Strongly Correlated Superconductivity: the case of the Iron Pnictides and Chalcogenides.

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Work done in collaboration with

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nature physics | LETTERS

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Spin dynamics and orbital-antiphase pairing symmetry in iron-based superconductors

Z. P. Yin*, K. Haule and G. Kotliar

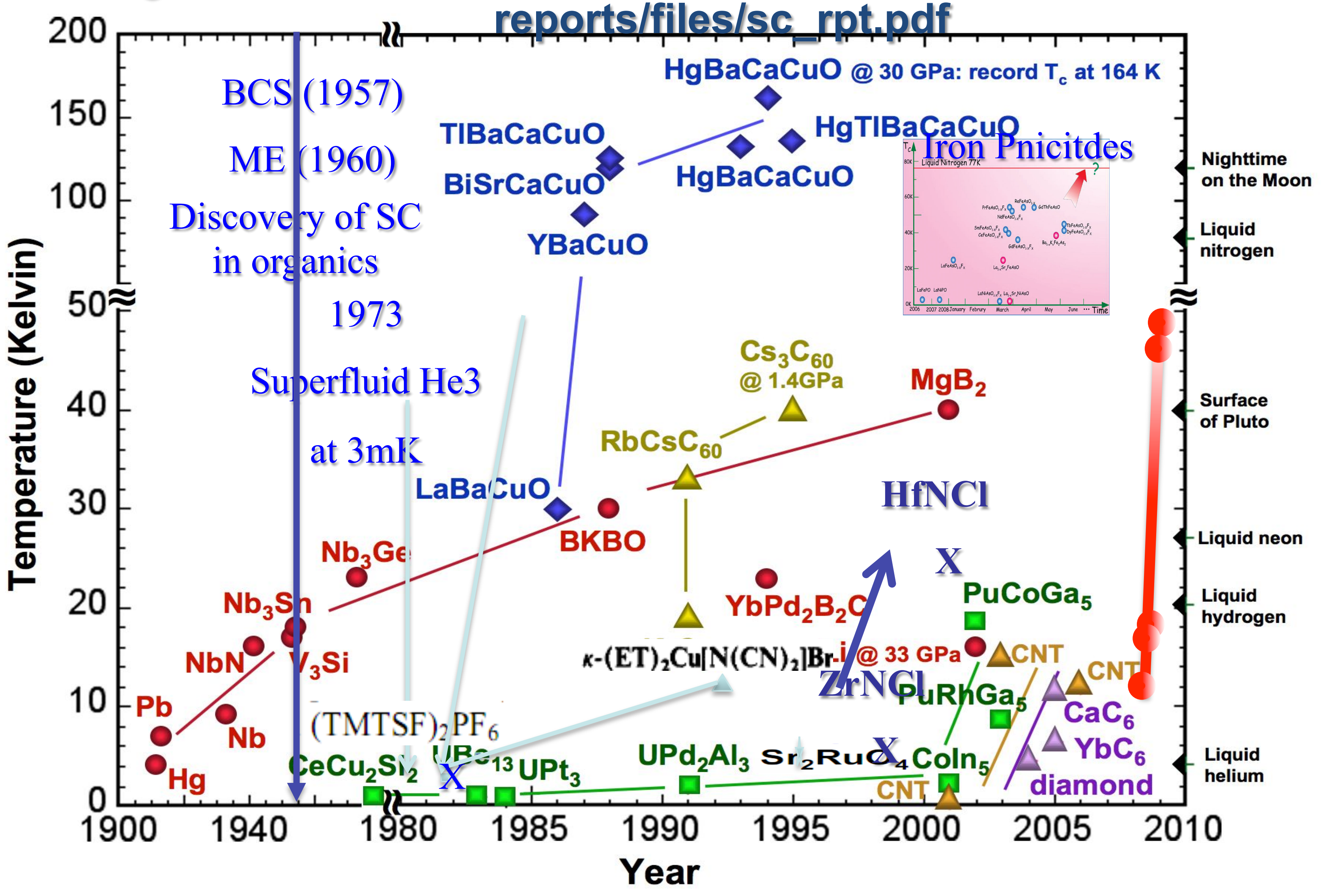
C. Aron and G. Kotliar arxiv: 1401.0331

Analytic theory of Hund's metals: a renormalization group perspective

Workshop on Probing and Understanding Exotic Superconductors and Superfluids

(Trieste, 27-31 October 2014).

"T_c vs. Time" http://science.energy.gov/~/media/bes/pdf/reports/files/sc_rpt.pdf



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

Band Theory. Fermi Liquid Theory (Landau 1957).

Density Functional Theory (Hohenberg Kohn Sham 1964)

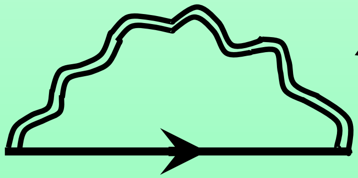
$$-\nabla^2/2 + V_{KS}(r)[\rho]\,\psi_{kj} = \varepsilon_{kj}\psi_{kj}$$

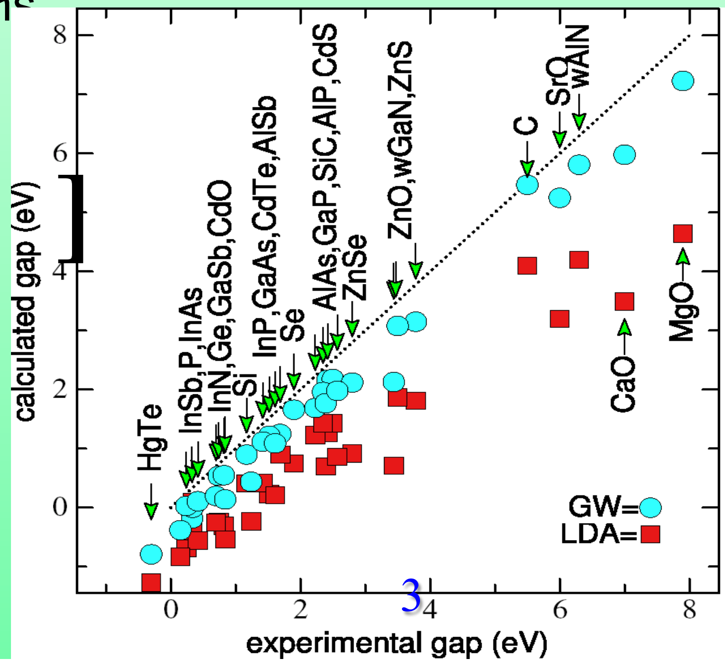
Reference Frame for Weakly Correlated Systems.

$$\rho(r) = \sum_{\varepsilon_{kj}<0} \psi_{kj}^*(r)\psi_{kj}(r)$$

Excellent binding energies and structures /Starting point for perturbation theoryGW (Hedin) in the screened Coulomb interactions

$$G^{-1} = G_{0KS}^{-1} + [\quad \Sigma \quad - V_{KS}]$$



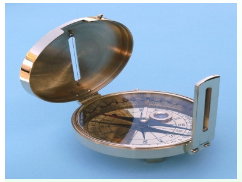


4)

Migdal Eliashberg. Controlled approximations as along as the coupling is not too strong and if

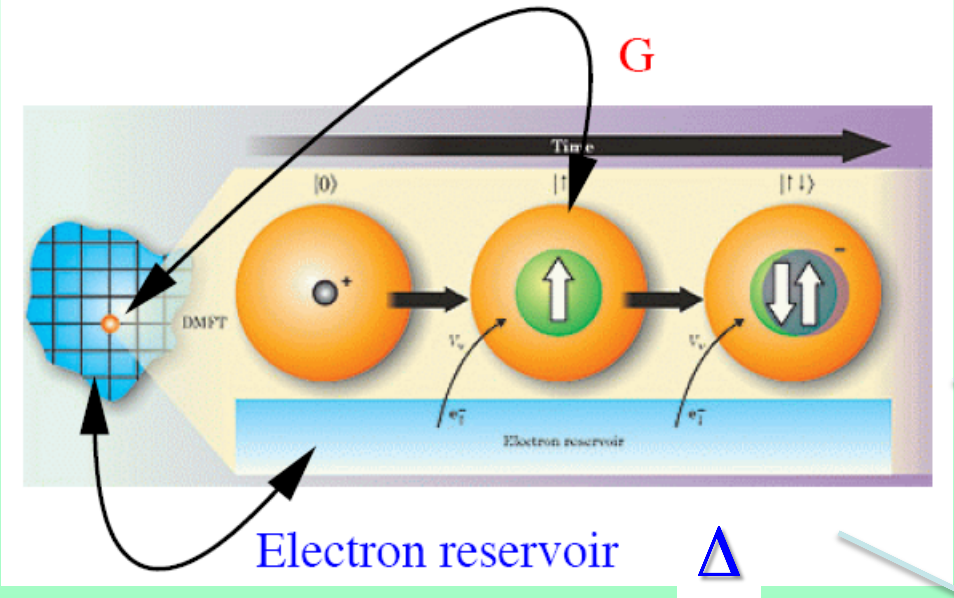
$$\omega_D << \varepsilon_F$$

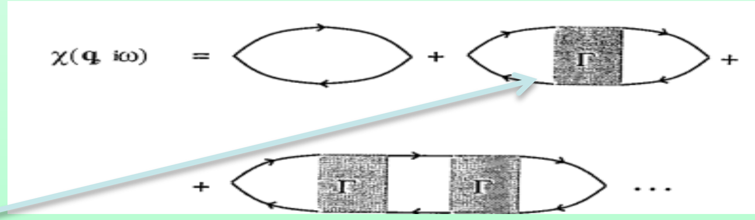
Weak copuling instabilities- BCS superconductivity…



DMFT Self consistent quantum impurity model. Reference system to study correlated electrons materials

A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, Rev. Mod. Phys. 68, 13 (1996)





Two particle irreducible vertex function

1 particle irreducible self energy

LDA+DMFT . Quantum Embedding. G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianetti, RMP. 78, 865 (2006)

$$G(\omega,r,r')=\frac{1}{[\omega+\nabla^2+\mu - V_{st} - \chi^*_{\alpha R}(r)\Sigma(i\omega)_{\alpha\beta}\chi_{\beta R}(r')]}$$

