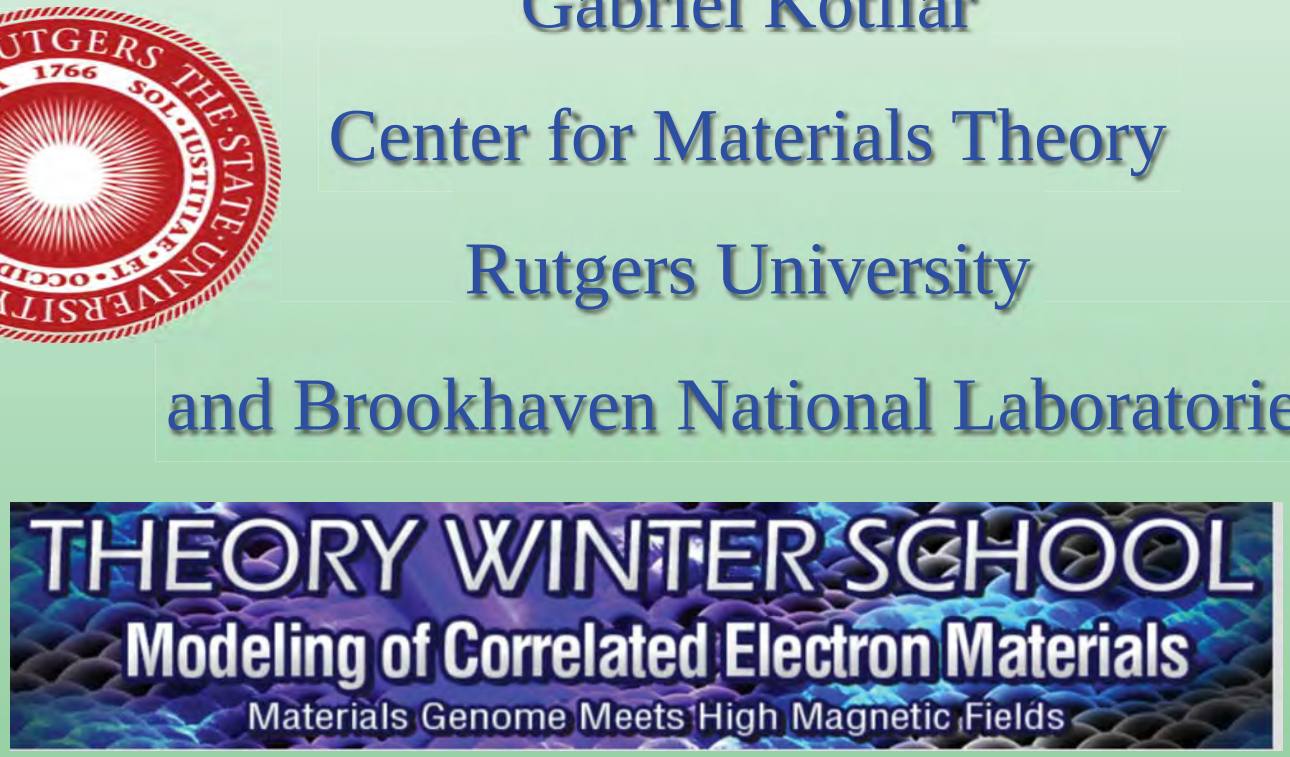
Electronic Structure and Correlated Electron Materials

Gabriel Kotliar

Center for Materials Theory

Rutgers University

and Brookhaven National Laboratories



January 9th-13th 2017

Outline

- Introduction to correlations in solids. Static and Dynamic Correlations.
- Brief introduction to DMFT + electronic structure.
- Roads to correlations, Mott vs Hund. Vanadium Oxides vs Iron pnictides and chalcogenides.
- Actinides.
- Static correlations, $BaBiO_3$ and their analogs.
- Conclusions.

Quantum Materials: Experiments and Theory

Eva Pavarini, Erik Koch, Jeroen van den Brink, and George Sawatzky (Eds.)

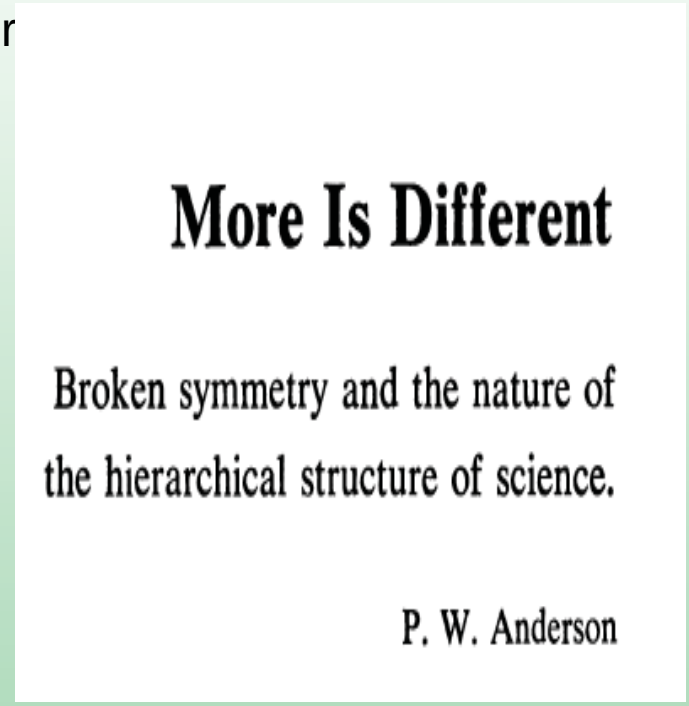
Preface

Quantum materials exhibit a spectacular variety of unusual emergent behavior that is practically impossible to predict from first-principles. Experiment is crucial for discovering phenomena such as the metal-insulator-transition, the Kondo effect, or superconductivity. Theory provides the paradigm for understanding these states of matter. Developing such understanding relies on the close interplay between theory and experiment, with experiments constantly putting theoretical ideas to a test. This year's school covers experimental techniques such as optics, photoemission, NMR, and tunneling spectroscopy. Understanding these experiments requires the realistic modeling of materials as well as approaches to solving them. Lectures ranging from the model building schemes to advanced many-body techniques provide the foundation to unraveling the mystery of these materials. Introductions to theoretical approaches for calculating spin, charge, and orbital structure as well as response functions provide direct contact to the experimental probes. The aim of the school is to introduce advanced graduate students and up to the essence of emergence and modern approaches for modeling strongly correlated matter.

Role of theory

SCIENCE :4 August 1972, Volume 177, Number

"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

Chemistry on the computer

Martin Head-Gordon and Emilio Artacho

Although exact descriptions of the quantum mechanics of molecules are computationally intractable, chemists and physicists have devised approximations that are efficient enough to be practical and accurate enough to be useful.

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"

58 April 2008 Physics Today

Role of theory, accelerate the pace of discovery

Materials Genome Initiative
for Global Competitiveness

June 2011

EXECUTIVE OFFICE OF THE PRESIDENT
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL
WASHINGTON, D.C. 20502

June 24, 2011

Dear Colleague:

In much the same way that silicon in the 1970s led to the modern information technology industry, the development of advanced materials will fuel many of the emerging industries that will address challenges in energy, national security, healthcare, and other areas. Yet the time it takes to move a newly discovered advanced material from the laboratory to the commercial market place remains far too long. Accelerating this process could significantly improve U.S. global competitiveness and ensure that the Nation remains at the forefront of the advanced materials marketplace. This *Materials Genome Initiative for Global Competitiveness* aims to reduce development time by providing the infrastructure and training that American innovators need to discover, develop, manufacture, and deploy advanced materials in a more expeditious and economical way.

The success of this initiative will require a sustained effort from the private sector, universities, and the Federal Government. I look forward to working with you to make this vision a reality.

Sincerely,

John P. Holdren

John P. Holdren
Assistant to the President for Science and Technology
Director, Office of Science and Technology Policy

Why can we even contemplate now the possibility of material design (in weakly correlated electron systems)?

Success based on having a good reference system

"Standard Model" of solids developed in the twentieth century. Reference System:Free electron waves in a periodic potential (Sommerfeld and Bloch) .

Works well for very weakly correlated materials, e.g. simple metals and insulators

Band Theory. Fermi Liquid Theory (Landau 1957).

Density Functional Theory (Kohn Sham 1964)

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

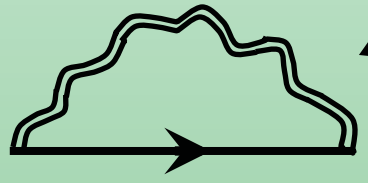
Reference Frame for Weakly Correlated Systems.

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

Starting point for perturbation theory in the screened Coulomb interactions

(Lars Hedin 1965)

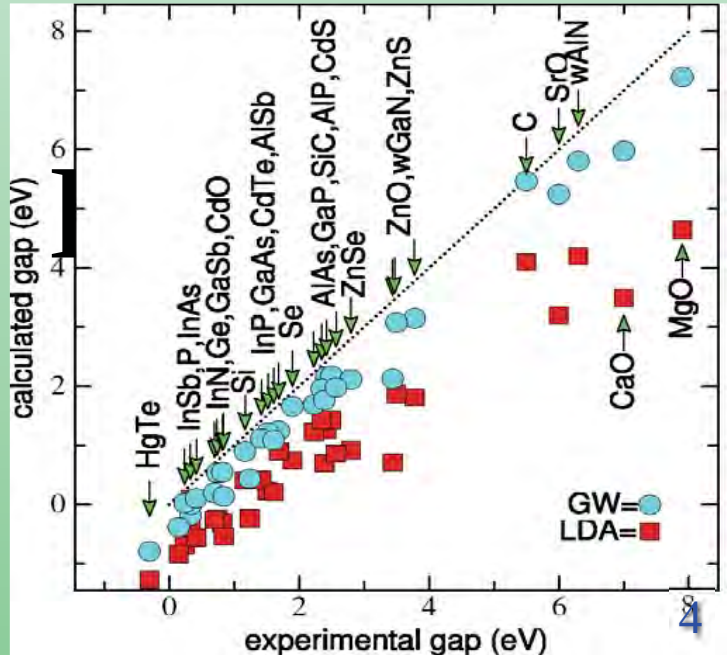
$$G^{-1} = G_{0KS}^{-1} + [\quad\quad - V_{KS}]$$



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

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

…..



Strongly correlated electron systems.[working definition]. Materials where the previous paradigm fails .

Results in “big things”. Metal to insulator transitions, heavy fermion behavior, high temperature superconductivity, colossal magnetoresistance, giant thermolectricity. Abnormal “ normal” state. Large resisitvities.

The Kohn Sham system cannot describe spectroscopic properties of correlated materials, because these retain atomic physics aspects. Mottness, Hundness. e.g. multiplets, transfer or spectral weight, high Tc’s) which are not perturbative

NEEDED: a new reference system to describe correlated materials and compute their properties.

Quantitfy correlations and locality

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

- Chemist

$$\Sigma(\omega) - \Sigma_{Hartree-Fock}$$ large

- Physicist

$$\Sigma(\omega) - Vxc_{LDA}$$ large

"Locality" is defined with respect to a basis

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

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

Vxc - Edc

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

- My definition of correlation is energy scale dependent, this is OK,, we are always interested in some limited energy range.
- Large, or small, maybe property dependent.
- Large or small depends on the reference system. The chemist use Hartree Fock not LDA as the reference.
- "Static" correlations Large k dependence of

$$\Sigma - Vxc_{LDA}$$

- "Dynamic" correlations, large frequency dependence on Σ

- The chemists exchanged terminology for “static” vs “dynamic’ correlation.
- In chemistry “static “ correlations, means that many slater determinants are needed to describe a state. In chemistry “ dynamical “ correlations, mean that a slater determinant is OK, but the DFT orbitals need improvement.

Cohen AJ, Mori-Sanchez P, Yang W (2008) Science 321:792–794 (2008) .

REFERENCE: G. Kotliar Chapter 2, of the proceedings of DMFT at 25. Pavarini et. al. editors. Springer Verlag.

http://www.cond-mat.de/events/correl14/

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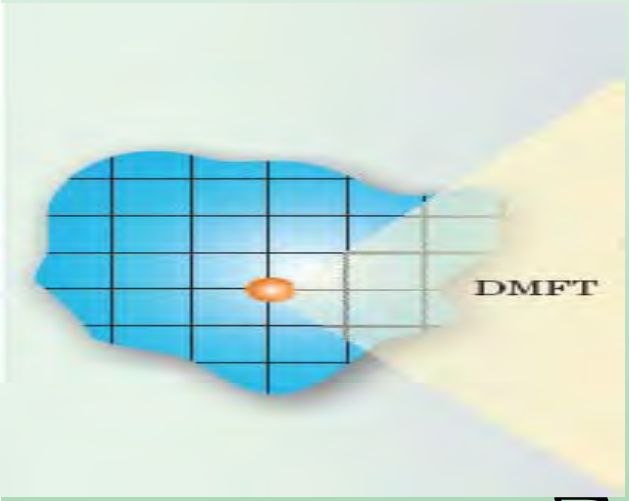
Mean Field Theories Replace a many body problem by a single site problem in an effective medium reference frame

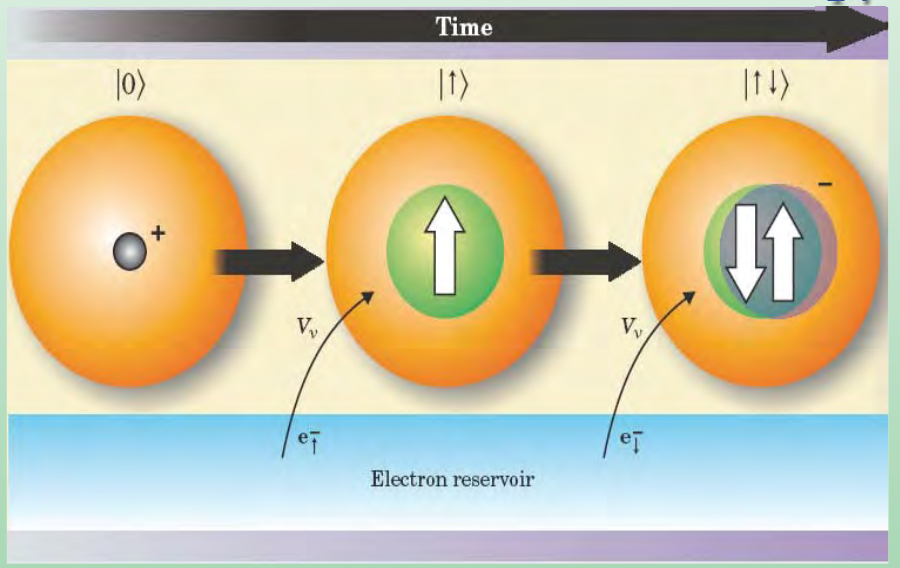
$$\sum_{<i,j>,q,j}(t_{ij}J_{ij}S_iS_j-\mu\delta_{ij})(c^{\dagger}_{i\sigma}c_{j\sigma}+c^{\dagger}_{j\sigma}c_{i\sigma})+U\sum_i n_{i\uparrow}n_{i\downarrow} \Rightarrow H_{MF}$$

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

$$H_{MF}=h_{eff}S_o$$



DMFT



$$\Delta(\omega)=\sum_\alpha \frac{V_\alpha^{*}V_\alpha}{\omega-\varepsilon_\alpha}$$

