

LDA+DMFT functional

$$\Gamma_{LDA + DMFT} [\rho(r) \mathbf{G}_{ab} V_{KS}(r) \Sigma_{ab}]$$

$$-Tr \log[i\omega_n + \nabla^2/2 - V_{KS} - \chi^{*}_{\alpha R}(r)\Sigma_{\alpha\beta}\chi_{\beta R}(r)] -$$

$$\int V_{KS}(r)\rho(r)dr - \sum_{i\omega_n} Tr\Sigma(i\omega_n)G(i\omega_n) +$$

$$\int V_{ext}(r)\rho(r)dr + \frac{1}{2}\int \frac{\rho(r)\rho(r')}{|r-r'|}drdr' + E_{xc}^{LDA}[\rho] +$$

$$\sum_R \Phi[G] - \Phi_{DC}$$

Sum of local 2PI graphs with local U matrix and local G

$$\Phi_{DC}[G] = Un(n-1)\frac{1}{2} - J\frac{n}{2}\left(\frac{n}{2}-1\right)$$

$$Edc = Un(n-\frac{1}{2}) - \frac{J}{2}(n-1)$$

$$n = T \sum_{abi\omega} \left(G_{ab}(i\omega) e^{i0^+} \right)$$

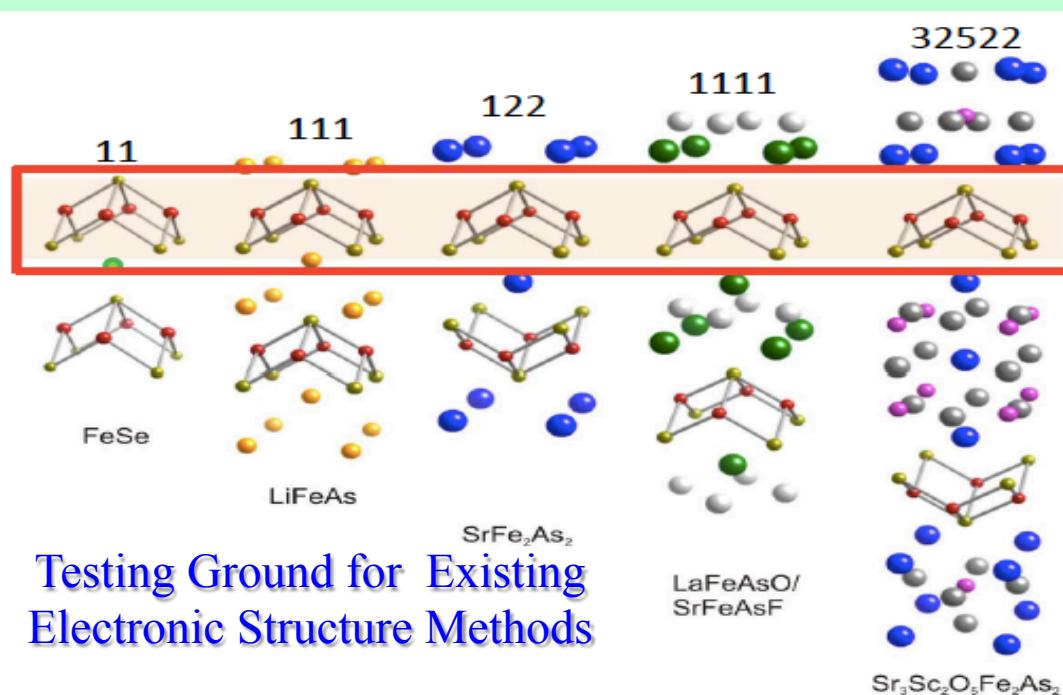
$$Edc = U(n_0 - \frac{1}{2}) - \frac{J}{2}(n_0 - 1) \quad \Phi_{DC}[G] = nE_{dc}[n_0]$$

Published on Web 02/23/2008

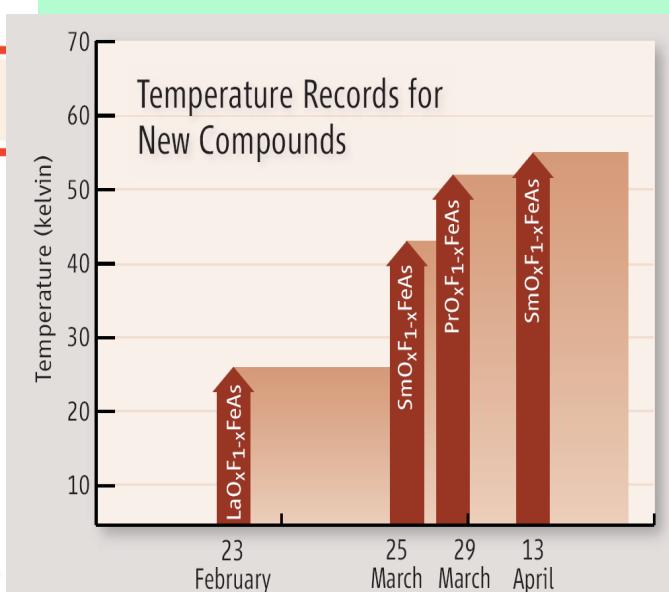
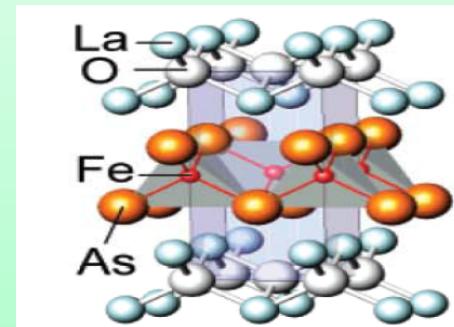
Iron-Based Layered Superconductor $\text{La}[\text{O}_{1-x}\text{F}_x]\text{FeAs}$ ($x = 0.05\text{--}0.12$) with $T_c = 26 \text{ K}$

Yoichi Kamihara,^{*,†} Takumi Watanabe,[‡] Masahiro Hirano,^{†,§} and Hideo Hosono^{†,‡,§}

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



Testing Ground for Existing
Electronic Structure Methods



2

Early DMFT predictions



PRL 100, 226402 (2008)

PHYSICAL REVIEW LETTERS



Correlated Electronic Structure of $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$

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

PRL 101, 026403 (2008)

PHYSICAL REVIEW LETTERS

week ending
11 JULY 2008

Is $\text{LaFeAsO}_{1-x}\text{F}_x$ an Electron-Phonon Superconductor?

L. Boeri,¹ O. V. Dolgov,¹ and A. A. Golubov²

¹Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany

²Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente,
7500 AE Enschede, The Netherlands

(Received 18 March 2008; published 8 July 2008)

In this Letter, we calculate the electron-phonon coupling of the newly discovered superconductor $\text{LaFeAsO}_{1-x}\text{F}_x$ using linear response. For pure LaFeAsO , the calculated electron-phonon coupling constant $\lambda = 0.21$ and logarithmic-averaged frequency $\omega_{\text{ln}} = 206$ K give a maximum T_c of 0.8 K, using the standard Migdal-Eliashberg theory. For the F-doped compounds, we predict even smaller coupling constants. To reproduce the experimental T_c , a 5–6 times larger coupling constant would be needed. Our

phonon coupling constants within the DF1, using the code of Ref. [5], gives a value too small to explain the observed critical temperature ($T_c < 1$ K).

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.