(2008)Superconductivity in $LaFeAsO_{1-x}F_x$

La+++   O--   (LaO)+ ionic-insulating

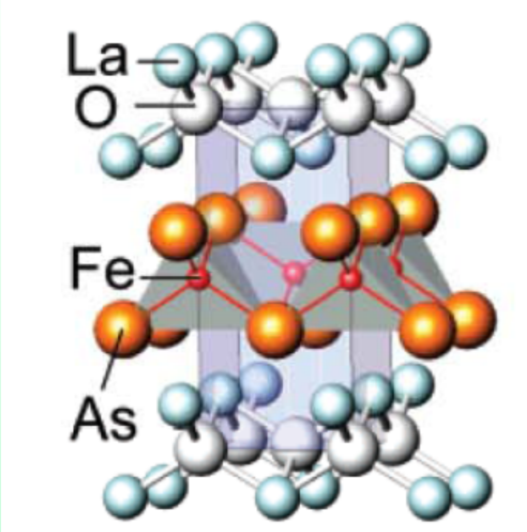
$(FeAs)^-$ layers   active block

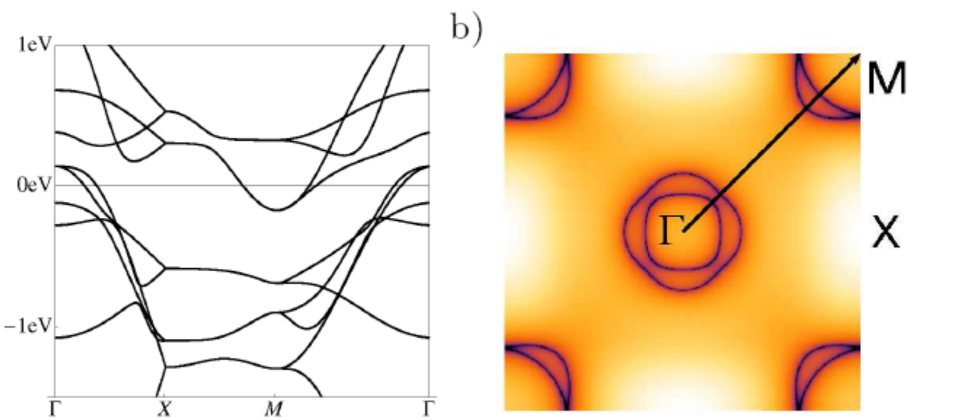
Atomic iron , **[Fe] 3d6 4s2. [As]**

Atomic arsenic [Ar] 3d10 4s2 4p3

Fe++ d6   As---   p6

Real Space Picture

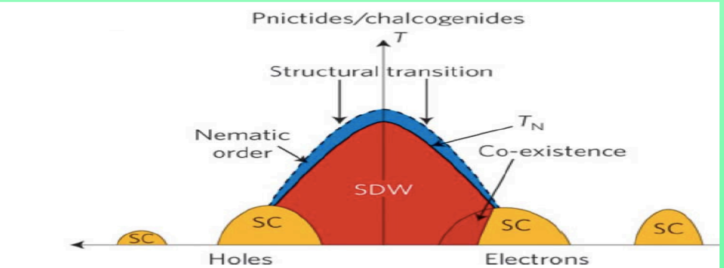




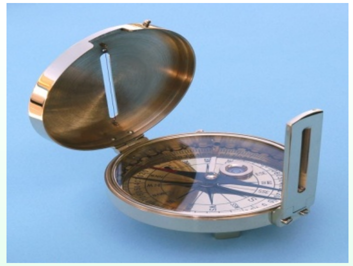
Momentum Space Picture

Doped Mott Insulators ?

Weakly correlated
Itinerant magnets?
Hunds metals ?



Early DMFT predictions



PRL **100,** 226402 (2008) PHYSICAL REVIEW LETTERS week ending 6 JUNE 2008

Correlated Electronic Structure of $LaO_{1-x}F_xFeAs$

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

Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA

(Received 9 March 2008; published 2 June 2008)

Parent Compound is a (bad)semi-metal.

phonon mediated. Indeed an explicit calculation of the phonon coupling constants within the DFT, using the code of Ref. [5], gives a value too small to explain the observed critical temperature ($T_c < 1$ K).

Unconventional SC

Phonon Tc<1K

Fermi level. The band velocity and effective mass are considerably enhanced (3–5 times) while the scattering rate still remains large. Finally, the hole pockets around Γ remain highly scattered.

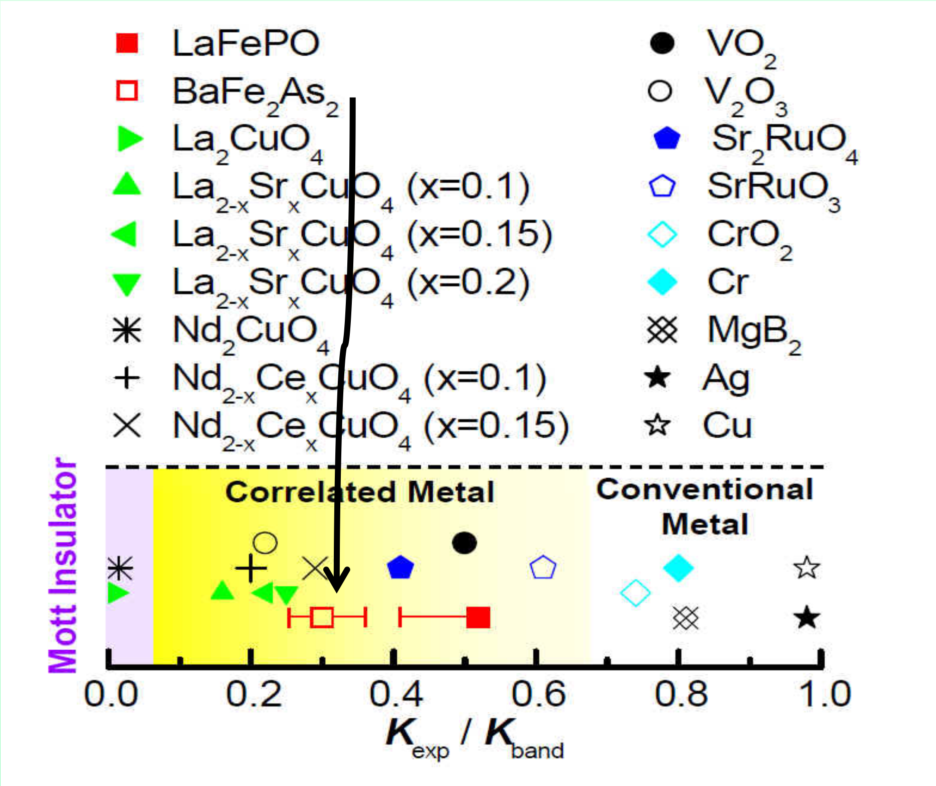
Importance of correlations

Mass enhancement 3-5

5 3d orbitals small X- fields

L. Boeri et. al. PRL , 101, 026403 (2008)

Optical Spectroscopy can be used to determine the mass enhancement relative to the band theory mass (LDA)



LDA+DMFT had predicted correlation effects m/m* ~.3 -.2 this WAS seen in OPTICS.

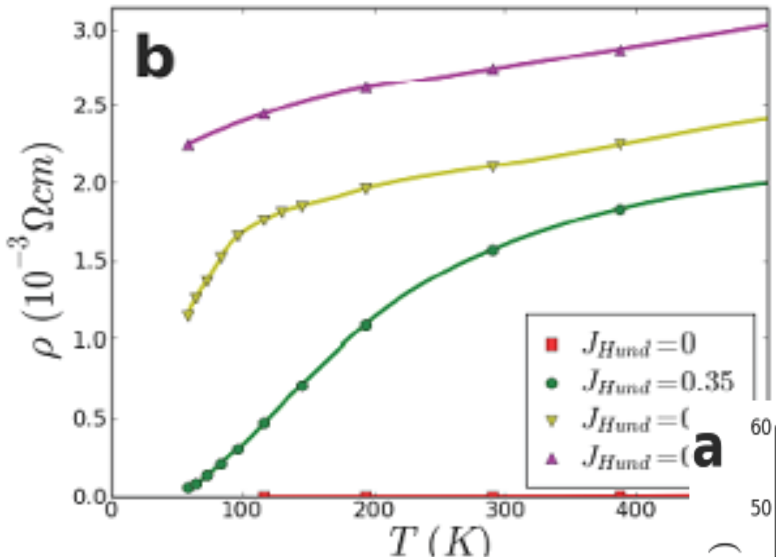
But proximity to the Mott transition can also induce Motness.

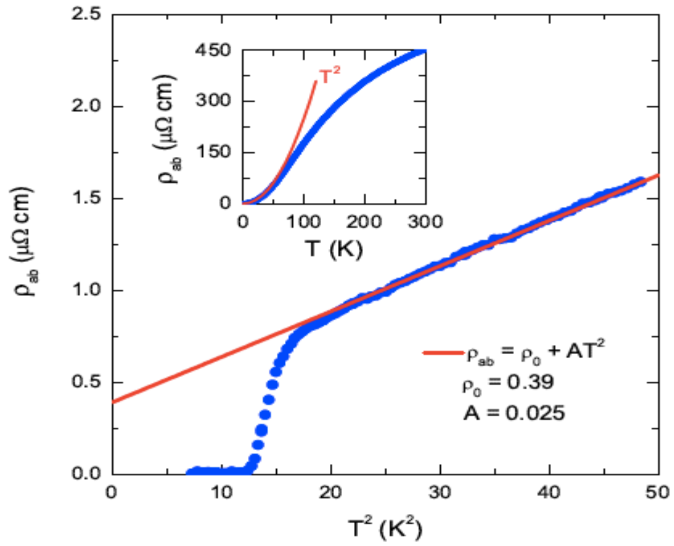
M. M. Qazilbash et. al. Nature Physics 5, 647 (2009)

Coherence–incoherence crossover in the normal state of iron oxypnictides and importance of Hund's rule coupling

K Haule[1] and G Kotliar
Department of Physics, Rutgers University, Piscataway, NJ 08854, USA
E-mail: haule@physics.rutgers.edu

New Journal of Physics **11** (2009) 025021





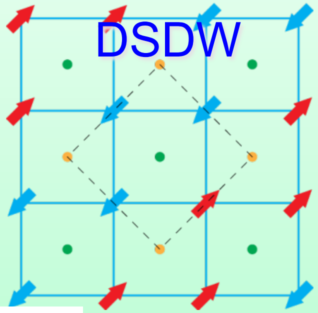
PRL 111, 027002 (2013) PHYSICAL REVIEW LETTERS week ending 12 JULY 2013

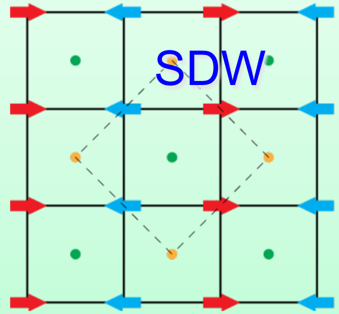
Evidence of Strong Correlations and Coherence-Incoherence Crossover in the Iron Pnictide Superconductor KFe_2As_2

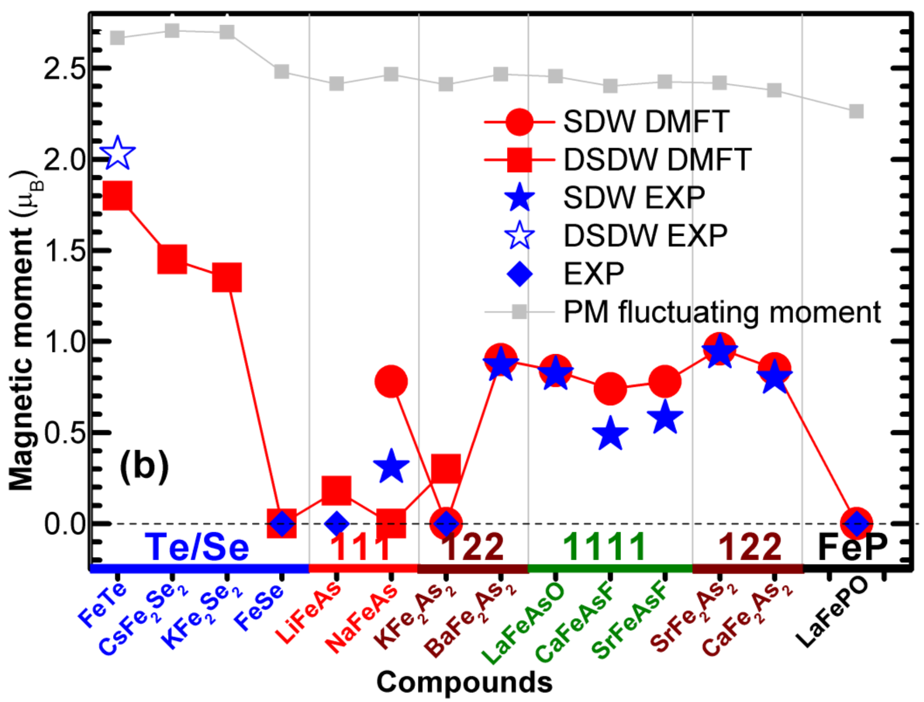
F. Hardy,[1,*] A. E. Böhmer,[1] D. Aoki,[2,3] P. Burger,[1] T. Wolf,[1] P. Schweiss,[1] R. Heid,[1] P. Adelmann,[1] Y. X. Yao,[4] G. Kotliar,[5] J. Schmalian,[6] and C. Meingast[1]

