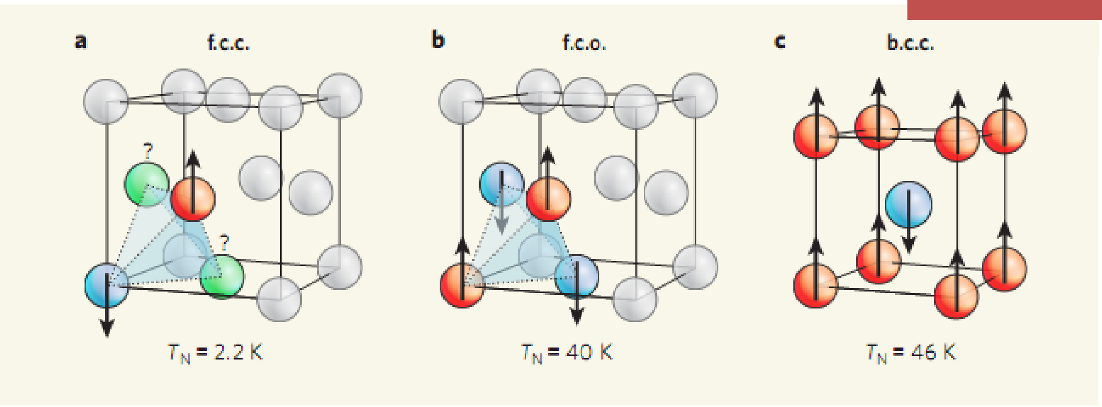
Cs$_3$C$_{60}$

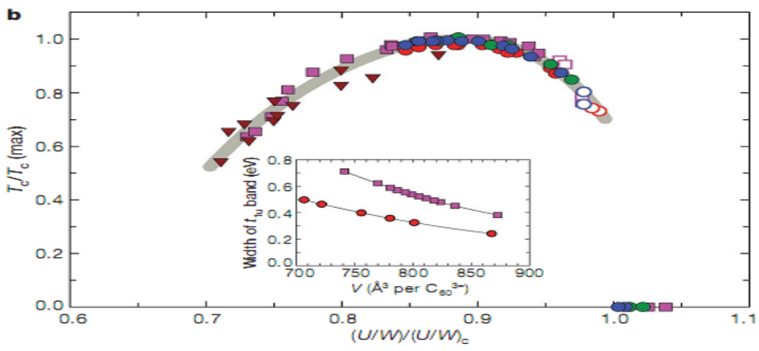


Ganin et. al. Nature (2010)

Predicted by strongly correlated superconductivity!! Capone Tossati Castellani Fabrizio

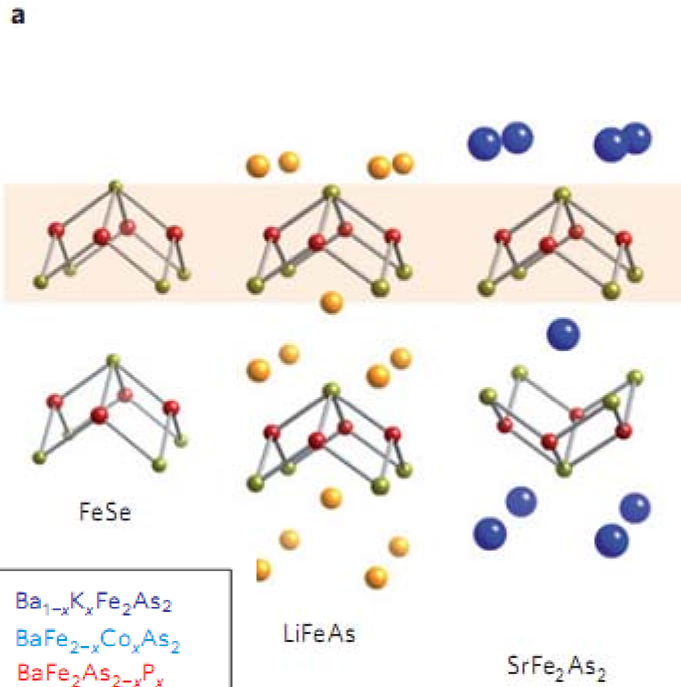
cc version is synthsized.
True Mottness .

