Electronic Structure of Correlated Materials:

Slave Boson Methods and Dynamical Mean

Field Theory. Introductory Comments and Perspectives.

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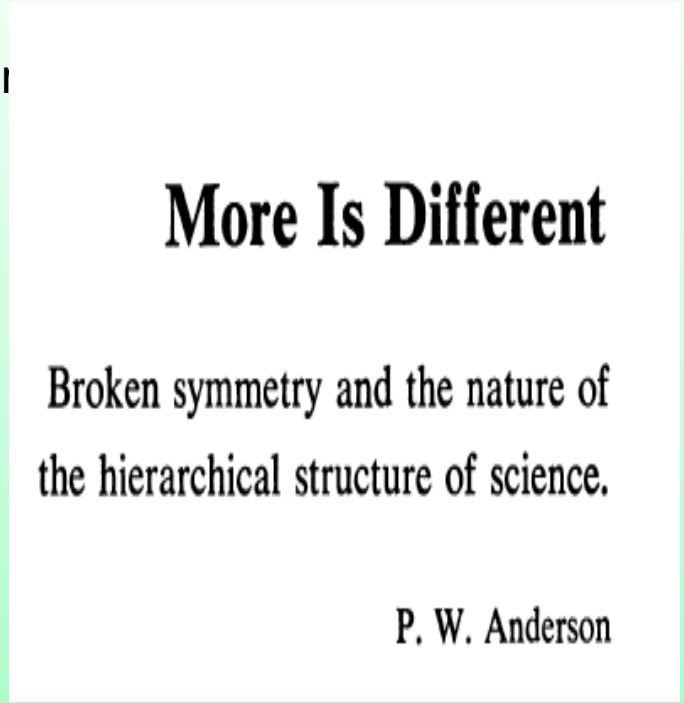
Autumn School on Correlated Electrons: DMFT at 25: Infinite Dimensions

Julich September 16th 2014

What is the role of theory ?

SCIENCE :4 August 1972, Volume 177, Numbe

"The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires research which I think is as fundamental in its nature as any other."



Role of theory: generate concepts and ideas.

The arrogance of the particle physicist and his intensive research may be behind us (the discoverer of the positron said "the rest is chemistry"), but we have yet to recover from that of some molecular biologists, who seem determined to try to reduce everything about the human organism to "only" chemistry, from the common cold and all mental disease to the religious instinct. Surely there are more levels of organization between human ethology and DNA than there are between DNA and quantum electrodynamics, and each level can require a whole new conceptual structure.

In closing, I offer two examples from economics of what I hope to have said. Marx said that quantitative differences become qualitative ones, but a dialogue in Paris in the 1920's sums it up even more clearly:

FITZGERALD: The rich are different from us.

HEMINGWAY: Yes, they have more money.

What is the role of theory ?

Paul Dirac (1929) "The underlying laws necessary for the mathematical theory of the whole chemistry are thus completely known and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble "

"Approximate practical methods of applying quantum mechanics should be developed which can lead to an explanation of the main features of complex atomic systems without too much computation"

In condensed matter theory both Dirac's and Anderson's dictum are intertwined. Both are needed and should be nurtured to make progress in the field.

Condensed Matter Theory continous interplay between theory and experiment.

Interplay of materials motivated problems, the development of theory , concepts and techniques.

- Highlight concepts and ideas
- Highlight development of techniques and material specific predictions.
- Examples. VanadiumSesquioxide, Plutonium Iron Pnictide and Chalcogenides…….

Model Hamiltonians and First Principles Methods

$$H = \sum_i \frac{\nabla_i^2}{2m_e} + \sum_\alpha \frac{\nabla_\alpha^2}{2m_\alpha} - \sum_{\alpha,i} \frac{Z_\alpha e^2}{|\vec{R}_\alpha - \vec{R}_i|} + \frac{1}{2}\sum_{i\neq j} \frac{e^2}{|\vec{R}_i - \vec{R}_j|} + \frac{1}{2}\sum_{\alpha\neq\beta} \frac{Z_\alpha^2 e^2}{|\vec{R}_\alpha - \vec{R}_\beta|}$$
$+$relativistic effects.

Theory of everything vs Hubbard model

$$H = \sum_{i,j} c_\alpha^\dagger(i) t_{ij}^{\alpha\beta} c_\beta(j) + \sum_i U_{\alpha\beta\gamma\delta} c_\alpha^\dagger(i) c_\beta^\dagger(i) c_\gamma(i) c_\delta(i).$$

Model Hamiltonians good to learn qualitative lessons common to many materials. TOE is needed to answer what each material does

Examples of ab initio methods

Density Functional Theory (Kohn Sham 1964)

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

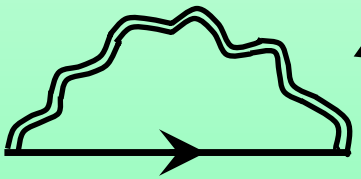
Reference Frame for Weakly Correlated Systems.

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

$$V_{KS} = V_{Hartree} + V_{cryst} + V_{xc}$$

Starting point for perturbation theory in the screened Coulomb interactions

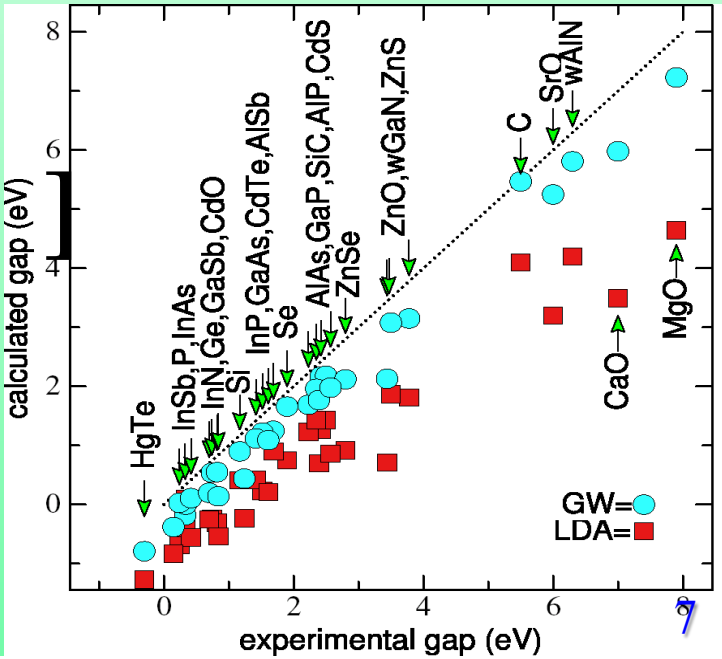
(Lars Hedin 1965)

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

M. VanSchilfgaarde Phys. Rev. Lett. 93, 126406 (2004)

Many other properties can be computed, structure , transport, optics, phonons, etc… Residual interactions

…..



Slave boson formalism

$$|n\rangle = (d_1^\dagger)^{n_1} \cdots (d_M^\dagger)^{n_M} |\mathrm{vac}\rangle$$

$$H_{\mathrm{loc}} = \sum_\alpha \varepsilon_\alpha^0 \hat{n}_\alpha + \sum_{\alpha\beta} U_{\alpha\beta} \hat{n}_\alpha \hat{n}_\beta$$

$$|n\rangle_f \equiv (f_1^\dagger)^{n_1} \cdots (f_M^\dagger)^{n_M} |\mathrm{vac}\rangle$$

$$|\underline{n}\rangle \equiv \phi_n^\dagger |\mathrm{vac}\rangle \otimes |n\rangle_f$$

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Constraints

$$\sum_n \phi_n^\dagger \phi_n = 1 \qquad \sum_n n_\alpha \phi_n^\dagger \phi_n = f_\alpha^\dagger f_\alpha, \quad \forall \alpha$$

$$\underline{d}_\alpha^\dagger = \sum_{nm} \langle n | f_\alpha^\dagger | m \rangle [\hat{\Delta}_\alpha]^{-1/2} \phi_n^\dagger \phi_m [1 - \hat{\Delta}_\alpha]^{-1/2} f_\alpha^\dagger$$

Physical content

Emergence of renormalized QP

$$\hat{\Delta}_\alpha[\phi] \equiv \sum_n n_\alpha \phi_n^\dagger \phi_n$$

$|\phi_n|^2$:

Probabilty of state n to be occupied

Coupling of fermions to local spin orbital charge modesl

Kinetic Part

$$\underline{H} = \sum_{ij} R_\alpha[\phi] f_\alpha^\dagger(i)\, t_{ij}^{\alpha\beta} R_\beta[\phi] f_\beta(j)\,.$$

Local Part

$$H_{loc} = \sum_n \phi_n{}^\dagger \phi_n \epsilon_n$$

$$\epsilon_n = \sum_\alpha (n_\alpha + \sum_\beta U_{\alpha\beta} n_\alpha n_\beta).$$

Interpretation in terms of self energies.

$$\Sigma_\alpha(\omega) = \Sigma_\alpha(0) + \omega\left(1 - \frac{1}{Z_\alpha}\right),$$

$$Z_\alpha = |R_\alpha|^2,$$

$$\Sigma_\alpha(0) = \lambda_\alpha/|r_\alpha|^2 - \epsilon_\alpha^0.$$

Rotationally invariant slave bosons

$$d_\alpha = \hat{R}_{\alpha\beta}[\phi] f_\beta.$$

Saddle point, Gutzwiller approximation to its wave function . Some references

- G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. 57, 1362 (1986).
- Benchmarks against QMC . L. Lilly, A. Muramatsu, and W. Hanke, Phys. Rev. Lett. 65, 1379 (1990).
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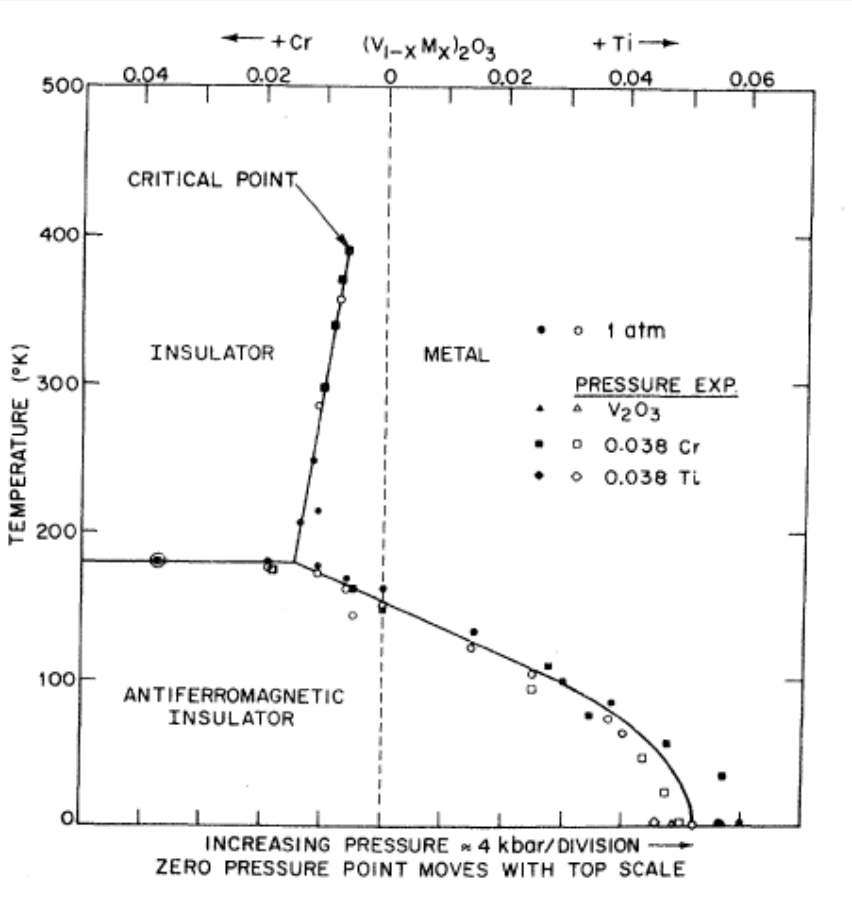
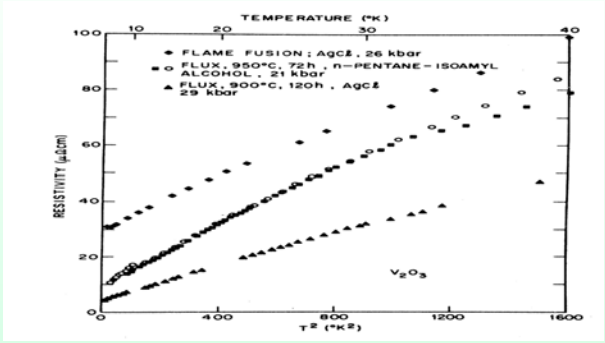
- T. Li, P. Wolfle,and P. J. Hirschfeld, Phys. Rev. B 40, 6817 (1989). Fluctuations.
- Lechermann and Georges Kotliar Parcollet PRB 76, 155102 (2007)

V2O3 MIT and transport



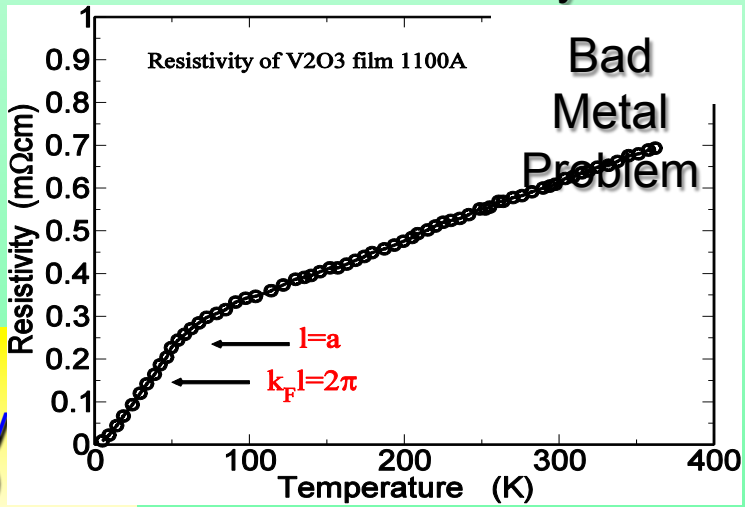
McWhan, PRL 23, 1834 (1969)



McWhan, PRB, 7, 1920 low T, Emergence of Fermi liquid T^2

Brinkman and **Rice**, **PRB** 2, 4302 (1970)

Natural consequence of the slave boson mean field theory.