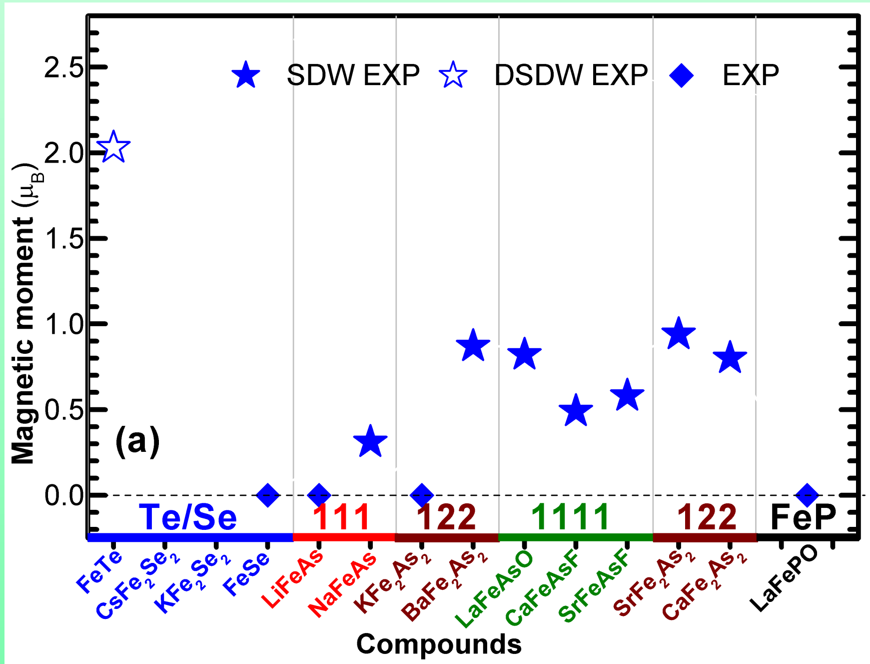
All families share the same FePn layers Fe d^6, similar bands

What governs the strength of the magnetims among the families ? Big window, same local interactions for all materials. Variations are in the one electron H0.

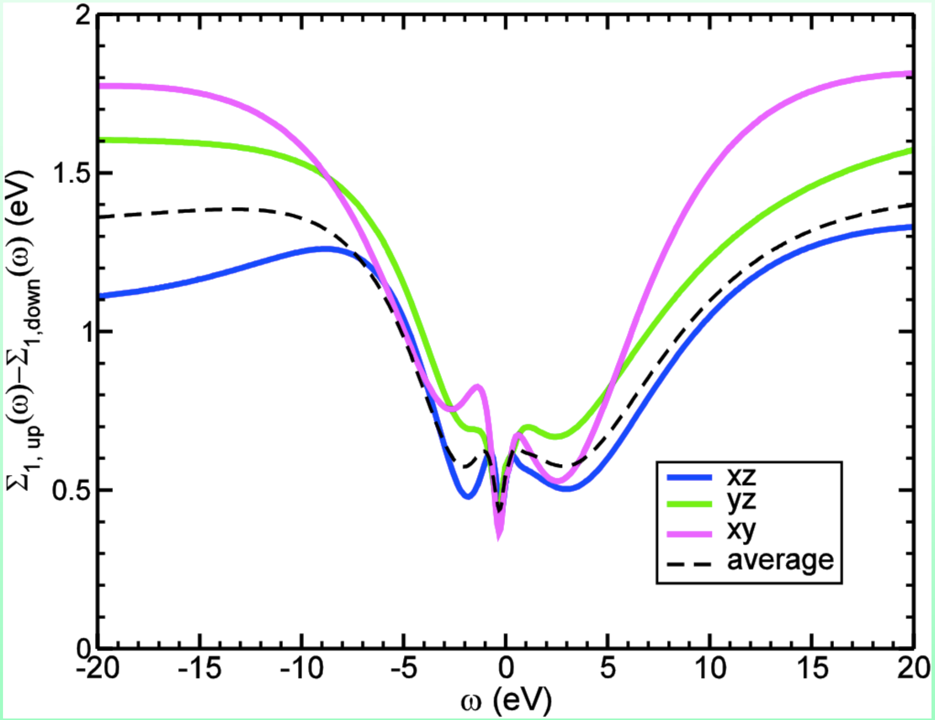


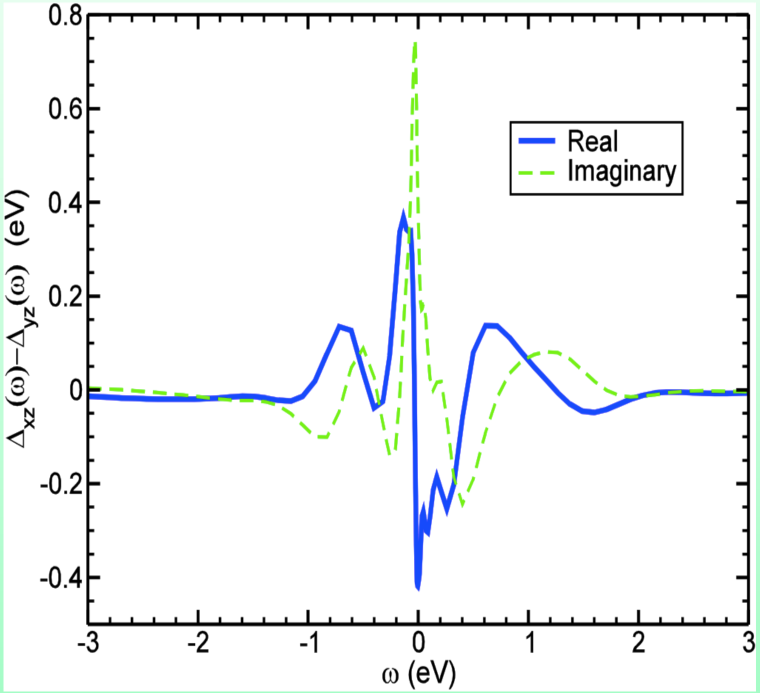






Understanding the Stripe Phase (and by extension the nematic phase above it)





Orbital polarization large at low energy (300 meV)

Spin polarization large at high energy

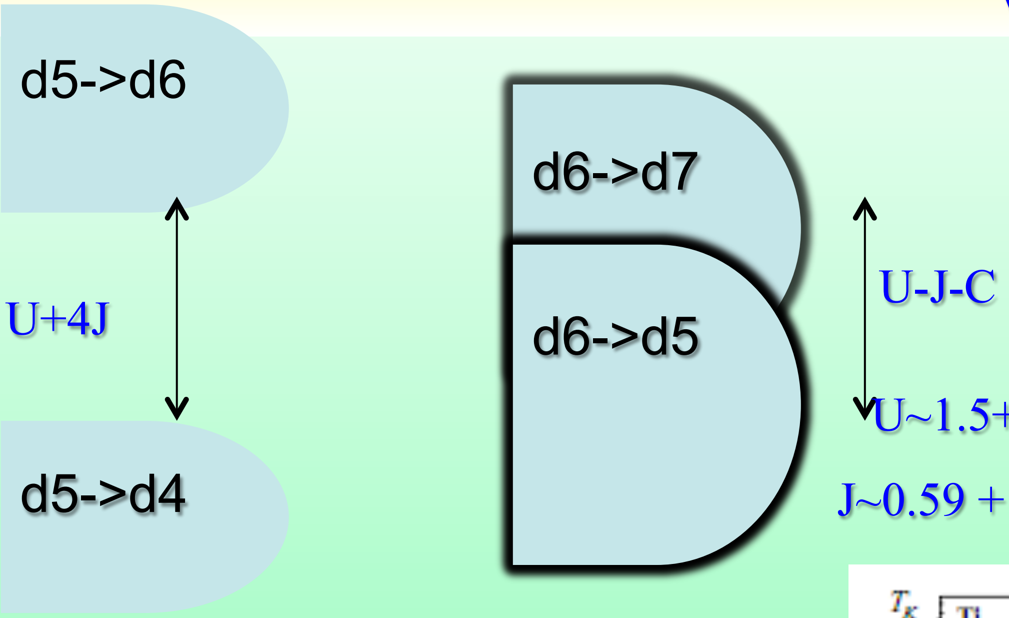
Spin moment lives at high energy and orbital polarization at low energy

DYNAMICAL NEMATICITY Yin Z Haule K and GK Nature Physics 7, 294–297 (2011)

Hundness 101 : Uc2 ~ N W, Uc1~N$^{.5}$ Orbitally degenerate systems tend to be metallic unless degeneracy is lifted

VanderMarel Sawatzky

PRB 37 , 10674 (1988)



U~1.5+0.21(Z—21)

J~0.59 + 0.075(Z—21)

Fe d6 confguration is much more metallic than the d5 configuration of Mn. No Mott blocking!!!

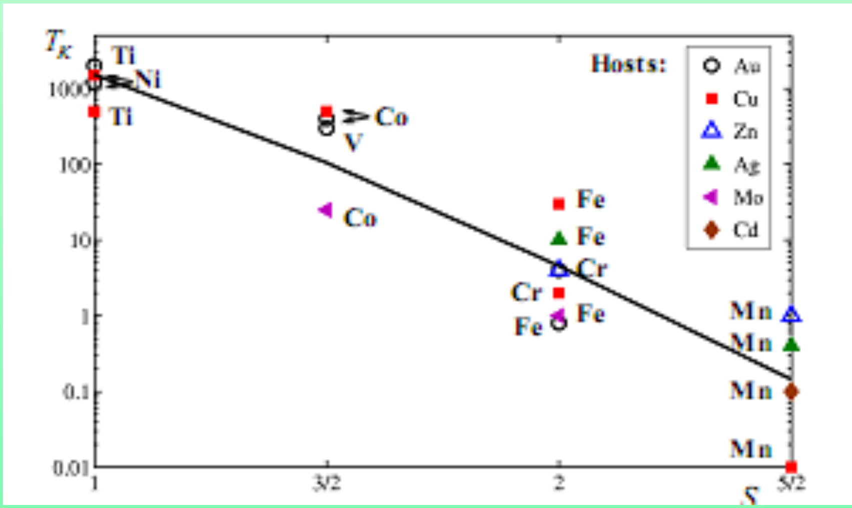
$$H_{Kondo} = \sum_{k\alpha,\beta k'} J_{\alpha\beta} d^+_\alpha \vec{\sigma} d_\beta . c^+_{\alpha k} \vec{\sigma} c_{\beta k'}$$

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

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

I. L... in ... (1973).

Extreme low energy scale Hundness reduce the coherence scale of the resonance by N^2



J. R. Schrieffer J. Applied Physics 32 , 1143 (1967)

Hundness 102 RG Eq for the Hunds metal. C. Aron and GK arxiv: 1401.0331 M orbitals N spins

Intermediate assymptotic multichannel fixed point K=2.N

FERROMAGNETIC SIGN

for hole doping!

$$H_{i\ldots} \ldots + J_0\, S^\alpha (\psi^\dagger_{m\sigma} \frac{\sigma^\alpha_{\sigma\sigma'}}{2} \psi_{m\sigma'}) \quad (4$$

$$+ K_0 T^a (\psi^\dagger_{m\sigma} \frac{T^a_{mm'}}{2} \psi_{m'\sigma}) + I_0 S \ldots \psi_{m'\sigma'})$$

Small Perturbation !