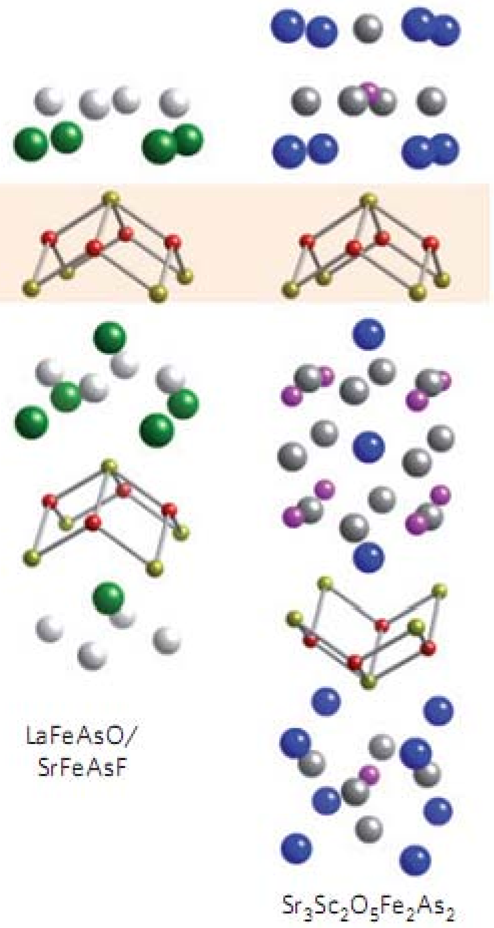


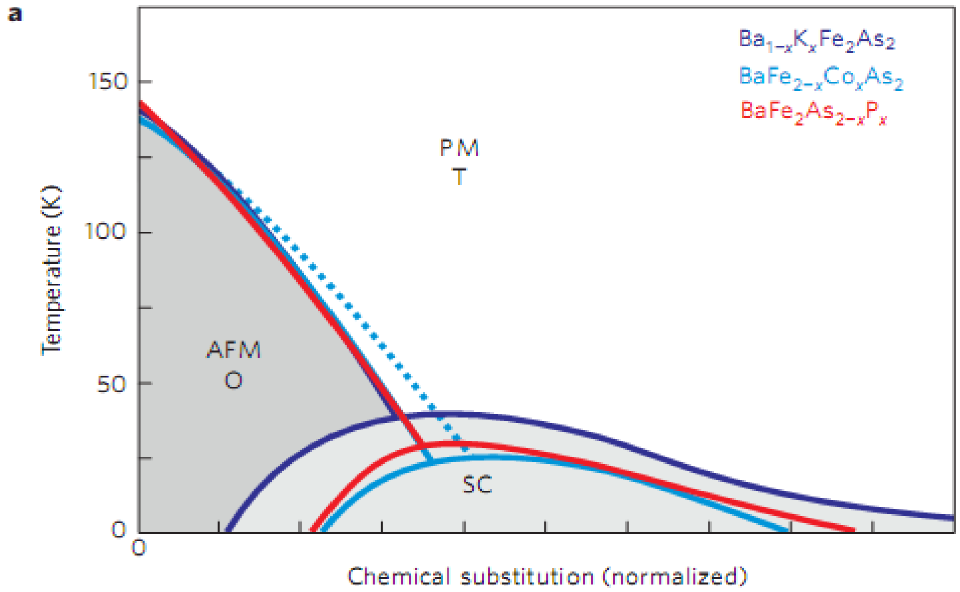


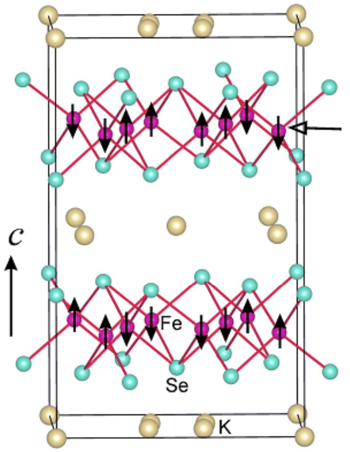
The “space of Fe pnictide/chalcogenide materials”

Simple itinerant metals ?
Localized Fe d electrons ?