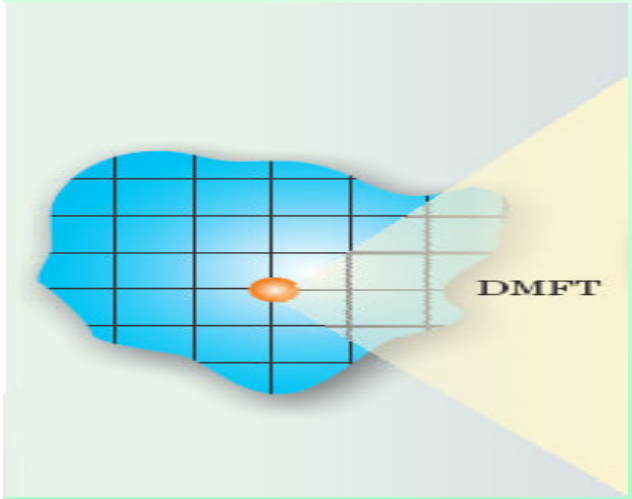
G. Grygiel et. al. Applied Phy Lett 91 , 262103 (2007)

Mean Field Theories Replace a many body problem by a single site problem in an effective medium reference frame

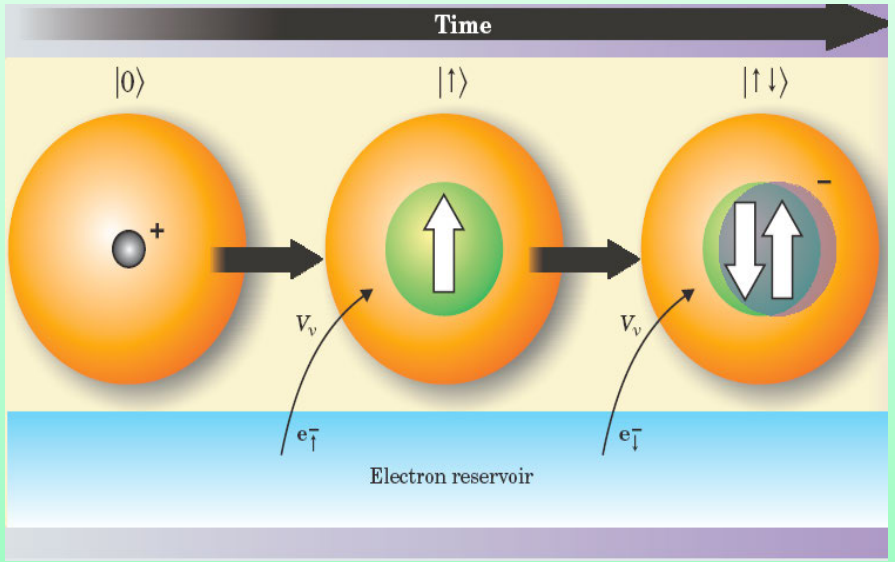
$$\sum_{<i,j>,\sigma} (t_{ij} + \mu\delta_{ij})(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

MODEL HAMILTONIAN

$$H_{\text{Anderson Imp}} = \sum_{\alpha,\sigma} (V_{\alpha} c^{\dagger}_{0\sigma} A_{\alpha\sigma} + \text{c.c}). + \sum_{\alpha,\sigma} \varepsilon_{\alpha} A^{\dagger}_{\alpha\sigma} A_{\alpha\sigma} + \sum_{\alpha,\sigma} \mu c^{\dagger}_{0\sigma} c_{0\sigma} + U c^{\dagger}_{0\uparrow} c_{0\uparrow} c^{\dagger}_{0\downarrow} c_{0\downarrow}$$



DMFT



Effective medium: quantifieds the notion of " metallicity" or itineracy

A. Georges and G. Kotliar PRB 45, 6479 (1992).

Exact in infinite dimensions Metzner Vollhardt PRL . **62, 324–327** (1989)

DMFT self consistency : medium to reproduce the exact (best) local spectral function of the problem.

$$G_{imp}(i\omega_n)[\Delta] = \sum_{k} \frac{1}{[i\omega_n + \mu + t(k) - \Sigma_{imp}(i\omega_n)[\Delta]]}$$

Optical Conductivity in Mott-Hubbard Systems

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(Received 13 March 1995)

We study the transfer of spectral weight in the optical spectra of a strongly correlated electron system as a function of temperature and interaction strength. Within a dynamical mean field theory of the Hubbard model that becomes exact in the limit of large lattice coordination, we predict an anomalous enhancement of spectral weight as a function of temperature in the correlated metallic state and report on experimental measurements which agree with this prediction in V_2O_3. We argue that the optical conductivity anomalies in the metal are connected to the proximity to a crossover region in the phase diagram of the model.

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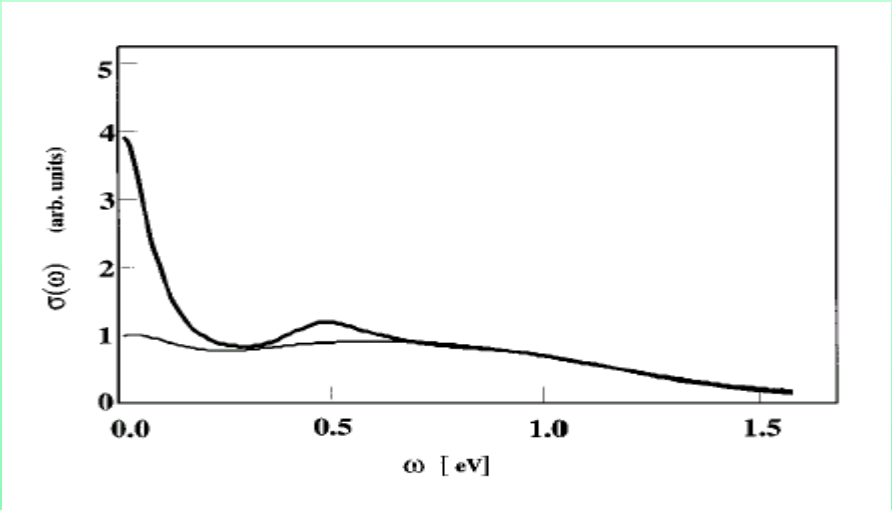

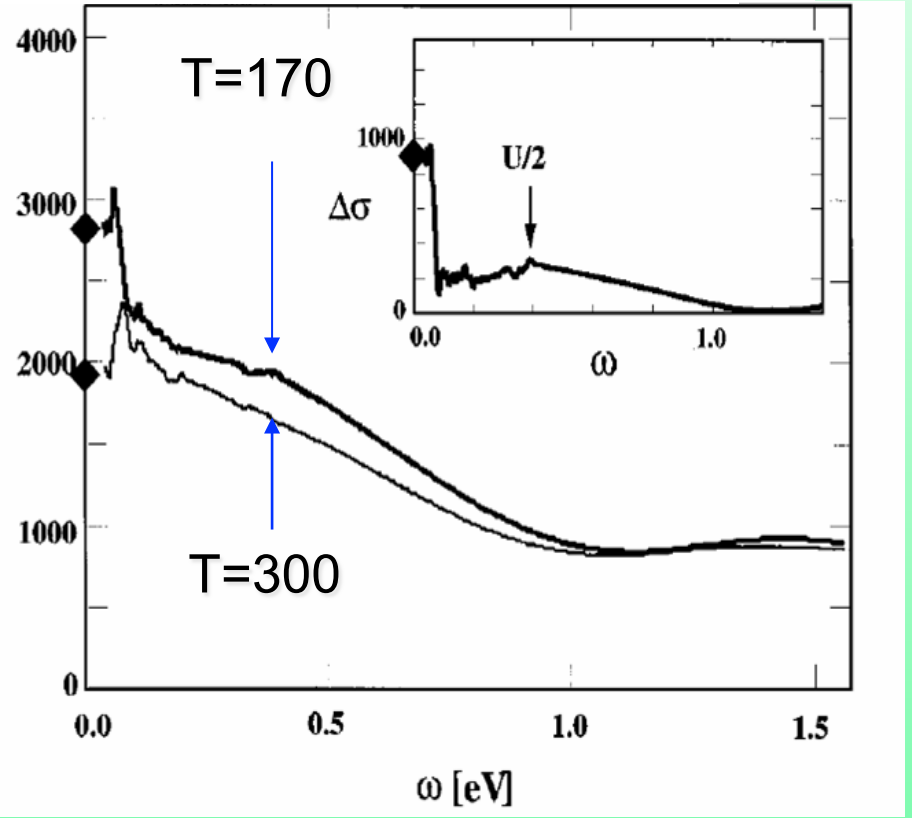

More realistic studies of vanadium oxides within LDA+DMFT followed over the last decade.

. K Held, G. Keller, V. Eyert, D. Vollhardt, and V. I. Anisimov, Phys. Rev. Lett. 86, 5345–5348 (2001).

. G. Keller, K. Held, V. Eyert, D. Vollhardt, and V. I. Anisimov, Phys. Rev. B 70, 205116 (2004).

. A. I. Poteryaev, J. M. Tomczak, S. Biermann, A. Georges, A. I. Lichtenstein, A. N. Rubtsov, T. Saha-Dasgupta, and

O. K. Andersen, Physical Review B (Condensed Matter

and Materials Physics) 76, 085127 (2007).

. J. M. Tomczak and S. Biermann, Phys. Rev. B 80, 085117 (2009).

. L. Baldassarre, A. Perucchi, D. Nicoletti, A. Toschi,

G. Sangiovanni, K. Held, M. Capone, M. Ortolani, L. Malavasi, M. Marsi, P. Metcalf, P. Postorino, and S. Lupi, Physical Review B 77, 113107 (2008)

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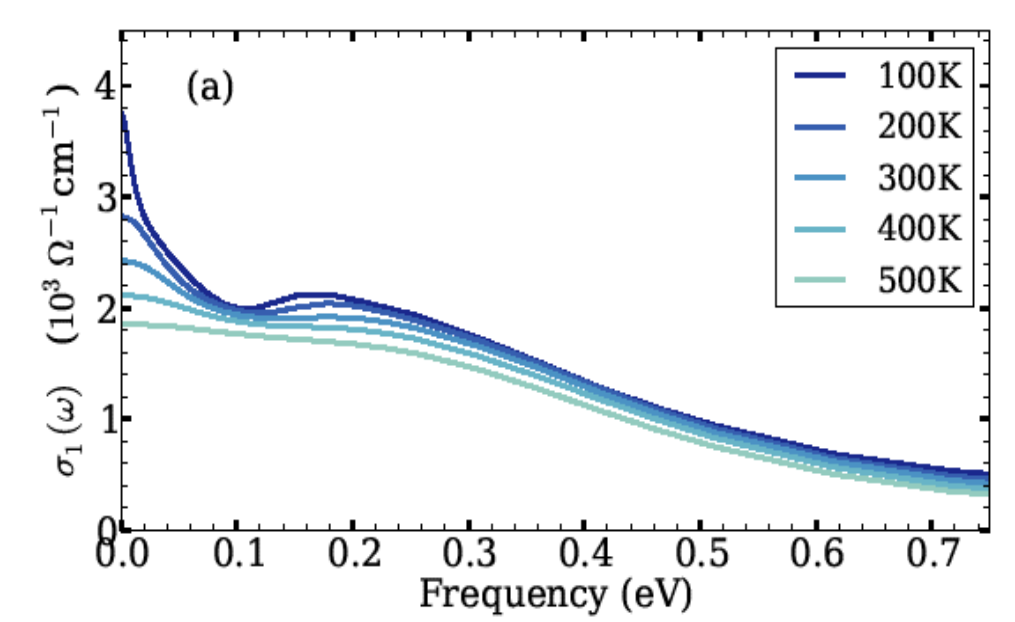
LDA+DMFT calculations of V2O3: Paramagnetic metallic phase



What is the origin of the bad metallic behavior ? Test recent ideas from DMFT model studies. X Deng, J Mravlje, M Ferrero, G Kotliar, A GeorgesPRL 110 (8), 086401 (2013)W Xu, K Haule, G Kotliar PRL 111 (3), 036401 (2013)

$$\sigma(T,\omega) = \sigma_1 + i\sigma_2 = \frac{{\omega_p}^{*2}}{4\pi(\omega + \frac{i}{\tau^*(T)})}$$

Deng. et.al. (2014) treats the oxygen degrees of freedom explicitly U=5.8 ev J=.7 ev

$$\frac{\omega_p^2}{8} = \int_0^{\Omega} \sigma_1(\omega) d\omega$$

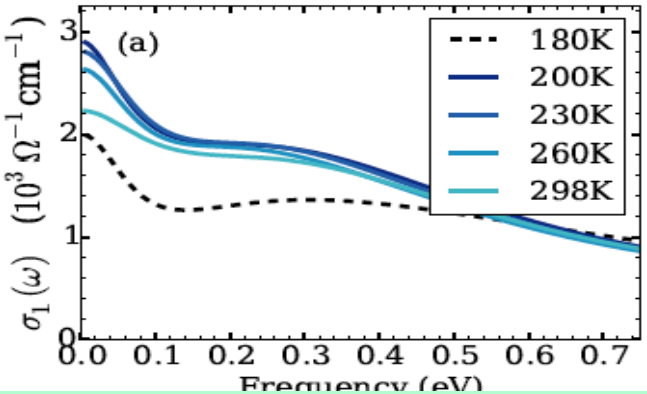
$\omega_p^2 \uparrow$ when T $\downarrow$ $\qquad$ $\omega_p^2{}^* \downarrow$ when $T \downarrow$

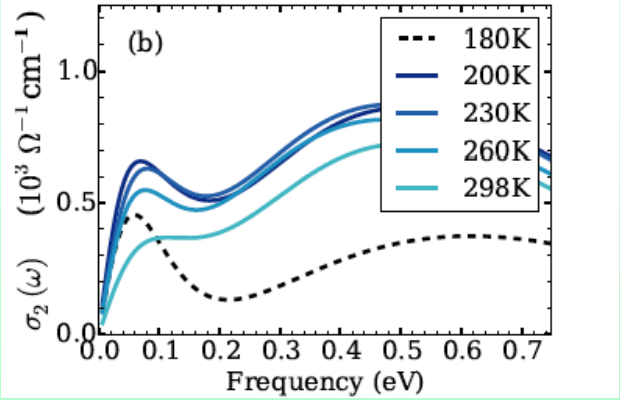
Resilient quasiparticles form a Hidden Fermi Liquid. $aT^2 + b$ law in $1/\tau^*$ at high temperatures not visible in ρ or $1/\tau$.