Flow to fermi liquid fixed point

is delayed

for a long time

Schrieffer effect

$$\beta_J = -\frac{N}{2}\left(1 - \frac{M}{2}J\right)\left(J^2 + \frac{C_2^T}{2M} I^2\right) + \ldots ,$$

$$\beta_K = -\frac{M}{2}\left(1 - \frac{N}{2}K\right)\left(K^2 + \frac{C_2^S}{2N} I^2\right) + \ldots ,$$

$$\beta_I = -\frac{MN}{4}\left[\left(\frac{4}{M}J + \frac{4}{N}K - J^2 - K^2\right) I + \left(\frac{C_3^T}{MC_2^T} + \frac{C_3^S}{NC_2^S}\right) I^2 + \left(\frac{1}{4} - \frac{C_2^T}{2M} - \frac{C_2^S}{2N}\right) I^3\right] + \ldots$$

$$J_0 = \frac{2}{M}\left[\frac{1}{\Delta E^-} - \frac{M - n_d}{n+1}\frac{1}{\Delta E^+}\right] V^2$$

$$K_0 = \frac{2}{N}\left[\frac{1}{\Delta E^-} + \frac{N + n_d}{n_d+1}\frac{1}{\Delta E^+}\right] V^2 ,$$

$$I_0 = 4\left[\frac{1}{n_d}\frac{1}{\Delta E^-} + \frac{1}{n_d+1}\frac{1}{\Delta E^+}\right] V^2 ;$$

See also Akahnjeee and Tsevlik PRB 87, 195137 (2013

and Tsen and Coleman PRL (2012)

Simple Impurity model

Explains the origin of the low energy scale in the model with Hunds coupling.

$T_K^K \approx \exp(-2/MK_0)D_0$, $T_K^I \approx \exp(-4/M^2I_0)D_0$
and $T_K^J \approx \exp(-2/NJ_0)D_0$ if $J_0 > 0$,

$q \equiv M/N$

$$T_K(d) \approx \exp(-q/d)\, T_K^K \ .$$

Explains the dependence of the coherence scale of the impurity on filling.

d distance from half filled shell.

- Explains particle hole asymmetry around d^6 Co doping on Fe vs K doping on Ba. d6. neq.d5

Explain the power laws observed in the optical conductivity of other Hunds metals SrRuO3 Y. S. Lee et al., Phys. Rev. B 67, 113101 (2003).and in DMFT studies of 3 band models (Werner P. Werner, E. Gull, M. Troyer, and A. J. Millis, Phys.Rev. Lett. 101, 166405 (2008).)

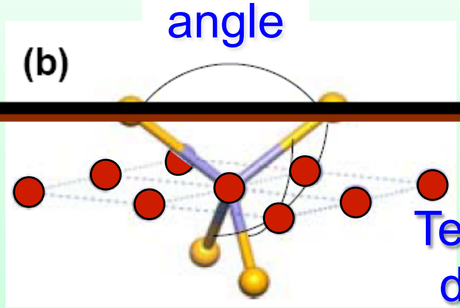
Explains the different ormalizations of the spin and orbital susceptibliities above the Fermi liquid coherence scale.

$$\chi_{S/T}(T) \sim \frac{1}{T} \exp\left(- \int_T^{D_0} \frac{\mathrm{d}D}{D}\, \gamma_{S/T}\left(J_i(D)\right) \right) ,$$

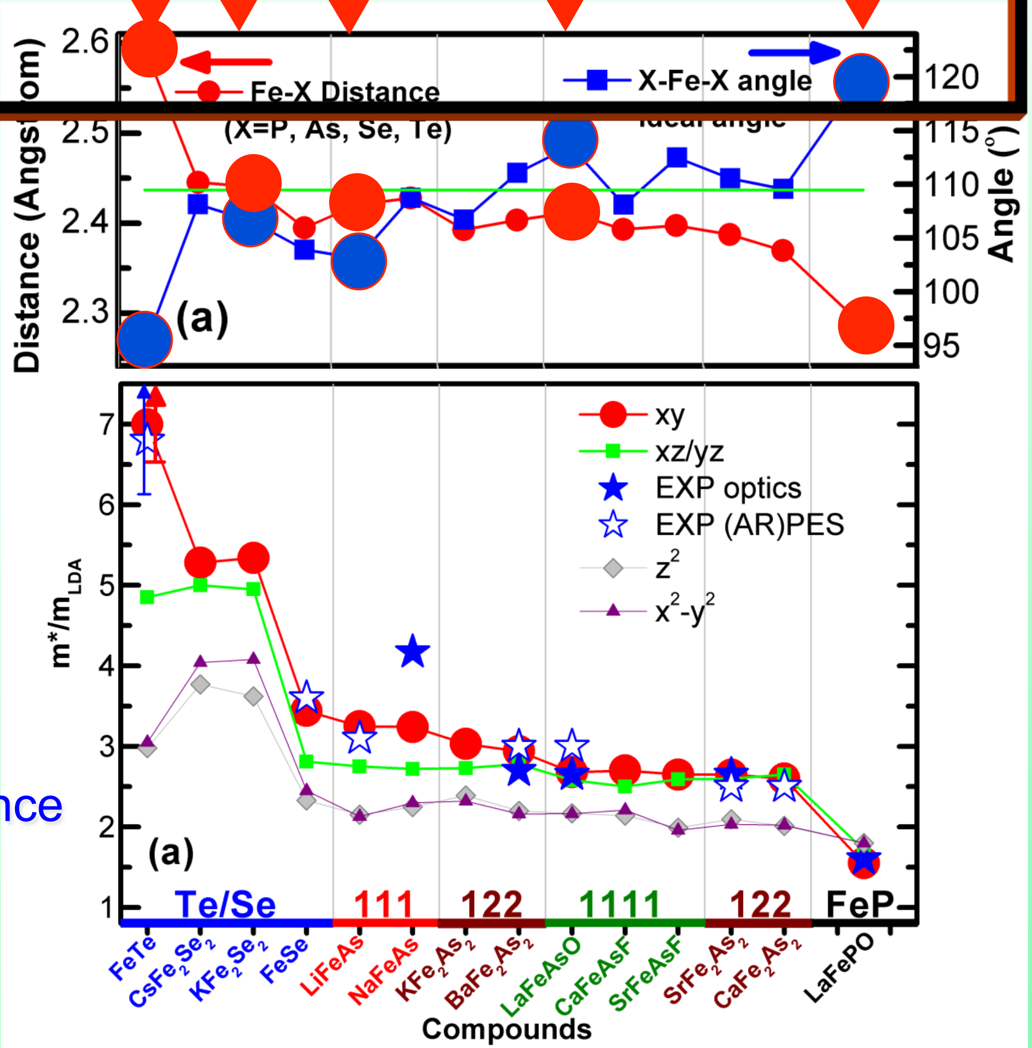
$MN(K^2 + C_2^S I^2/2)/2.$

$MN(J^2 + C_2^T I^2/2)/2$

Landscape of Materials: Nature Materials 10,:932–935:(2011)



Tendency to orbital differentiation as correlations increase.

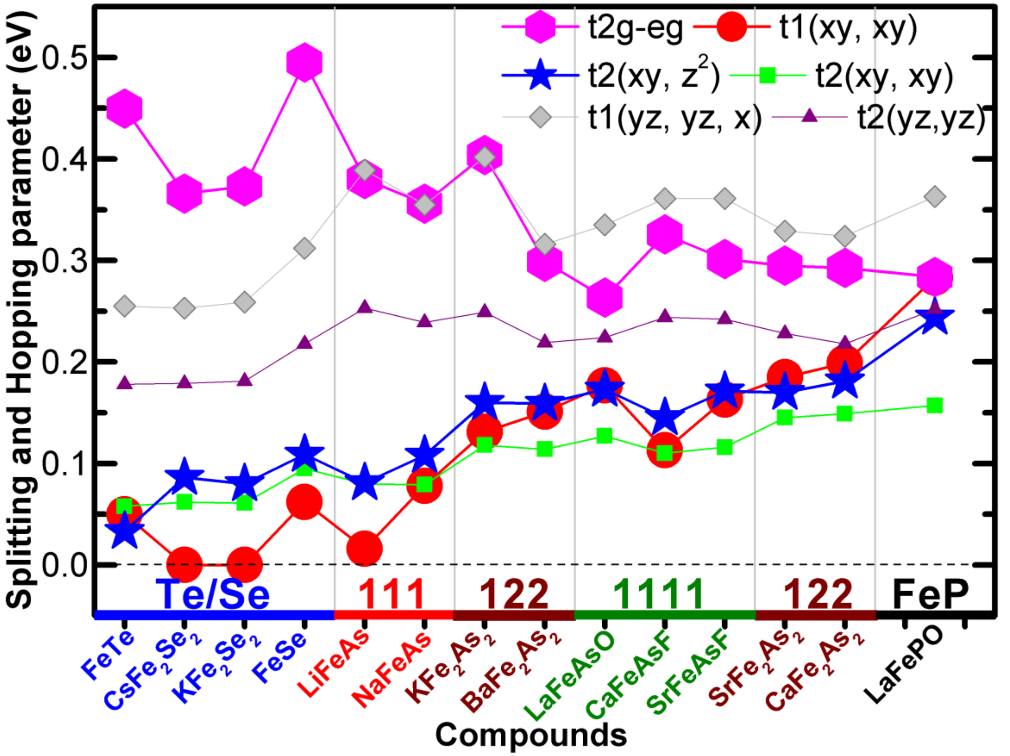


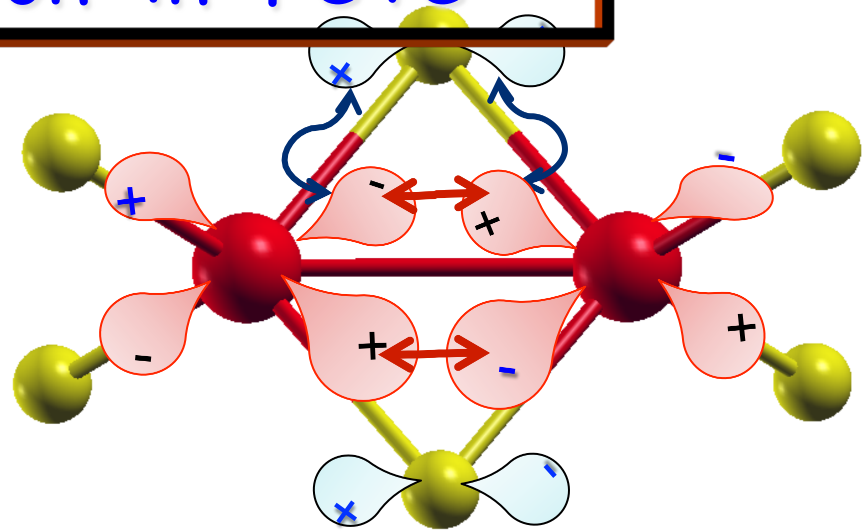
Overall trend consistent with Fe-As distance

Hybridization with pnictogen

Orbital Differentiation and Kinetic frustration in FeTe

Effective low energy hoppings





$$t^{direct}_{xy,xy} < 0$$

$$t^{As}_{xy,xy} > 0$$

t^{As} usually larger, but not when pnictogen height large!