Phonon $T_c < 1$ K

Importance of correlations

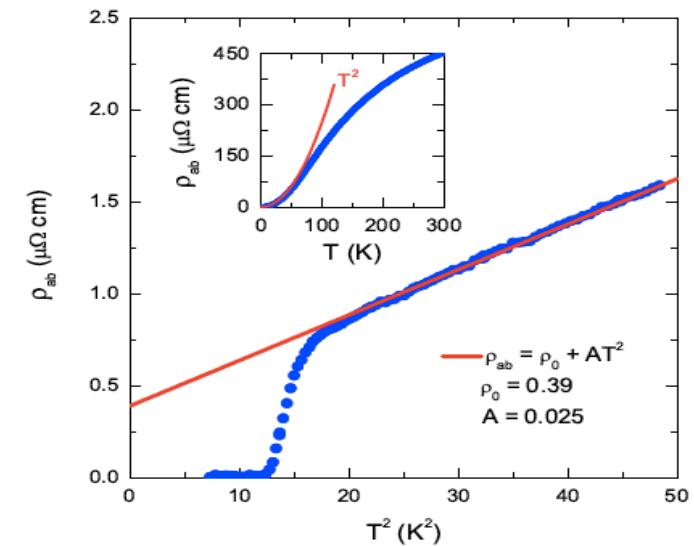
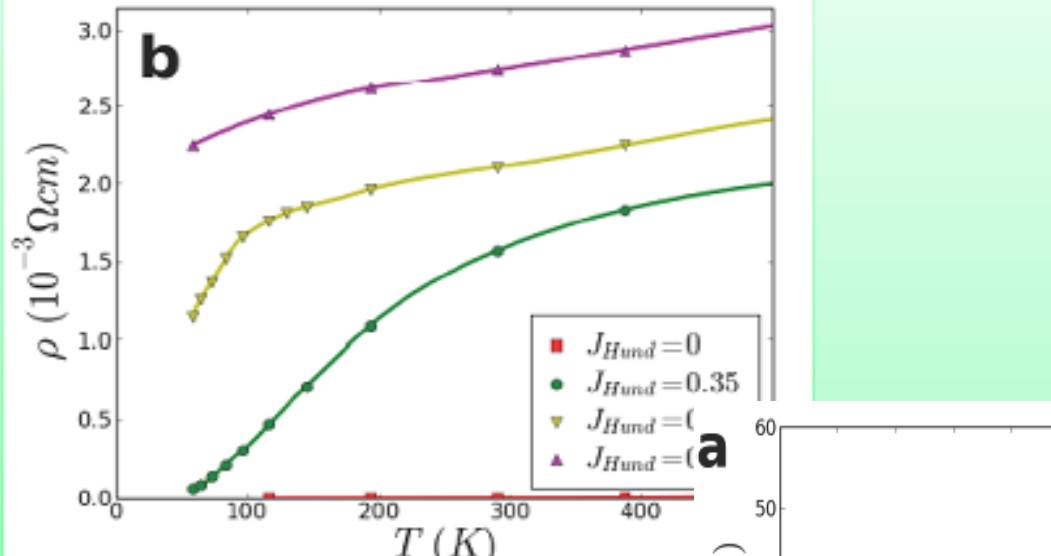
Mass enhancement 3-5

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

K Haule¹ 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. Meingast¹

Weak correlations ? Itinerant magnets ?

Evidence for weak electronic correlations in iron pnictides

W. L. Yang,¹ A. P. Sorini,² C-C. Chen,^{2,3} B. Moritz,² W.-S. Lee,² F. Vernay,⁴ P. Olalde-Velasco,^{1,5} J. D. Denlinger,¹ B. Delley,⁴ J.-H. Chu,^{2,6,7} J. G. Analytis,^{2,6,7} I. R. Fisher,^{2,6,7} Z. A. Ren,⁸ J. Yang,⁸ W. Lu,⁸ Z. X. Zhao,⁸ J. van den Brink,^{2,9} Z. Hussain,¹ Z.-X. Shen,^{2,3,6,7} and T. P. Devereaux^{2,7}



Selected for a Viewpoint in *Physics*

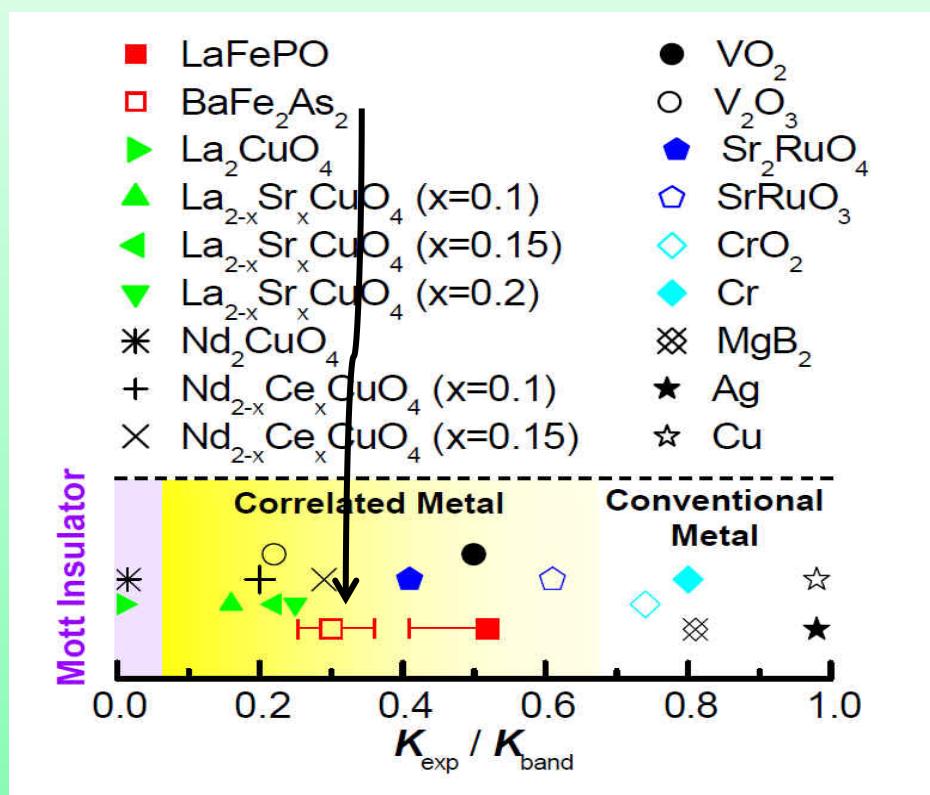
PHYSICAL REVIEW B **80**, 014508 (2009)

PHYSICAL REVIEW B **81**, 104518 (2010)

C. Parks Cheney,¹ F. Bondino,² T. A. Callcott,¹ P. Vilmercati,¹ D. Ederer,³ E. Magnano,² M. Malvestuto,⁴ F. Parmigiani,^{2,5} A. S. Sefat,⁶ M. A. McGuire,⁶ R. Jin,⁶ B. C. Sales,⁶ D. Mandrus,⁶ D. J. Singh,⁶ J. W. Freeland,⁷ and N. Mannella^{1,*}

states, which are found to contribute substantially at the Fermi level. The energies and detailed orbital character of Fe and As derived unoccupied *s* and *d* states are found to be in remarkably good agreement with the predictions of standard density-functional theory.

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

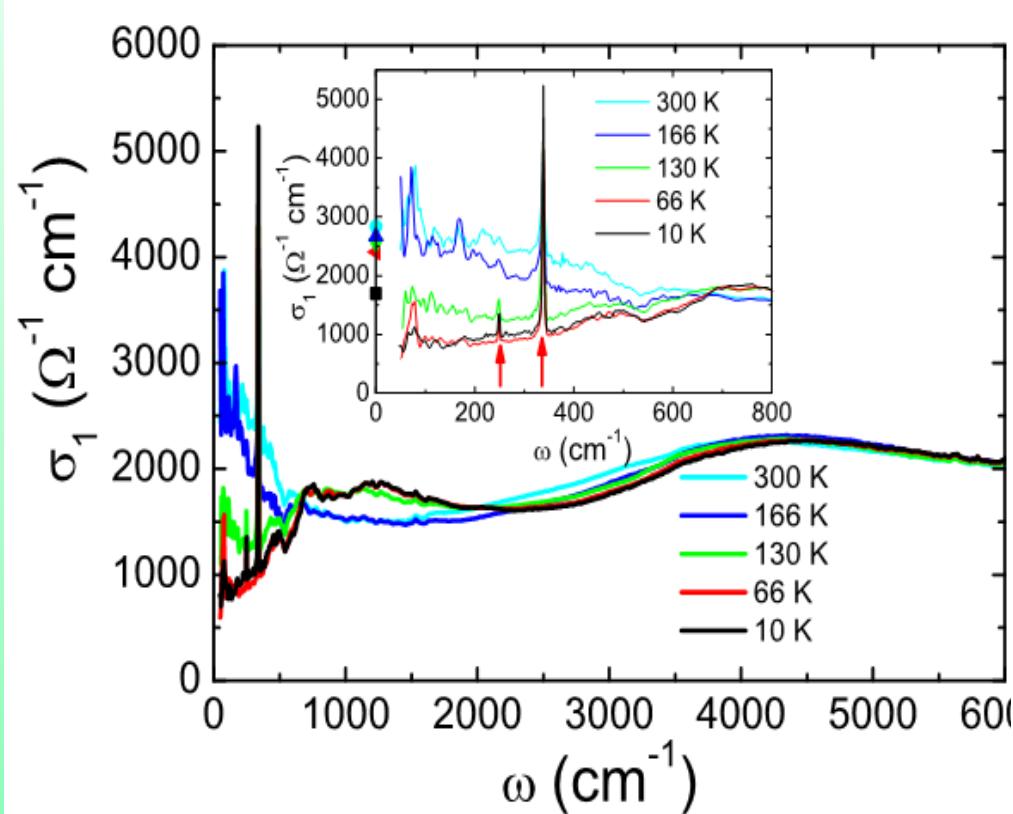


LDA+DMFT had predicted correlation effects $m/m^* \sim .3 - .2$ this WAS seen in OPTICS.