HIDDEN non-Landau Fermi Liquid Found in V2O3 case from experimentX. Deng A. Sternbach K. Haule D. Basov GK

arXiv:1404.6480 integrate to 140 mev to get ω_p^2

analyze low freq get ω^{*2}_p ,τ^*





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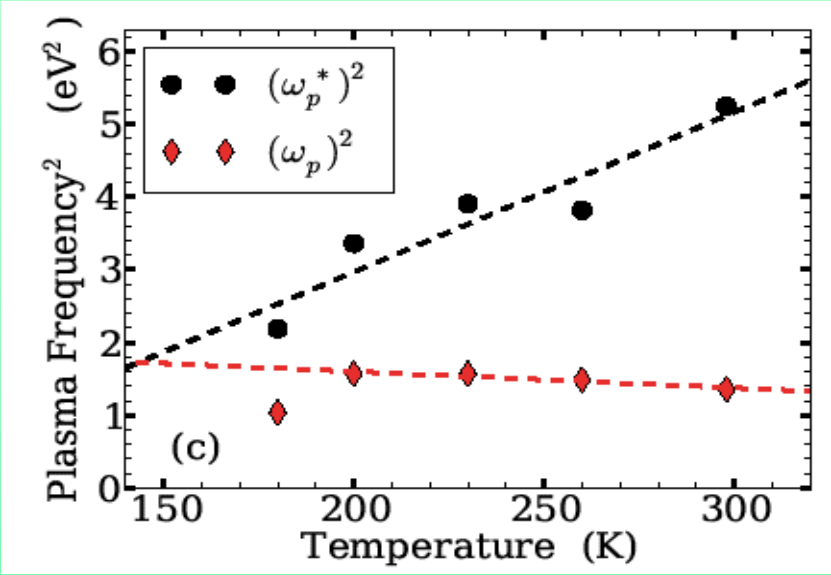
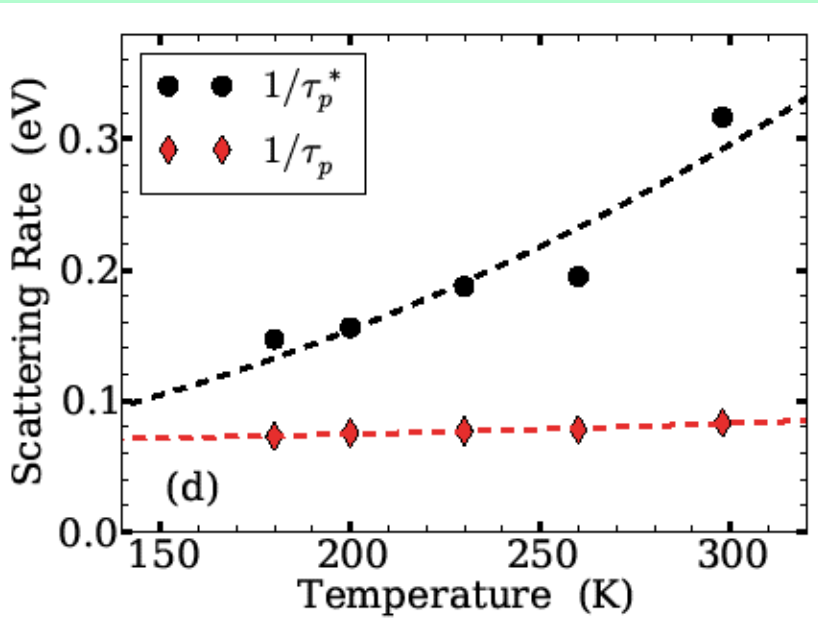
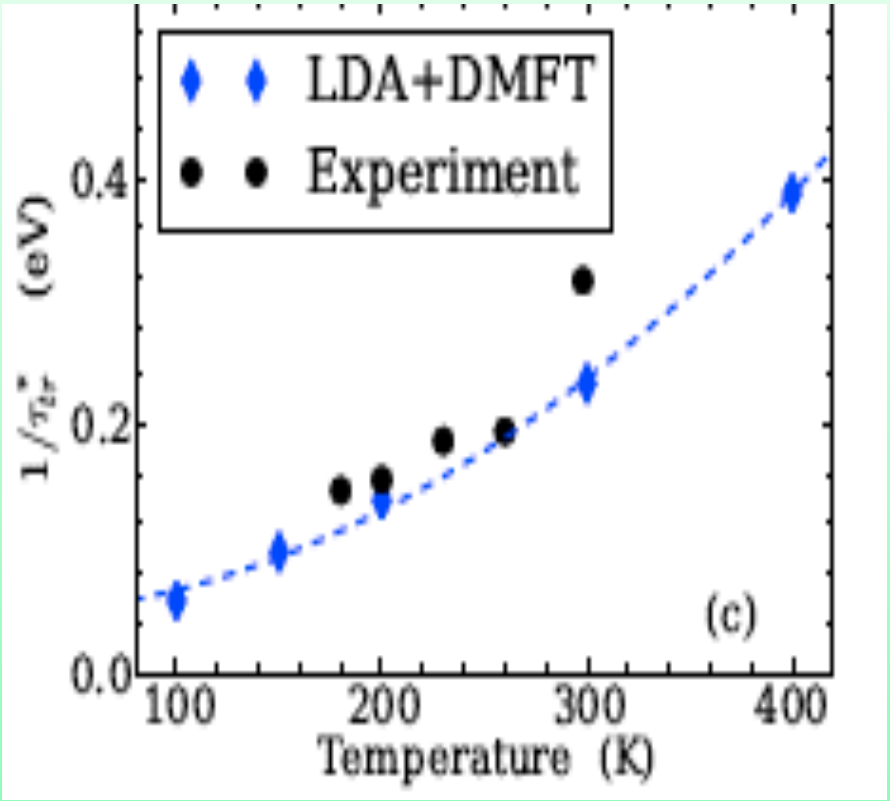
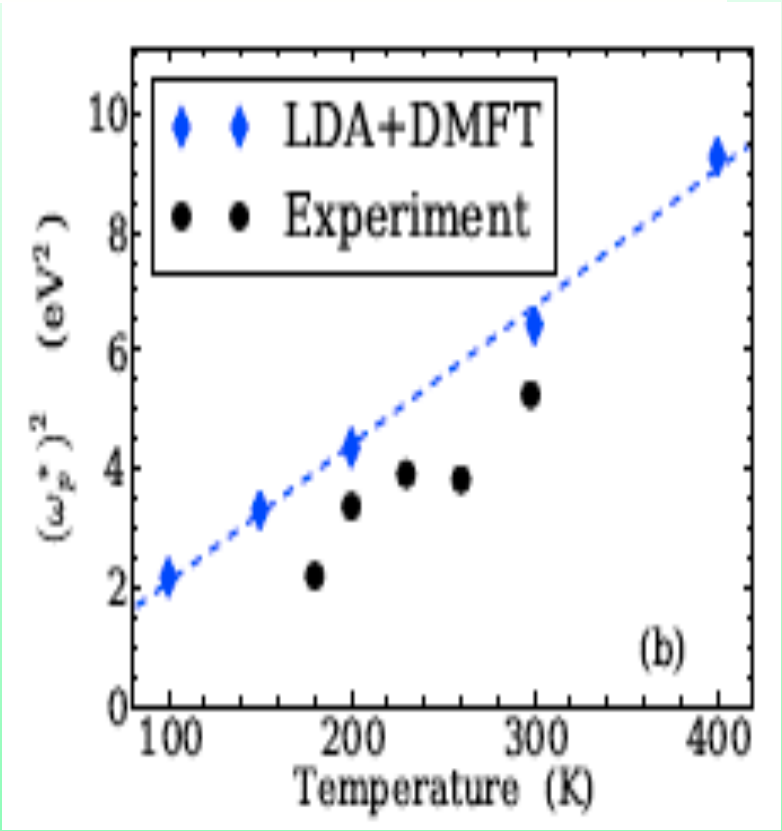




Hidden Fermi Liquid in V2O3: the case from theory (and experiment)





$1/\tau^* \sim a + b\,T^2$

Quantitfy correlations and locality

$$G(\omega,k)=\frac{1}{[\omega+\nabla^2+\mu-V_{Hartree}-V_{cryst}]-\Sigma(k,\omega)}$$

- Chemist

$$\Sigma(k,\omega)-\Sigma(k)_{Hartree-Fock}$$ large

- Physicist

$$\Sigma(k,\omega)-V(k)xc_{LDA}$$ large

"Locality" is defined with respect to a basis

$$\Sigma(r,r')=\chi^{*}{}_{\alpha R}(r)\Sigma(i\omega_n)_{\alpha R\beta R'}\chi_{\beta R'}(r') \qquad Zn<R,\beta|\Sigma|R',\alpha>\lll<R,\beta|\Sigma|R,\alpha>$$

Challenge : Finding optimal truncations to get right spectra and total energies.

Vxc - Edc

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

DFT+DMFT V. Anisimov, A. Poteryaev, M. Korotin, A. Anokhin and G. Kotliar, J. Phys. Cond. Mat. 35, 7359 (1997).

- The light, SP (or SPD) electrons are extended, well described by LDA .The heavy, D (or F) electrons are localized treat by DMFT.
- LDA Kohn Sham Hamiltonian already contains an average interaction of the heavy electrons, subtract this out by shifting the heavy level (double counting term)

❑ Kinetic energy is provided by the Kohn Sham Hamiltonian (sometimes after downfolding). The U matrix can be estimated from first principles of viewed as parameters. Solve resulting model using DMFT.

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

Local Self-Energy Approach for Electronic Structure Calculations

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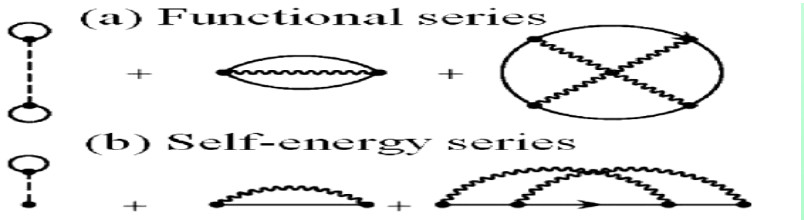
(Received 29 November 2005; published 7 June 2006)

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

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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.

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

LDA+DMFT functional

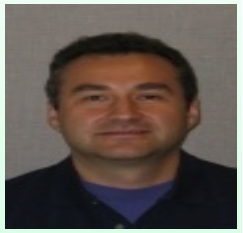
$$\Gamma_{LDA+DMFT}[\rho(r)\ G_{ab}\ V_{KS}(r)\ \Sigma_{ab}]$$

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

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

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

$$\sum_R \Phi[G_{\alpha\beta R}\ Uabcd]-\Phi_{DC}$$



Φ **Sum of local 2PI graphs**

local U matrix and local G

Explicit Dependence on : U , DC, and Projectors [Orbitals], and Independence of basis

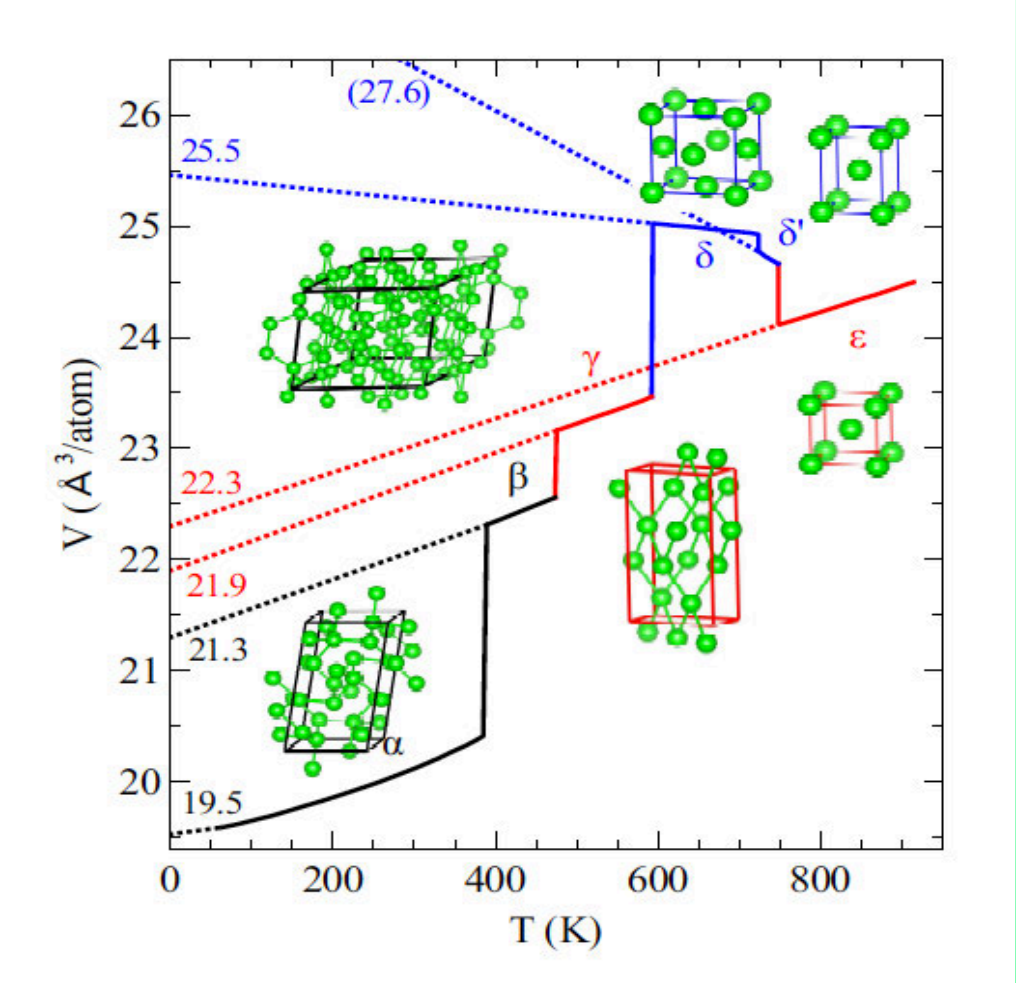
Input parameters can be in principle computed (constrained RPA,Ariasetiawan, Imada Miyake) or can be adjusted to fit one experiment in one compound, and use to predict results of multiple spectroscopies in multiple materials within a family of compounds.