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

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

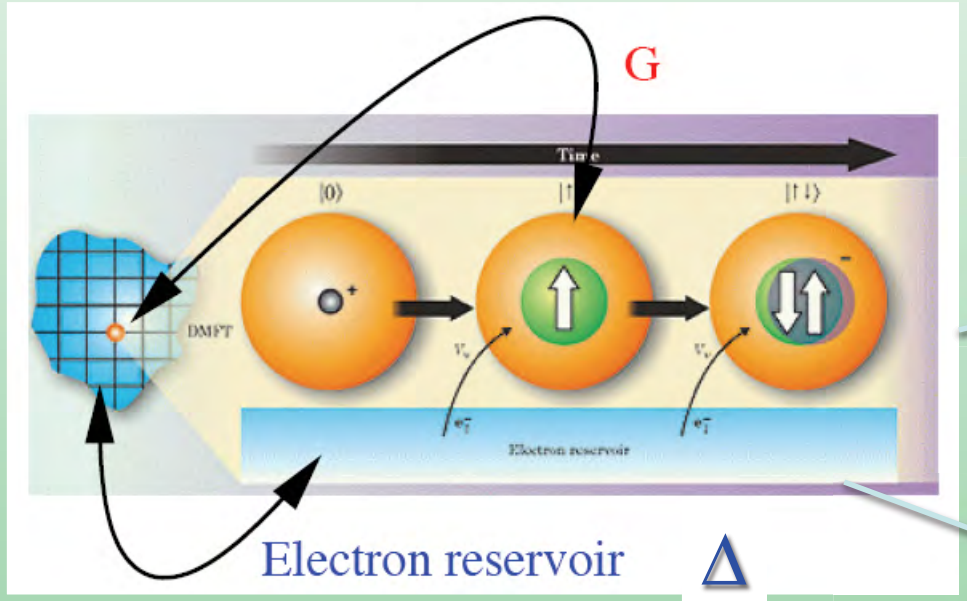
$$G_{imp}(i\omega_n)[\Delta]=\sum_k \frac{1}{[i\omega_n+\mu+t(k)-\Sigma_{imp}(i\omega_n)[\Delta]]}$$

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

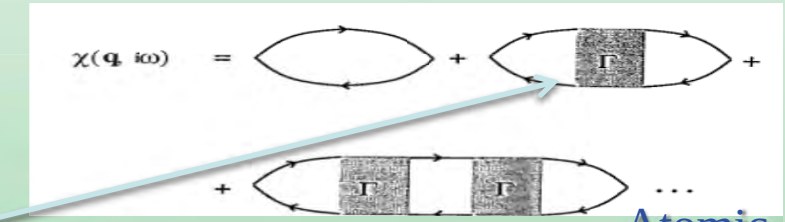
DMFT impurity model in self consistent medium. Embedding +Truncation

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

Formalism derived from functionals



LDA+DMFT. V. Anisimov, A. Poteryaev, M. Korotin, A. Anokhin and G. Kotliar, J. Phys. Cond. Mat. 35, 7359 (1997) 15



Two particle irreducible vertex function

Atomic parameters and dc determined from constrained RPA or GW

$$G(\omega) = \frac{1}{[\omega + \nabla^2 + \mu - V_{Hartree} - V_{cryst}] - V_{static} - \Sigma_{R\alpha\beta} |R\alpha\rangle \Sigma_{locRR}(\omega) \langle R\beta|}$$

LDA+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.

❑ See also Lichtenstein and Katsenelson Phys. Rev. B **57**, 6884 (1998)

LDA+DMFT functional

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

$$-Tr\log[i\omega_n + \nabla^2/2 - V_{KS} \quad] -$$

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

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

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

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

Notice Explicit Dependence on : U , DC, and Projectors

[Orbitals], and Independence of basis set.

R. Chitra and Gkotliar Phys.Rev.B62:12715 (2000).

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

For each choice of orbitals (projector) there is a choice of ineraction U. Localized orbitals, have proved to be transferable.

A great deal of progress has been made to develop methods to solve impurity models over the last two decades.
CTQMC Review : E. Gull A Millis A. Lichtenstein A. Rubtsov, M . Troyer, P. Werner Rev. Mod. Phys. 83, 349-404 (2011) . Talk by Andy Millis.

NRG Review Ralf Bulla, Theo Costi, Thomas Pruschke Rev. Mod. Phys. 80, 395 (2008). Talk by K. Ingersent

DMRG : Ulrich Schollwoeck Annals of Physics 326, 96 (2011) . Talks Friday .

Kohn Sham self energy is local in space and time. GW corrections brings spatial non locality from inscreened Coulomb interactions. Mott physics rquires non locality in time.

Model Hamiltonians. DMFT is exact in infinite dimensions Metzner and Vollhardt PRL 62, 324 (1989) Kinetic energy ~ onsite repulsion

How can we tell if and when a local approach is OK ?

Cluster DMFT Studies ***DCA*** M Hettler M. Jarrell H. Krishnamrthy et. al. Phys. Rev. B 58, 7475 (1998) CDMFT kotliar et. al. Phys. Rev. Lett. 87, 186401 (2001).

Compare experiments with multiple theoretical and experimental spectroscopies

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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

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

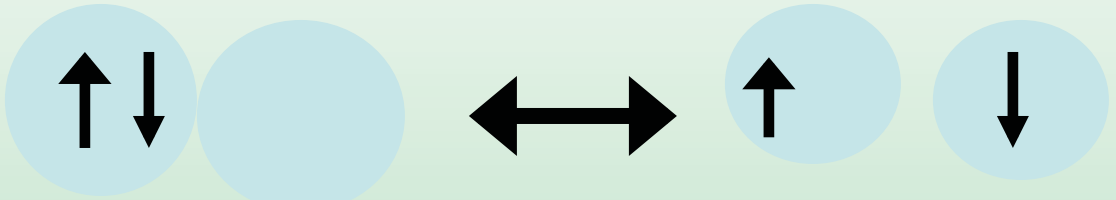
Questions to ask ?

Model Hamiltonians spirit qualitative issues common themes to many materials. TOE is needed to answer what material does what.

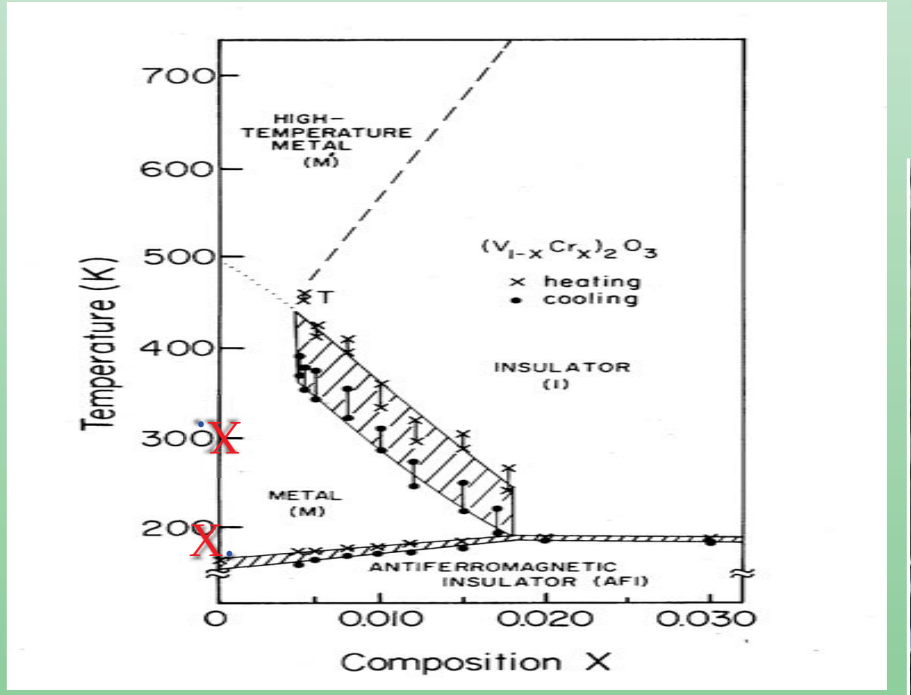
Mott Hubbard Mechanism and V2O3

Hubbard Model Kinetic Energy~t vs CoulombEnergy U

$$Hatom = \frac{1}{2}U(N-1)^2$$



$$(E(N+1)-E(N))\text{-}(E(N)-E(N-1))=U$$



Mott Insulator U >> t

Charge Blocking

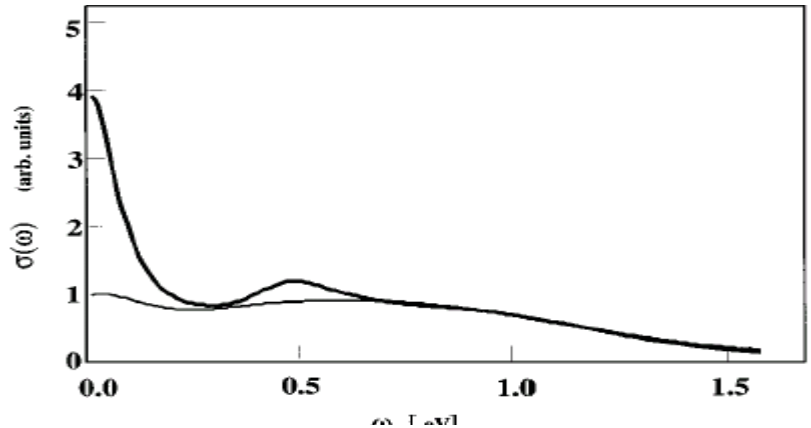
Optical Conductivity in Mott-Hubbard Systems

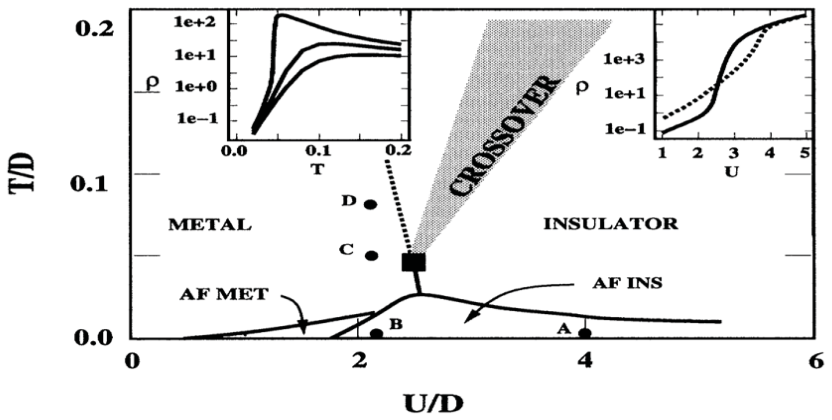
M. J. Rozenberg,* G. Kotliar, and H. Kajueter
Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08855-0849

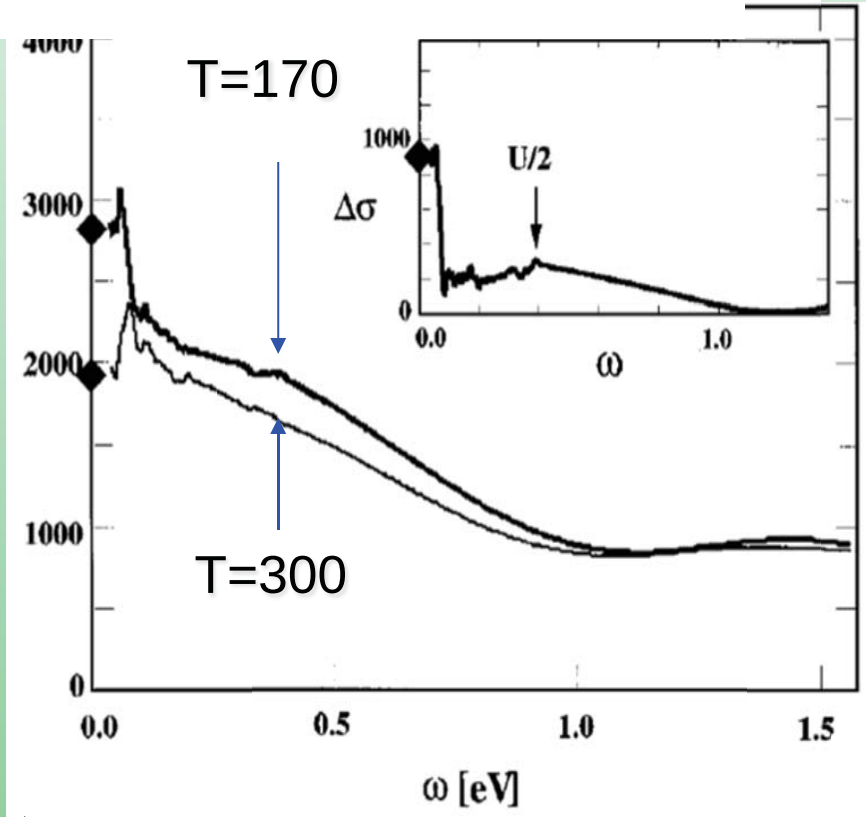
G. A. Thomas and D. H. Rapkine
AT&T Bell Laboratories, Murray Hill, New Jersey 07974-0636

J. M. Honig and P. Metcalf
Department of Chemistry, Purdue University, West Lafayette, Indiana 47907
(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.