Destructive interference leads to kinetic frustration

Factors that govern the correlation ndLiebsch Ishida Phys. Rev. B 81, 054513 (2008) Yin Haule and Kotliar Phys. Rev. B 86, 195141 (2012)

ORBITAL DIFFERENTIATION

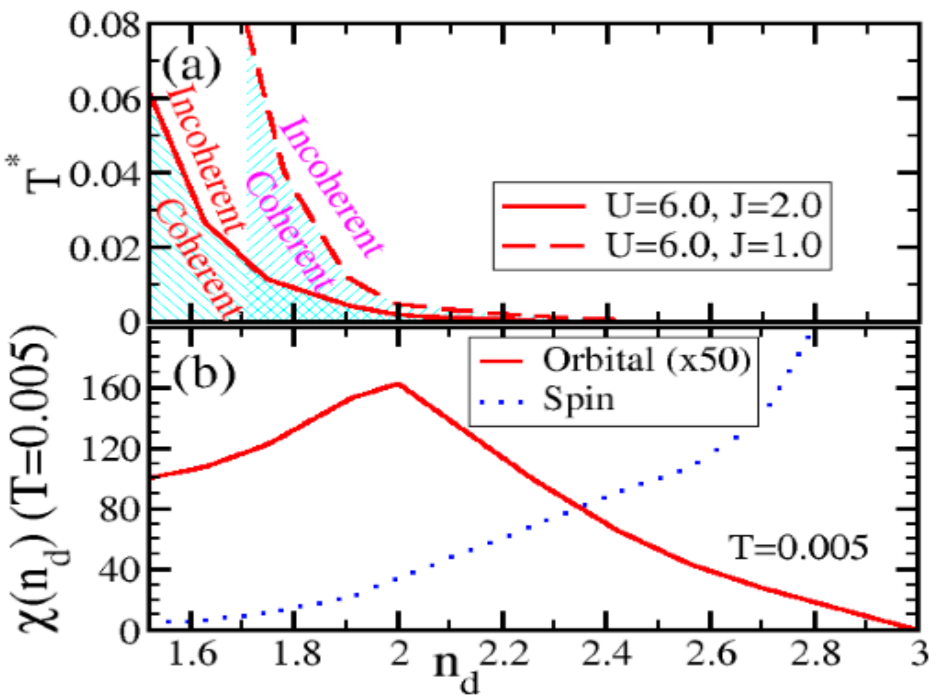
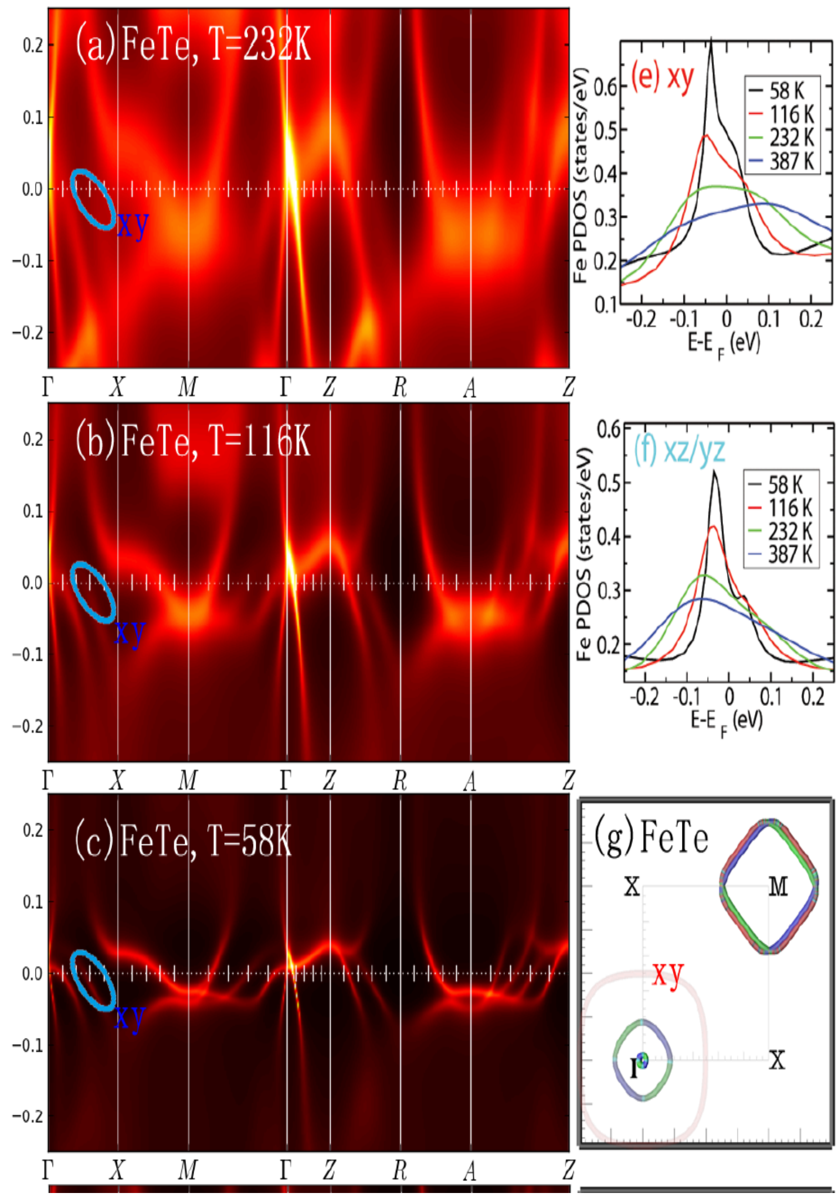


FIG. 4: (color online) (a) The coherent temperature; and (b) the spin and orbital susceptibility, as a functional of n_d for a three band model with $J_H = 2.0$ (solid lines) and $J_H = 1.0$ (dash lines).

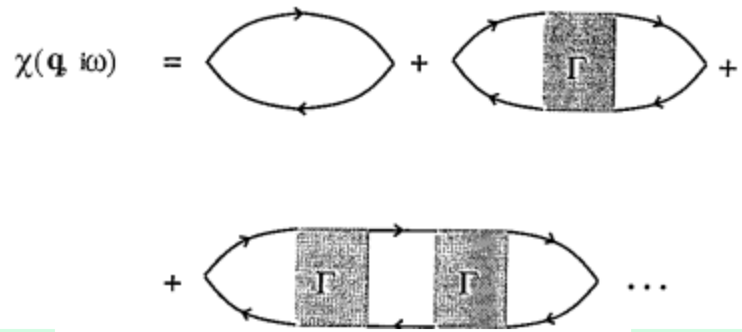


Theory: H. Park , K. Haule and GK

Phys. Rev. Lett. 107, 137007 (2011).

L Harriger H. Luo M. Liu T. Perring C Frost H. Ju M. Norman and Pengcheng Dai : PRB 84, 054544

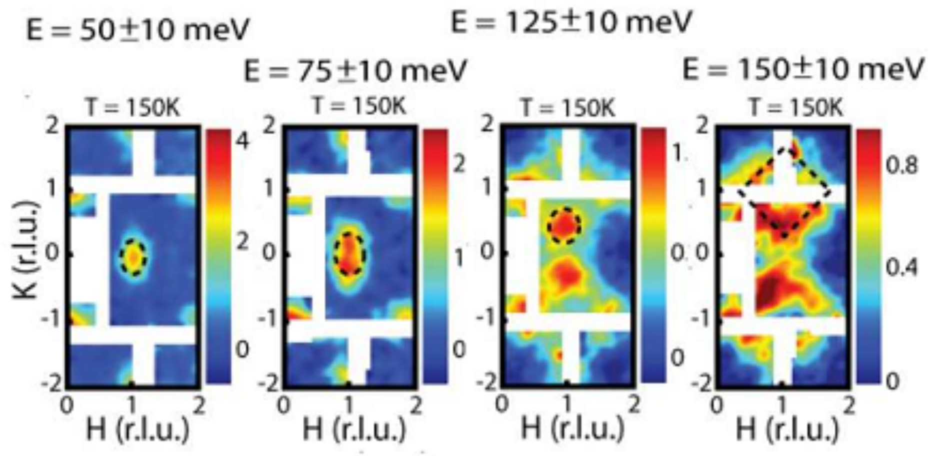
$$S(\mathbf{Q},\hbar\omega) = |F(Q)|^2 \frac{\chi''(\mathbf{Q},\hbar\omega)}{1-\exp(-\hbar\omega/k_B T)}.$$

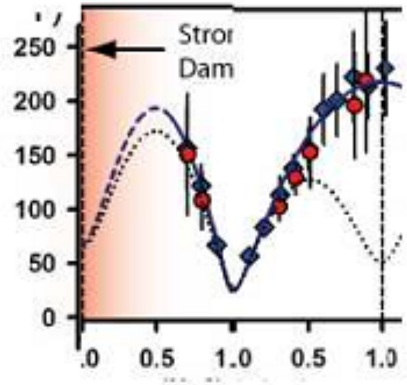


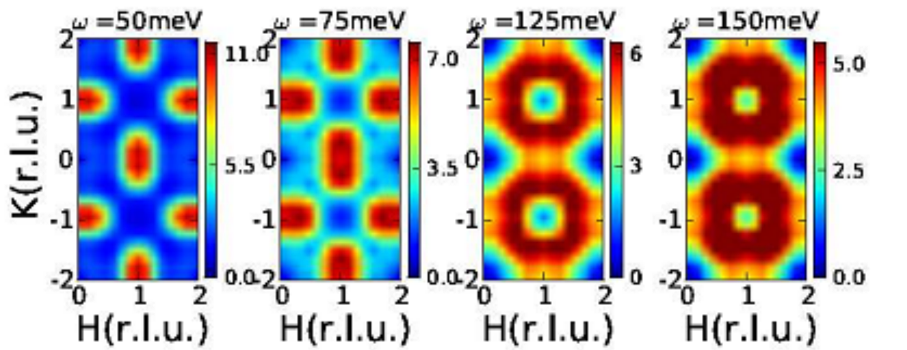
$SJ_{1a} \approx 59.2meV$

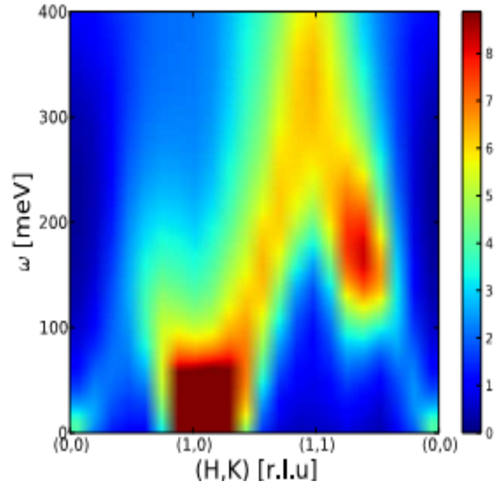
$SJ_{1b} \approx -9.2meV$

$SJ_2 \approx 13.6meV$





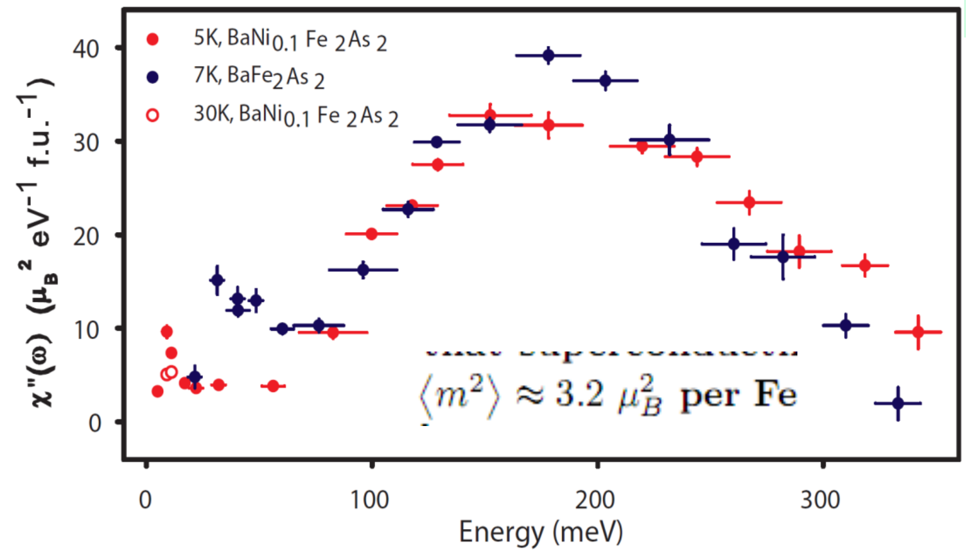


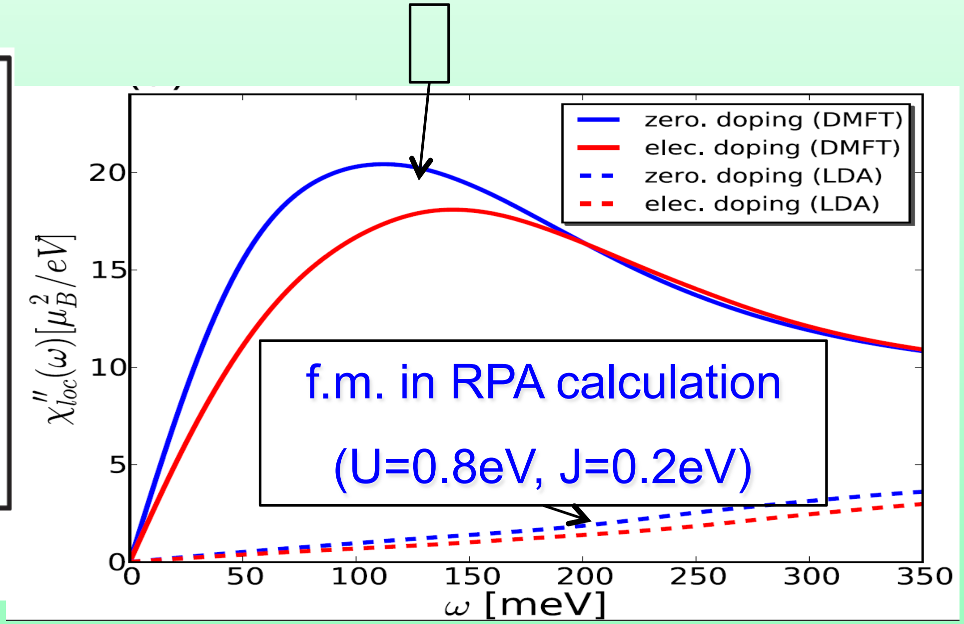


Needed absolute intensities

Fluctuating moment by neutrons: $u^2\rangle = \int \frac{d\omega}{\pi} n(\omega)\chi''(\omega)$

Experiment by Liu …Pengcheng Dai





Large fluctuating moment can not be explained by a purely itinerant model- doping dependence different than in localized model. Understandable in the Hunds metal picture.