R. Chitra and G. Kotliar, Phys. Rev. B 62, 12715 (2000)

S. Y. Savrasov and G. Kotliar, Phys. Rev. B 69, 245101 (2004)

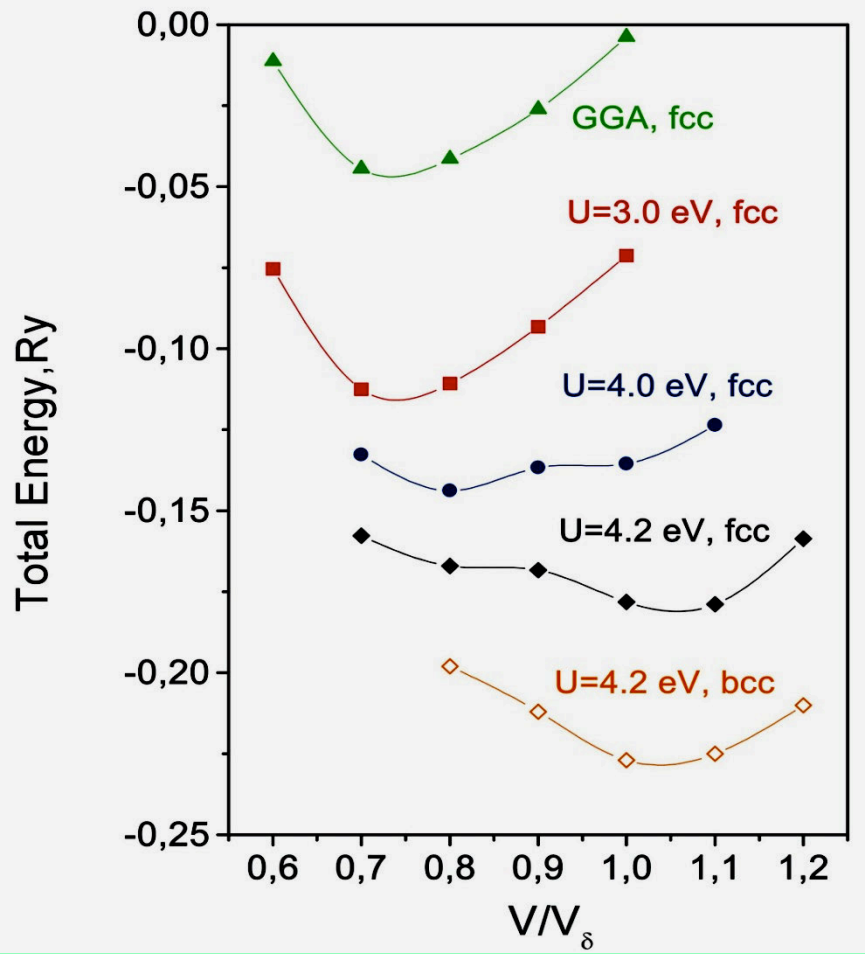
Spectral Density Functional

Strong Correlation in an Element Pu



- Spin Density functional theory (i.e. LSDA) **predicts** that Pu , Am, magnetic, **large orbital and spin moments**.
- Experimentδ **Pu is non magnetic. No static or fluctuating moments.**
- Paramagnetic LDA underestimates Volume of δ Pu. by more than 30 %

Total Energy as a function of volume for Pu



Paramagnetic Calculation

f Valence close to nf~ 5.2

Competing views:

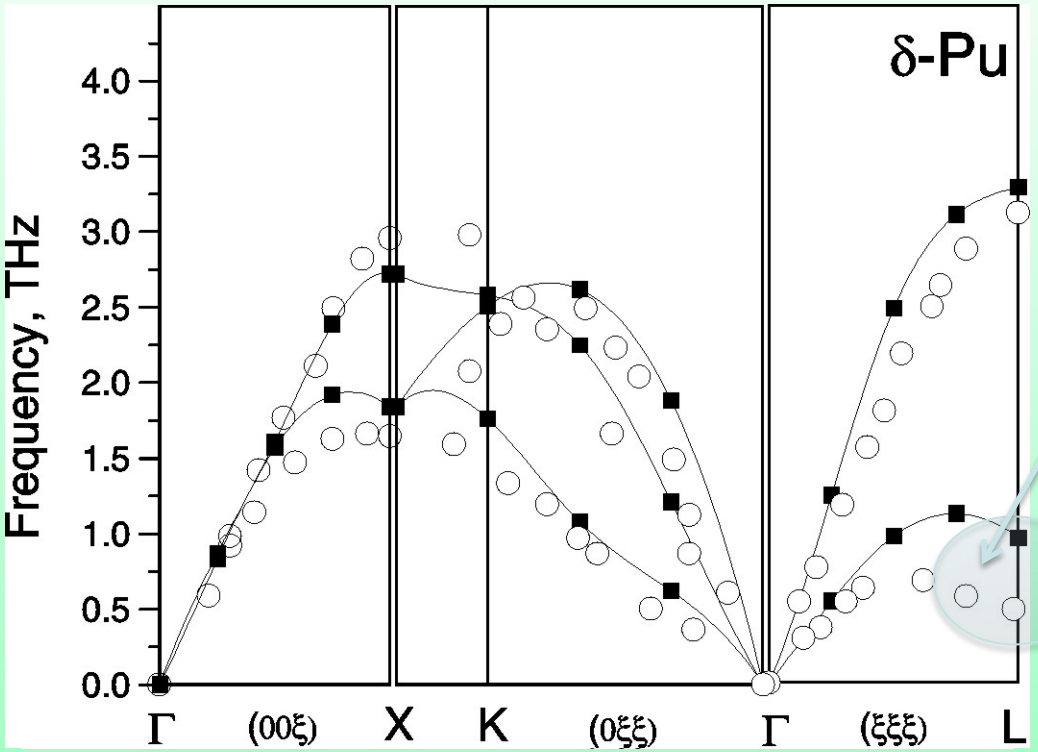
nf~ 4 nf~ 6

The f electron in δ-phase is only slightly more localized than in the α-phase which has larger spectral weight in the quasiparticle peak and smaller weight in the Hubbard bands

(Savrasov, Kotliar, Abrahams, Nature (2001)

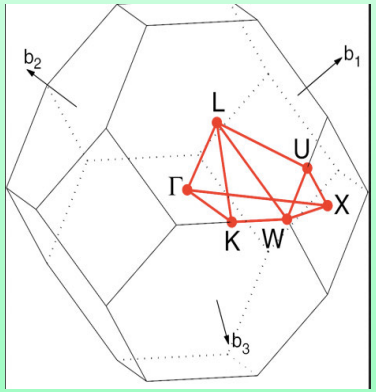
Non magnetic correlated state of fcc Pu.

DMFT Phonons in fcc δ-Pu. Inelastic X ray scattering



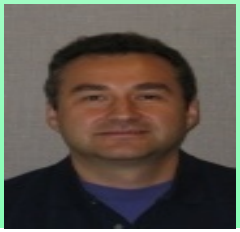
Theory

Experiment



Recent phenomenological ideas: Z. Yin, X Deng
K Basu Q. Yin and G. Kotliar

Philosophical Magazine Letters, 2014
http://dx.doi.org/10.1080/09500839.2014.953617



(Dai, Savrasov, Kotliar,Ledbetter, Migliori, Abrahams, Science, 9 May 2003)

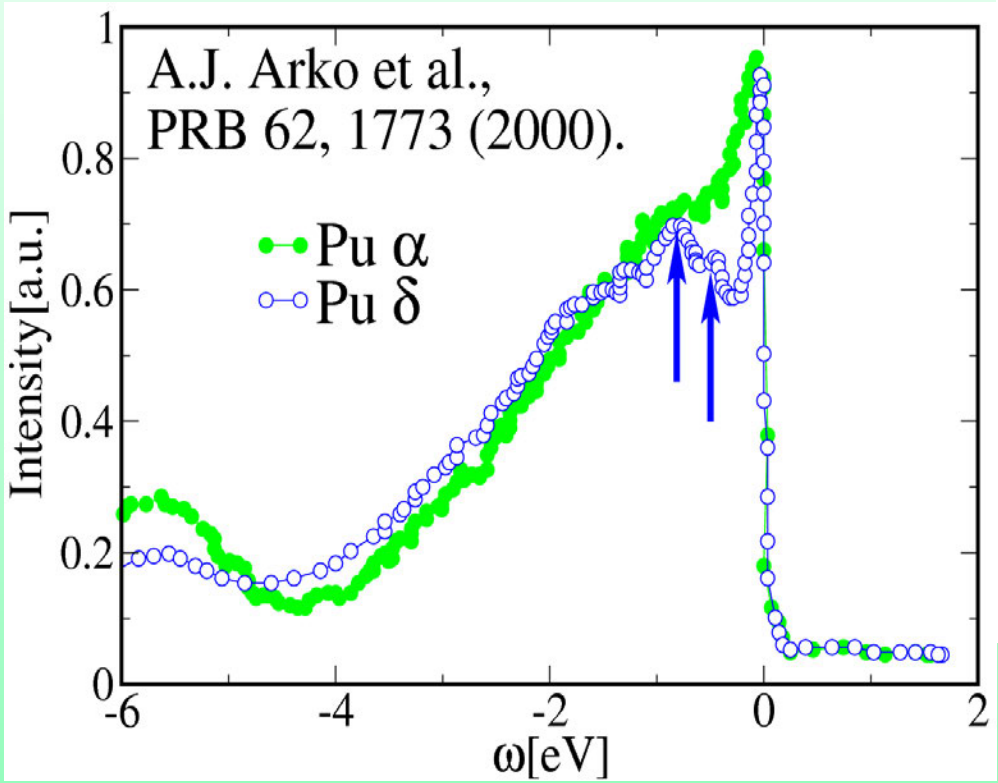
(experiments from Wong et.al, Science, 22 August 2003)

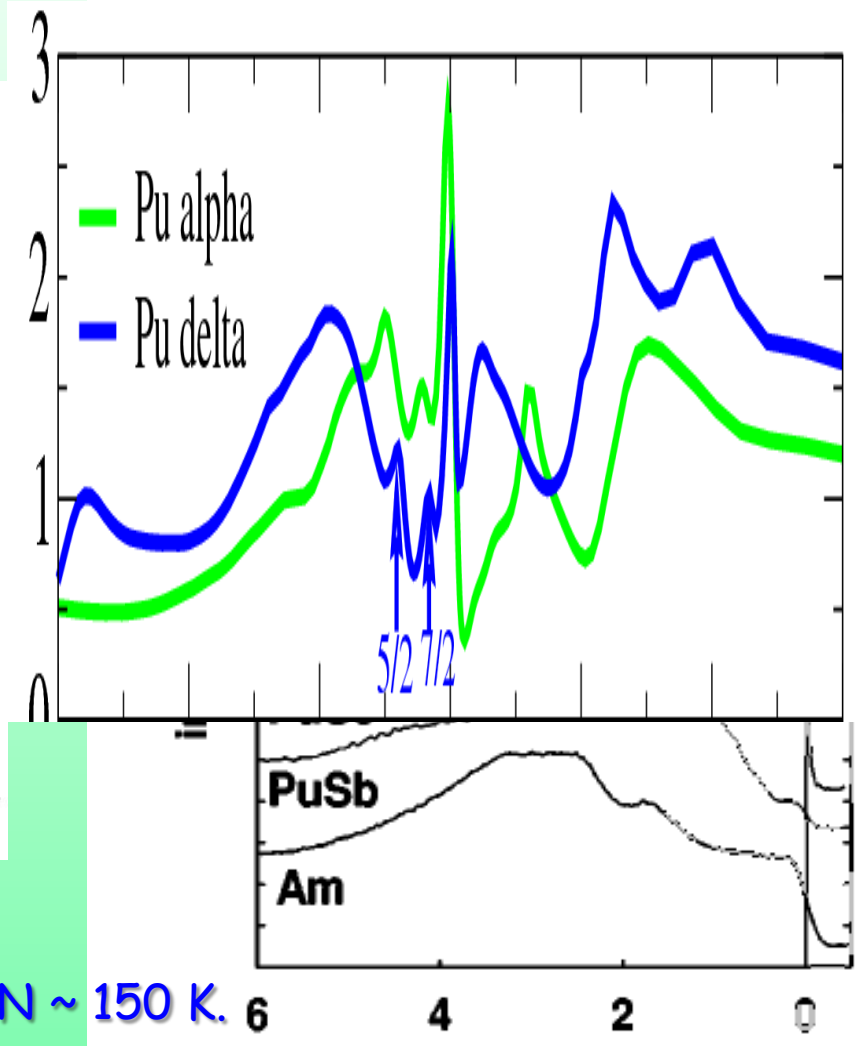
Photoemision and Magnetism

Havela et. al. Phys. Rev. B 68, 085101 (2003)

QP multiplets : C. Yee G. Kotliar K. Haule

Phys. Rev. B 81, 035105 (2010)

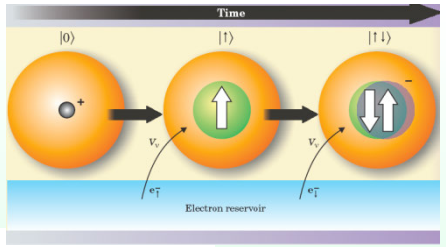




Pu is non magnetic – Cm is magnetic TN ~ 150 K.

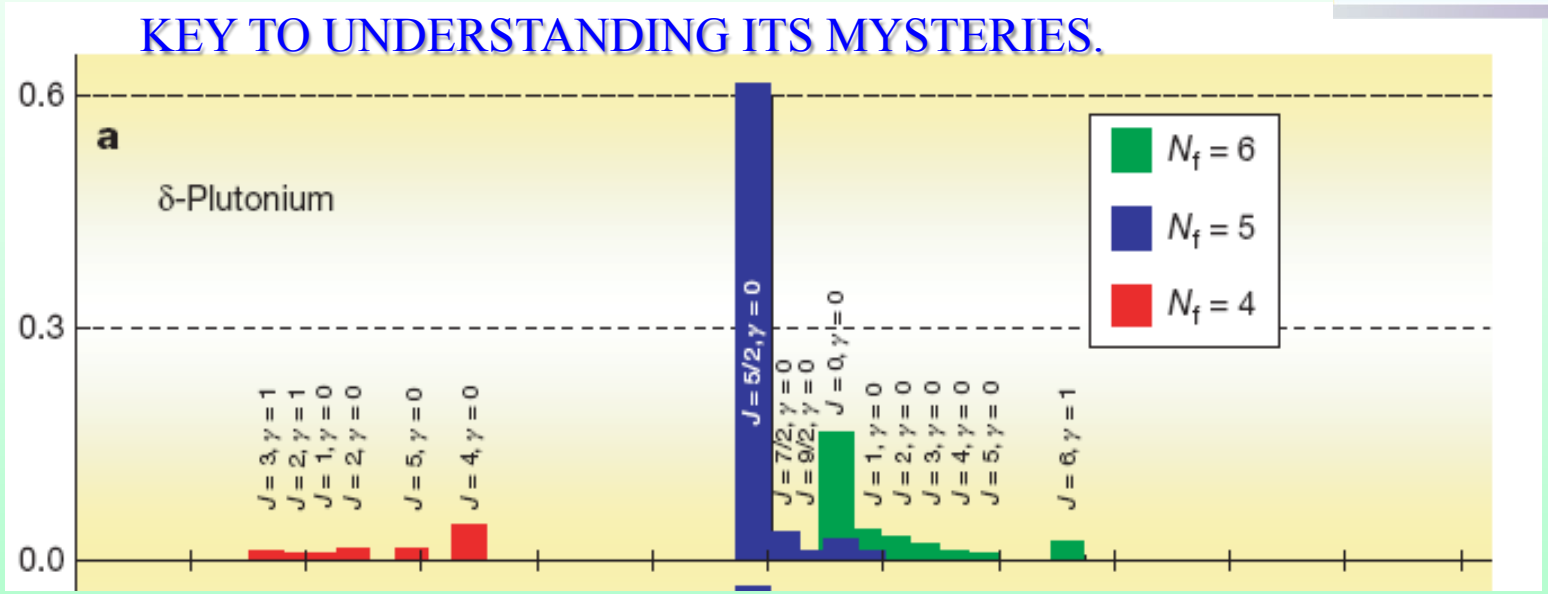
K.Haule J. Shim and GK Nature 446, 513 **(2007)**