Is the enhancement due to proximity to the Mott transition???

Z. G. Chen, R. H. Yuan, T. Dong, and N. L. Wang

Phys. Rev. B 81, 100502(R) (2010)



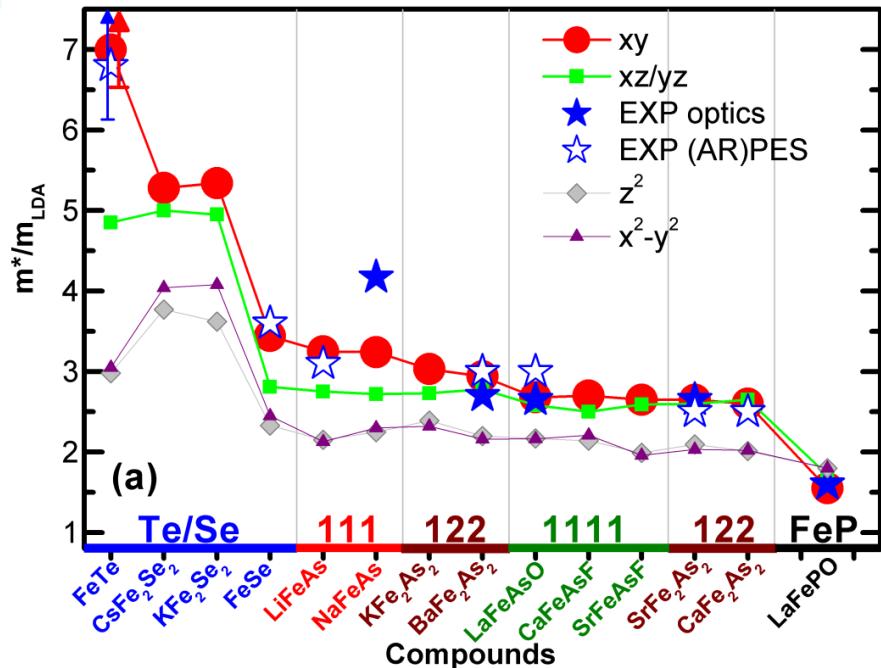
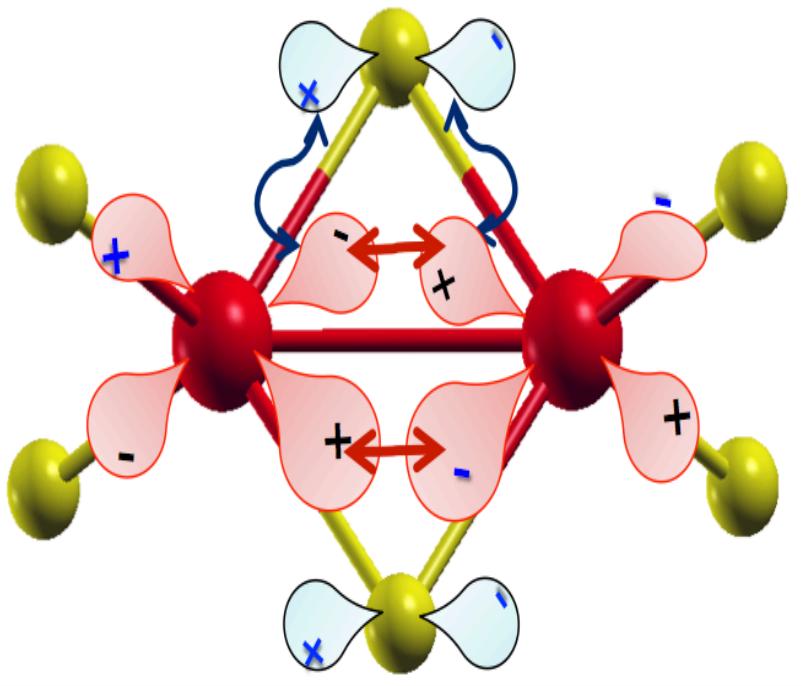
$$\omega_p \approx 1.01 \times 10^4 \text{ cm}^{-1} \text{ for } T=300 \text{ K.}$$

Remarkable effort in single crystal synthesis!

Cleaned up theoretical confusion which argued that 1111 were weakly correlated materials.

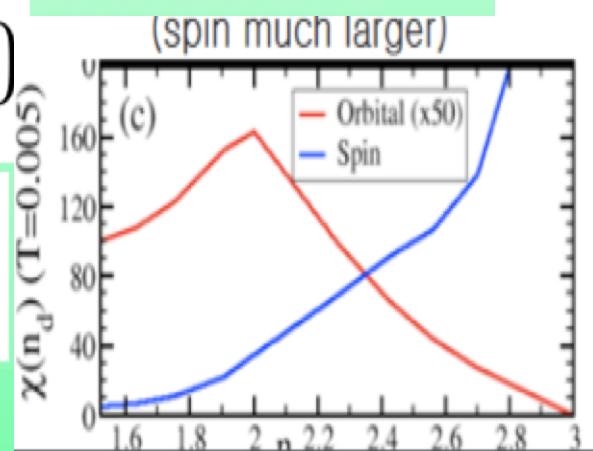
obtained by the sum-rule analysis. Note that the plasma frequency for BaFe_2As_2 is around $1.3 \times 10^4 \text{ cm}^{-1}$ in the nonmagnetic phase.¹³ So LaFeAsO has a slightly smaller plasma frequency. The band-structural calculations give the ab plane plasma frequency of $2.1\text{-}2.3 \text{ eV}$.^{10,17} Then we can estimate that $K_{exp}/K_{band} = \omega_{p,exp}^2/\omega_{p,band}^2 \approx 0.30\text{-}0.38$. This value is smaller than LaFePO,¹¹ indicating a stronger reduction in the kinetic energy of the electrons with respect to the band theory. This yields evidence that LaFeAsO is more strongly correlated than LaFePO.

Hund Metal Correlations and Orbital Differentiation



$$t_{xy,xy}^{direct} < 0$$

$$t_{xy,xy}^{As} > 0$$



i.e Window of Frequencies, same U
J and dc for all materials.

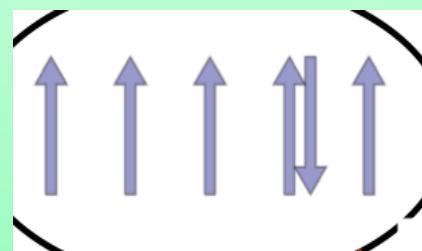
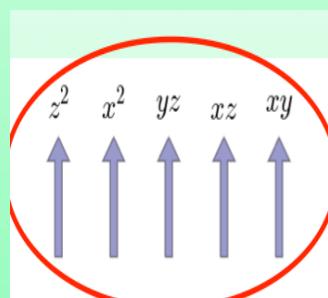
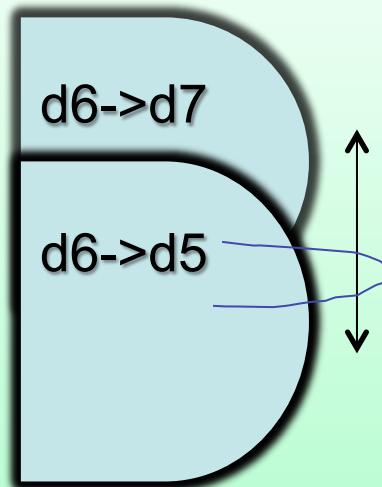
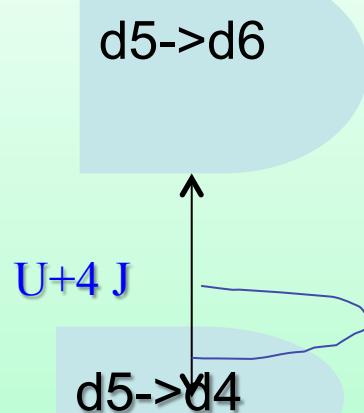
Yin ZP, Haule K, Kotliar G.
(2011). Nat. Mater. 10:932–935