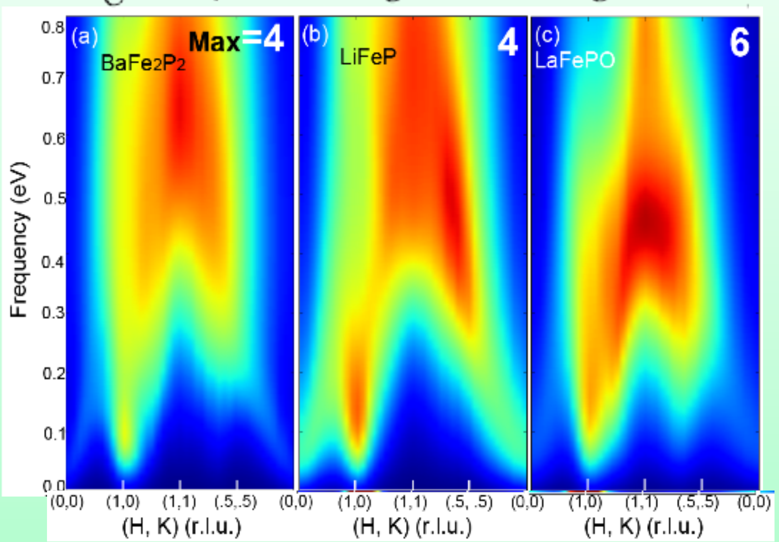
Nature Physics 8, 376-381 (2012)

Nature of magnetic excitations in superconducting $BaFe_{1.9}Ni_{0.1}As_2$

Mengshu Liu,[1] Leland W. Harriger,[1] Huiqian Luo,[2] Meng Wang,[2,1] R. A. Ewings,[3] T. Guidi,[3] Hyowon Park,[4] Kristjan Haule,[4] Gabriel Kotliar,[4] S. M. Hayden,[5] and Pengcheng Dai[1,2,6,*]

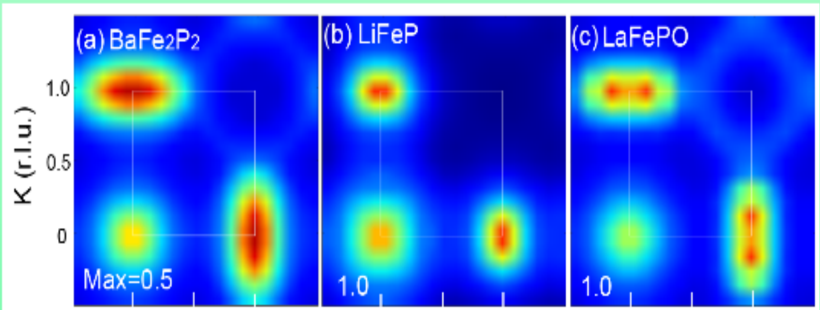
Evaluation of S(q, ω) for many families

$T_C^{max} < 2K \quad T_C = 6K \quad T_C = 7K$

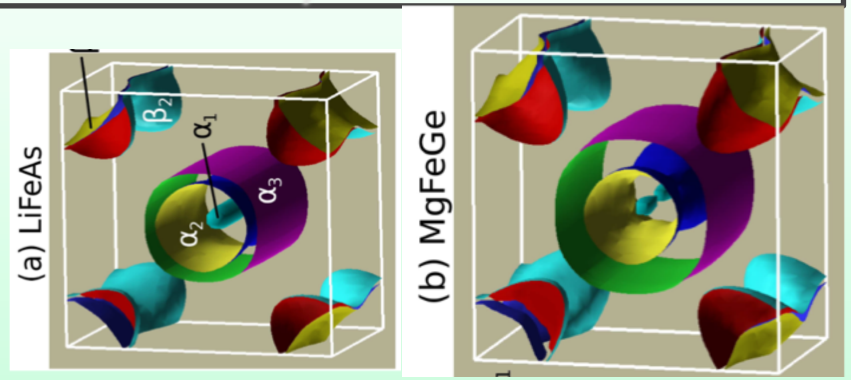


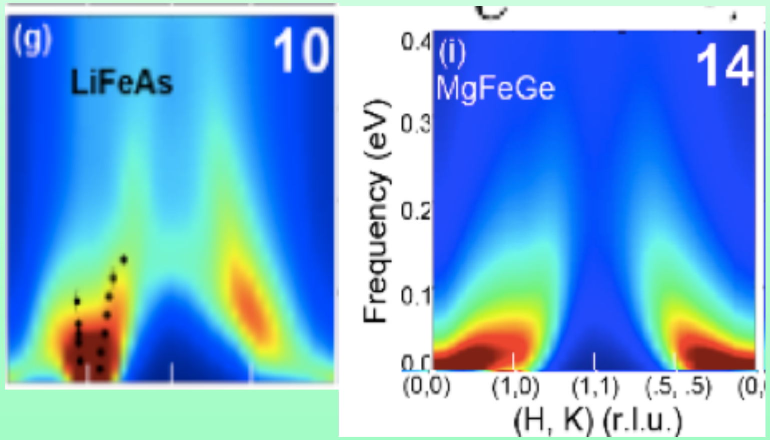
Very small low energy intensity

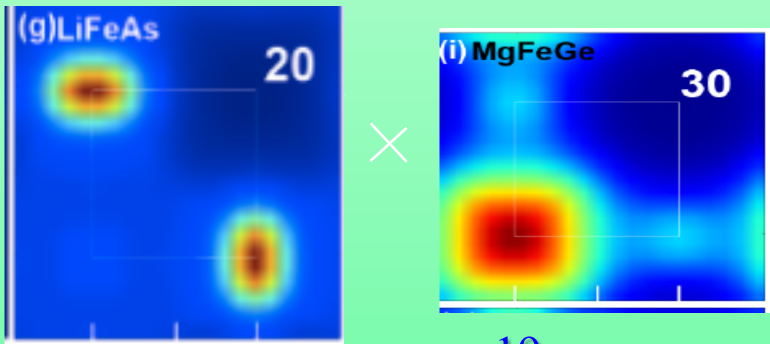
competing order at (0,0)!



Z. Yin K. Haule and G. Kotliar Nature Physics Letters (2014)

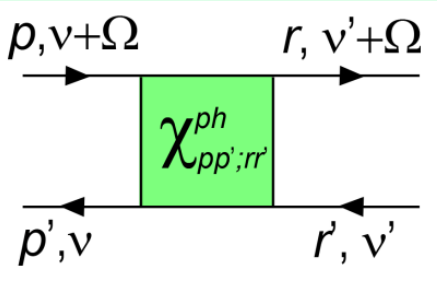


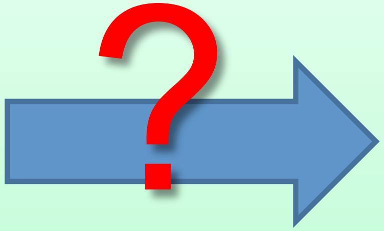




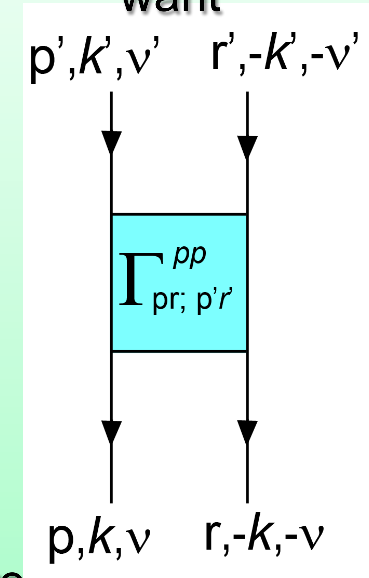
Z. Yin K. Haule and G. Kotliar
Nature Physics Letters (2014)

have particle hole

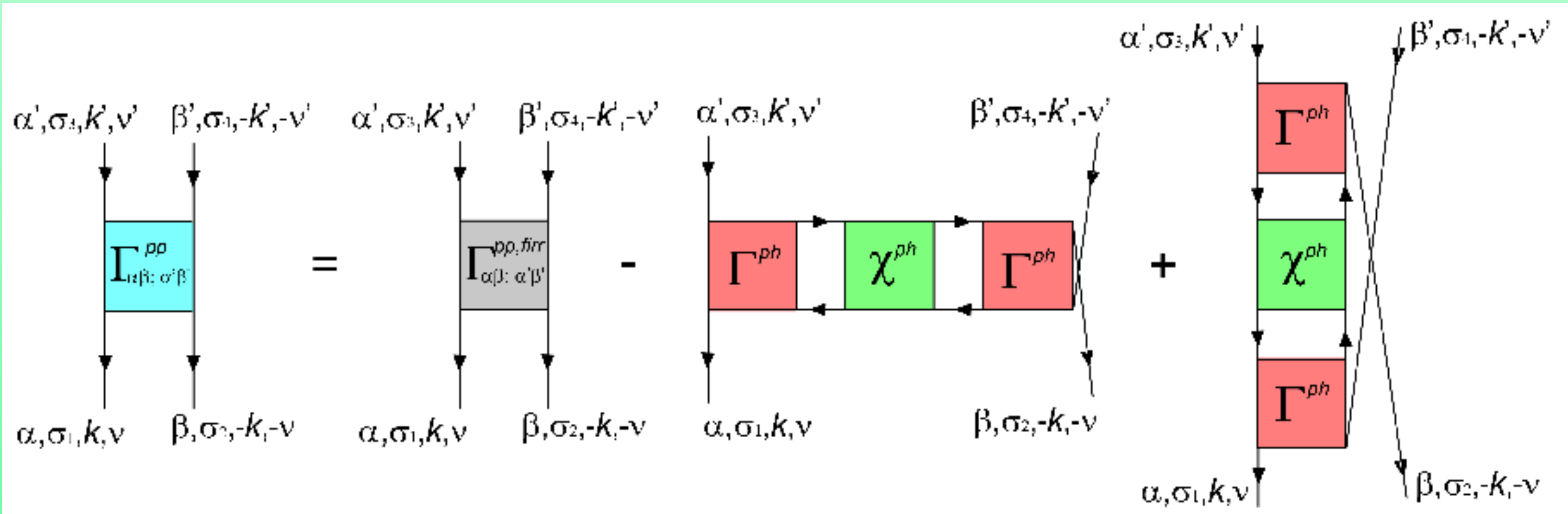




want



We can compute particle-particle vertex using local irreducible objects. :