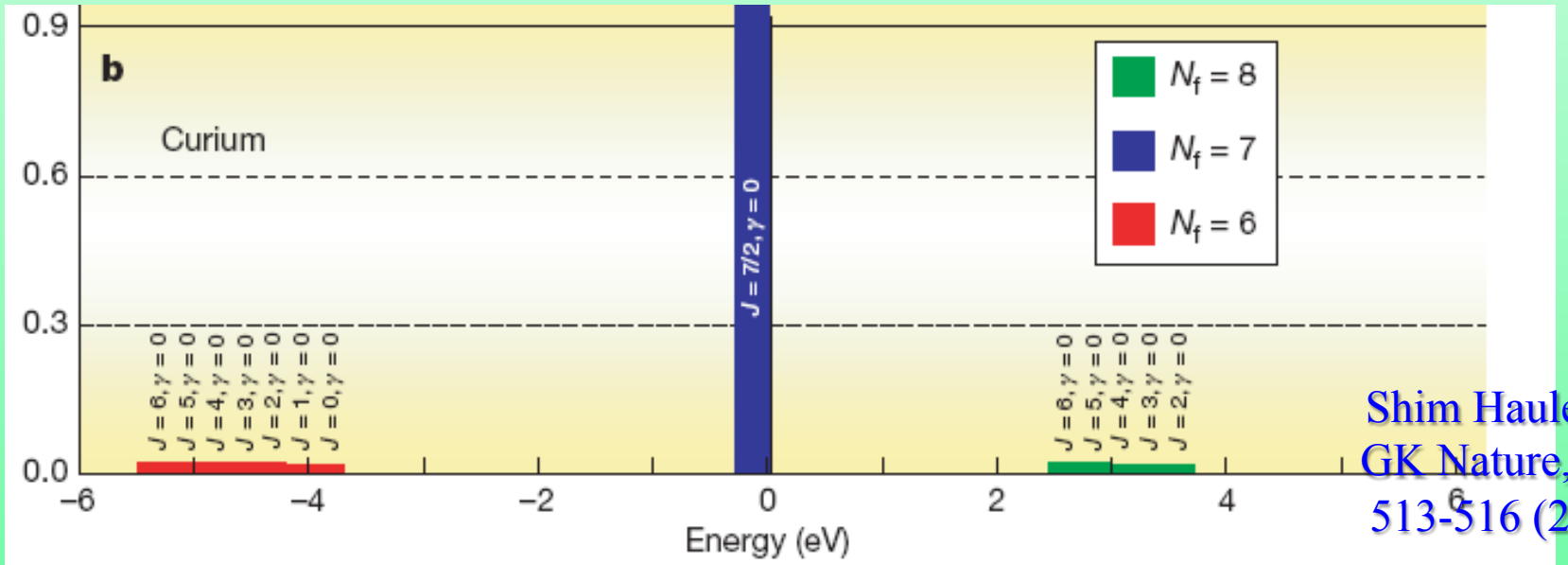
What is the meaning of valence in a solid ?



Plutonium is MIXED VALENCE. DMFT valence histogram.

KEY TO UNDERSTANDING ITS MYSTERIES.



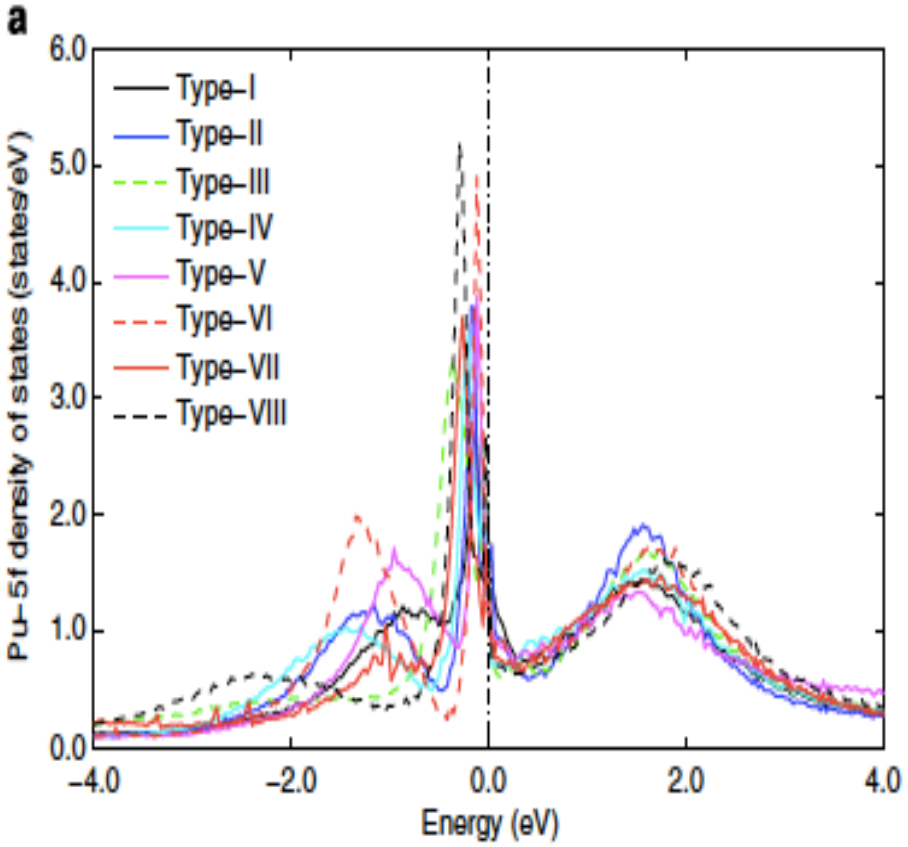


Shim Haule and GK Nature, 446, 513-516 (2007)

Site-selective electronic correlation in α-plutonium metal

Jian-Xin Zhu[1], R.C. Albers[1], K. Haule[2], G. Kotliar[2] & J.M. Wills[1]

Nat. Commun. 4, 2644 (2013)



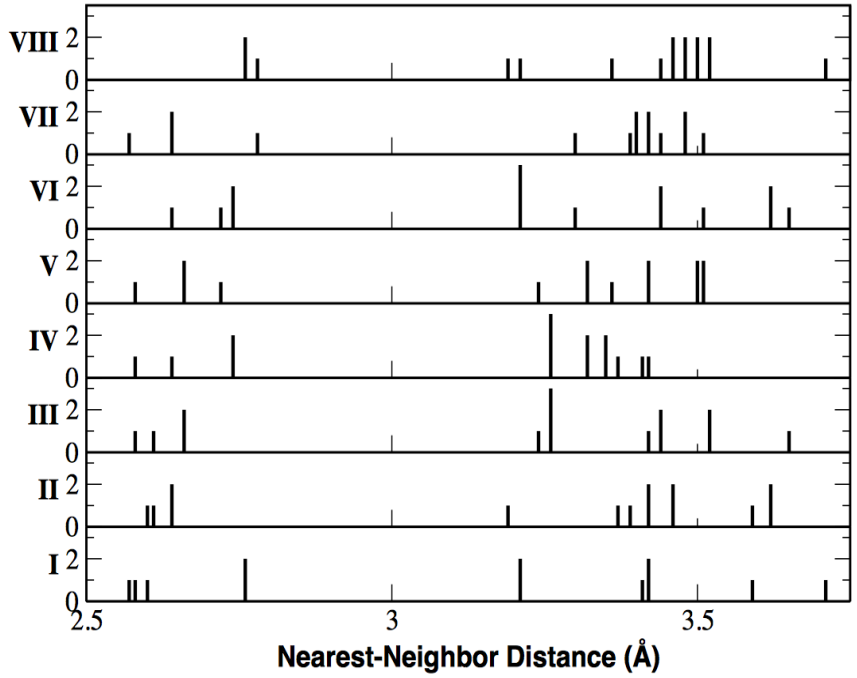
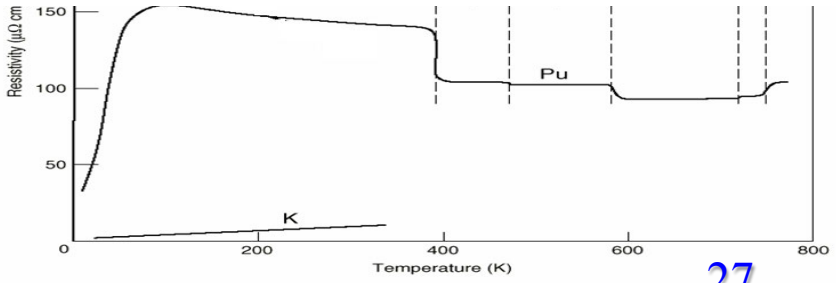
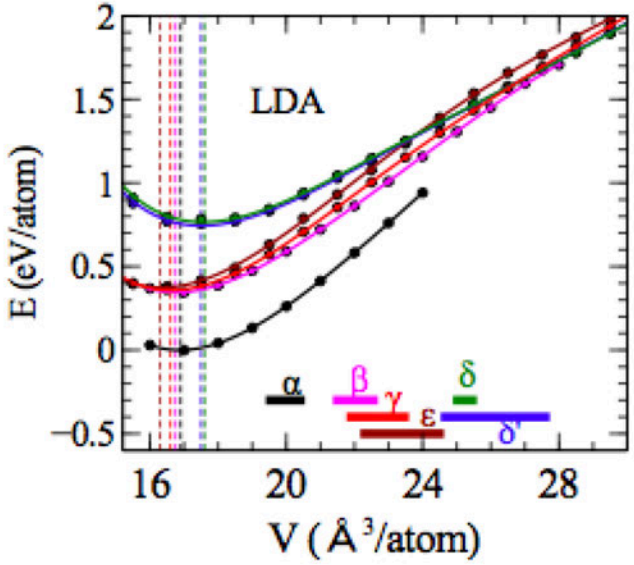
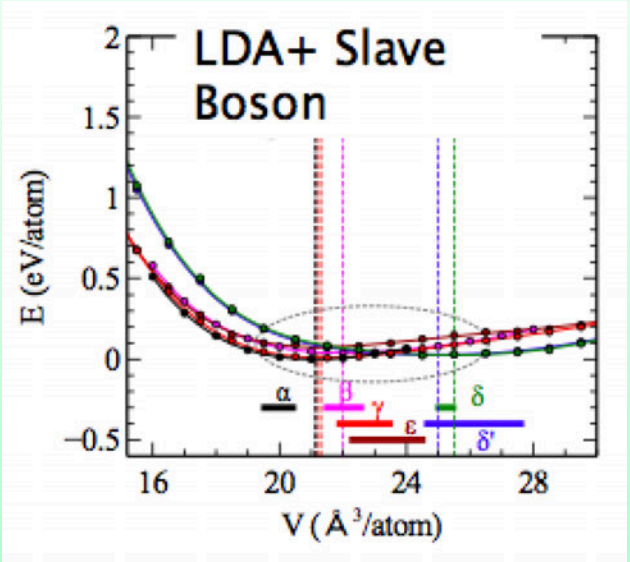


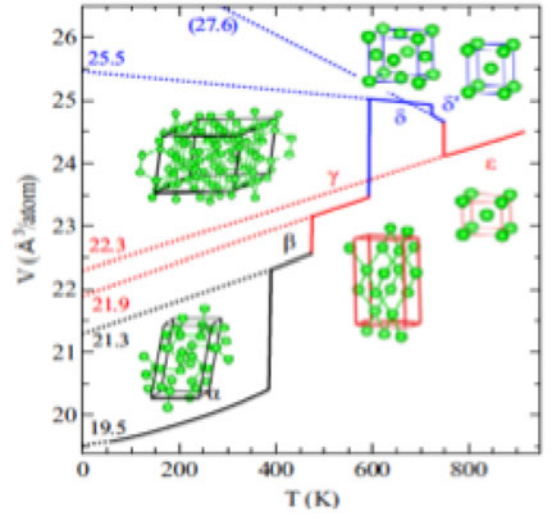
FIG. 2. **Bond lengths.** Distribution of interatomic distances for eight crystallographically nonequivalent atoms in α-Pu. The height of the lines measures the number of neighbors at the given distance.



In all the phases correlation energy is weakly dependent on structure !!!







28

Calculations with the rotationally invariant slave boson formulation of F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, Phys. Rev. B 76, 155102 (2007) N. Lanat`a, Y. X. Yao, C. Z. Wang, K. M. Ho, and G. Kotliar, arXiv:1407.4862

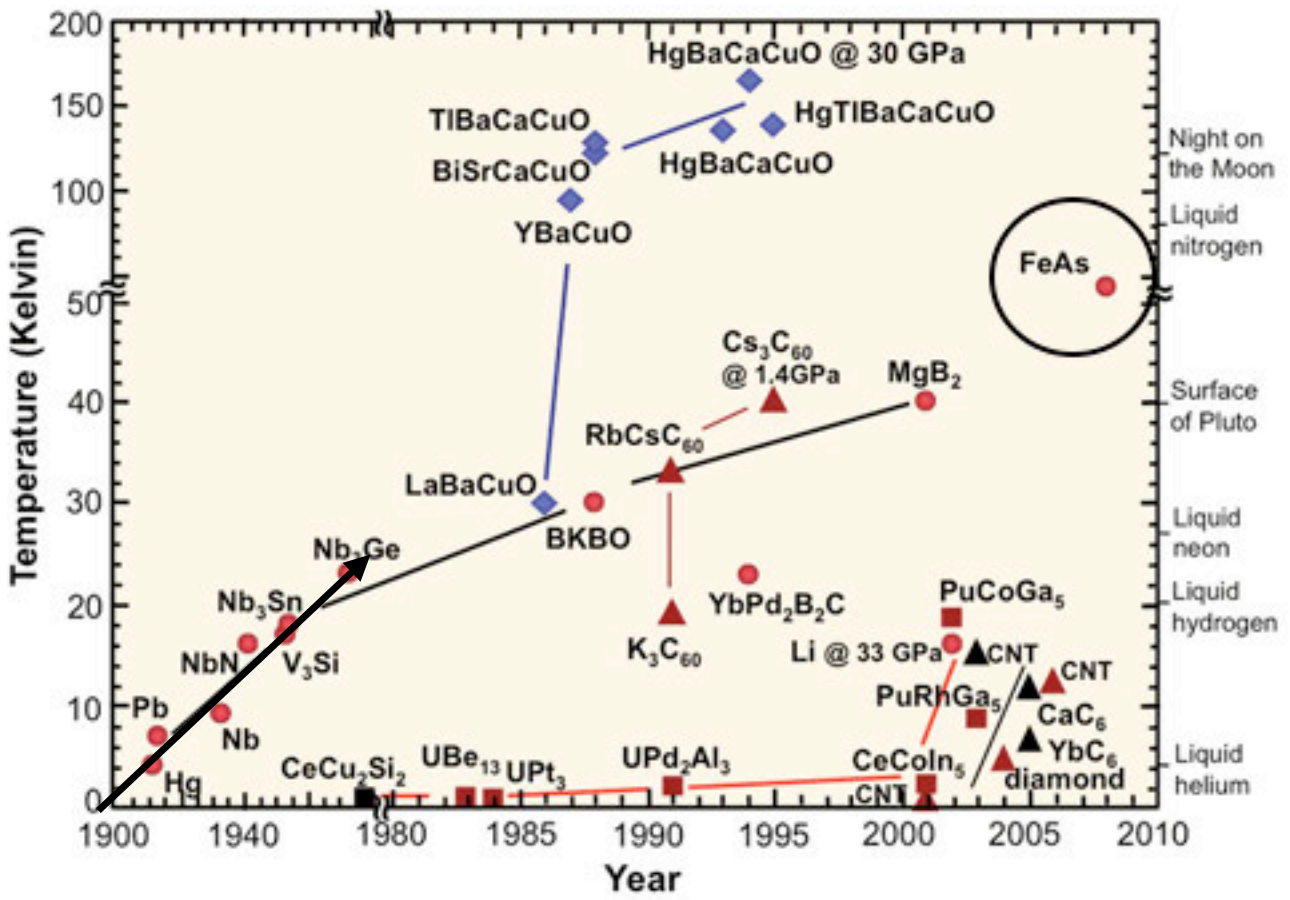
Predicted / explained observations

- Phonon spectra , f occupations
- Quasiparticle Multiplets
- Valence Histograms
- Mixed valent metal
- Continuous increase in our capability of describing a very challenging system.