Hund's Metals

Hundness 101

$$H_{\text{atom}} = \frac{1}{2}U(N)^2 - \frac{1}{2}J(S)^2$$

Friedrich Hund



$$E(N+1) + E(N-1) - 2E(N)$$

N= 5, U+4J

N= 5 See work with M. Aronson's group, e.g. LaMnPO

See Liebsch and Ishida, DeMedicis Giovannetti and Capone

U-J

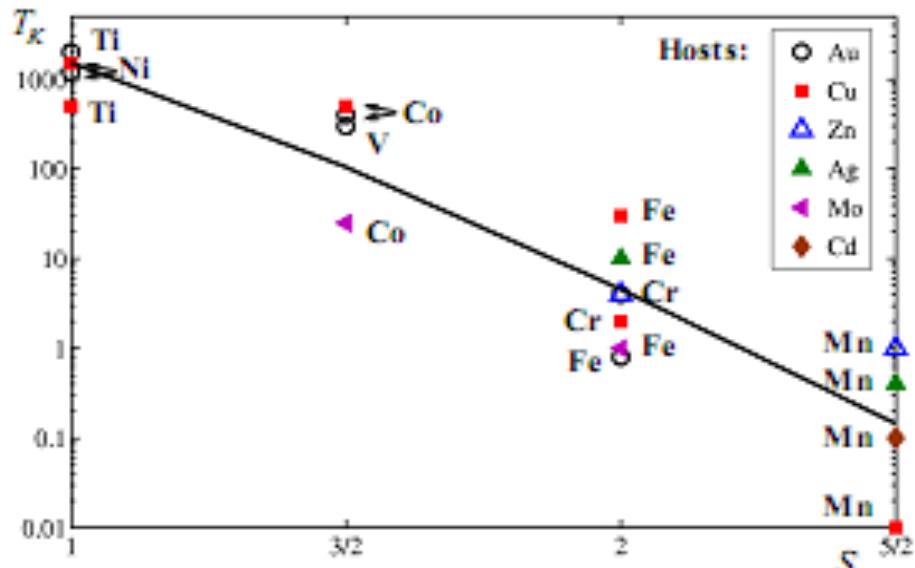
VanderMarel Sawatzky
PRB 37 , 10674 (1988)

9

Empty bus seat rule



Hundness 102 . Single Impurity Physics.



Extreme low energy Kondo impurity scale

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).

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

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

$$\begin{aligned} J_{\alpha\beta} &= J & T_K &= e^{-\frac{1}{\rho J N}} & 10 \\ J_{\alpha\beta} &= J \delta_{\alpha\beta} & T_K &= e^{-\frac{N}{\rho J}} \end{aligned}$$

TK depends strongly
on filling !!

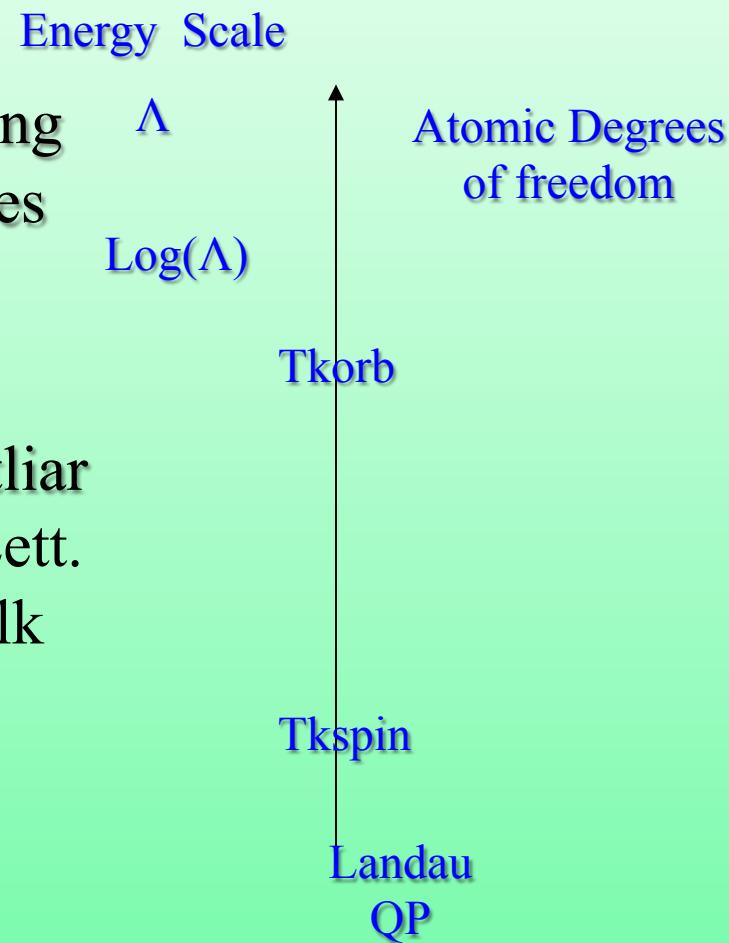
Hundness (103) :Origin of normal state anomalies: Z. Yin K. Haule and GK Phys. Rev. B 86, 195141 (2012) Orbital-Spin Separation

Full solution of the puzzle

Weak coupling RG analysis, involving
Spin, Orbital and Spin-Orbital degrees
of freedom C. Aron and G. Kotliar
PRB 91, 041110 (2015)

K. Stadler Z. Yin J. von Delft G. Kotliar
and A. Weichselbaum Phys. Rev. Lett.
115, 136401 (2015) . K. Stadler's talk
in this conference. Origin of apparent
power laws.

The DMFT self consistency is NOT
essential to understand Hundness!





Lytic theory of Hund's metals: A renormalization group perspective

Camille Aron^{1,2} and Gabriel Kotliar¹

Intermediate
assymptotic
multichannel fixed
point K=2.N

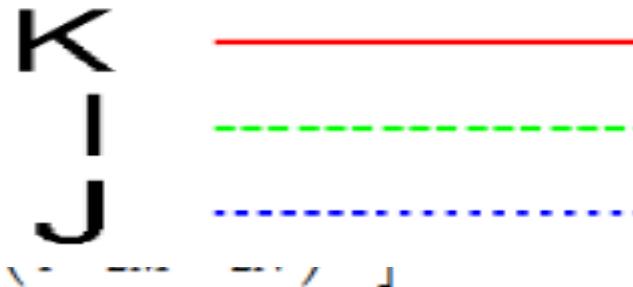
$$H_{\text{int}} = \dots + J_0 S^\alpha (\psi_{m\sigma}^\dagger \frac{\sigma_{\sigma\sigma'}^\alpha}{2} \psi_{m\sigma'}) \quad (4)$$

$$+ K_0 T^a (\psi_{m\sigma}^\dagger \frac{\tau_{mm'}^a}{2} \psi_{m'\sigma}) + I_0 S^\alpha T^a (\psi_{m\sigma}^\dagger \frac{\sigma_{\sigma\sigma'}^\alpha}{2} \frac{\tau_{mm'}^a}{2} \psi_{m'\sigma'})$$

$$\beta_J = -\frac{N}{2} \left(1 - \frac{M}{2} J\right) \left(J^2 + \frac{C_2^T}{2M} I^2\right) + \dots, \quad \begin{matrix} \text{Flow to fermi} \\ \text{liquid fixed} \\ \text{point} \end{matrix}$$

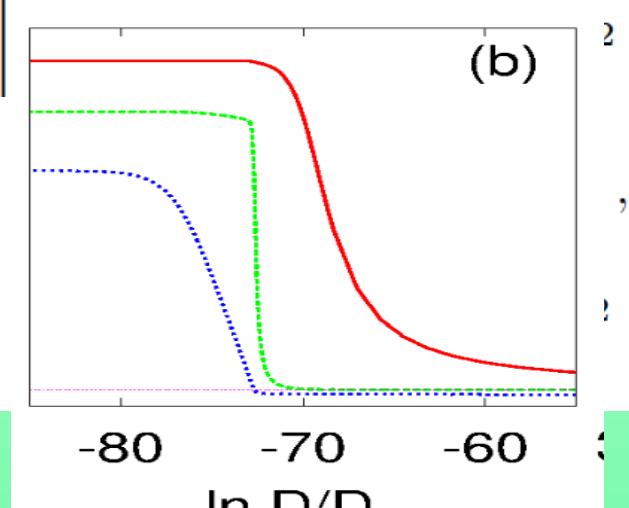
$$\beta_K = -\frac{M}{2} \left(1 - \frac{N}{2} K\right) \left(K^2 + \frac{C_2^S}{2N} I^2\right) + \dots, \quad \text{is delayed} \quad J_0 = \frac{2}{M}$$

$$\begin{aligned} \beta_I &= -\frac{MN}{4} \left[\left(\frac{4}{M} J + \frac{C_3^T}{MC_2^T} + \frac{C_3^S}{NC_2^S}\right) I \right. \\ &\quad \left. + \left(\frac{C_3^T}{MC_2^T} + \frac{C_3^S}{NC_2^S}\right) I^2 \right] \end{aligned}$$



FERROMAGNETIC SIGN!

12



12

Schrieffer's puzzle of Tkondo vs nd finally solved!!!