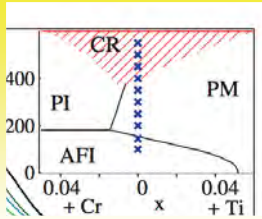


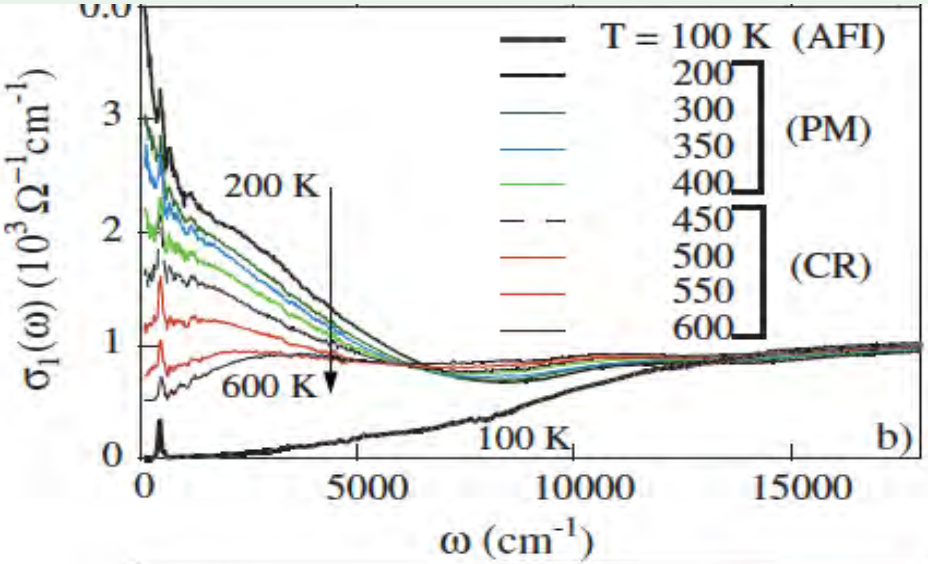


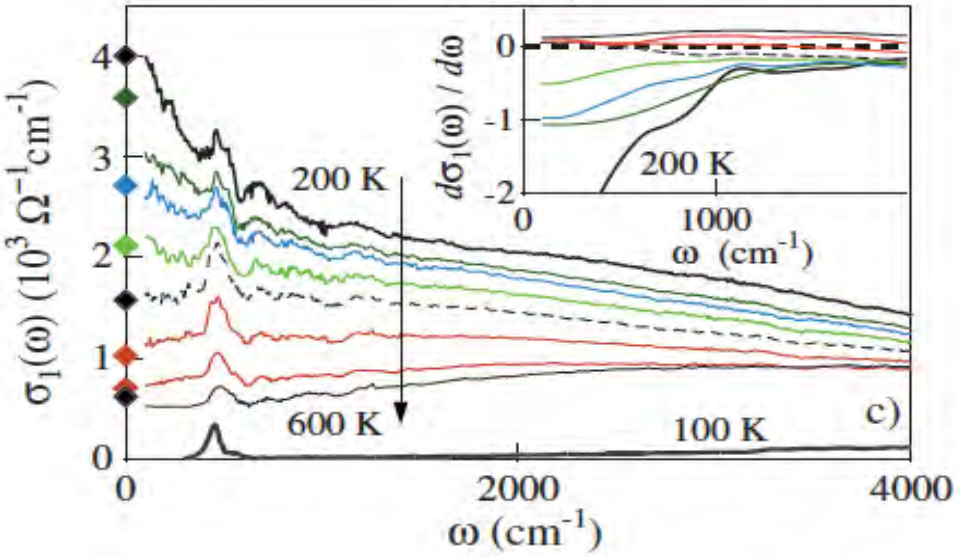


$$\int_0^{\Lambda} \sigma(\omega)\, d\omega = Neff\ (T, \Lambda)$$

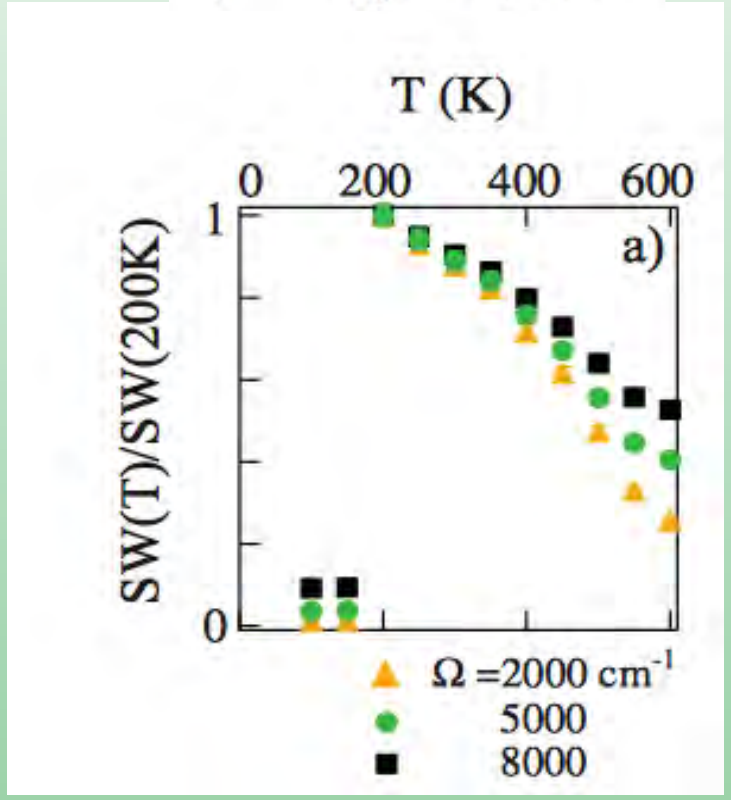
Signatures of correlations: Optical conductivity. Plasma frequency increases with decreasing T.







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



Baldassarre et.al

PRB **77, 113107 (2008)**

More realistic studies of vanadium oxides within LDA+DMFT followed over the last decade, very incomplete list

. 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)

- Lo Veccchio et. al. Phys. Rev. Lett. 117, 166401 (2016)

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PRL 113, 246404 (2014) PHYSICAL REVIEW LETTERS week ending 12 DECEMBER 2014

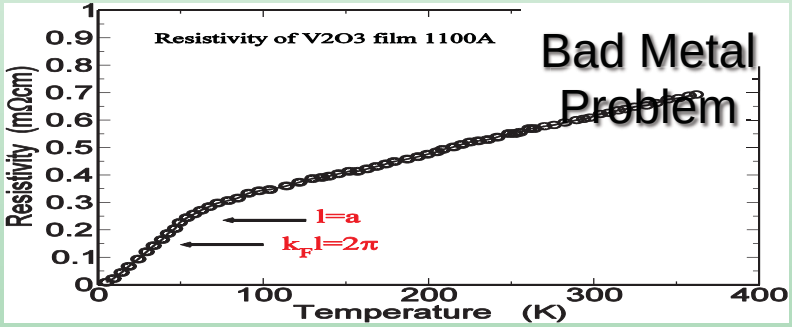
Shining Light on Transition-Metal Oxides: Unveiling the Hidden Fermi Liquid

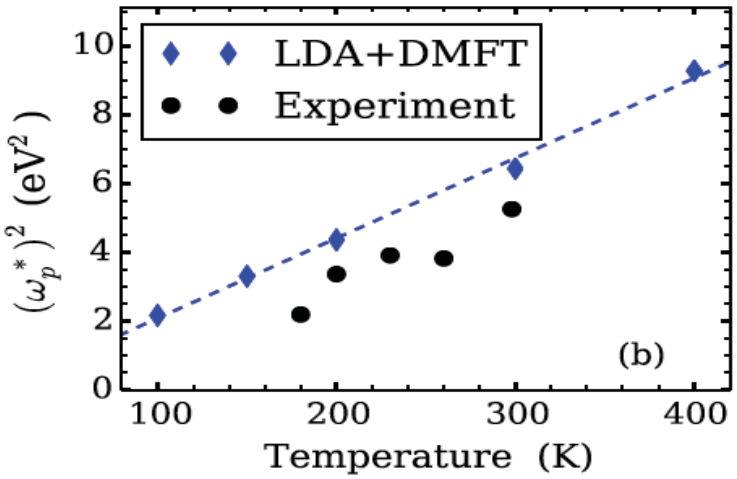
Xiaoyu Deng,[1] Aaron Sternbach,[2] Kristjan Haule,[1] D. N. Basov,[2] and Gabriel Kotliar[1]
[1]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*
[2]*Department of Physics, University of California San Diego, La Jolla, California 92093, USA*
(Received 25 April 2014; published 8 December 2014)

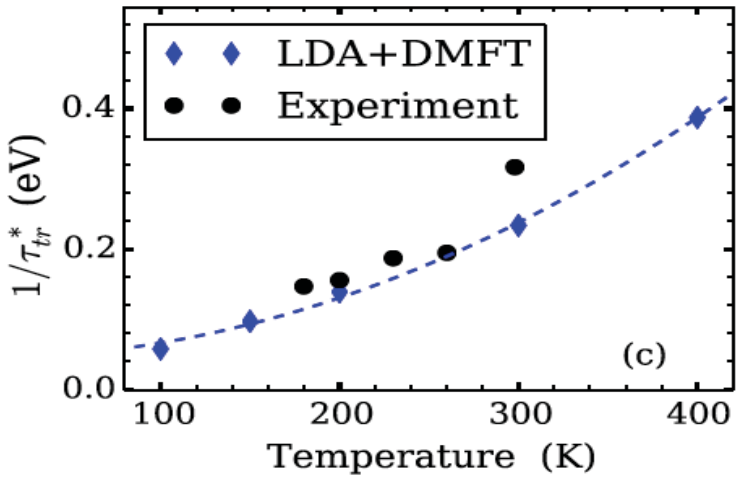
We use low energy optical spectroscopy and first principles local density approximation plus dynamical mean field theory calculations to test the hypothesis that the anomalous transport properties of strongly correlated metals originate in the strong temperature dependence of their underlying resilient quasiparticles. We express the resistivity in terms of an effective plasma frequency ω_p^* and an effective scattering rate $1/\tau_{tr}^*$. We show that in the archetypal correlated material V_2O_3, ω_p^* increases with increasing temperature, while the plasma frequency from the partial sum rule exhibits the opposite trend. $1/\tau_{tr}^*$ has a more pronounced temperature dependence than the scattering rate obtained from the extended Drude analysis. The theoretical calculations of these quantities are in quantitative agreement with experiment. We conjecture that these are robust properties of all strongly correlated metals, and test the conjecture by carrying out a similar analysis on thin film $NdNiO_3$ on a $LaAlO_3$ substrate.

$$\rho = \frac{h}{e^2}\, a\, \frac{1}{l k_F} \qquad \rho_{3d\,\min} << 125 \mu Ohm\ cm$$

$$\sigma(\omega) = \frac{(\omega_p^*)^2}{4\pi}\,\frac{1}{-i\omega + 1/\tau^*}$$







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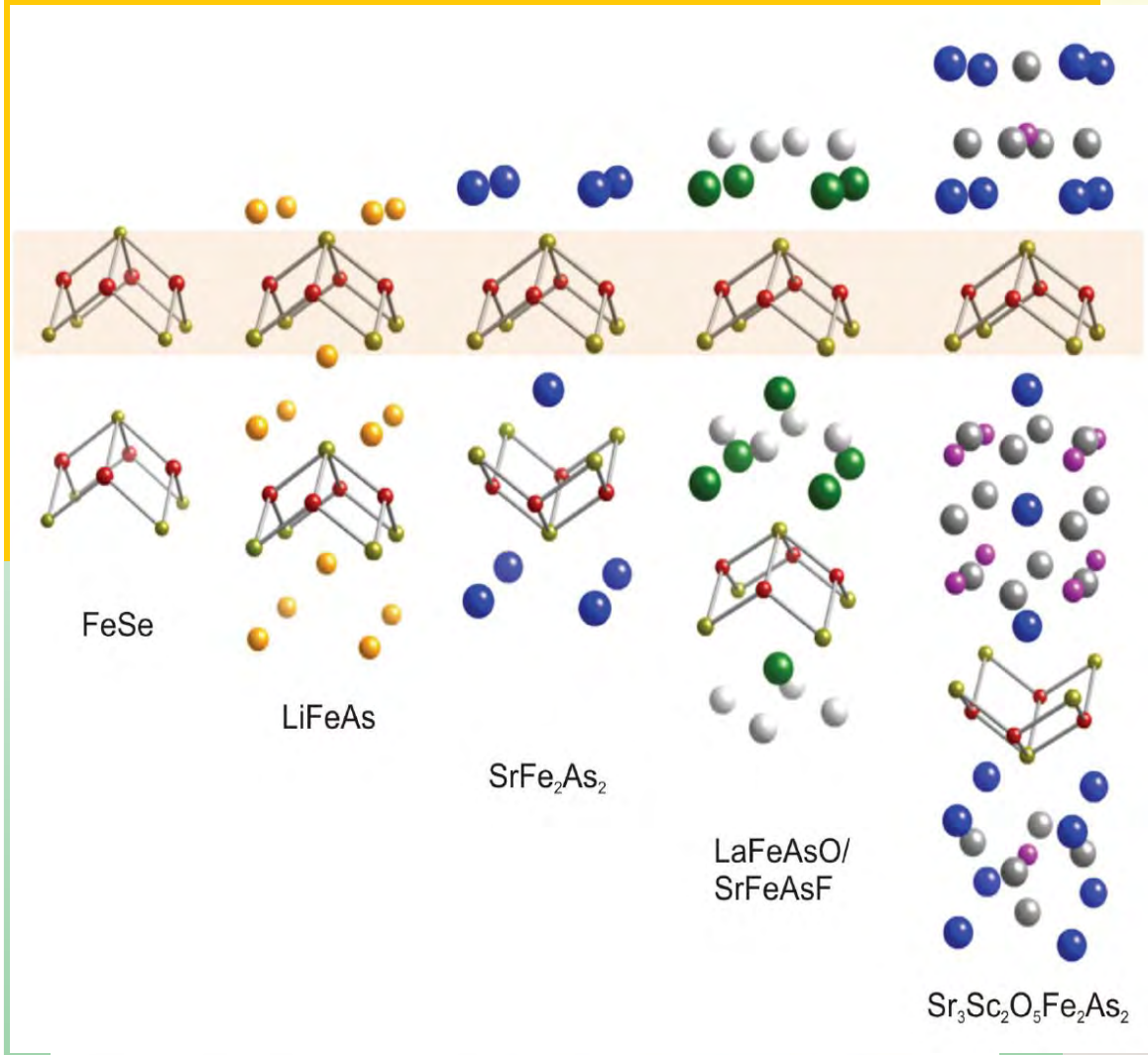
2008 Superconductivity in $LaFeAsO_{1-x}F_x$



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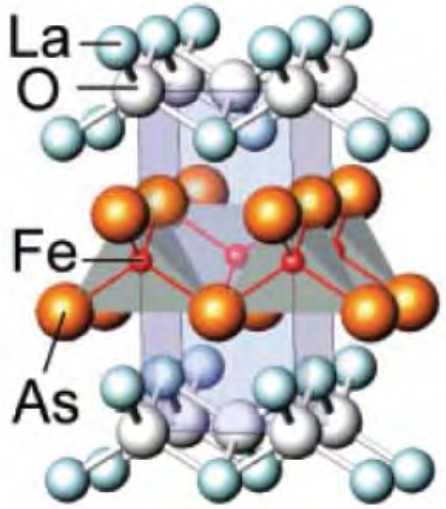
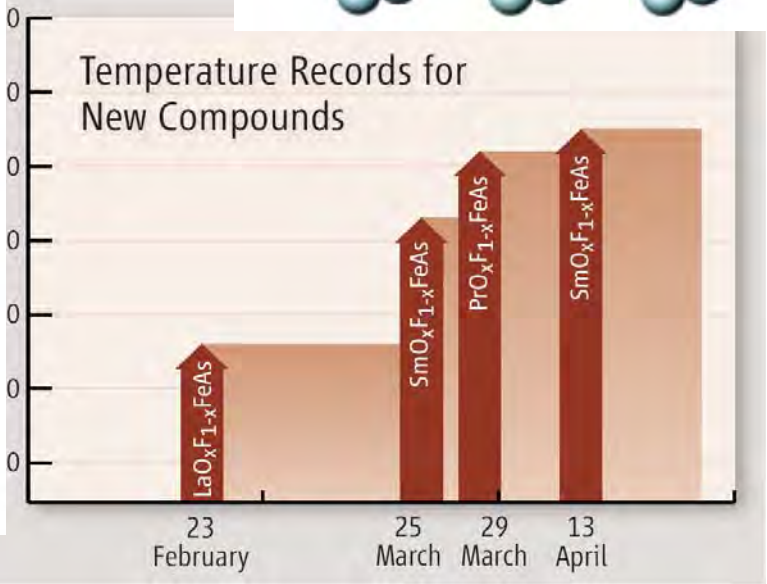




Hosono et.a.., Tokyo, JACS (2008)

28

Address Predictive power of state of the art methods
Predictive power of realistic DMFT and its extensions, LDA+DMFT .

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.

PHYSICAL REVIEW B **80**, 085101 (2009)

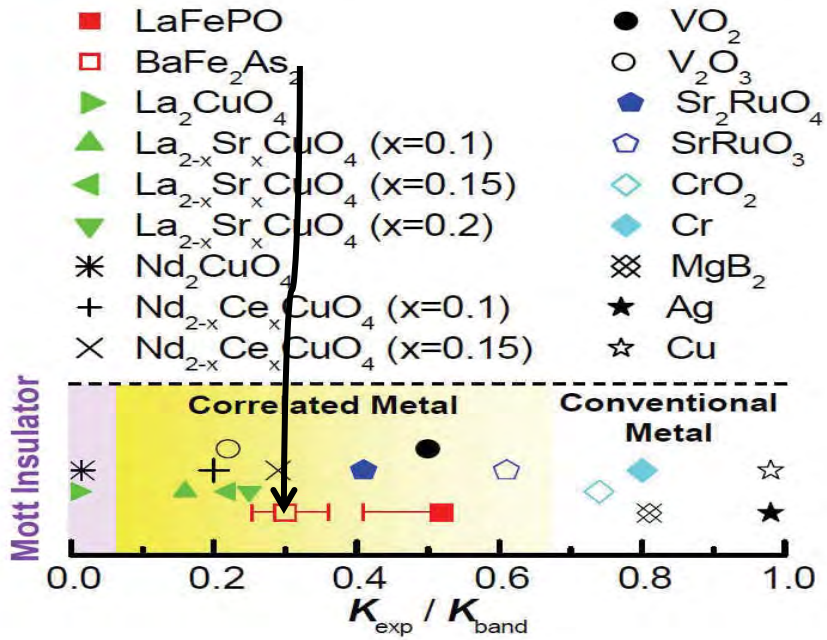
Dynamical mean-field theory within an augmented plane-wave framework: Assessing electronic correlations in the iron pnictide LaFeAsO

Markus Aichhorn,[1] Leonid Pourovskii,[1] Veronica Vildosola,[1,2,3] Michel Ferrero,[1,4] Olivier Parcollet,[4] Takashi Miyake,[3,5,6] Antoine Georges,[1,3,7] and Silke Biermann[1,3]

Our LDA+DMFT results indicate that LaFeAsO is a moderately correlated metal with an average value for the mass renormalization of the Fe 3*d* bands about 1.6. This value is in reasonable agreement with estimates from photoemission experiments.