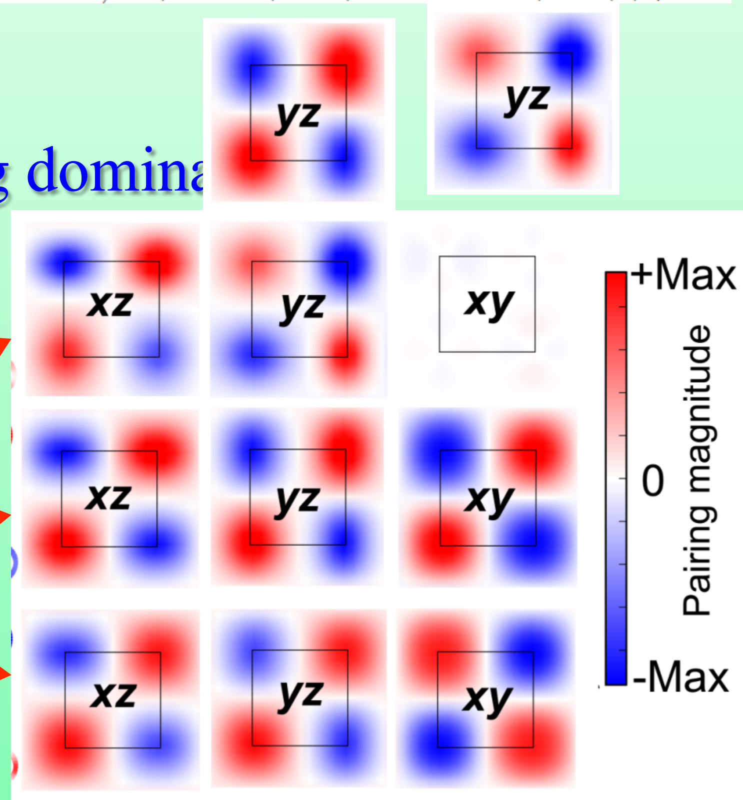
Pairing function $\Delta(k)\alpha\beta = < d_\alpha(-k) d_\beta(k) >$

$\Delta_{\alpha\beta}(k)$ is diagonal $\Delta_{\alpha\beta}(k) = \Delta_{\alpha\alpha}(k)\delta_{\alpha\beta}$ $\begin{bmatrix} \Delta_{eg} & 0 & 0 & 0 \\ 0 & \Delta_{xz} & 0 & 0 \\ 0 & 0 & \Delta_{yz} & 0 \\ 0 & 0 & 0 & \Delta_{xy} \end{bmatrix}$

$$\Delta_\alpha(kx, ky) = \Delta_{nnn,\alpha} cos(kx)cos(ky) + \Delta_{nn,\alpha}(cok(kx) + cos(ky))/2$$

$$|\Delta_{nn,\alpha}| << |\Delta_{nnn,\alpha}|$$

- Second nearest neighbor pairing domina



Different combinations of the signs $\Delta_{nnn,\alpha}$ of the (xz, yz, xy) orbitals produce different pairing symmetry on the Fermi surface.

d-wave: (1, -1, 0)

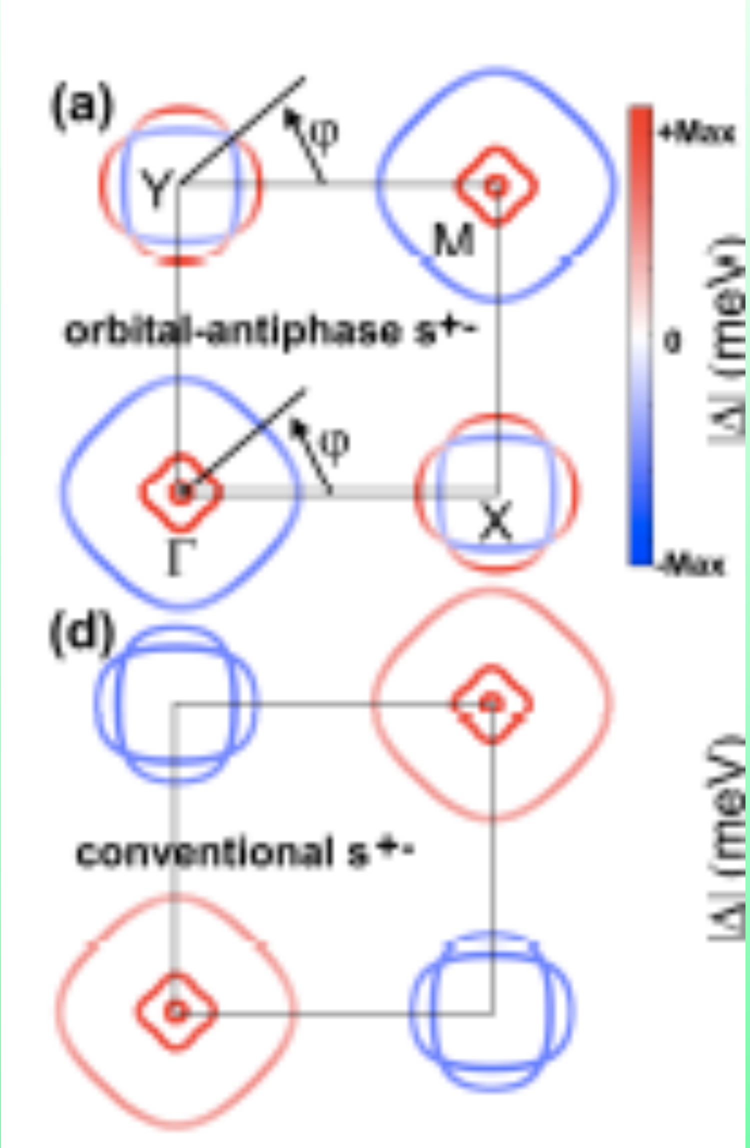
Kuroki - Mazin S^{+-} : (1, 1, 1)

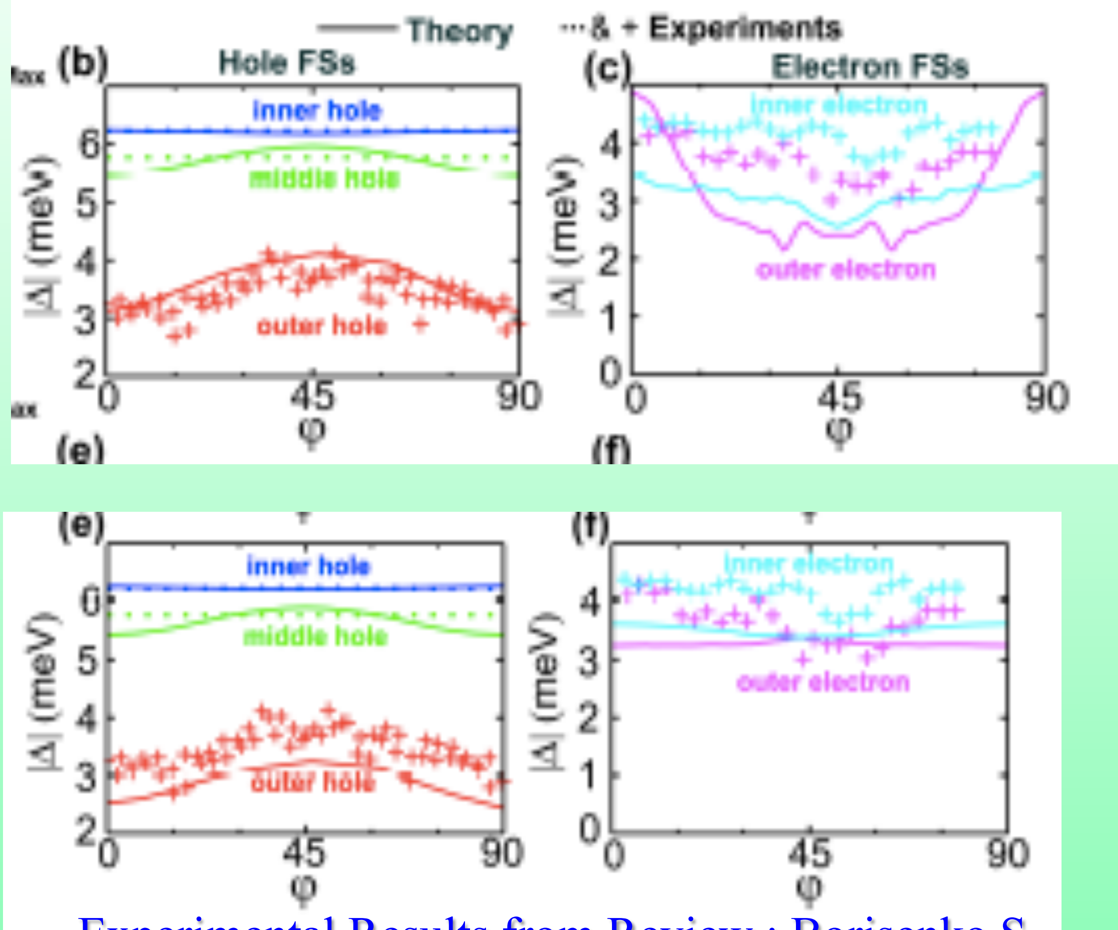
A new antiphase S^{+-} : (1, 1, -1)

They are very close in energy and almost degenerate!

Z.P. Yin, K. Haule, G. Kotliar, Nature Physics Letters 2014

Conventional vs antiphase orbital s+- the case of LiFeAs





Experimental Results from Review : Borisenko,S. V. et al Symmetry 4, 251-264 (2012).:

Theory: Yin Haule and GK, Nature Physics Letterss (2014)

PRL **96,** 226403 (2006) PHYSICAL REVIEW LETTERS week ending 9 JUNE 2006

Local Self-Energy Approach for Electronic Structure Calculations

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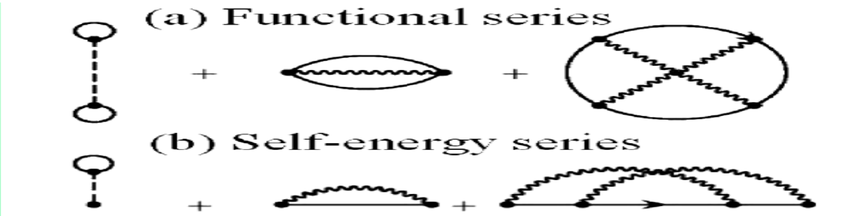
(Received 29 November 2005; published 7 June 2006)

Using a novel self-consistent implementation of Hedin's *GW* perturbation theory, we calculate space- and energy-dependent self-energy for a number of materials. We find it to be local in real space and rapidly convergent on second- to third-nearest neighbors. Corrections beyond *GW* are evaluated and shown to be completely localized within a single unit cell. This can be viewed as a fully self-consistent implementation of the dynamical mean field theory for electronic structure calculations of real solids



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PRL **109,** 237010 (2012) PHYSICAL REVIEW LETTERS week ending 7 DECEMBER 2012

Many-Body Effects in Iron Pnictides and Chalcogenides: Nonlocal Versus Dynamic Origin of Effective Masses

Jan M. Tomczak,[1] M. van Schilfgaarde,[2] and G. Kotliar[1]
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(Received 7 September 2012; published 5 December 2012)

We apply the quasiparticle self-consistent *GW* approximation (QS*GW*) to some of the iron pnictide and chalcogenide superconductors. We compute Fermi surfaces and density of states, and find excellent agreement with experiment, substantially improving over standard band-structure methods. Analyzing the QS*GW* self-energy we discuss nonlocal and dynamic contributions to effective masses. We present evidence that the two contributions are mostly separable, since the quasiparticle weight is found to be essentially independent of momentum. The main effect of nonlocality is captured by the static but nonlocal QS*GW* effective potential. Moreover, these nonlocal self-energy corrections, absent in, e.g., dynamical mean field theory, can be relatively large. We show, on the other hand, that QS*GW* only partially accounts for dynamic renormalizations at low energies. These findings suggest that QS*GW* combined with dynamical mean field theory will capture most of the many-body physics in the iron pnictides and chalcogenides.