ARPES view of orbitally resolved quasiparticle lifetimes in iron pnictides

Véronique Brouet,^{1,*} David LeBoeuf,¹ Ping-Hui Lin,¹ Joseph Mansart,¹ Amina Taleb-Ibrahimi,² Patrick Le Fèvre,² François Bertran,² Anne Forget,³ and Dorothée Colson³

¹*Laboratoire de Physique des Solides, Université Paris-Sud, UMR 8502, Bâtiment 510, 91405 Orsay, France*

²*Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin-BP 48, 91192 Gif-sur-Yvette, France*

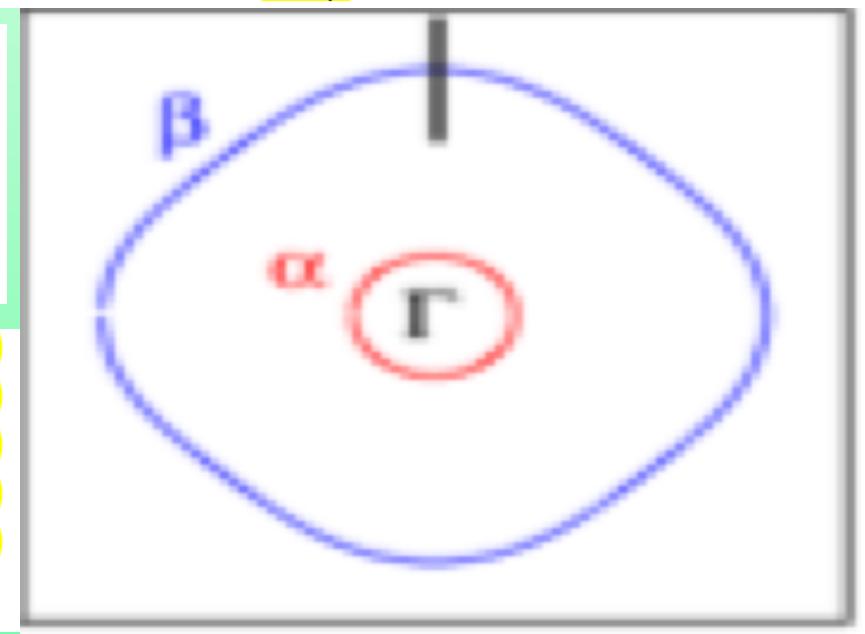
³*Service de Physique de l'Etat Condensé, Orme des Merisiers, CEA Saclay, CNRS-URA 2464, 91191 Gif-sur-Yvette Cedex, France*

(Received 13 November 2015; revised manuscript received 8 February 2016; published 25 February 2016)

We study with angle-resolved photoemission spectroscopy (ARPES) the renormalization and quasiparticle lifetimes of the d_{xy} and d_{xz}/d_{yz} orbitals in two iron pnictides, LiFeAs and Ba(Fe_{0.92}Co_{0.08})₂As₂ (Co8). We find that both quantities depend on orbital character rather than on the position on the Fermi surface (for example, hole or electron pocket). In LiFeAs, the renormalizations are larger for d_{xy} , while they are similar for both types of orbitals in Co8. The most salient feature, which proved robust against all the ARPES caveats we could think of, is that the lifetimes for d_{xy} exhibit a markedly different behavior than those for d_{xz}/d_{yz} . They have smaller

hand, LiFeAs appears slightly more correlated in dynamical mean-field theory (DMFT) calculations [3,21]. This is mainly due to the elongation of the Fe tetrahedra along z , which tends to reduce the hopping between neighboring Fe and enhance correlations, especially for the in-plane d_{xy} orbital.

Here, holes are mainly transferred from d_{xz}/d_{yz} to d_{xy} (see Table I and Sec. IV for more details). This transfer is induced by correlations and was correctly predicted by DMFT [3] and was already observed by ARPES [25,26]. This puts d_{xy} closer to half filling, which is one of the reasons why it is predicted to get more correlated [4].



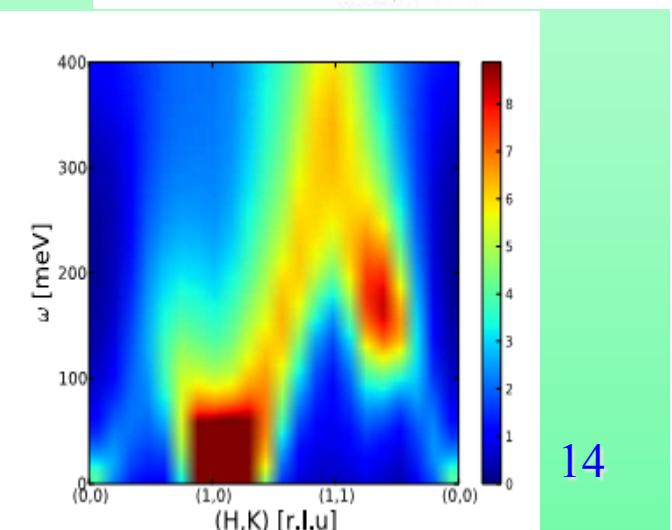
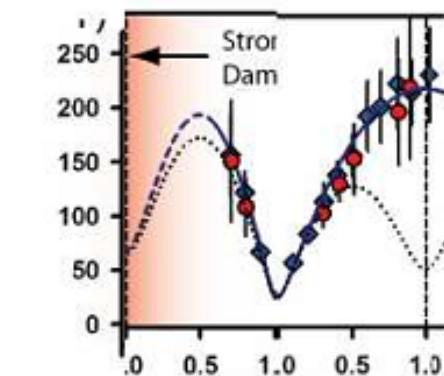
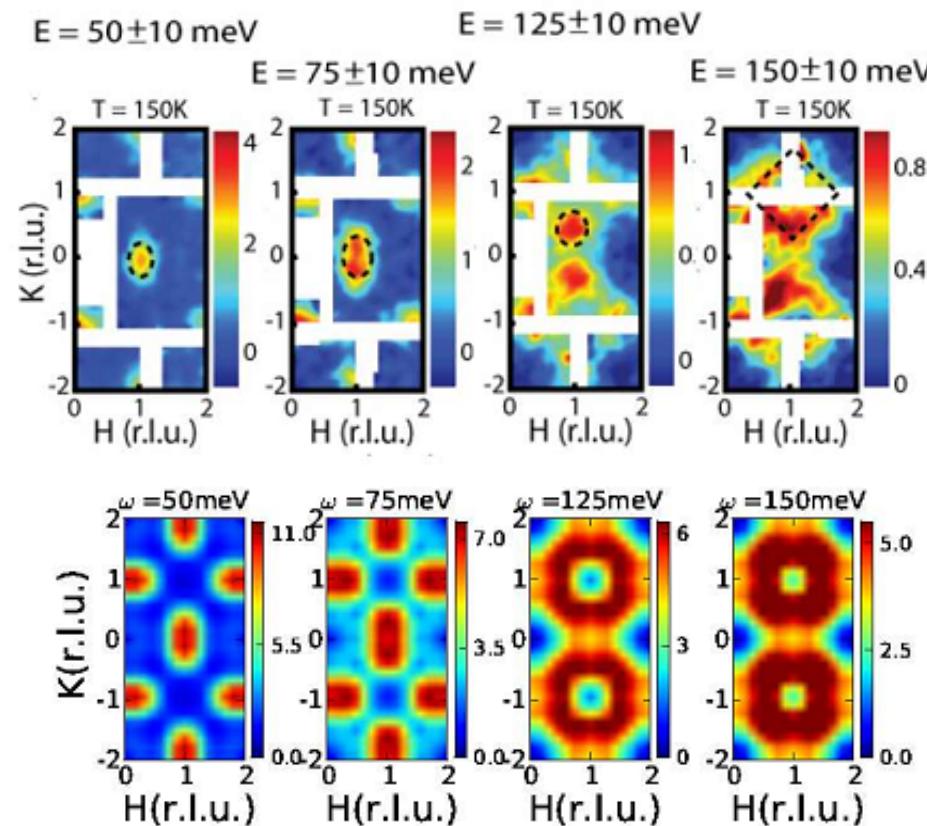
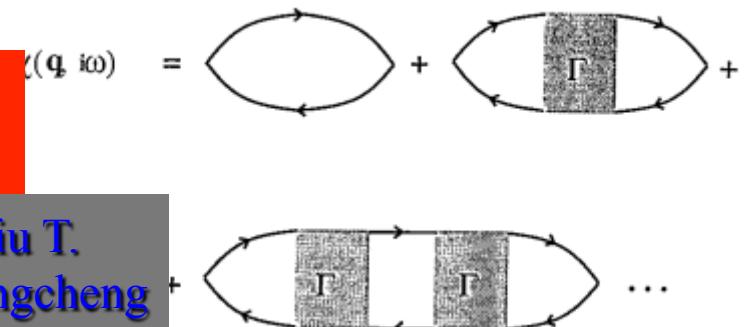
Neutron spectroscopy with LDA +DMFT