Early DMFT predictions

PHYSICAL REVIEW LETTERS



ture of $LaO_{1-x}F_xFeAs$

and G. Kotliar

Piscataway, New Jersey 08854, USA

iblished 2 June 2008)

Parent Compound is

a (bad)semi-metal.

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

lculation 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

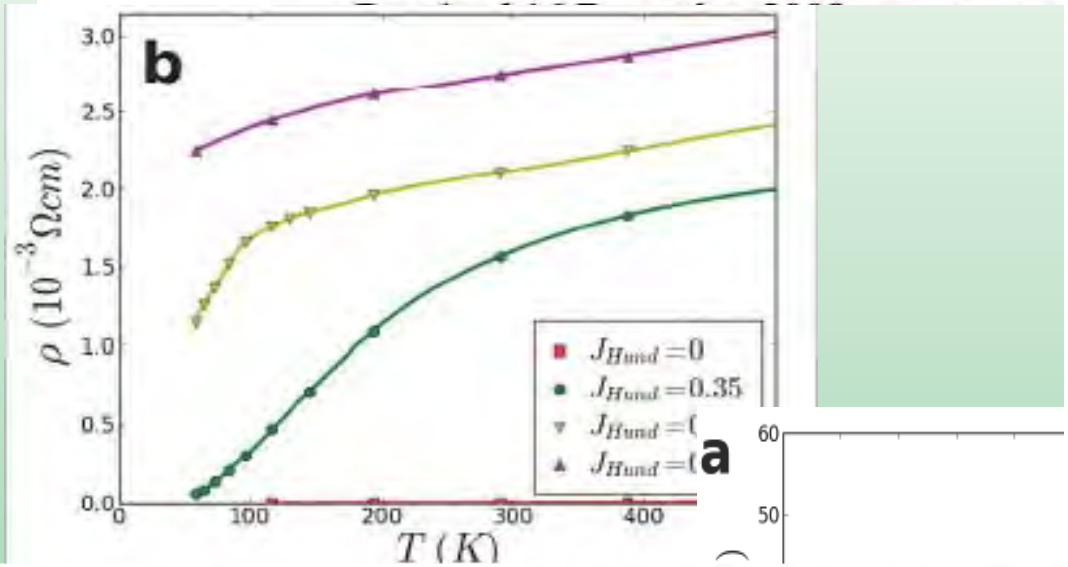
Mass enhancement 3-5

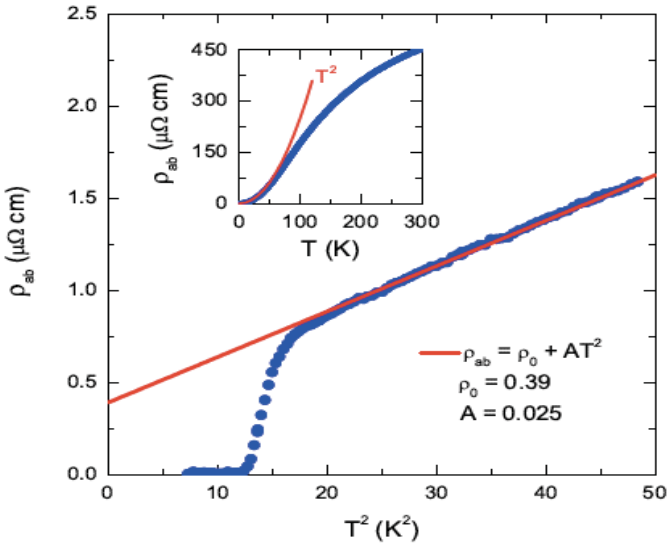
5 active d orbitals

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]

Hund's metals come out of the closet!

PRL **106,** 096401 (2011) PHYSICAL REVIEW LETTERS 4 MARCH 2011

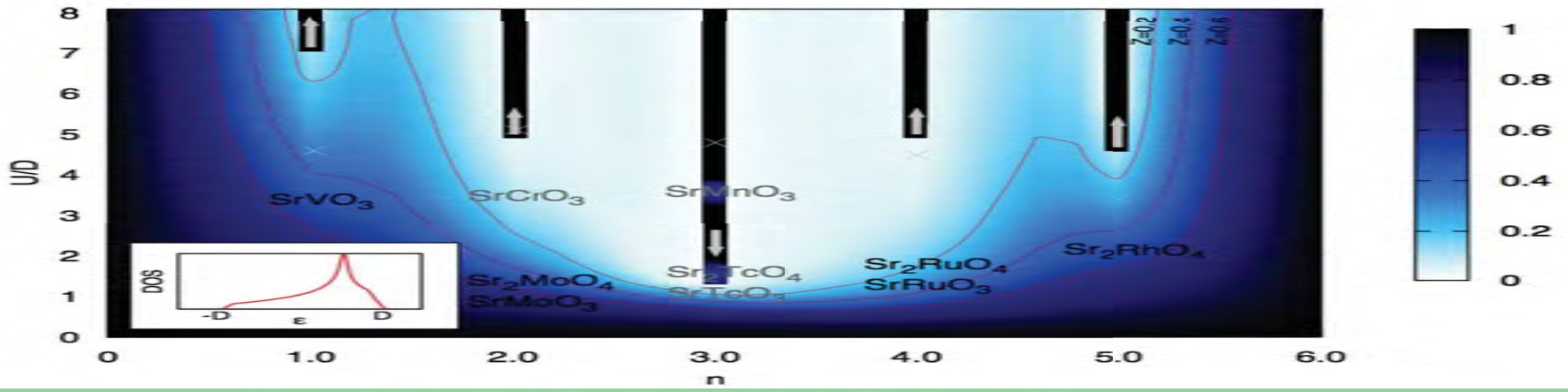
Coherence-Incoherence Crossover and the Mass-Renormalization Puzzles in Sr_2RuO_4

Jernej Mravlje,[1,2] Markus Aichhorn,[3,1] Takashi Miyake,[4,5] Kristjan Haule,[6] Gabriel Kotliar,[6] and Antoine Georges[1,7,5]

[1]*Centre de Physique Théorique, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France*
[2]*Jožef Stefan Institute, Jamova 39, Ljubljana, Slovenia*
[3]*Institute of Theoretical and Computational Physics, TU Graz, Petersgasse 16, Graz, Austria*
[4]*Nanosystem Research Institute, AIST, Tsukuba 305-8568, Japan*
[5]*Japan Science and Technology Agency, CREST, Kawaguchi 332-0012, Japan*
[6]*Physics Department and Center for Materials Theory, Rutgers University, Piscataway New Jersey 08854, USA*
[7]*Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France*

(Received 27 October 2010; published 2 March 2011)

We calculate the electronic structure of Sr_2RuO_4, treating correlations within dynamical mean-field theory. The approach successfully reproduces several experimental results and explains the key properties of this material: the anisotropic mass renormalization of quasiparticles and the crossover into an incoherent regime above a low temperature scale. While the orbital differentiation originates from the proximity of the van Hove singularity, strong correlations are caused by the Hund's coupling.



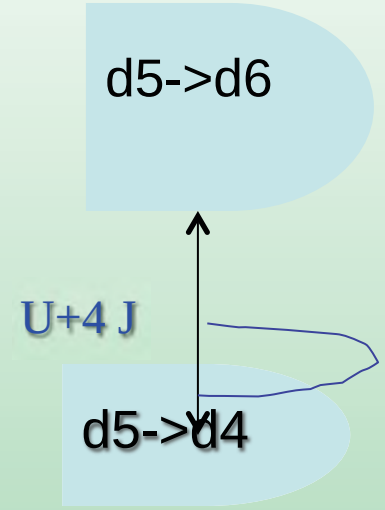
Antoine Georges, Luca de' Medici, Jernej Mravlje

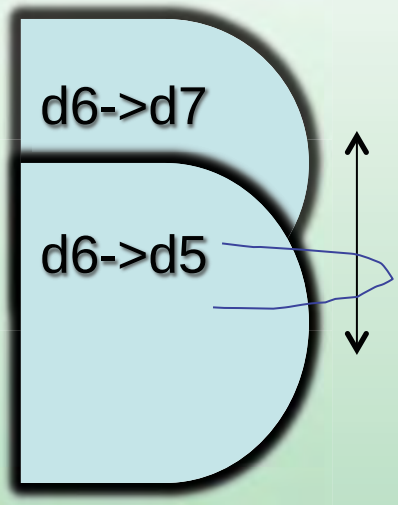
Annual Reviews of Condensed Matter Physics 4, 137-178 (2013

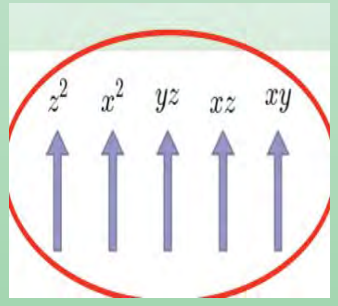
Hundness 101

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

Friedrich Hund







VanderMarel Sawatzky

J survives in the solid U is screened

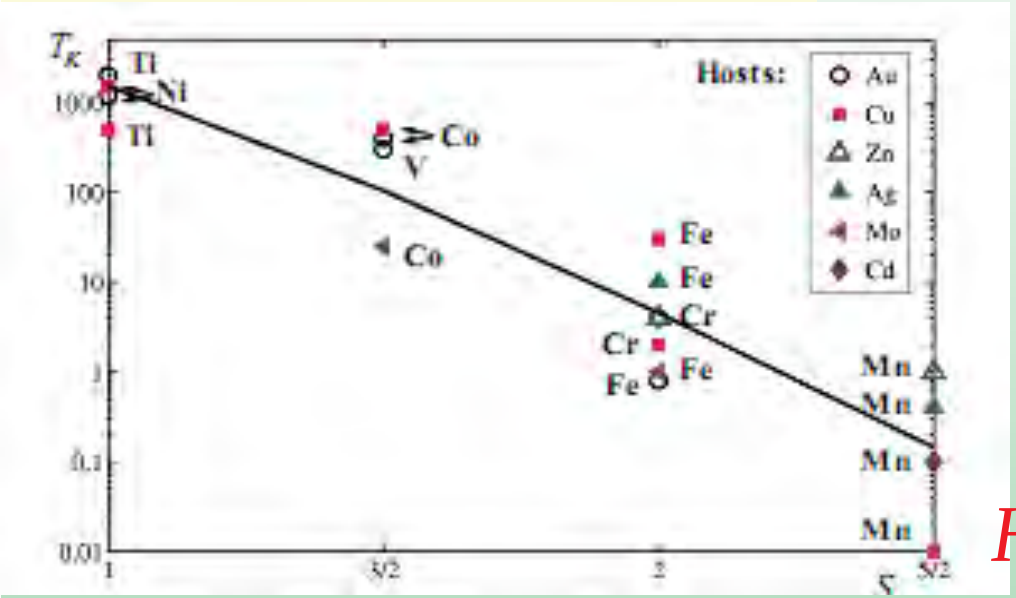
PRB 37 , 10674 (1988)

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

N= 5, U+4J

N=6, U-J

TK depends strongly on filling !



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

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

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).

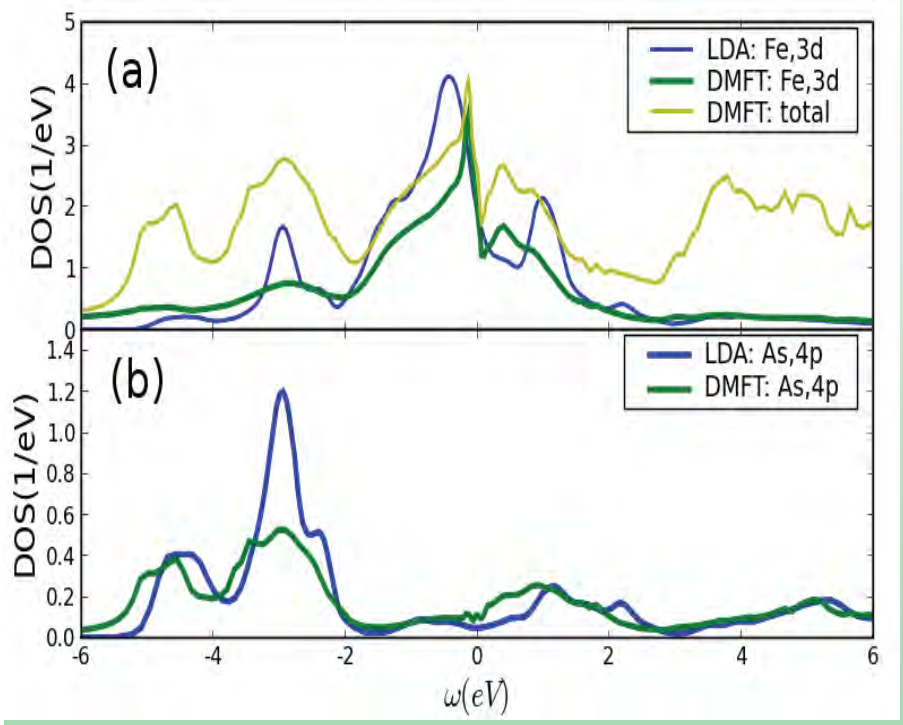
$$J_{\alpha\beta} = J$$

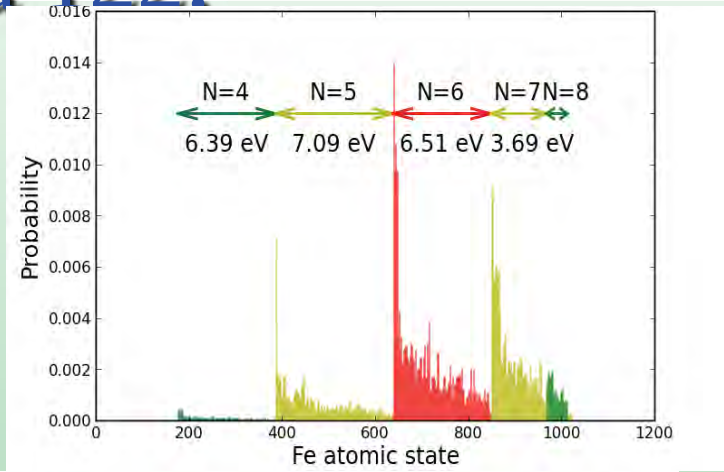
$$J_{\alpha\beta} = J\delta_{\alpha\beta}$$

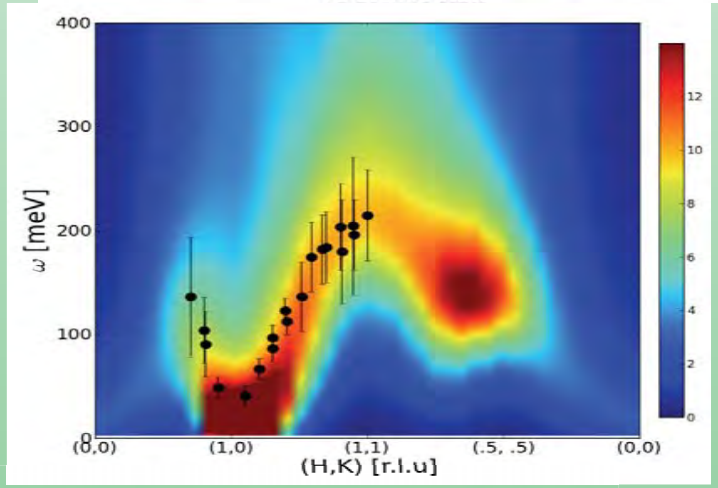
$$T_K = e^{-\frac{1}{\rho JN}}$$

$$T_K = e^{-\frac{N}{\rho J}}$$

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







A. Kutepov, K. Haule, S.Y. Savrasov, G. Kotliar, Phys. Rev. B 82, 045105 (2010).

Theory: H Park. K. Haaule and GK Phys. Rev. Lett. 107, 137007 (2011)

Many experiments.