Against the backdrop of many other competing theories.

Dominance of 5f6 conf, quantum criticality, Kondo lattice, dominance of 5f4 conf (mixed level model), ……

Superconducting Tc as a function of time



H. Hosono

DOE map of Superconductors

Real time test of electronic structure methods and their implementation

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

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

$(FeAs)^-$ layers active block

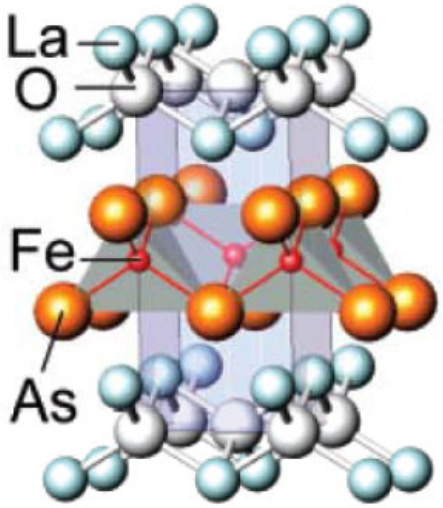
Atomic iron , **[Fe] 3d6 4s2. [As]**

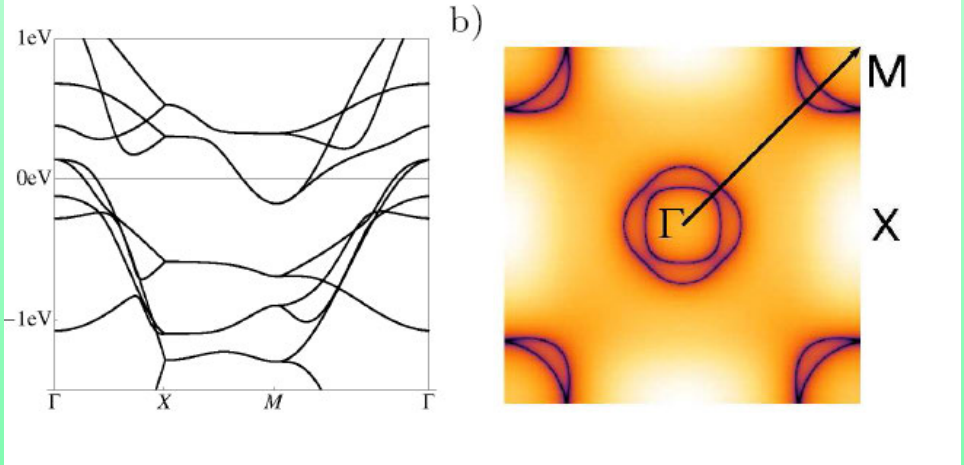
Atomic arsenic [Ar] 3d10 4s2 4p3

Fe++ d6 As--- p6

Doping with fluorine (electrons) F, d7

Real Space Picture





Momentum Space Picture

Address Predictive power of state of the art methods

Basic Questions/Normal State

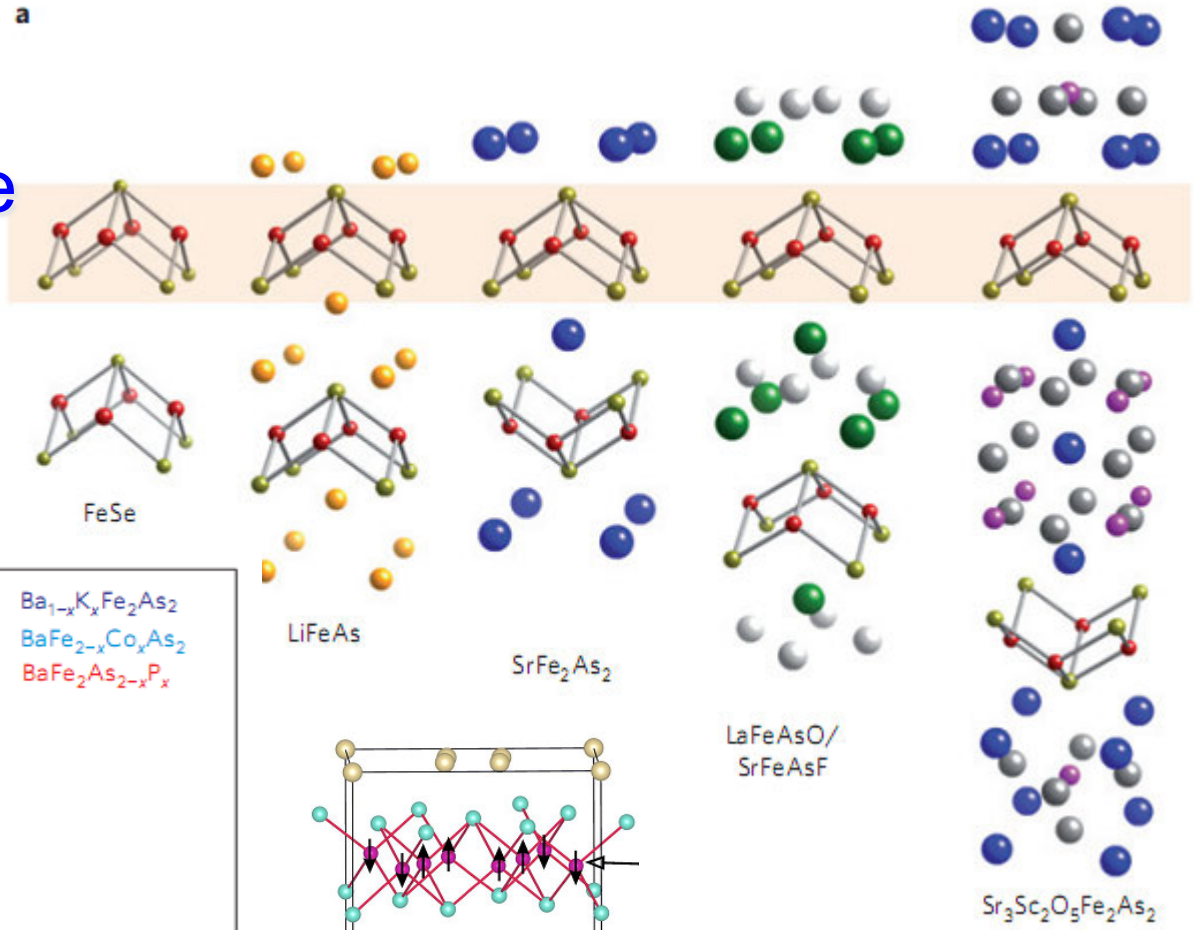
- Strength and origin of the electronic correlations.
- "What are the parameters, or "chemical handles" that control the low energy physics.
- Pairing Mechanism and Role of Spins and their Fluctuations: Glue or Fabric ?
- Playground for testing electronic structure methods

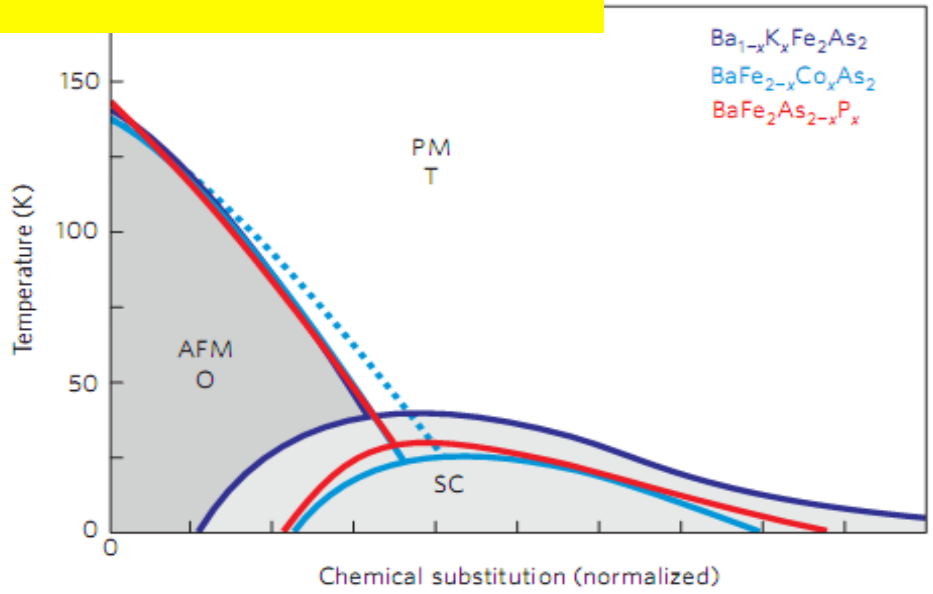
VIEWPOINTS:

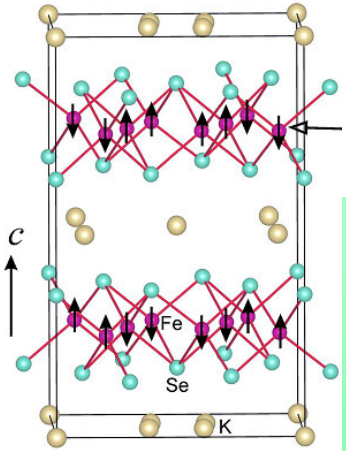
- Itinerant Magnets (LDA + RPA corrections)
- Doped Mott Insulators (t-J models)
- Hunds Metals
- Quantum Criticality

The "space of Fe pnictide/chalcogenide materials"

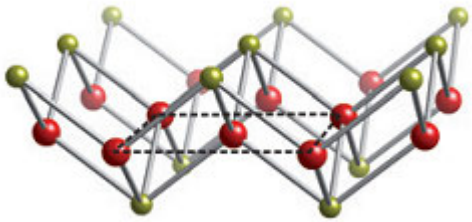
Is there physics common ot the tetrahedrally coordinated Fe d6 layers ?

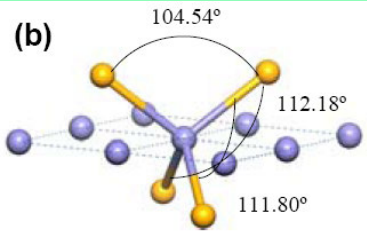


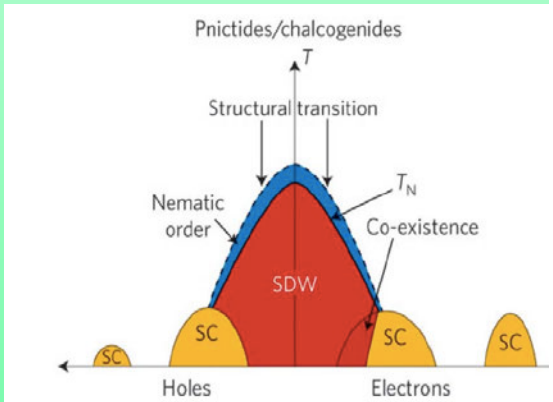




$K_{1-x}Fe_{2-2x}Se_2$







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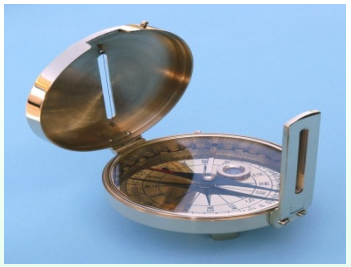
Paglione and Greene Nature Physics 6, 645(2010)

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).

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.