Theory: H Park, K. Haud and GK
[Phys. Rev. Lett. 107, 137007 \(2011\)](#)

Experiments: L Harriger H. Luo M. Liu T.
 Perring C Frost H. Ju M. Norman and Pengcheng
 Dai :PRB 84 054544 (2011)

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



Neutron absolute intensities

NATURE PHYSICS | LETTER



Nature of magnetic excitations in superconducting $\text{BaFe}_{1.9}\text{Ni}_{0.1}\text{As}_2$

Mengshu Liu, Leland W. Harriger, Huiqian Luo, Meng Wang, R. A. Ewings, T. Guidi, Hyowon Park, Kristjan Haule, Gabriel Kotliar, S. M. Hayden & Pengcheng Dai

Affiliations | Contributions | Corresponding author

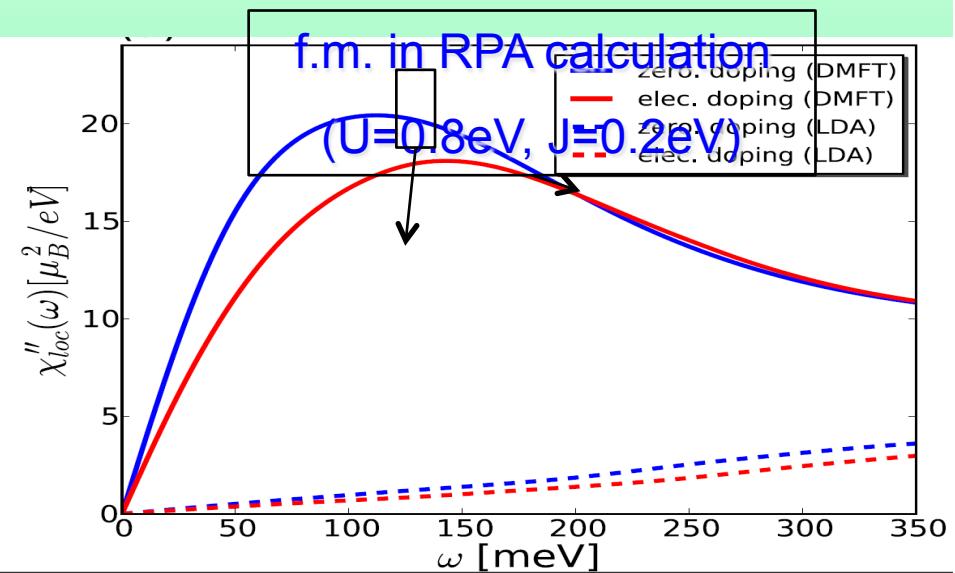
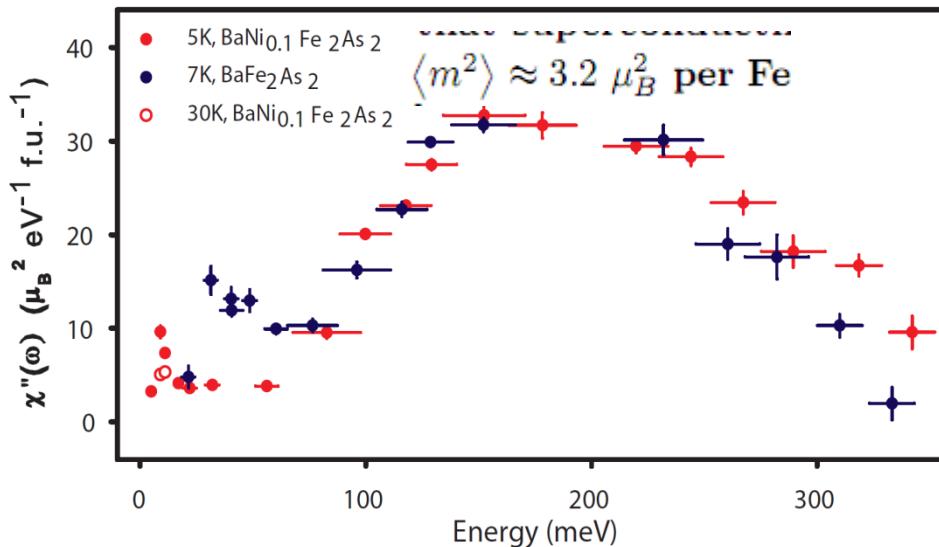
Nature Physics 8, 376–381 (2012) | doi:10.1038/nphys2268

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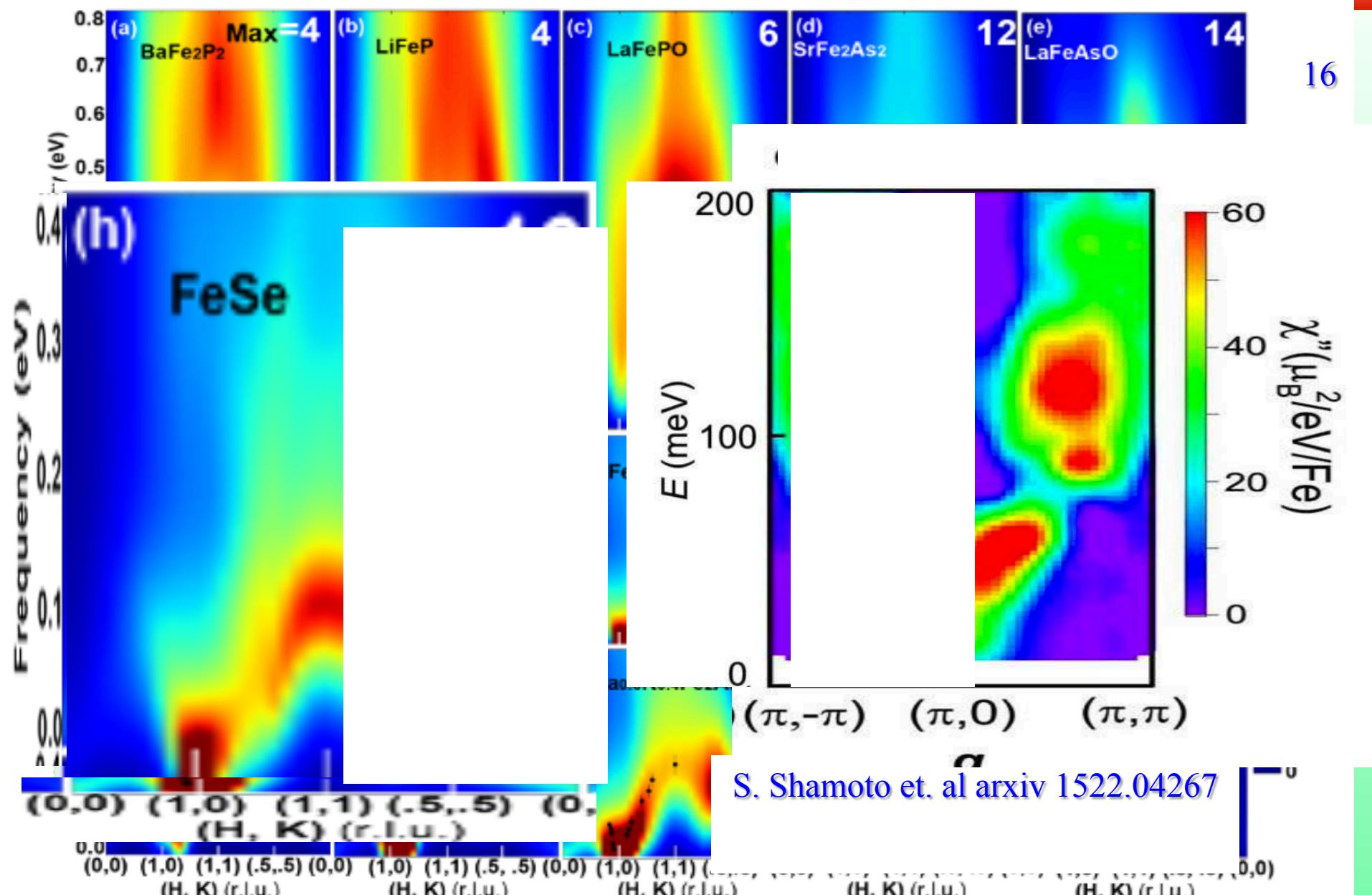
Fluctuating moment by neutrons:

$$\langle \mu^2 \rangle = \int \frac{d\omega}{\pi} n(\omega) \chi''(\omega)$$

Experiment by Liu ... Pengcheng Dai

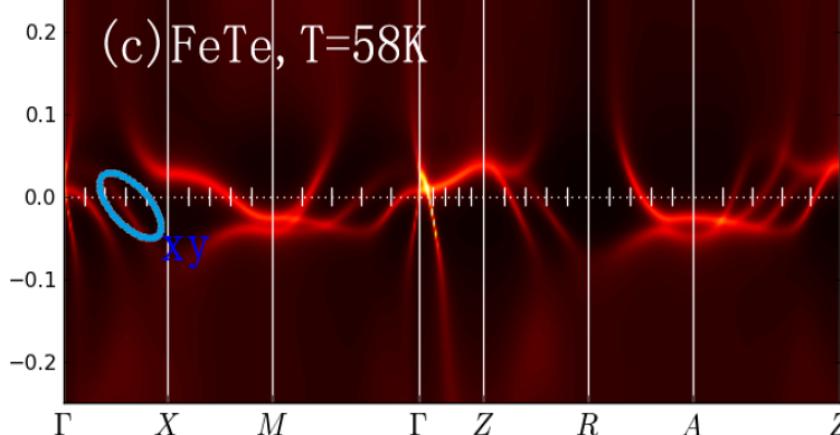
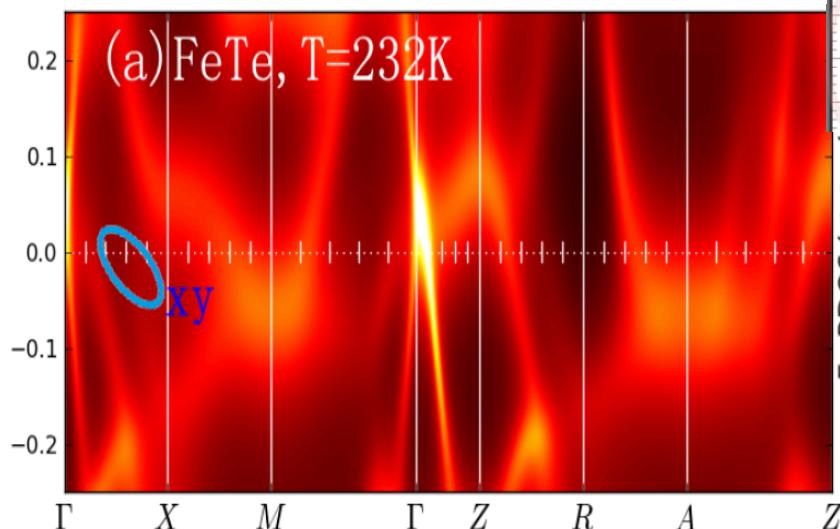
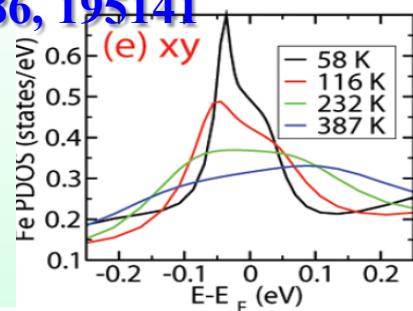


Z. Yin K. Haule and GK Nature Physics 10, 845-850 (2014)

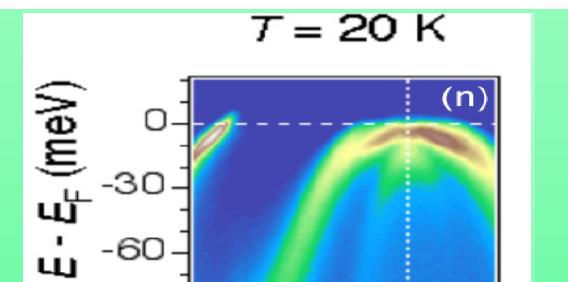
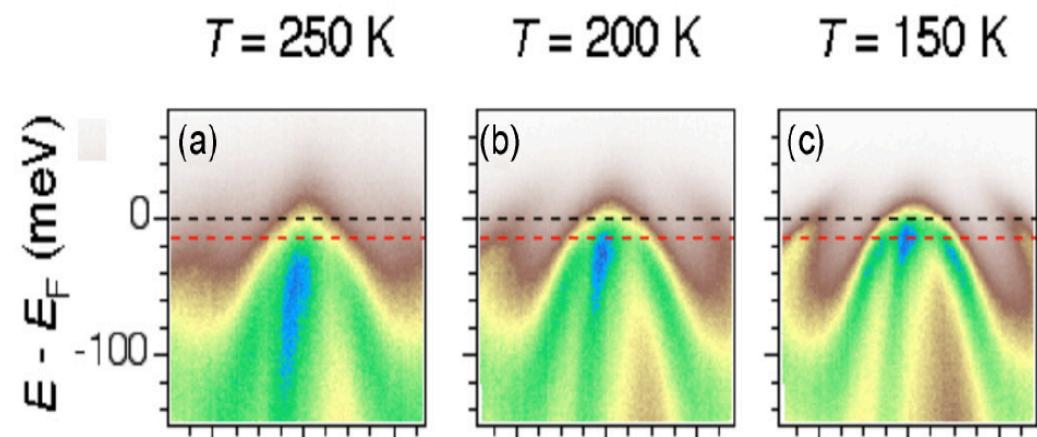
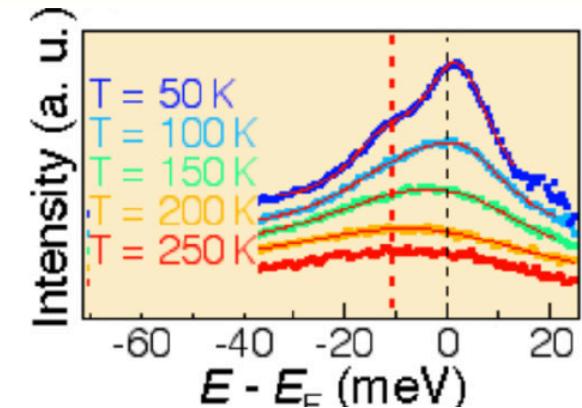
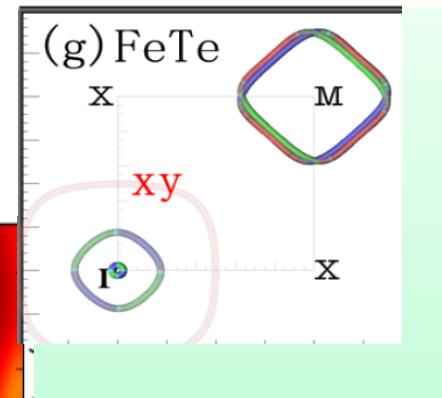


Yin Haule and GK (2012)

Phys. Rev. B 86, 195141



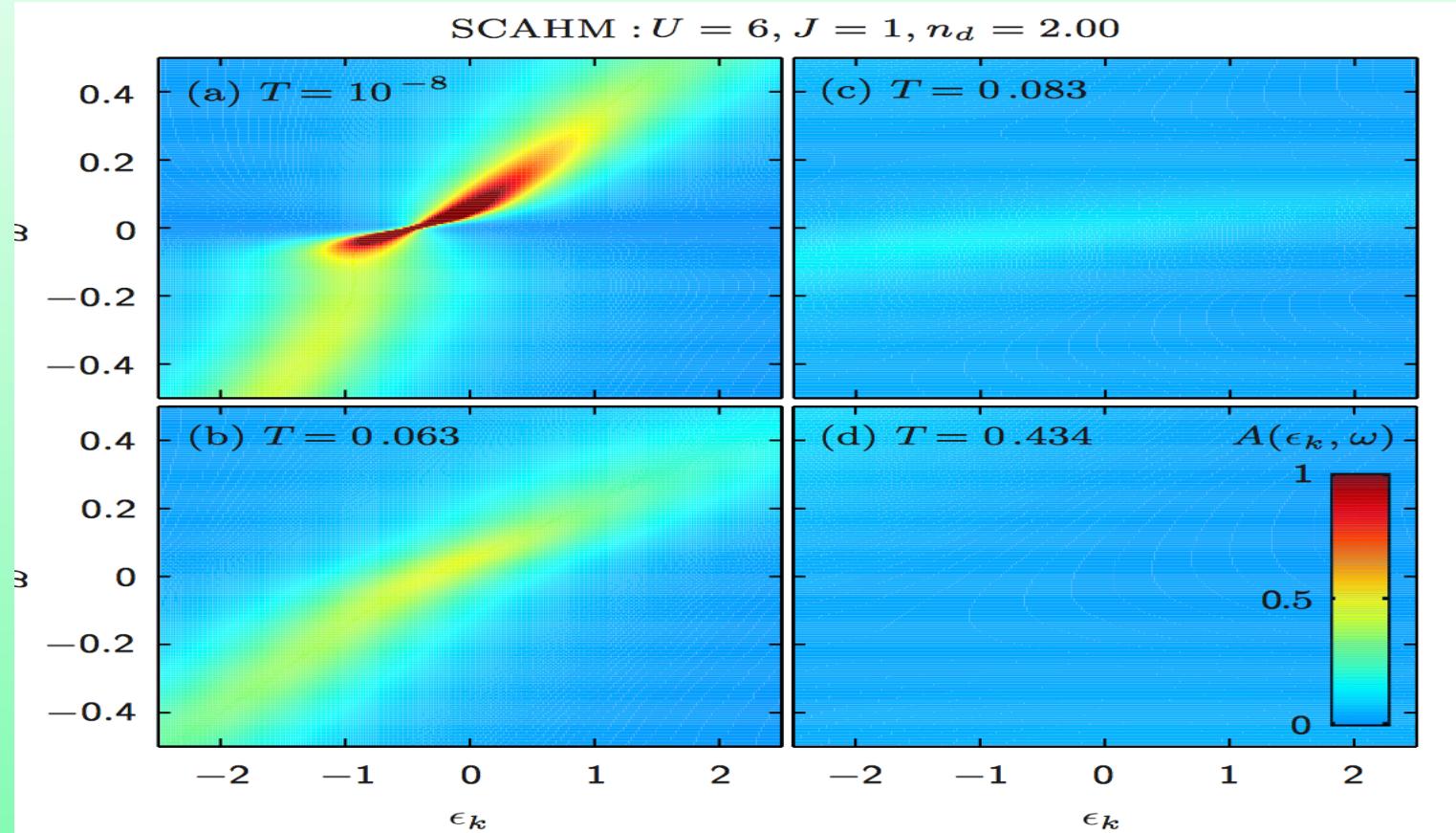
LiFeAs H. Miao et. al., PRB 89, 220503(R) (2014) 17