$$\Sigma(k,\omega) \approx \Sigma(k) + \left|R\alpha\right\rangle \Sigma_{locRR\alpha\beta}(\omega) \left\langle R\beta\right|$$

Studying the d^5 : the case of LaMnPO. [Mn analog of LaFePO]

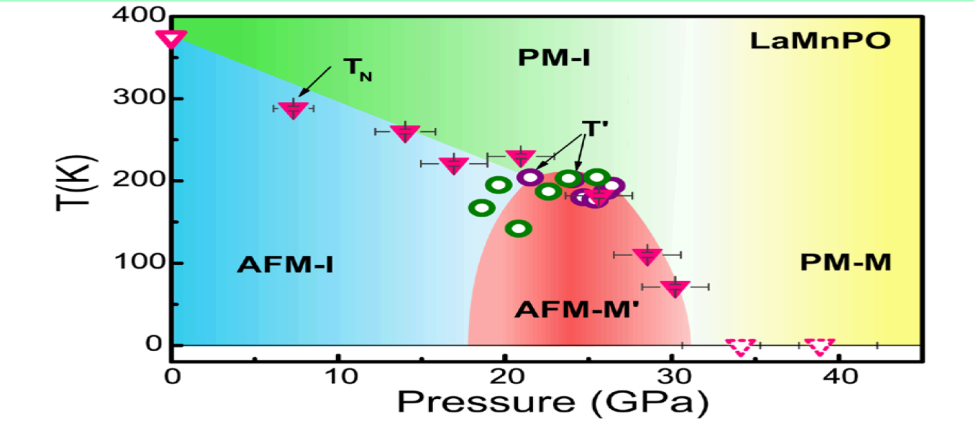
Observation of antiferromagnetic order collapse in the pressurized insulator LaMnPO

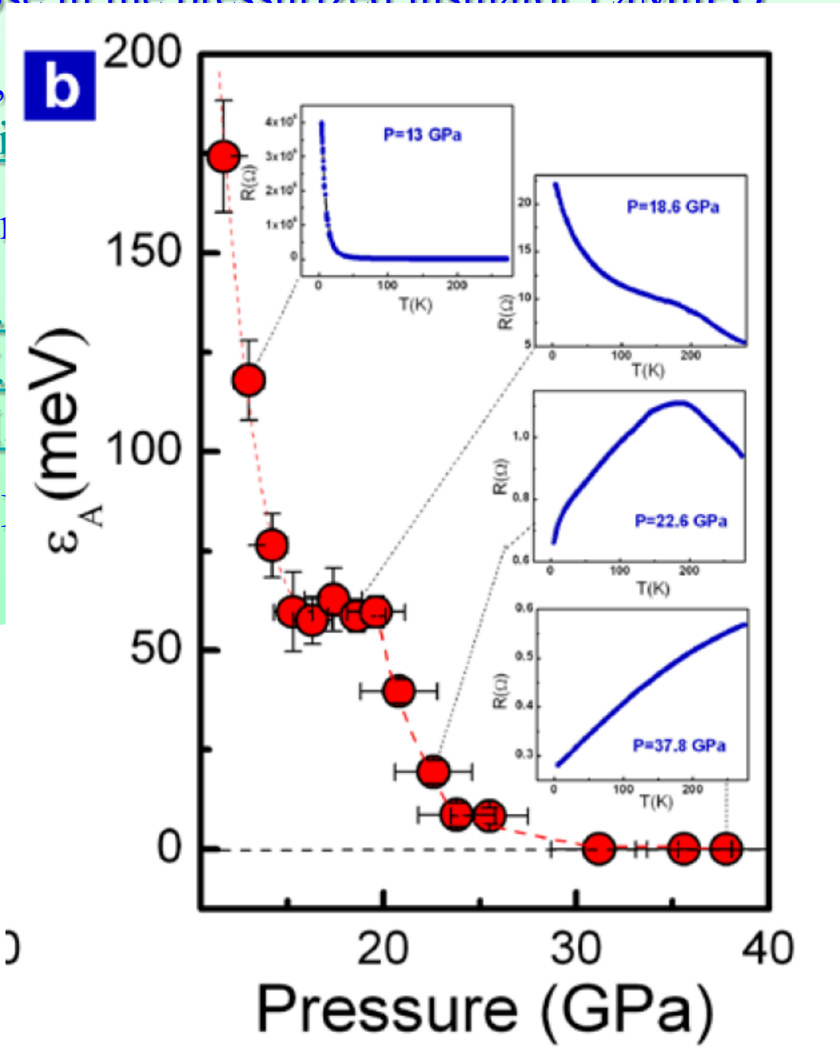
Jing Guo, J. W. Simonson, Liling Sun, Qi Wu,
Gabriel Kotliar, Meigan Aronson, Zhongxi

From antiferromagnetic insulator to correlated

J. W. Simonson, Z. P. Yin, M. Pezzoli, J. Guo, J.
Z. Hu, H.-J. Lin, C. T. Chen, C. Marques, V.
G. Kotliar, D. N. Basov, L. H

Proc. Natl. Acad. Sci 109,

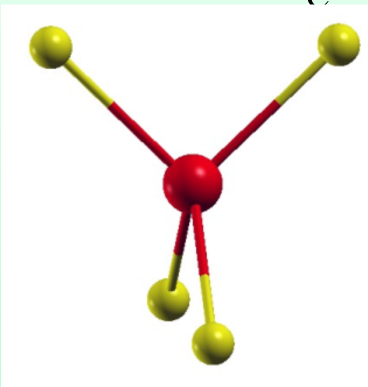


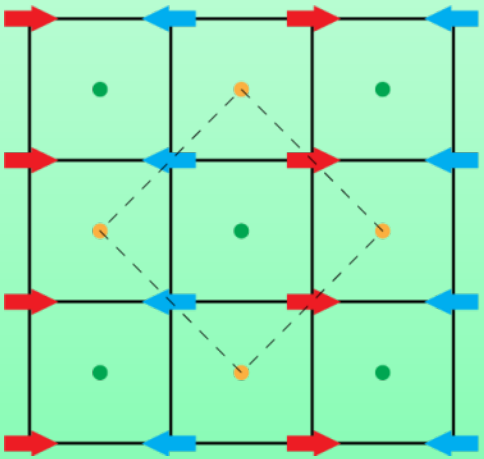


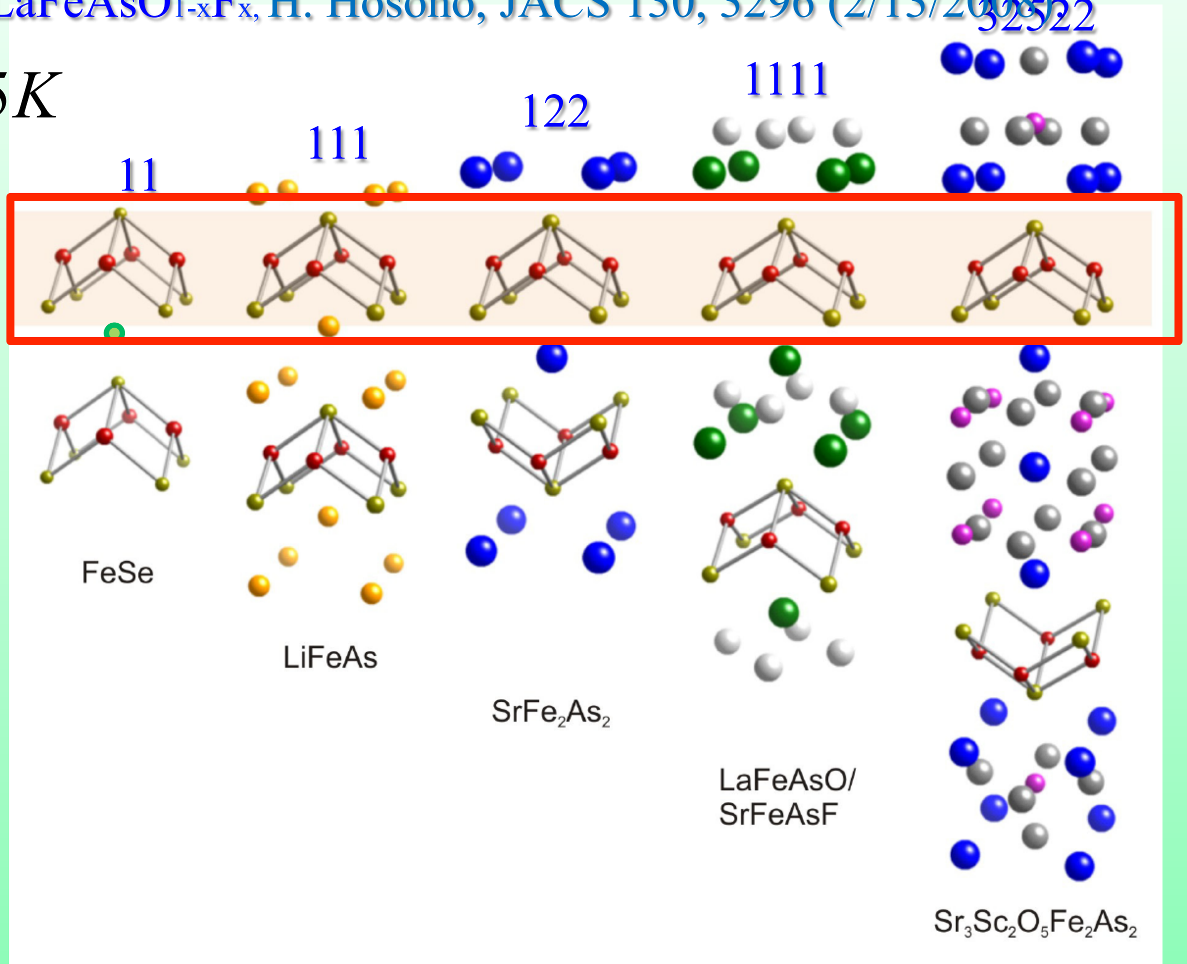
Landscape of Fe based SC

First discovery in 2008: $LaFeAsO_{1-x}F_x$, H. Hosono, JACS 130, 3296 (2/13/2008)

$$T_C^{max} \sim 65K$$







J. Paglione and R L. Greene, Nature Physics 6, 645-658 (2010).

Density-functional calculations of the electronic structures and magnetism of the pnictide superconductors $BaFeAs_2$ and $BaFeSb_2$

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

Phys. Rev. B **79**, 060501(R) – Published 1 February 2009

We investigate the structural, electronic, and magnetic properties of the hypothetical compound $BaFePn_2$ (Pn = As and Sb), which is isostructural to the parent compound of the high-temperature superconductor $LaFeAsO_{1-x}F_x$. Using density-functional theory, we show that the Fermi surface, electronic structure, and spin-density wave instability of $BaFePn_2$ are very similar to the Fe-based superconductors. Additionally, there are very dispersive metallic bands of a spacer Pn layer, which are almost decoupled from $FePn$ layer. Our results show that experimental study of $BaFePn_2$ can test the role of charge

internal coordinates of Ba (0.25, 0.25, z_{Pn}), Fe (0.75, 0.25, ... , z_{Pn}). ... is ex-

Journal of the Physical Society of Japan **83**, 025001 (2014)

http://dx.doi.org/10.7566/JPSJ.83.025001

Enhanced Superconductivity up to 43 K by P/Sb Doping of $Ca_{1-x}La_xFeAs_2$

Kazutaka Kudo[1,2*], Tasuku Mizukami[1], Yutaka Kitahama[1], Daisuke Mitsuoka[1], Keita Iba[1], Kazunori Fujimura[1], Naoki Nishimoto[1], Yuji Hiraoka[1,2], and Minoru Nohara[1,2]

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Thanks for your attention!

Z

$upport NSF

Pengcheng Dai (Rice)

Dimitri Basov (UCSD)

Meigan Aronson (Stony Brook)

Experimentalists .

Zhiping Yin Kristjan Haule Hyowon. Park Camille Aron Jihoon Shim