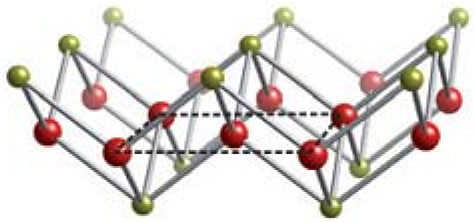


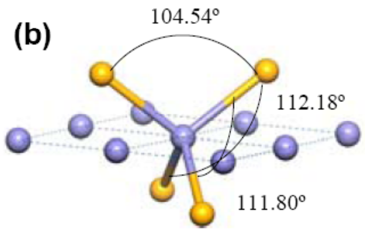




$K_{1-x}Fe_{2-2x}Se_2$

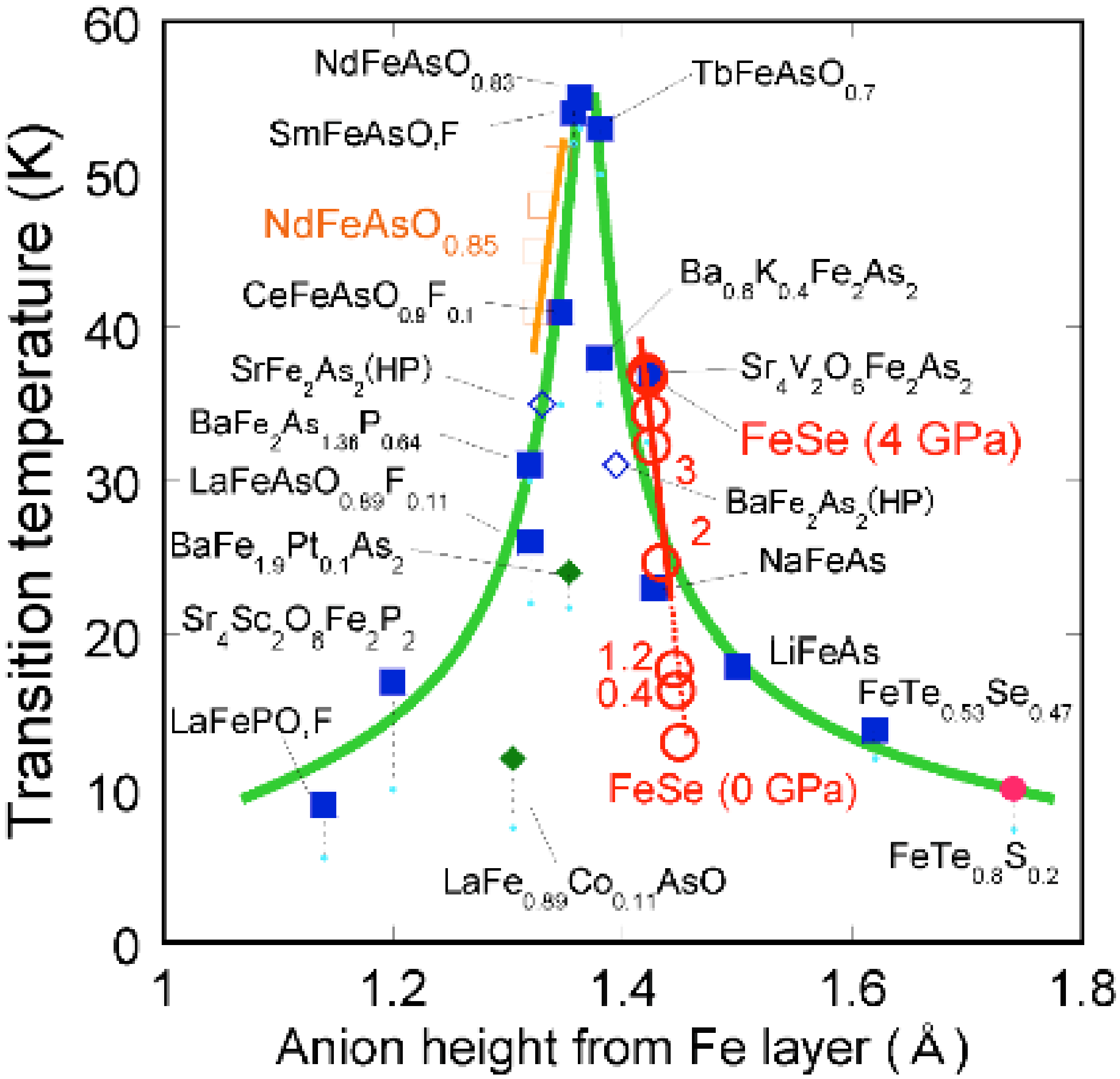
Mechanism of superconductivity ?
Real time test for methodologies