PHYSICAL REVIEW B 91, 041110(R) (2015)

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

Camille Aron[1,2] and Gabriel Kotliar[1]

ntermediate assymptotic multichannel fixed point K=2.N

FERROMAGNETIC SIGN!

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

$$+K_0T^a(\psi^\dagger_{m\sigma}\frac{\tau^a_{mm'}}{2}\psi_{m'\sigma})+I_0S^\alpha T^a(\psi^\dagger_{m\sigma}\frac{\sigma^\alpha_{\sigma\sigma'}}{2}\frac{\tau^a_{mm'}}{2}\psi_{m'\sigma'})$$

Flow to fermi liquid fixed point is delayed

36

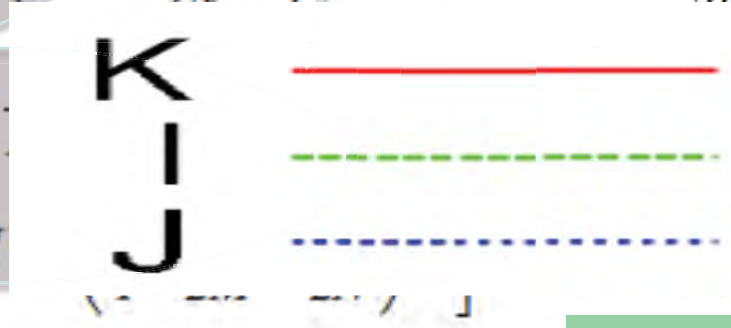
$$\beta_J = -\frac{N}{2}\left(1-\frac{M}{2}J\right)\left(J^2+\frac{C_2^T}{2M}I^2\right)+\dots,$$

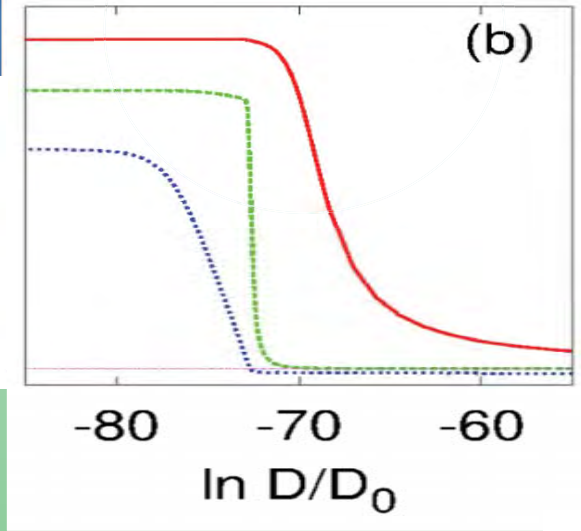
$$\beta_K = -\frac{M}{2}\left(1-\frac{N}{2}K\right)\left(K^2+\frac{C_2^S}{2N}I^2\right)+\dots,$$

$$\beta_I = -\frac{MN}{4}\left[\left(\frac{4}{M}J+\dots\right)\right.$$

$$\left.+\left(\frac{C_3^T}{MC_2^T}+\frac{C_3^S}{NC_2^S}\right)I\right.$$

$$J_0 = \frac{2}{M}\left[$$





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

36

Hundness (102) :Transmuting atoms into quasiparticles, Orbital-Spin Separation

Z. Yin K. Haule and GK Phys. Rev. B 86, 195141 (2012)

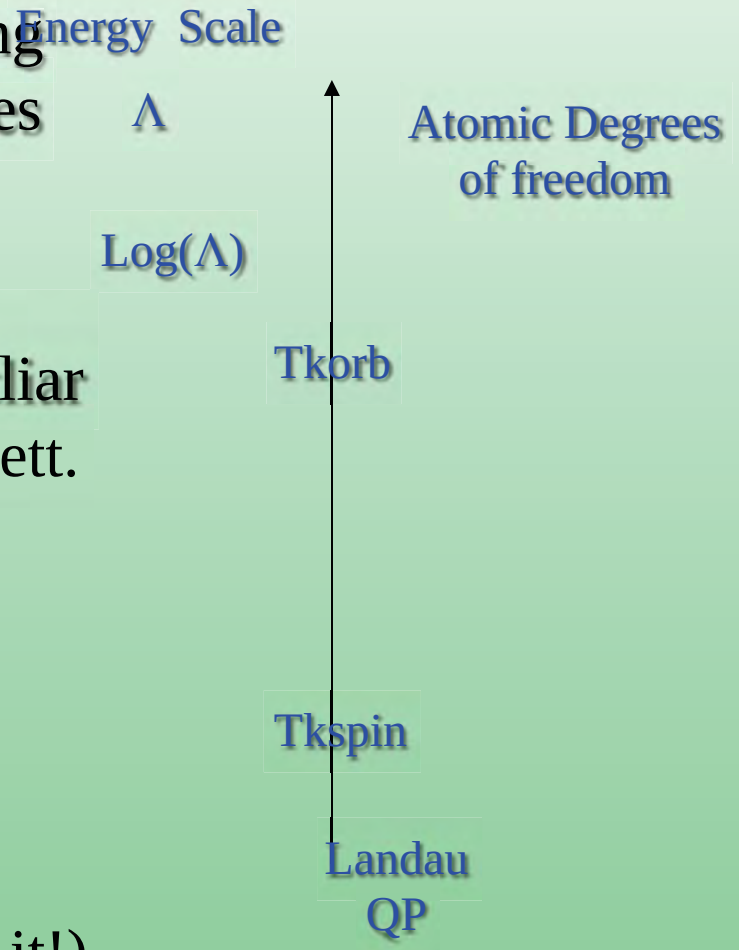
Weak coupling RG analysis, involving Spin, Orbital and Spin-Orbital degrees of freedom C. Aron and G. Kotliar PRB 91, 041110 (2015)

K. Stadler Z. Yin J. von Delft G. Kotliar and A. Weichselebaum Phys. Rev. Lett. 115, 136401 (2015)

Origin of aparent power laws.

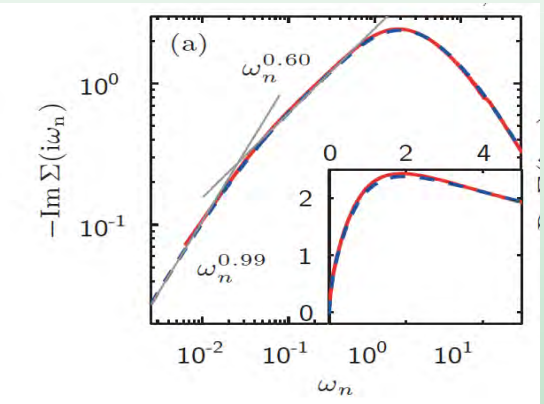
The DMFT self consistency is NOT essential to understand Hundness!

(unlike Mottness which is driven by it!)



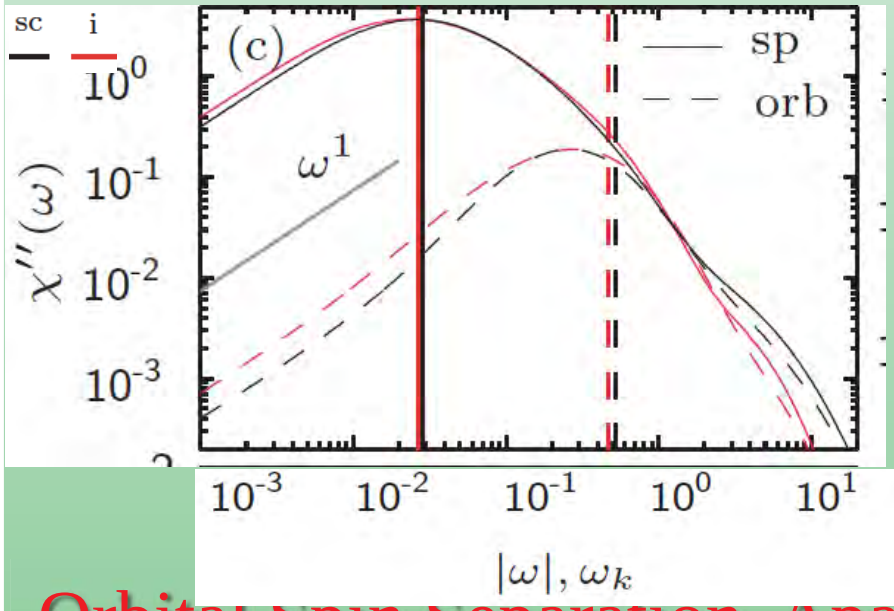
NRG: Stadler et. al. Manifestations of Hundness.

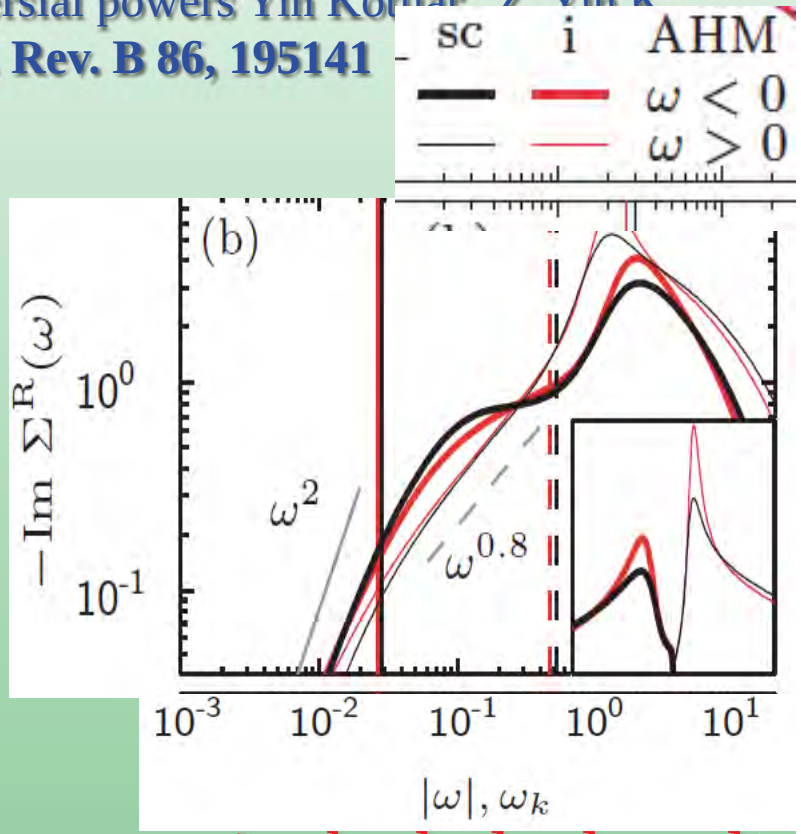
Power law in the self energy on the Matsubara axis.



½ power law in self energy Werner P, Gull E, Troyer M, Millis AJ. 2008. Phys. Rev. Lett. 101:166405.

Apparent Non Universial powers Yin Kotliar, Z. Yin K. Haule and GK **Phys. Rev. B 86, 195141**

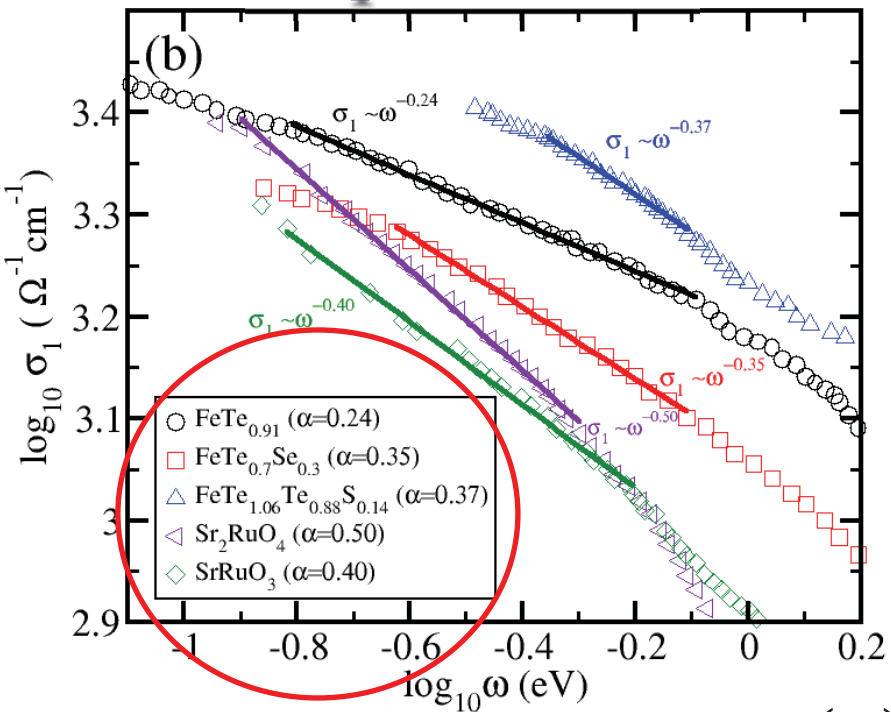




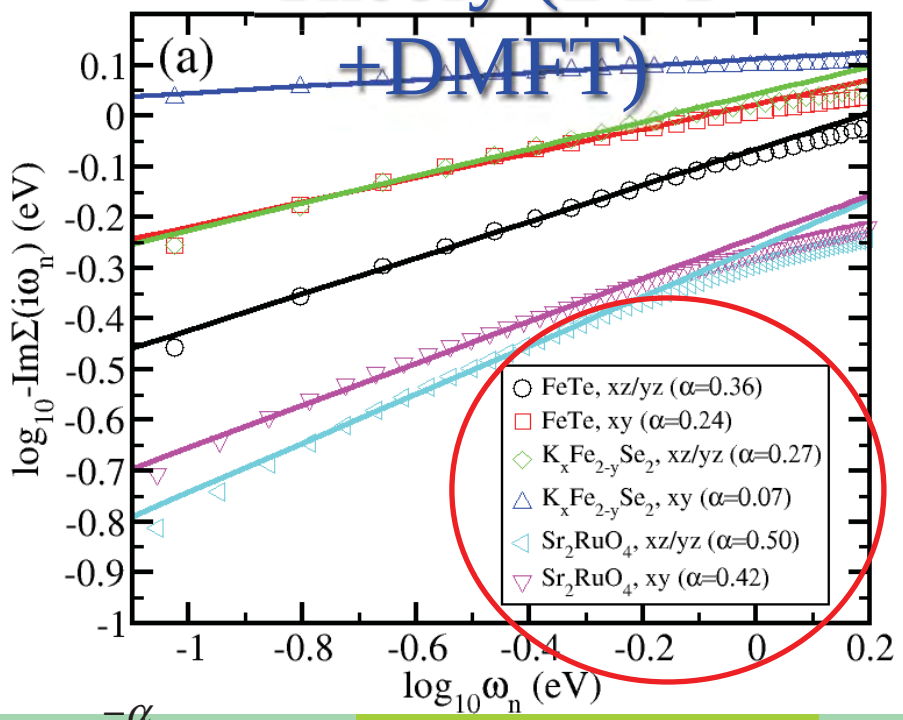
Orbital Spin Separation. Aparent exponents in the hole doped side or the self energy.