Unconventional SC

Phonon Tc<1K

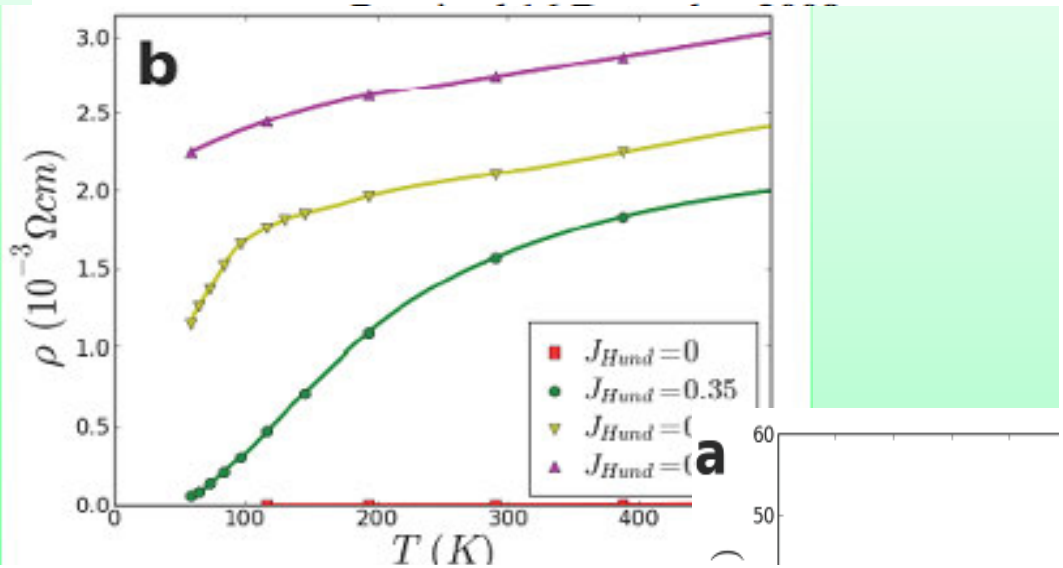
Importance of correlations

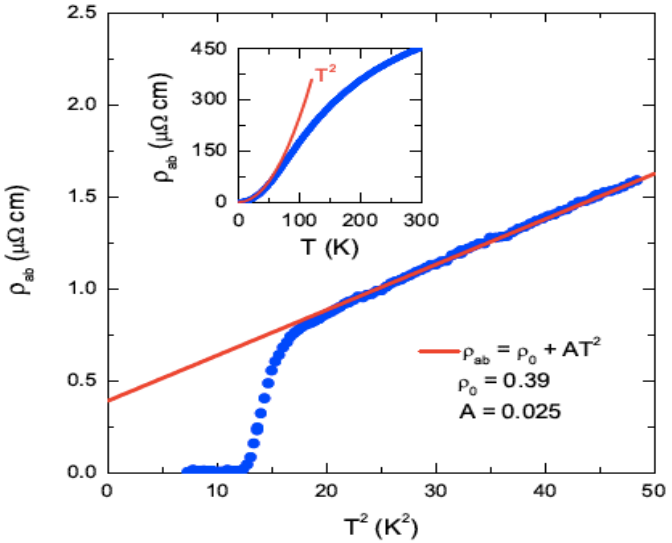
Mass enhancement 3-5

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

K 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





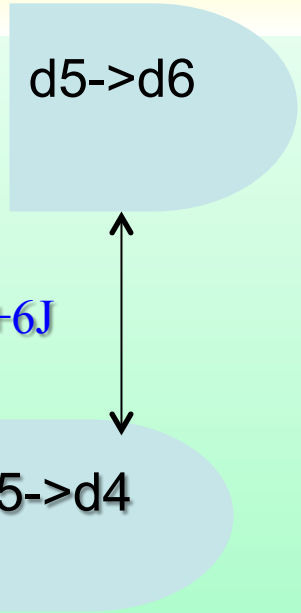
PRL 111, 027002 (2013) PHYSICAL REVIEW LETTERS week ending 12 JULY 2013

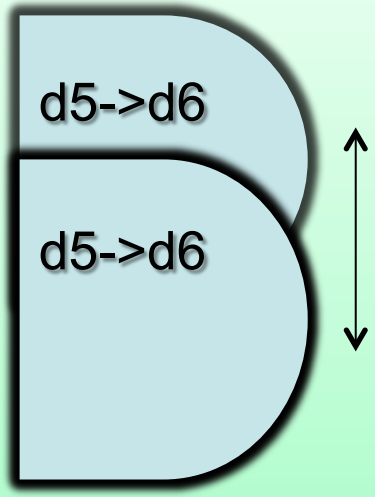
Evidence of Strong Correlations and Coherence-Incoherence Crossover in the Iron Pnictide Superconductor KFe_2As_2

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]

Hundness 101 . Uc2 ~ N² W. Orbitally

degenerate systems tend to be metallic unless degeneracy is lifted





U-J-3C

Fe d6 confguration is much more metallic

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

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

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

I. Okada, *Localized in Metals*, (1973).

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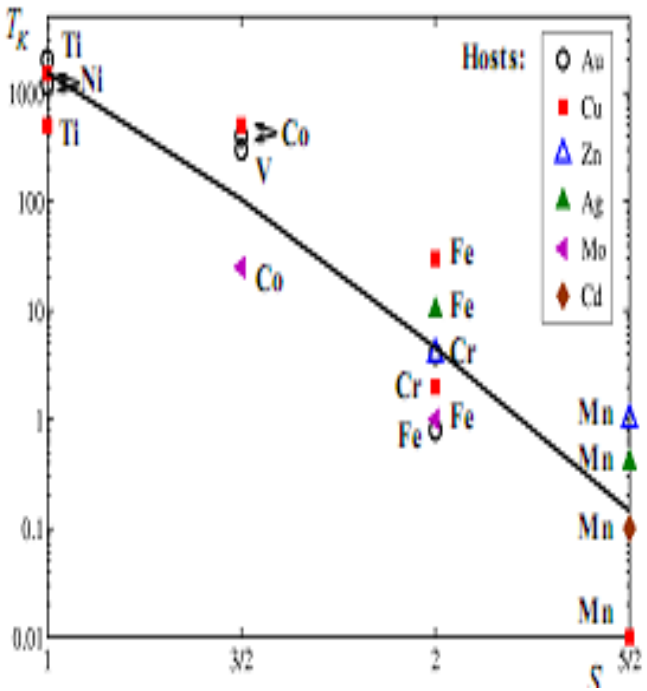
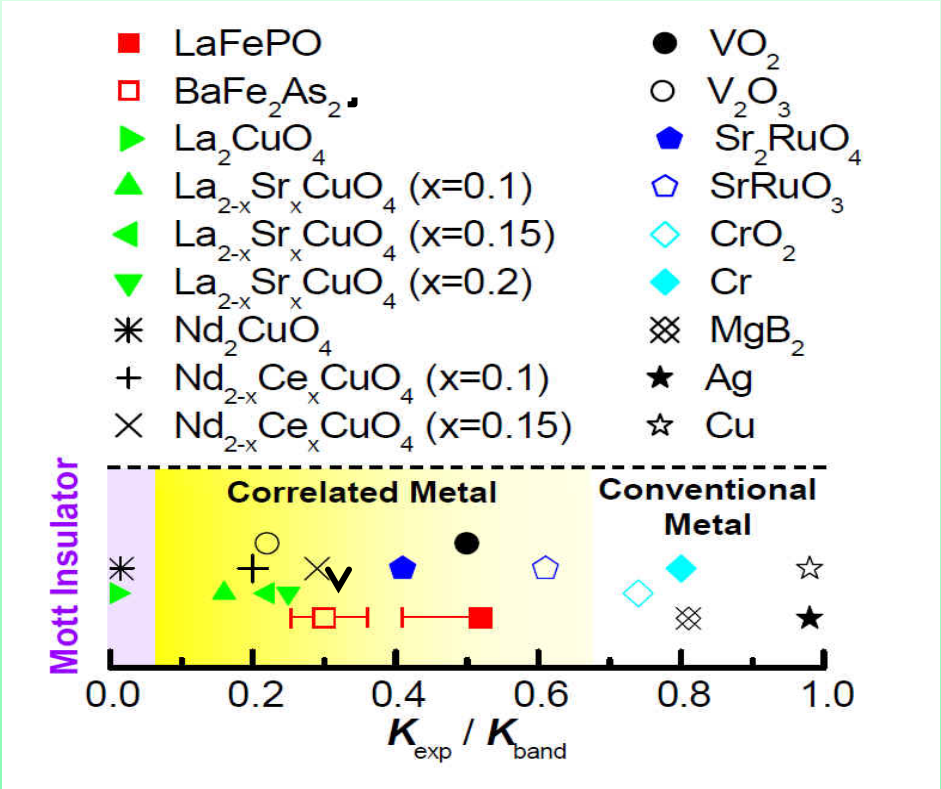


Extreme low energy scale Hundness reduce the coherence sc resonance by N2

. J. R. Schrieffer J. Applied Physics 32 , 1143 (19

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)

Evidence for weak correlations in experiments

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*

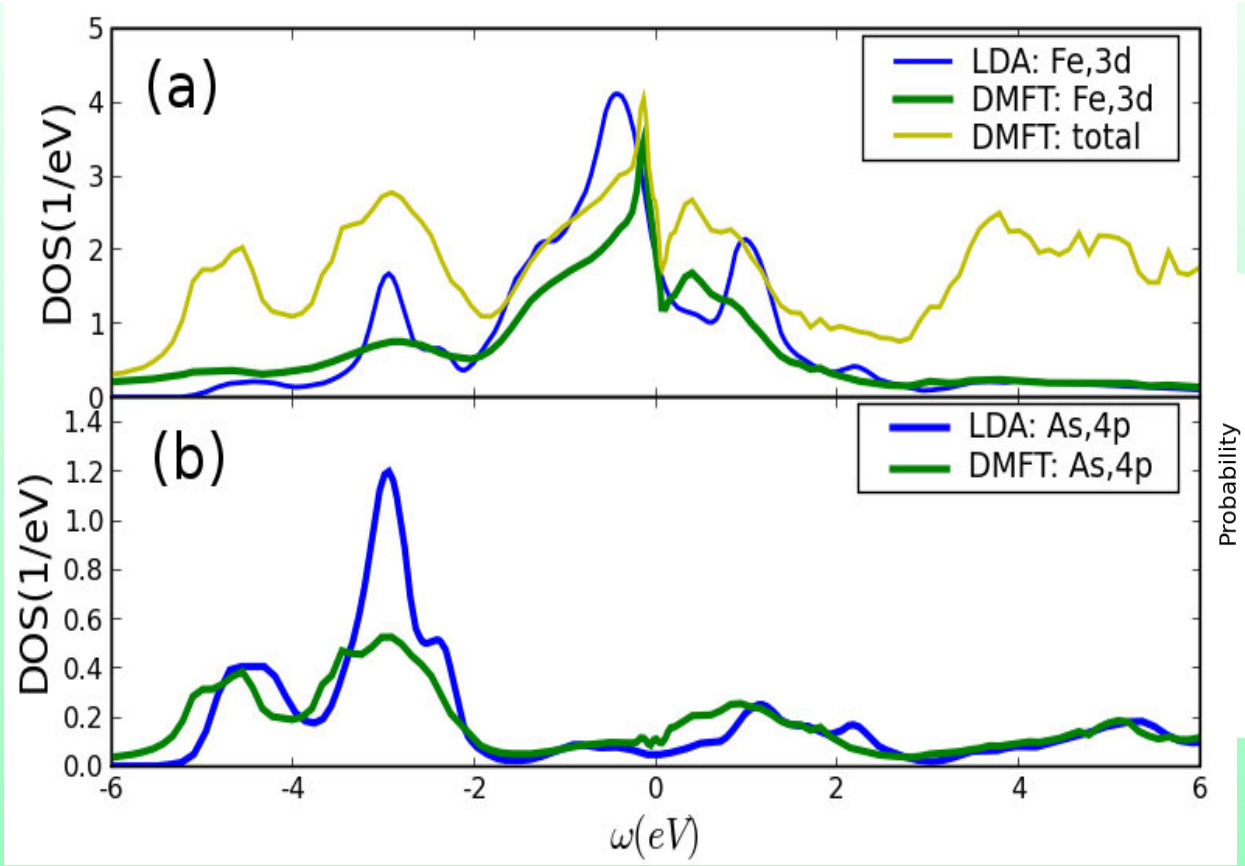
PHYSICAL REVIEW B **80**, 014508 (2009)

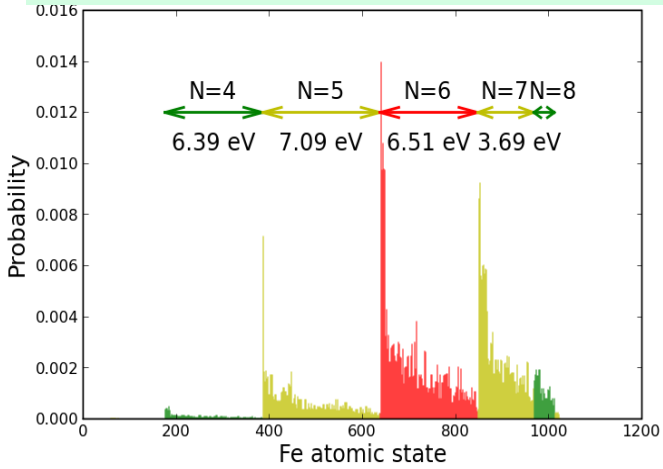
PHYSICAL REVIEW B **81**, 104518 (2010)

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.

DOS and valence histogram





There is transfer of spectral weight to high energies, spectral weight is conserved. But the DOS is featuresless no satellites, and resembles the LDA! Strong Correlations without Hubbard bands. Kutepov Haule and GK PRB (2011)Big difference between oxides and pnictides important role of As

PHYSICAL REVIEW B **84**, 054544 (2011)

Nematic spin fluid in the tetragonal phase of $BaFe_2As_2$

L. W. Harriger,[1] H. Q. Luo,[2] M. S. Liu,[1] C. Frost,[3] J. P. Hu,[4,2] M. R. Norman,[5] and Pengcheng Dai[1,2,6,*]

[1]*Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996-1200, USA*

[2]*Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

[3]*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire OX11 0QX, United Kingdom*

[4]*Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA*

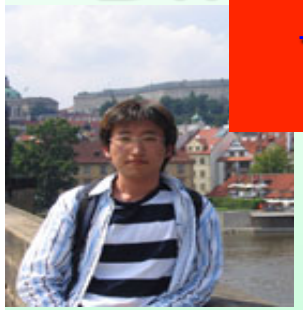
[5]*Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*

[6]*Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

(Received 26 November 2010; revised manuscript received 29 June 2011; published 24 August 2011)

We use inelastic neutron scattering to study spin waves below and above T_N in iron-arsenide $BaFe_2As_2$. In the low-temperature orthorhombic phase, we find highly anisotropic spin waves with a large damping along the antiferromagnetic *a*-axis direction. On warming the system to the paramagnetic tetragonal phase, the low-energy spin waves evolve into quasi-elastic excitations, while the anisotropic spin excitations near the zone boundary persist. These results strongly suggest the presence of a spin nematic fluid in the tetragonal phase of $BaFe_2As_2$, which may cause the electronic and orbital anisotropy observed in these materials.