Paglione and Greene Nature Physics 6, 645(2010)

Tc ≈ Anion Height in Fe-based SCs

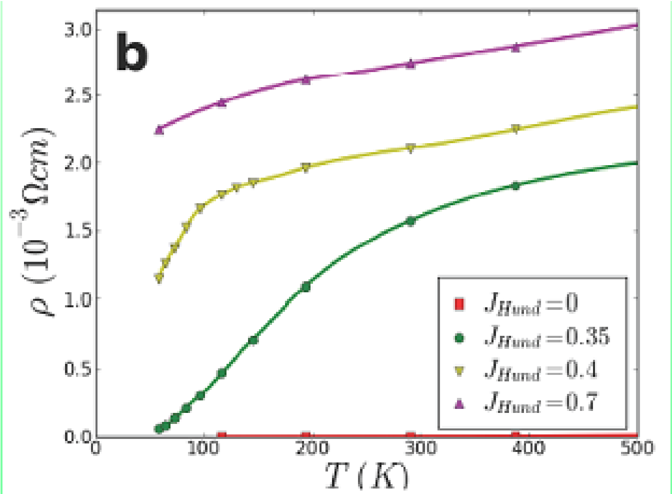


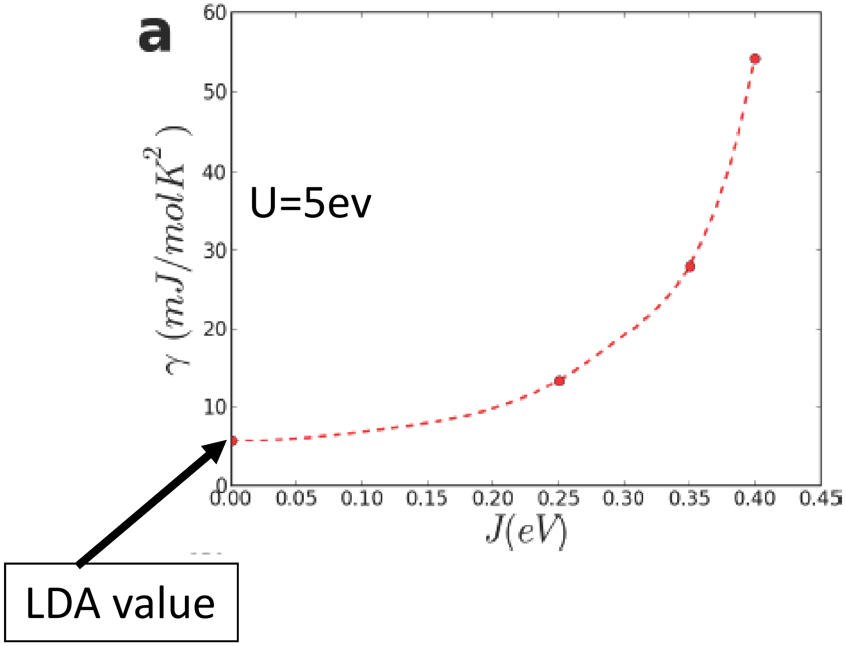
Mizuguhci et al, (2010)

Hunds Metals not doped Mott Insulators. Strength of correlations are due to Fe Hunds rule J not to Hubbard U.