Self-energy at intermediate energies: Fractional power-law behavior. Old puzzle optics in ruthenatesL. Klein, J. S. Dodge, C. H. Ahn, G. J. Snyder, T. H. Geballe, M. R. Beasley, and A. Kapitulnik, PRL 77, 2774 (1996)

Experiments



Theory (DFT +DMFT)



$$\sigma_1(\omega) \sim \omega^{-\alpha} \quad \Longleftrightarrow \quad \Sigma''(\omega) \propto -\omega^{\alpha}$$

$$\sigma_1(\omega) \propto \mathrm{Re}\left[\frac{1}{\omega + i\Sigma''(\omega) + \Sigma'(\omega) - \Sigma'(\omega=0)}\right]$$

ZPY *et al.*, PRB **86**, 195141 (2012).

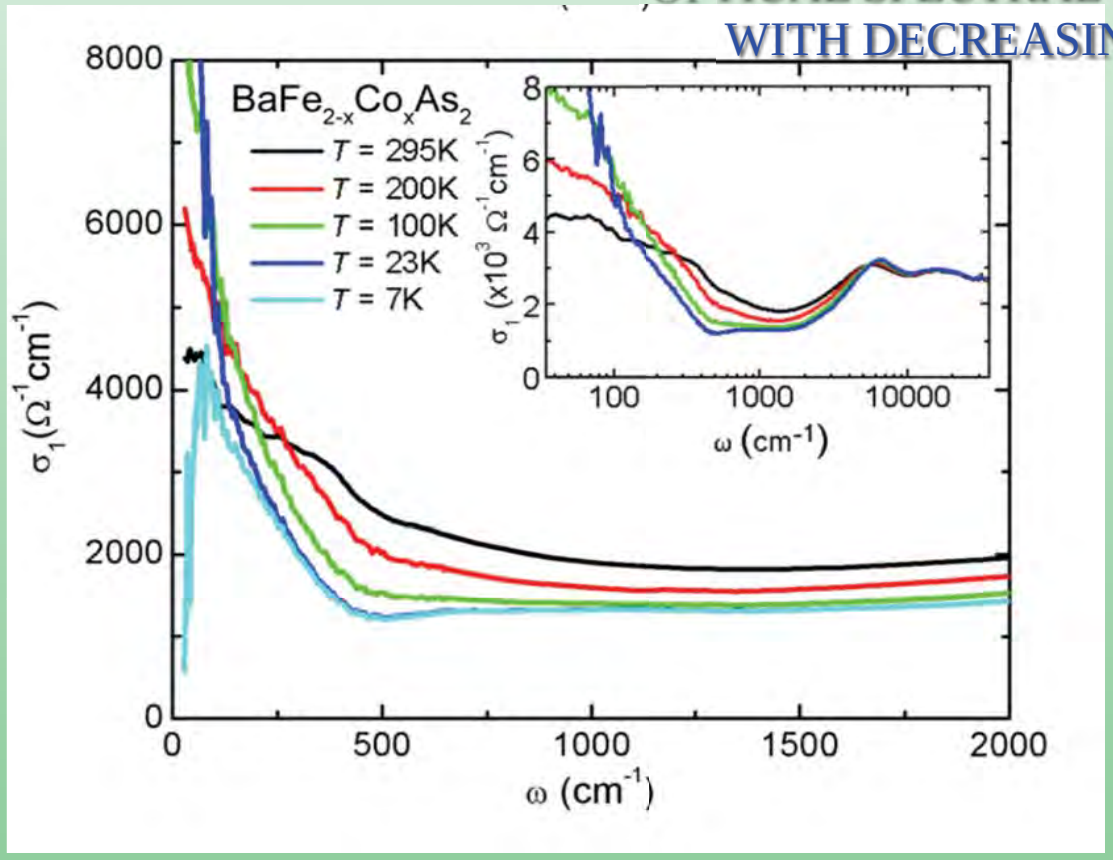
a is orbital and material dependent, not necessarily 1/2.

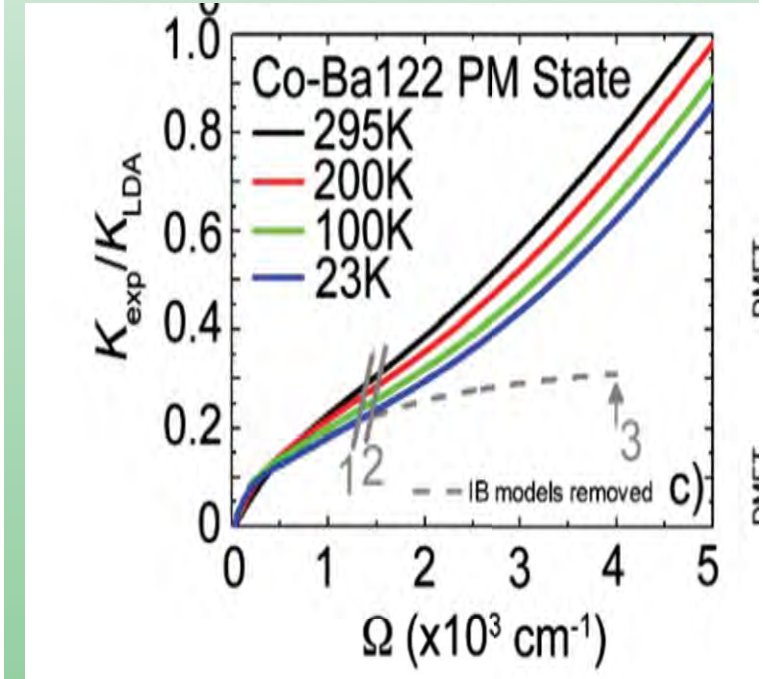
PRL 108, 147002 (2012) PHYSICAL REVIEW LETTERS week ending 6 APRIL 2012

Electronic Correlations and Unconventional Spectral Weight Transfer in the High-Temperature Pnictide $BaFe_{2-x}Co_xAs_2$ Superconductor Using Infrared Spectroscopy

A. A. Schafgans,[1,*] S. J. Moon,[1] B. C. Pursley,[1] A. D. LaForge,[1] M. M. Qazilbash,[2] A. S. Sefat,[3] D. Mandrus,[3,4] K. Haule,[5] G. Kotliar,[5] and D. N. Basov[1]

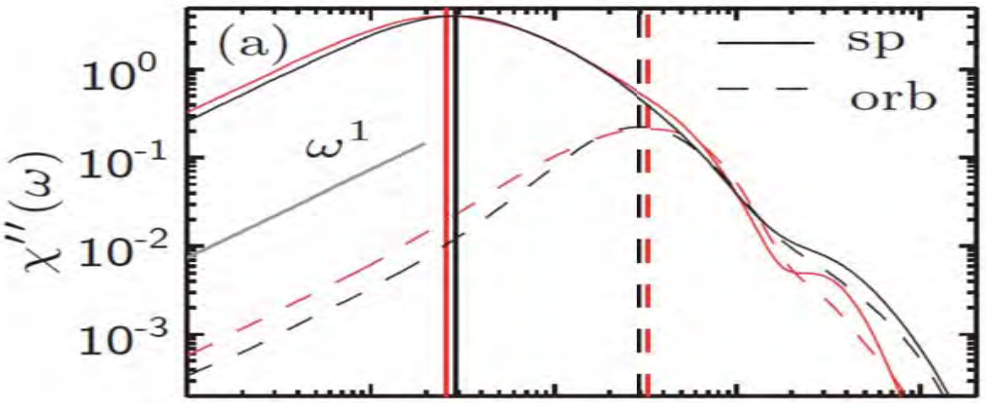
OPTICAL SPECTRAL WEIGHT DECREASES WITH DECREASING TMPERATURE!

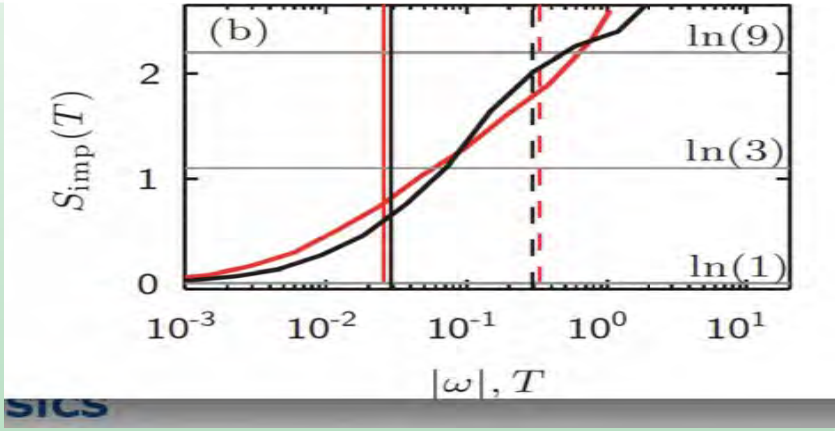




Dynamical Mean-Field Theory Plus Numerical Renormalization-Group Study of Spin-Orbital Separation in a Three-Band Hund Metal

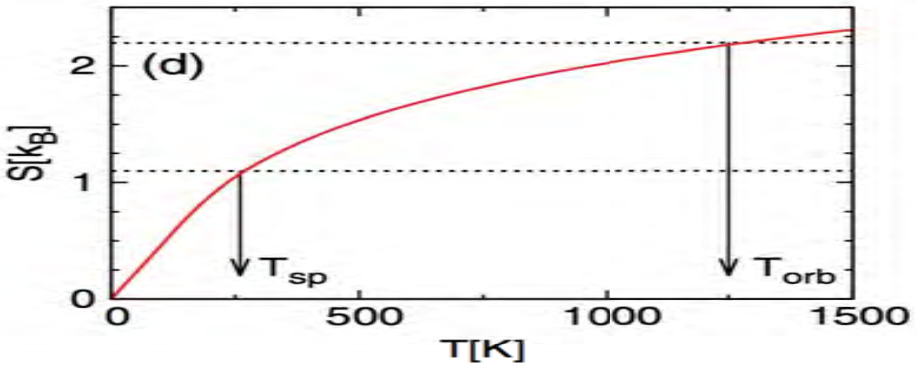
K. M. Stadler,[1] Z. P. Yin,[2] J. von Delft,[1,*] G. Kotliar,[2] and A. Weichselbaum[1]

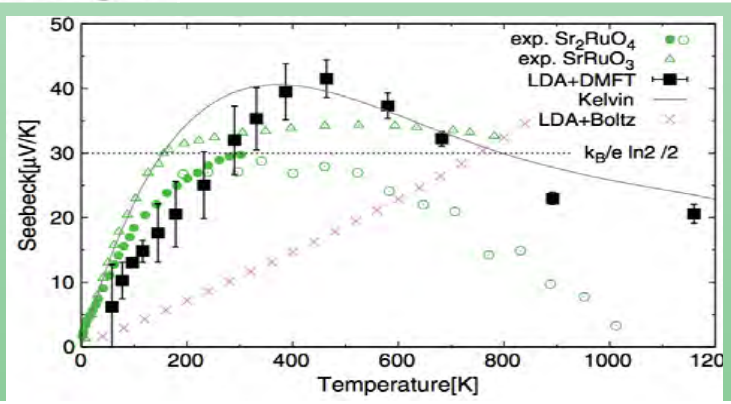




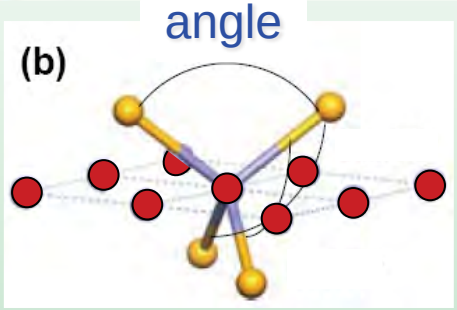
Thermopower and Entropy: Lessons from Sr_2RuO_4

Jernej Mravlje[1] and Antoine Georges[2,3,4]





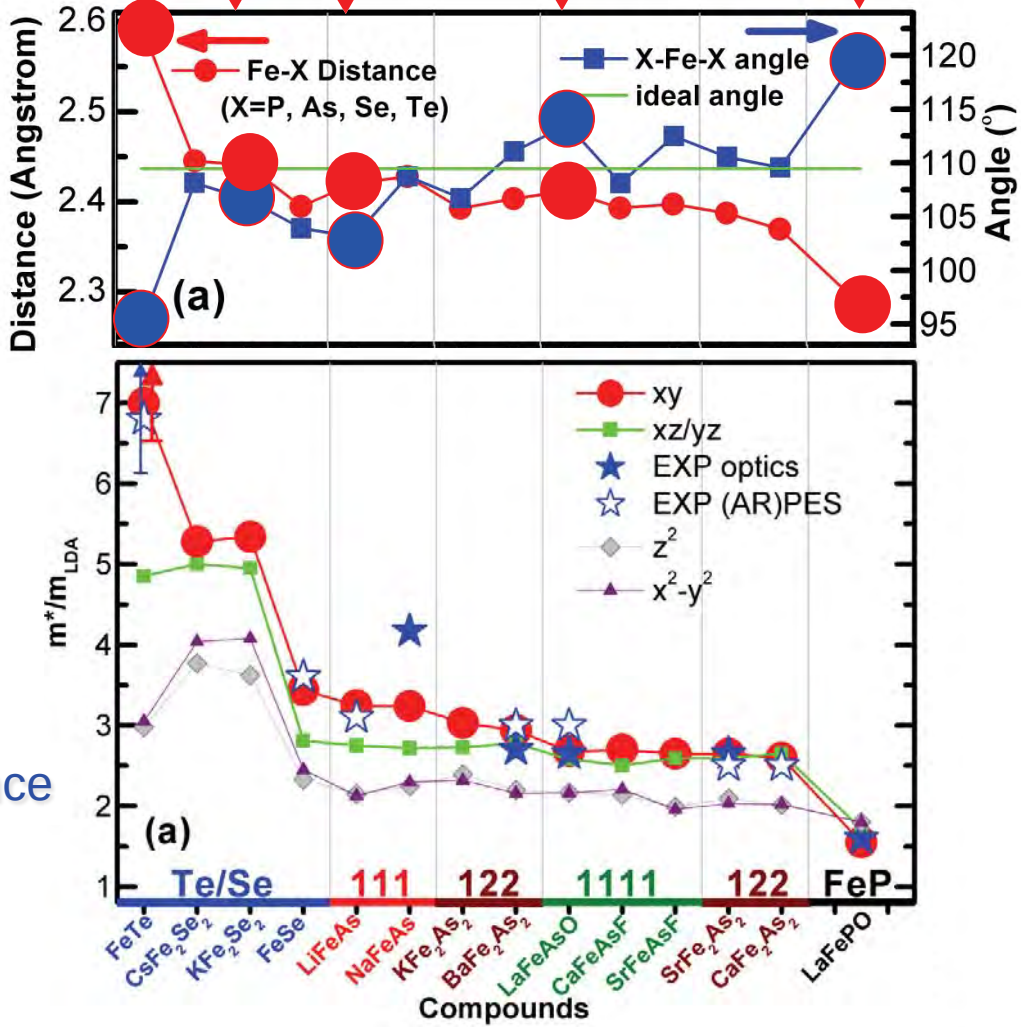
Landscape of Materials: Yin Haule GK Nature Materials (2011)



Tendency to orbital differentiation as correlations increase.