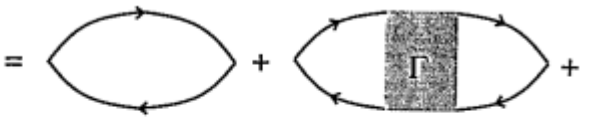
Neutron spectroscopy with LDA +DMFT

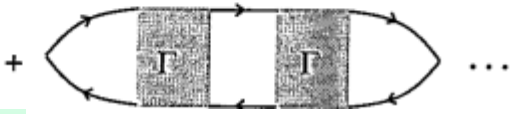


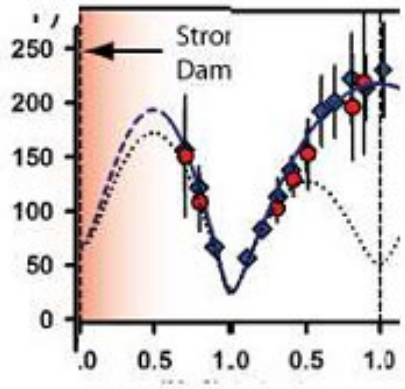
Theory: H. Park , K. Haule and GK PRL in press

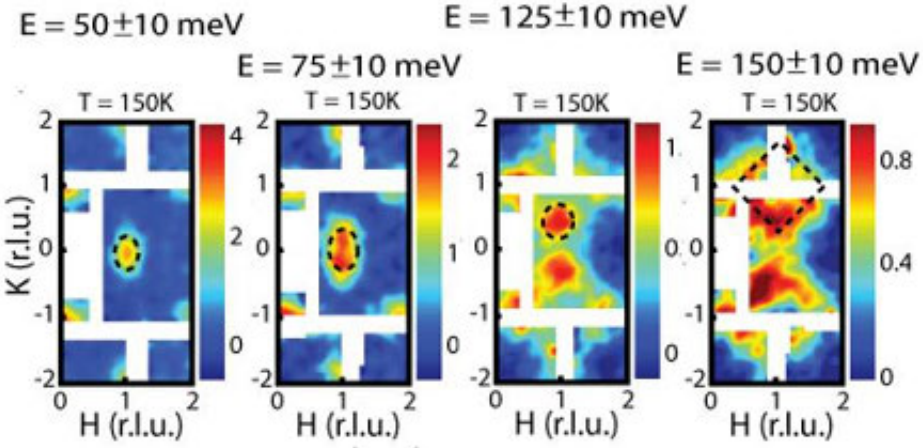
Experiments: L Harriger H. Luo M. Liu T. Perring C Frost H. Ju M. Norman and Pengcheng Dai : arXiv:1011.3771

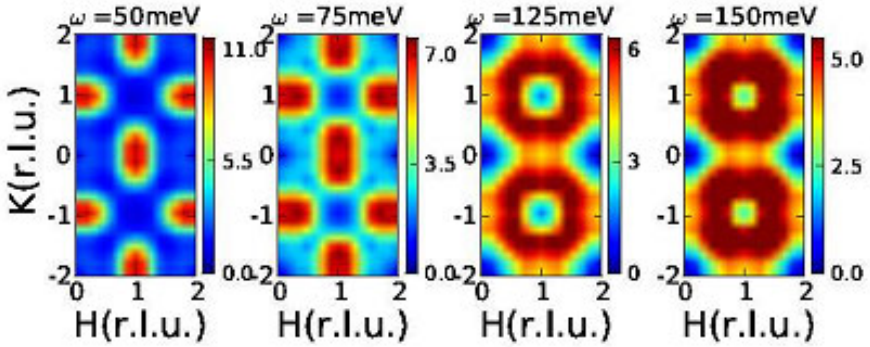
$$S(\mathbf{Q},\hbar\omega) = |F(Q)|^2 \frac{\chi''(\mathbf{Q},\hbar\omega)}{1-\exp(-\hbar\omega/k_B T)}.$$

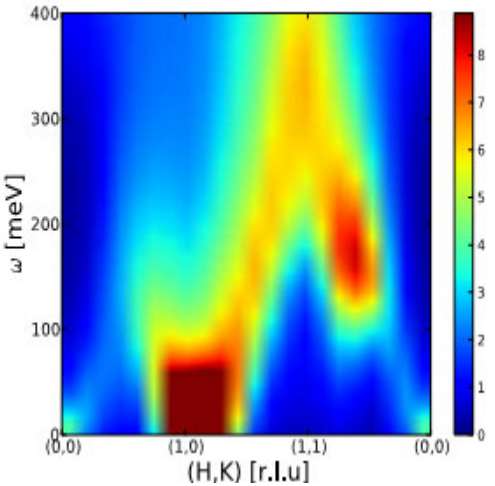






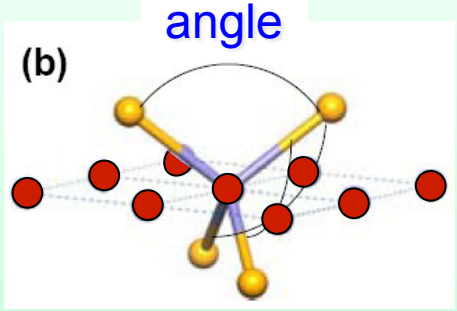




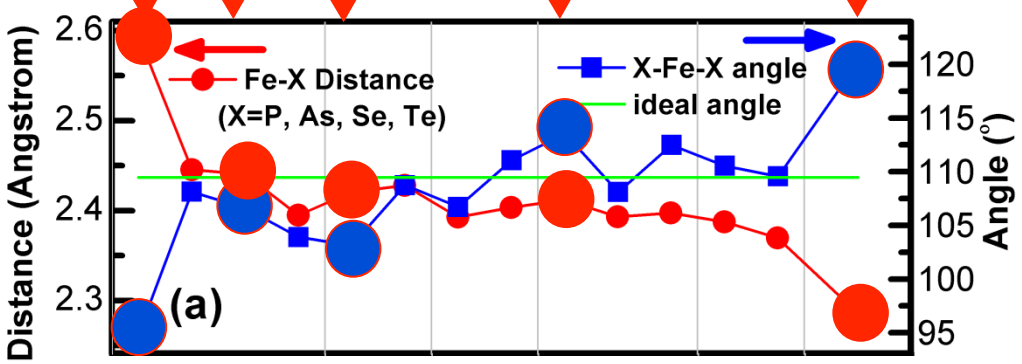


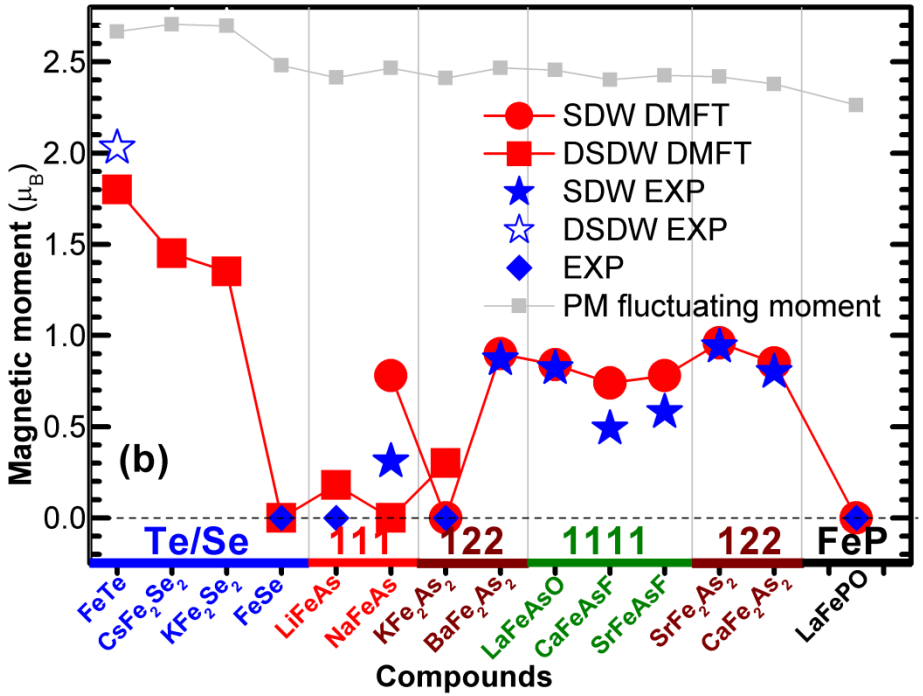
Landscape of Materials: Yin Haule GK Nature Materials (2011)

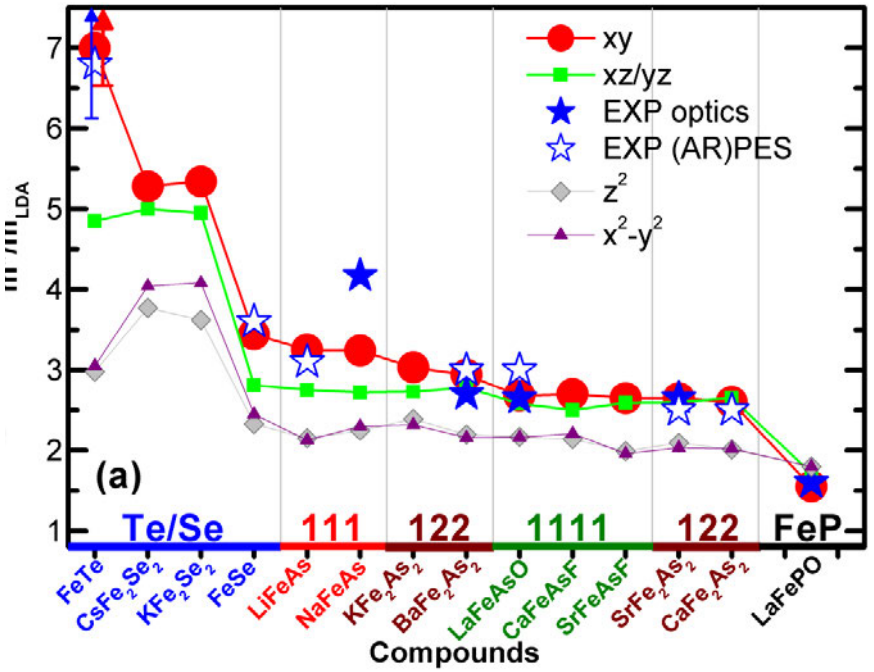
angle



Tendency to orbital differentiation as correlations increase.

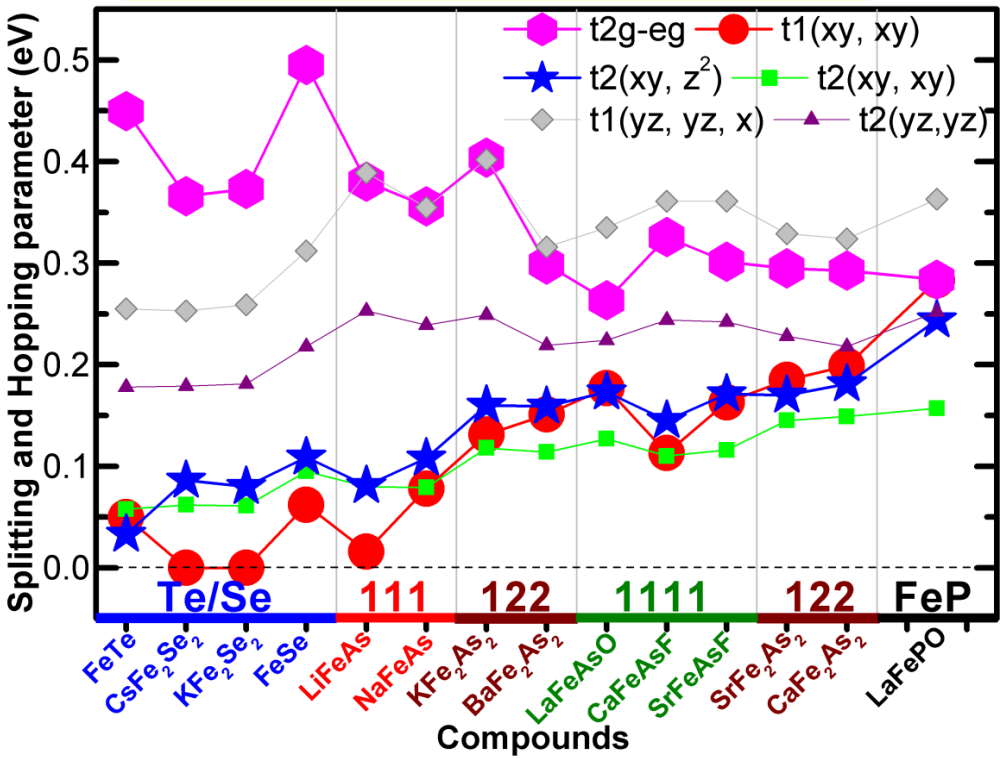


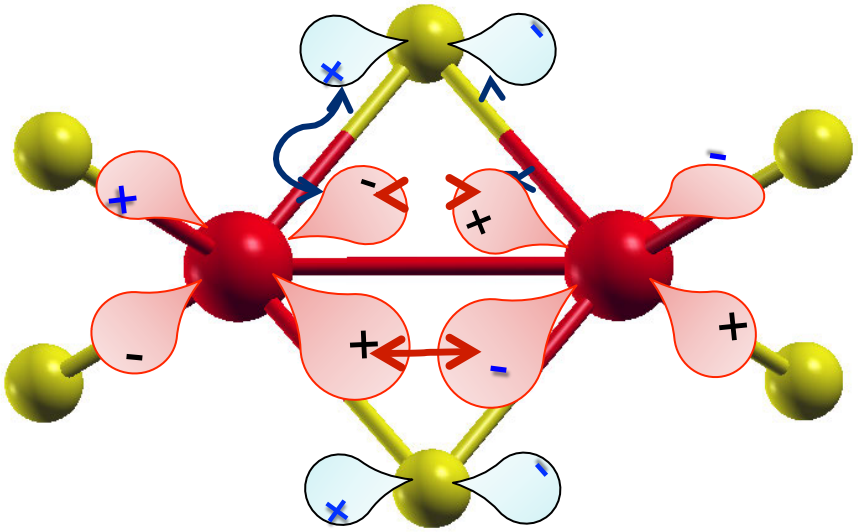




xy orbital, kinetic frustration and FeTe

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

Main Points

- Iron pnictides and chalcogenides are strongly correlated by virtue of the Hunds rule coupling J rather than the Hubbard U. Hunds metals not (doped) Mott insulators

•Subtle but (for me clear) experimental signatures of Hundness in iron pnictides.Neither itinerant nor localized framework account for the data. Interplay of spin and orbit is different than in oxides and itinerant magnets.

DMFT based methods can now study physical changes within a FAMILY of materials

- Implications for superconductivity.

Conclusions

- Materials, Theory, Concepts, Techniques
- Example: V2O3 three peak structure of DOS, transfer of spectral weight, resilient quasiparticles, hidden fermi liquid.
- Example: Plutonium, energy scale compression giving rise to multiple phases, quasiparticle multiplets and mixed valence, phonon spectra, f occupancy, S(q, omega)
- Example: Hunds metals, iron pnictides, new class of correlated materials

Looking Ahead

- Conceptual and technical developments enabled the community to catch up with a trove of deep puzzles in the field of strongly correlated electron materials
- Many of them have been solved, including the anomalous properties of the copper oxide and iron pnictide layers, except for the quantitative elucidation of their high Tc.
- The next challenge will be to speed up the discovery of new remarkable phenomena.

- ‘It (society) always sets itself only such problems as it can solve; since, looking at the matter more closely it will always be found that the problem itself arises only when the material conditions for its solution are already present or are at least understood to be in the process of emergence.

But there is another level of urgency and complexity for the problems society will need to address in the 21st century.

Schools, international colaborations, organization of science from the bottom up, will be essential.

I hope you all will contribute to this challenge!

Thank you for your attention !!