K. Haule and G. Kotliar **cond-mat arXiv:0805.0722**

New Journal of Physics 11 (2009) 025021.





$$H_{Kondo} = \sum_{k\alpha,\beta k'} J_{\alpha\beta} d^{+}_{\alpha} \vec{\sigma} d_{\beta} . c^{+}_{\alpha k} \vec{\sigma} c_{\beta k'}$$

$$J_{\alpha\beta} = J \qquad T_K = e^{-\frac{1}{\rho JN}}$$

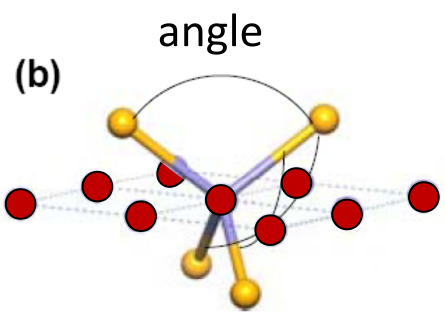
$$J_{\alpha\beta} = J\delta_{\alpha\beta} \qquad T_K = e^{-\frac{N}{\rho J}}$$

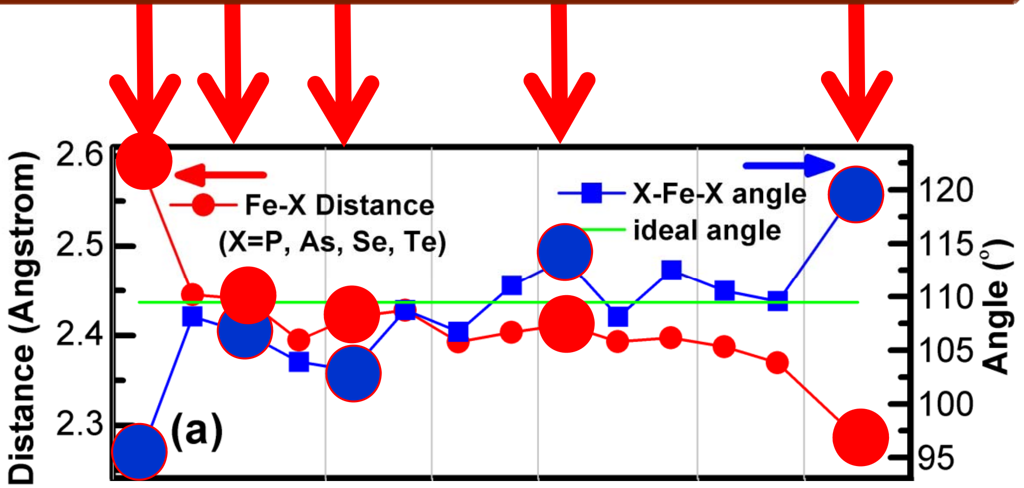
I. Okada, and K. Yosida, *Singlet Ground State of the Localized d-Electrons Coupled with Conduction Electrons in Metals*, Progress of Theoretical Physics **49**, No.5, 1483 (1973).