Dynamical Mean-Field Theory Plus Numerical Renormalization-Group Study of Spin-Orbital Separation in a Three-Band Hund Metal

Supplementary Material

K. M. Stadler,¹ Z. P. Yin,² J. von Delft,¹ G. Kotliar,² and A. Weichselbaum¹



Model ARPES: 3 band Hubbard model, no crystal fields!!!

Local Self-Energy Approach for Electronic Structure Calculations

N. E. Zein,^{1,2} S. Y. Savrasov,² and G. Kotliar^{3,4}

¹RRC “Kurchatov Institute”, Moscow 123182, Russia

²Department of Physics, University of California, Davis, California 95616, USA

³Center for Material Theory, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

⁴École Polytechnique, 91128 Palaiseau Cedex, France
(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

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. Kotliar¹

¹Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

²Department of Physics, Kings College London, Strand, London WC2R 2LS, United Kingdom

(Received 7 September 2012; published 5 December 2012)

We apply the quasiparticle self-consistent *GW* approximation (QSGW) 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 QSGW 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 QSGW 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 QSGW only partially accounts for dynamic renormalizations at low energies. These findings suggest that QSGW combined with dynamical mean field theory will capture most of the many-body physics in the iron pnictides and chalcogenides.

19

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

Validity of the Local Approximation in Iron- Pnictides and Chalcogenides

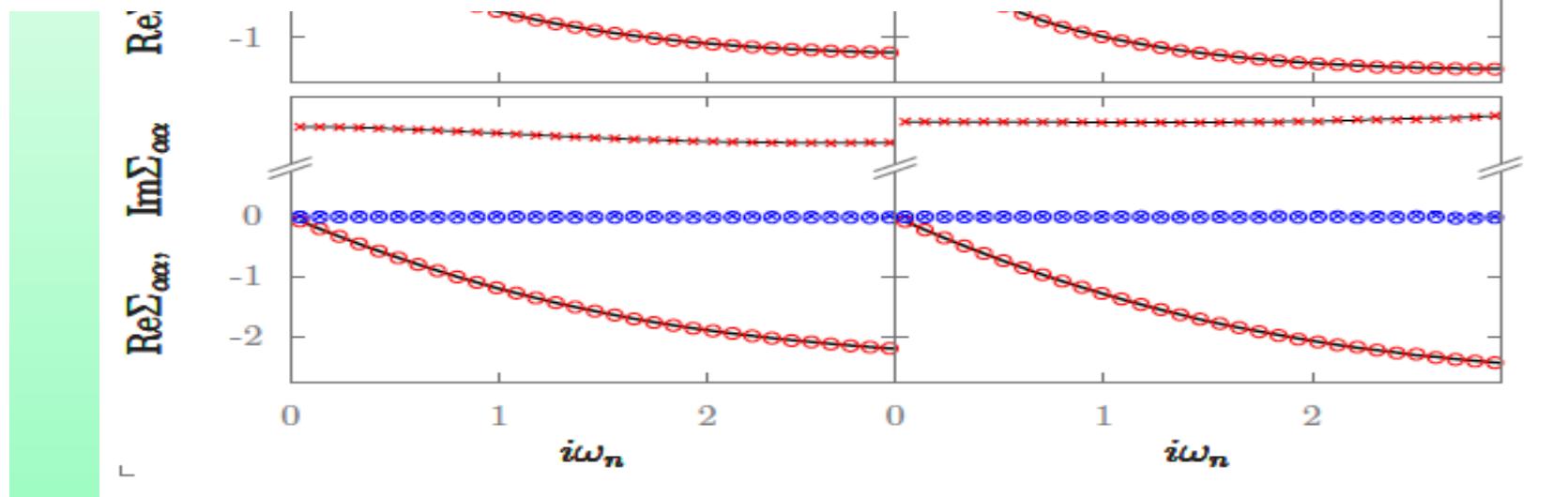
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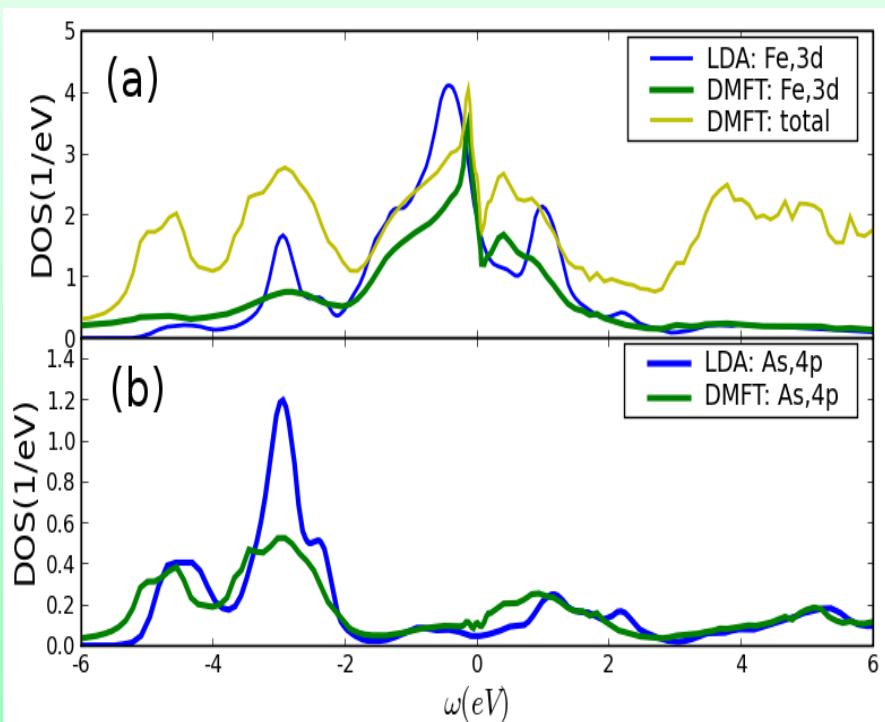
We carry out cluster DMFT for a model describing the normal state of the iron pnictides and chalcogenides. In the regime of moderate mass renormalizations, the self-energy all orbitals is surprisingly local justifying the success of single site DMFT in the iron pnictides and for other Hunds metals



FIG. 2. (Color online) Comparison of the t_{2g} self-energy obtained by DMFT (real/imaginary part with thin/bold lines) and DCA (local/non-local part in red/blue and real/imaginary part with crosses/circles). In the upper panel $(U, \tilde{U}) = (4.5, 4.5)$ and $(J, \tilde{J}) = (0.45, 0.375)$ while in the lower panel $(U, \tilde{U}) = (10.125, 9)$ and $(J, \tilde{J}) = (0, 0)$. The temperature is $T = 174K$.



Hunds metals: correlations without satellites – localized magnetism at intermediate scales without spins Ba 122.



BOTH ITINERANT MODELS
AND LOCALIZED MODELS ARE RIGHT!!!

FOR SOME THINGS, HUND'S METALS HAVE LOCALIZED SPINS BUT
ITINERANT CHARGE AND ORBITALS . HUNDS METAL PHYSICS IS LOCAL
LDA+DMFT SUCCESS