Overal trend consistent with Fe-As distance

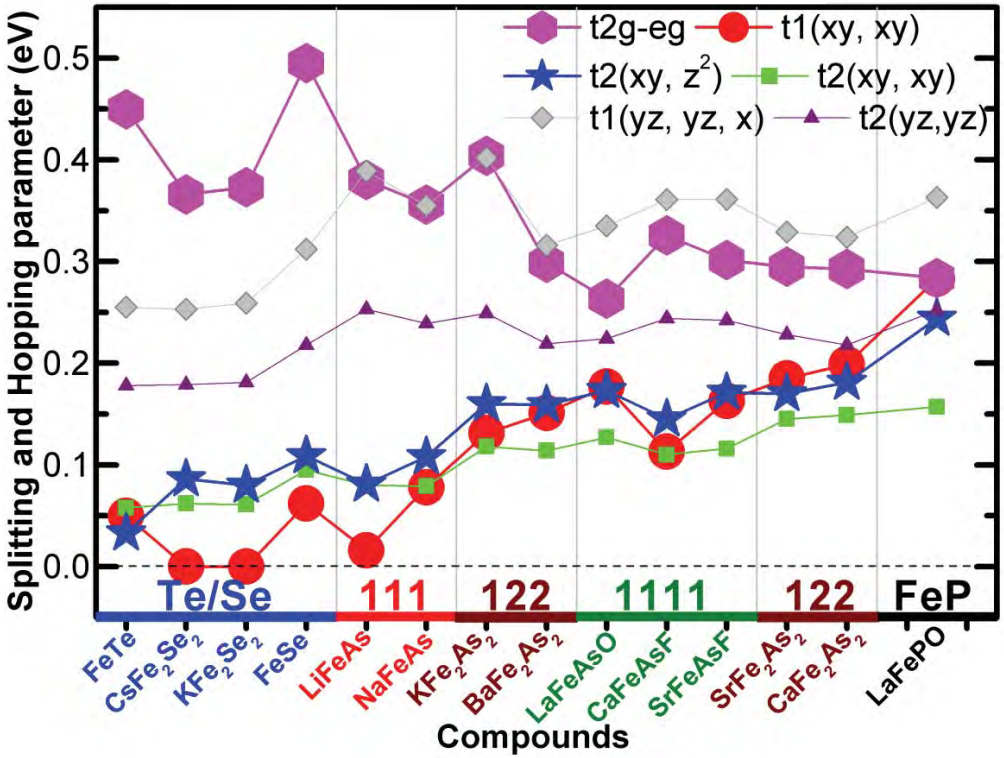
Hybridization with pnictogen

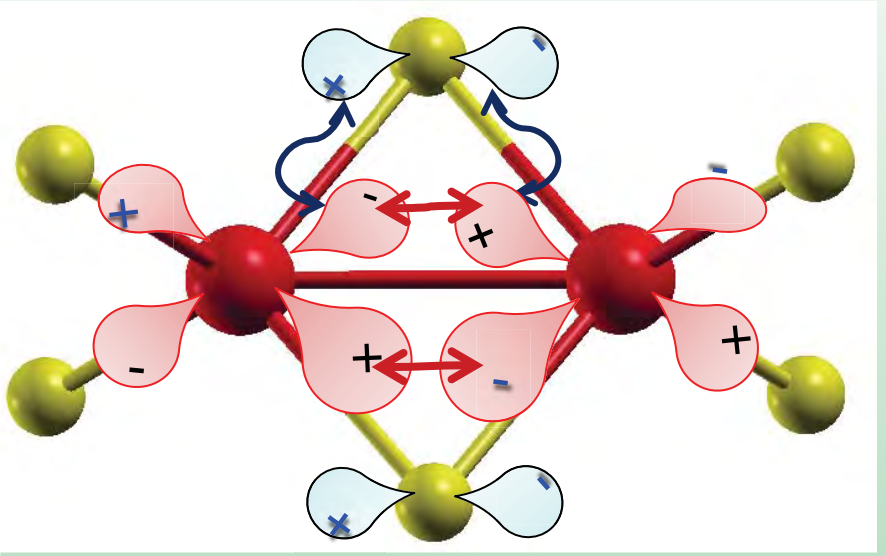


xy orbital, kinetic frustration and FeTe

Yin ZP, Haule K, Kotliar G. 2011.
Nat. Mater. 10:932-935.

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!

Neutron absolute intensities

NATURE PHYSICS | LETTER

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

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

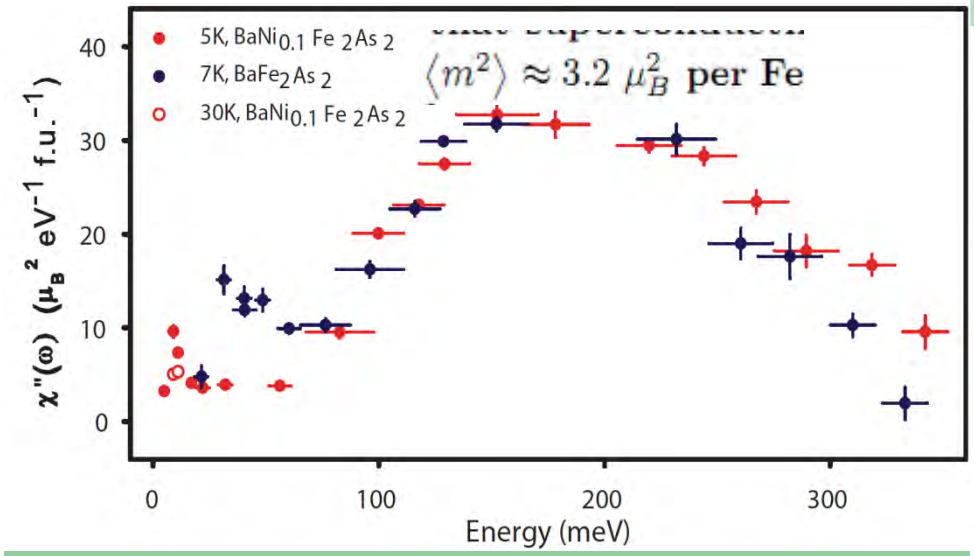
Affiliations | Contributions | Corresponding author

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

Fluctuating moment by neutrons:

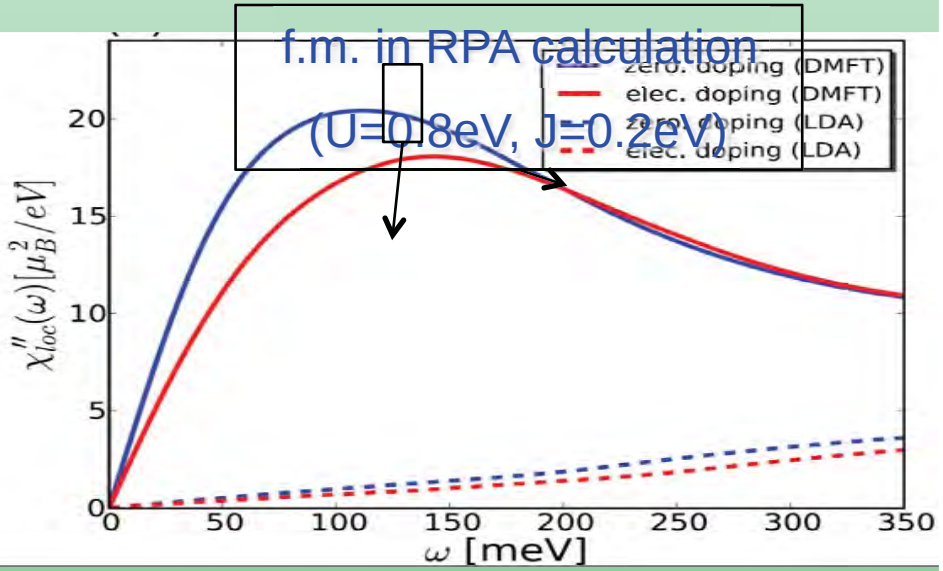
$$\langle \mu^2 \rangle = \int \frac{d\omega}{\pi} n(\omega) \chi''(\omega)$$

Experiment by Liu …Pengcheng Dai

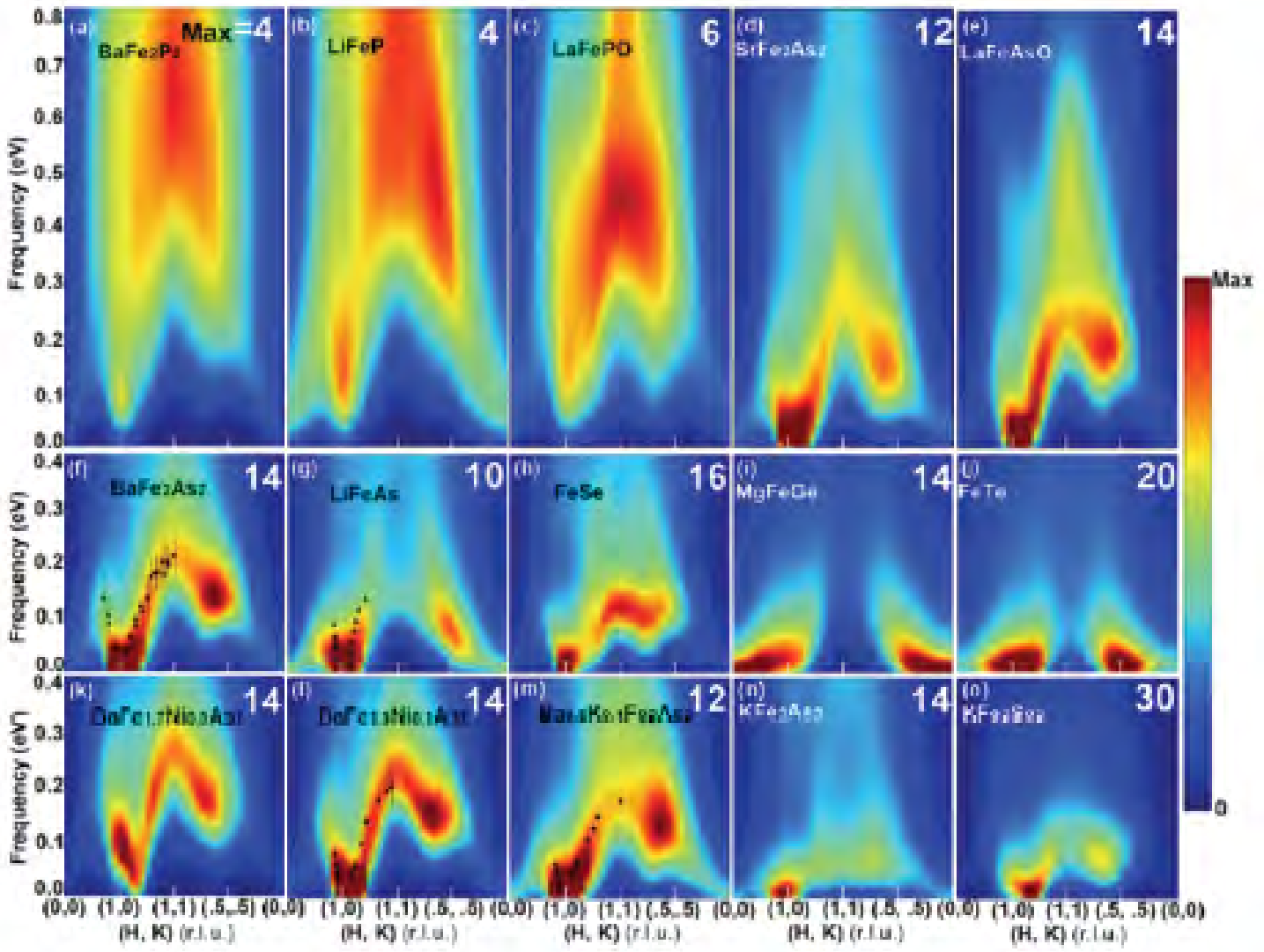


f.m. in RPA calculation

(U=0.8eV, J=0.2eV)



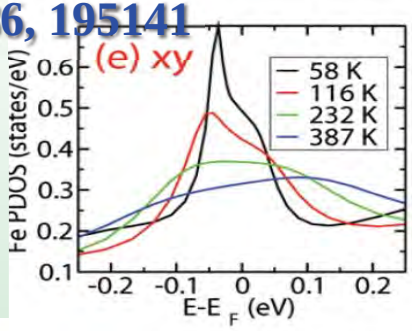
Spin Fluctuation Spectrum, ZYin K Haule and GK et. al. Nature Physics (2014)

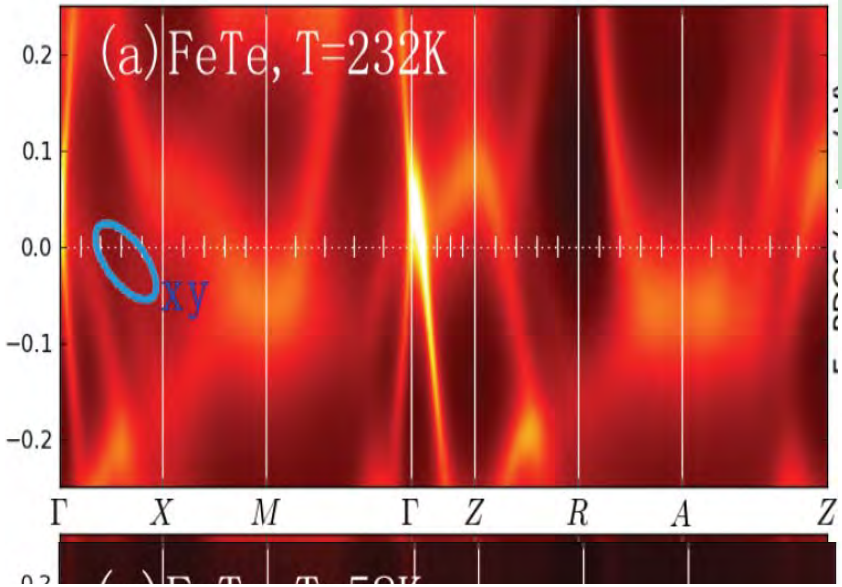


Yin Haule and GK (2012)