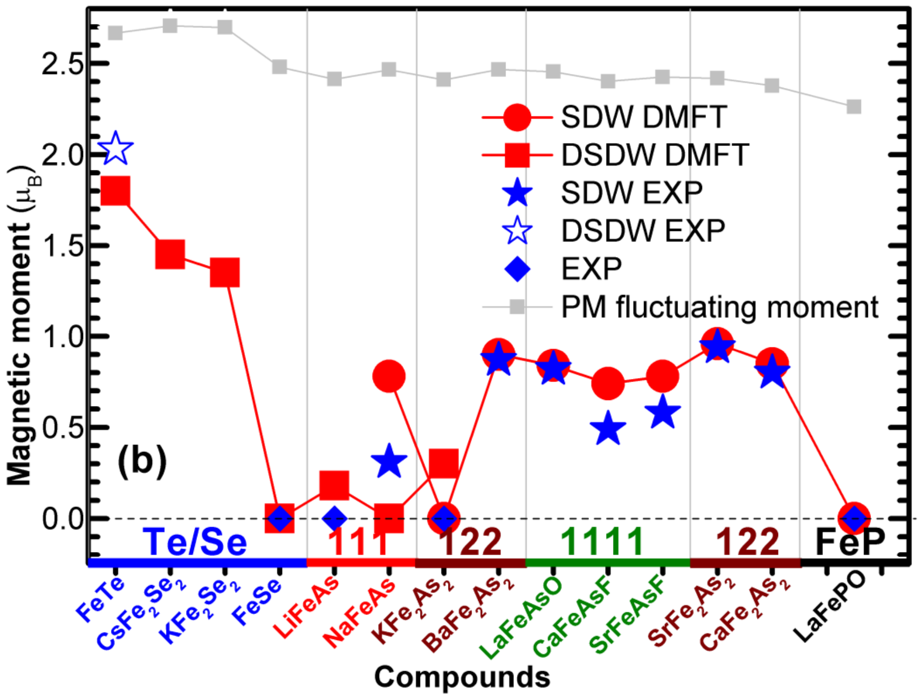
Orbital blocking. In d^6 configuration exponential amplification is regulated by x-fields. Very different than oxides. Yin et. al.

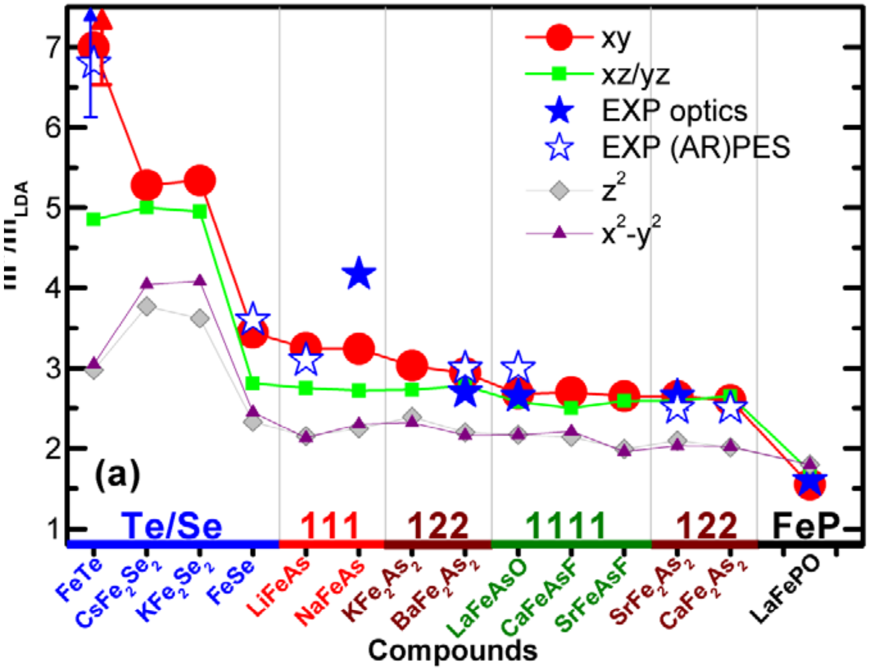
Later work by other DMFT groups now support this, Liebsch and Ishida, Sangiovanni and Held, Aichorn et. al

Yin Haule GK nature materials 2011









Same F0 F2 F4 were used for all materials

On this and most of the questions raised in this series of lectures the jury is still out, and the researchers are working their way into the mysteries of the high Tc landscape.

Many surprises are still ahead.

THANK YOU FOR YOUR ATTENTION!!!