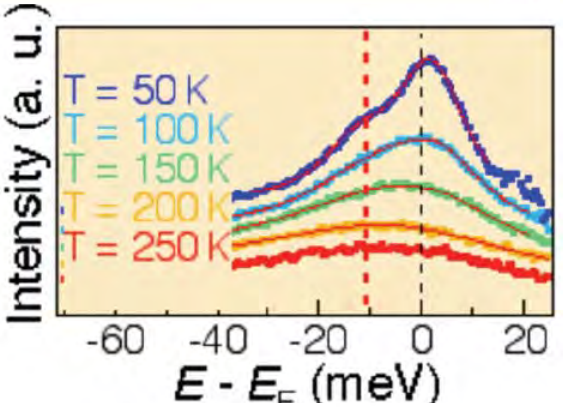
Phys. Rev. B 86, 195141

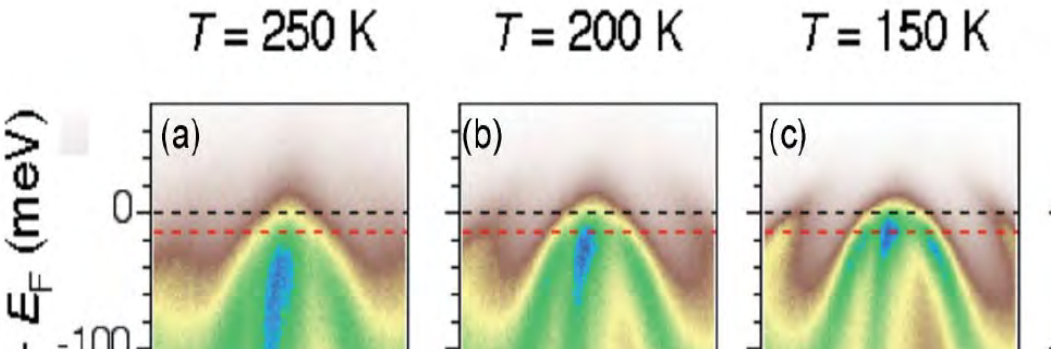
46





LiFeAs H. Miao et. al.. PRB 89, 220503(R) (2014) 46





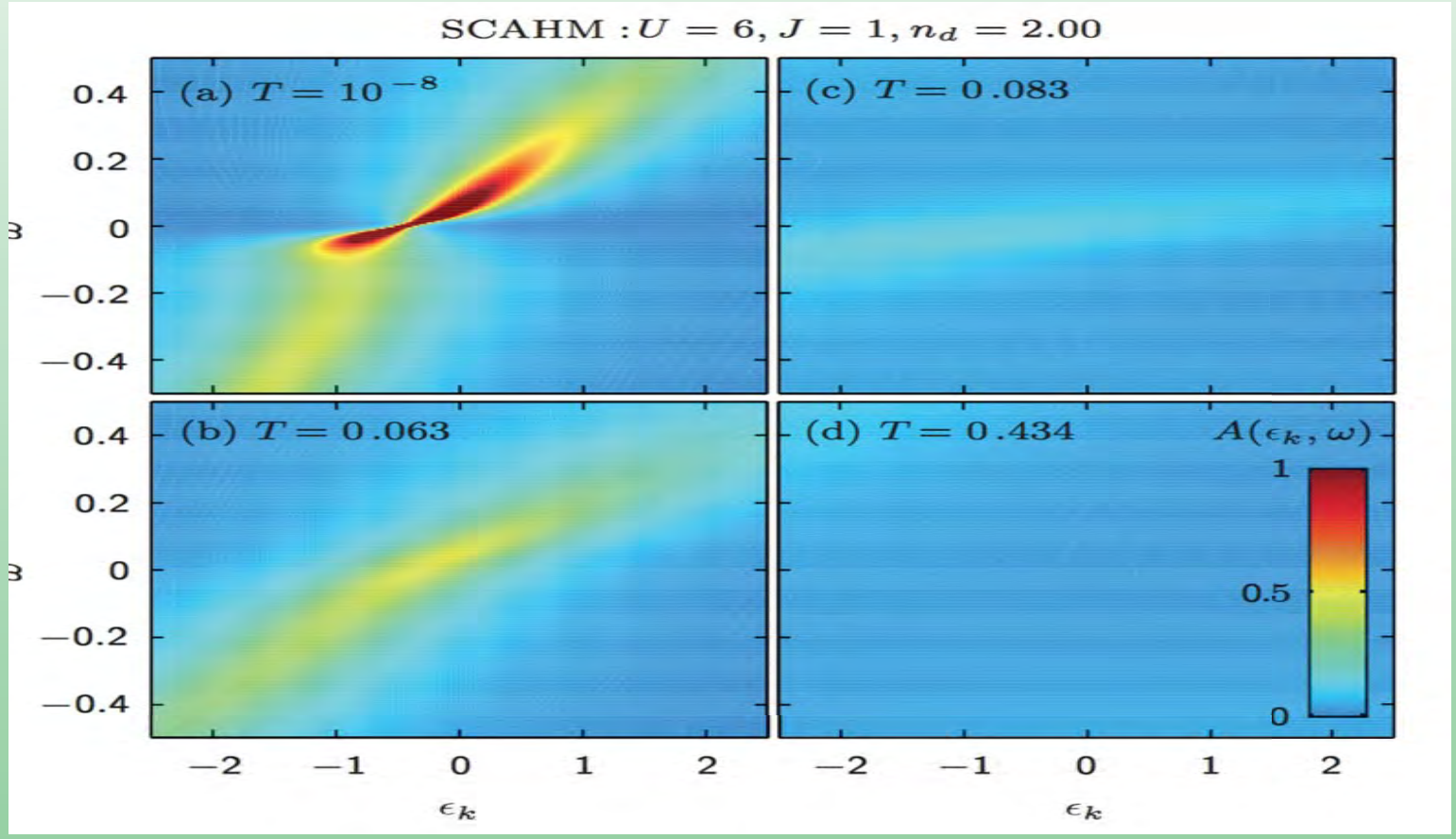
Experimental Observation of Incoherent-Coherent Crossover and Orbital Dependent Band Renormalization in Iron Chalcogenide Superconductors

Z. K. Liu[1,2], M. Yi[1,2], Y. Zhang[1,3], J. Hu[4], R. Yu[5,6], J.-X. Zhu[7], R.-H. He[8], Y. L. Chen[9], M. Hashimoto[10], R. G. Moore[1], S.-K. Mo[3], Z. Hussain[3], Q. Si[6], Z. Q. Mao[4], D. H. Lu[10,*], Z.-X. Shen[1,2,*]

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

Supplementary Material

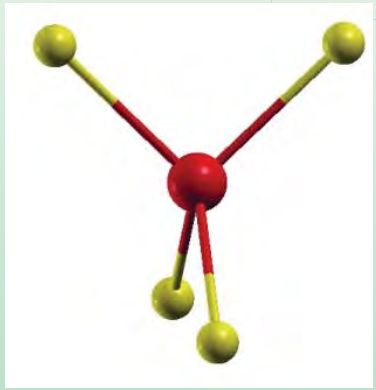
K. M. Stadler,[1] Z. P. Yin,[2] J. von Delft,[1] G. Kotliar,[2] and A. Weichselbaum[1]

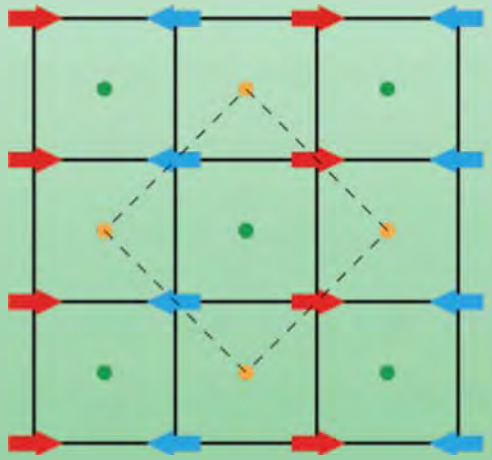


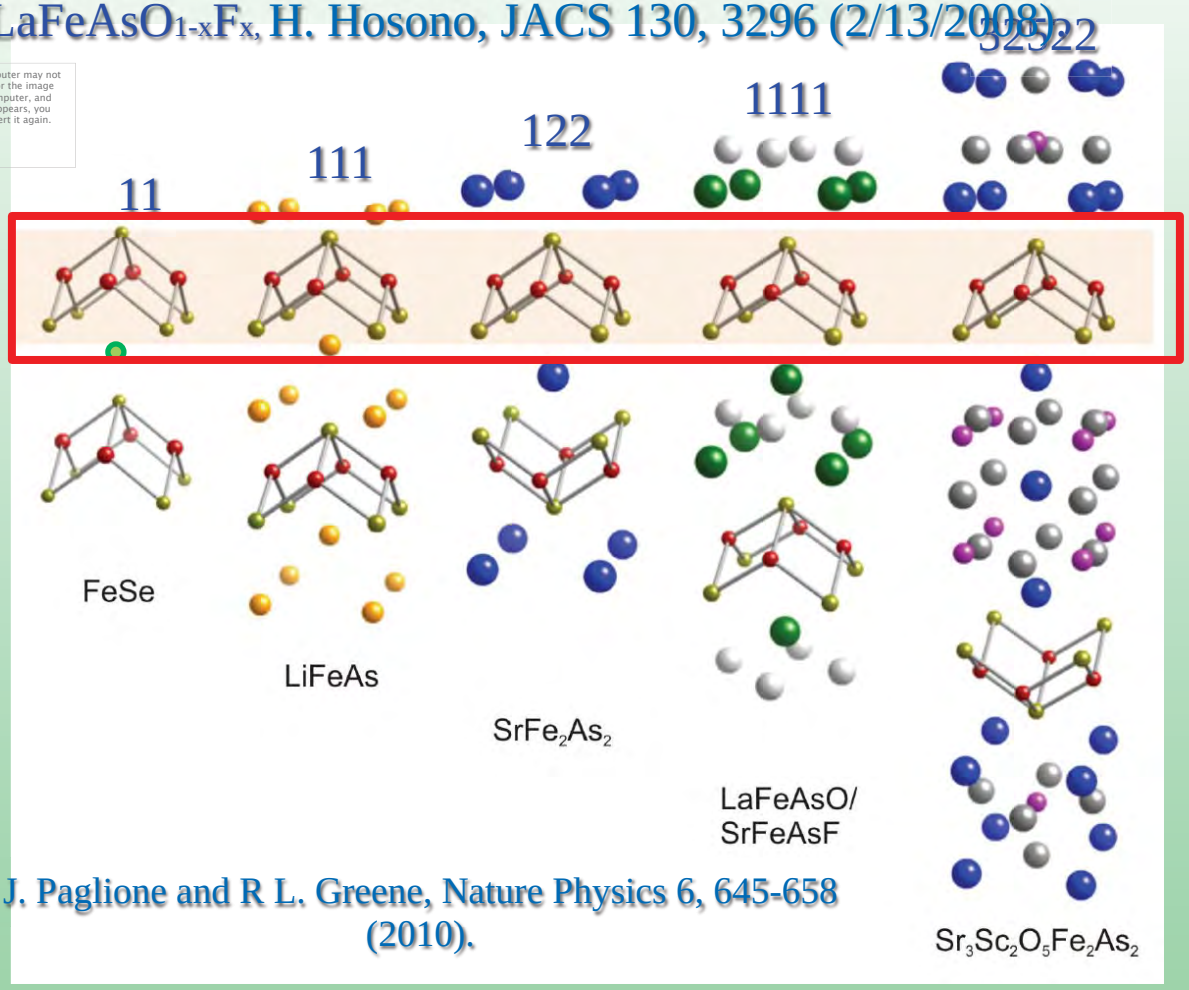
Model ARPES: 3 band Hubbard model, no crystal fields!!!

Landscape of Fe based SC

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







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

17

Theoretical understanding: iron pnictides as Hunds metals.

Various properties were predicted, using LDA+DMFT !

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

(1995

Journal of the Physical Society of Japan **83**, 025001 (2014)
http://dx.doi.org/10.7566/JPSJ.83.025001

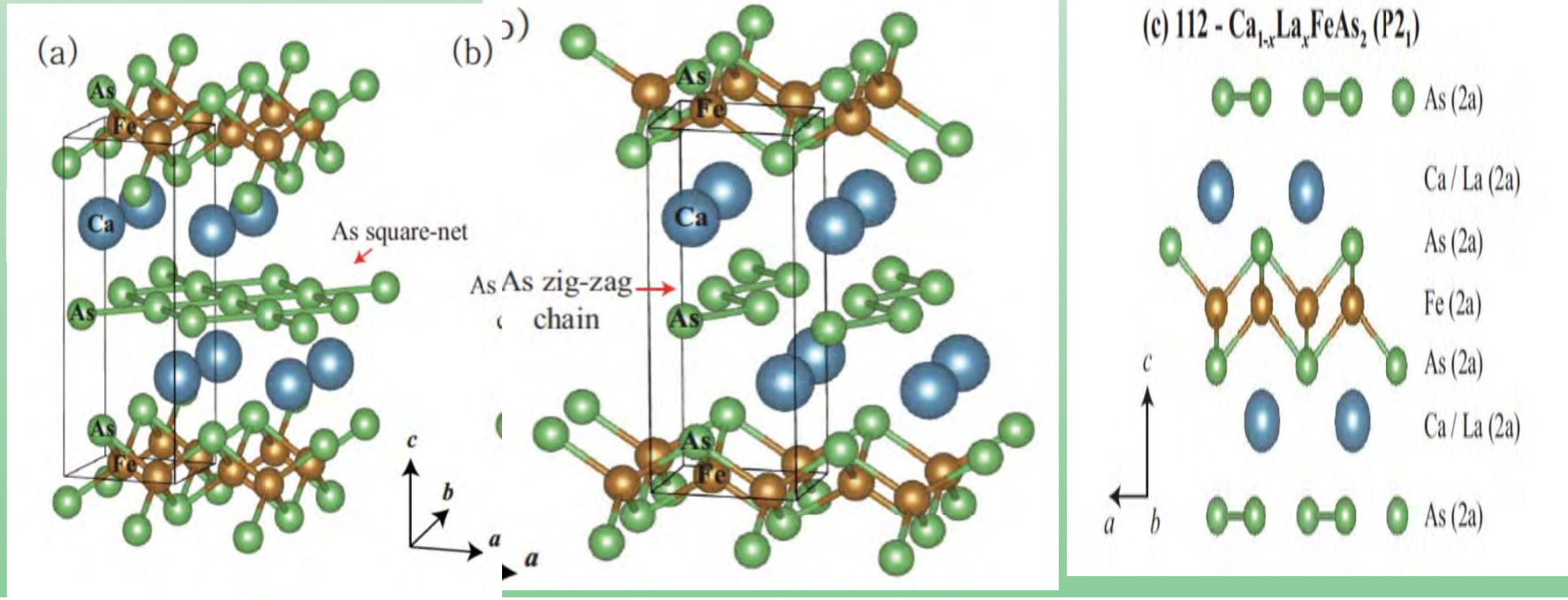
Enhanced Superconductivity up to 43 K by P/Sb Doping of $Ca_{1-x}La_xFeAs_2$

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]

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]



Search for TM in the 112 structure

[FeAs][CaAs]-[MnBi][SrBi]

PHYSICAL REVIEW B **84**, 064428 (2011)

Layered transition-metal pnictide $SrMnBi_2$ with metallic blocking layer

Jiakui K. Wang,[1] Liang L. Zhao,[1] Quan Yin,[2] G. Kotliar,[2] M. S. Kim,[3,4] M. C. Aronson,[3,4] and E. Morosan[1]
[1]*Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA*
[2]*Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA*
[3]*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973, USA*
[4]*Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York 11794, USA*
(Received 13 May 2011; revised manuscript received 21 June 2011; published 25 August 2011)

The physical properties and the band structure of the layered pnictide $SrMnBi_2$ were investigated. This compound has a crystal structure similar to that of the superconducting Fe pnictides, and is a bad metal with large residual resistivity. Magnetic order sets in at very high temperatures, around 290 K, as shown by magnetization, resistivity, and specific heat data. Band structure calculations using density functional theory (DFT) are consistent with the thermodynamic and transport measurements, suggesting a checkerboard antiferromagnetic (cAFM) ground state and a localized picture for the magnetism. Moreover, DFT results indicate that the Mn 3*d* electrons are strongly correlated, and that, unlike in the known superconductors, the Sr-$Bi_{(1)}$ layer is metallic. One more notable feature of the DFT calculation is the multiple Dirac-cone-like dispersion close to the Fermi level.

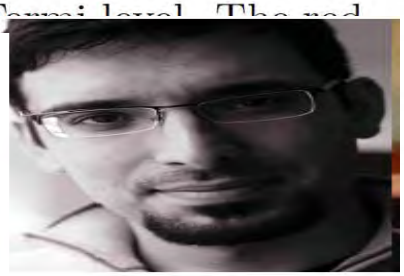
5402 (2011) PHYSICAL REVIEW LETTERS we 16 SEPT

Anisotropic Dirac Fermions in a Bi Square Net of $SrMnBi_2$

bum Park,[1] G. Lee,[2] F. Wolff-Fabris,[3] Y. Y. Koh,[4] M. J. Eom,[1] Y. K. Kim,[4] M. A. Farhan,[2] Y. J. C. Kim,[4] J. H. Shim,[2,*] and J. S. Kim[1,†]
[1]*Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Korea*
[2]*Department of Chemistry, Pohang University of Science and Technology, Pohang 790-784, Korea*
den High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germ
[4]*Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea*
[5]*Department of Physics, Kyungpook National University, Daegu 702-701, Korea*
(Received 27 April 2011; published 16 September 2011)

We report the observation of highly anisotropic Dirac fermions in a Bi square net of $SrMnBi_2$, based on a first-principles calculation, angle-resolved photoemission spectroscopy, and quantum oscillations for high-quality single crystals. We found that the Dirac dispersion is generally induced in the $(SrBi)^+$ layer containing a double-sized Bi square net. In contrast to the commonly observed isotropic Dirac cone, the Dirac cone in $SrMnBi_2$ is highly anisotropic with a large momentum-dependent disparity of Fermi velocities of ~8. These findings demonstrate that a Bi square net, a common building block of various layered pnictides, provides a new platform that hosts highly anisotropic Dirac fermions.

Chang LIu



T. Birol

FIG. 3. (a)The ARPES constant energy map of the $Ca_{0.73}La_{0.27}FeAs_2$ at the Fermi level. The red

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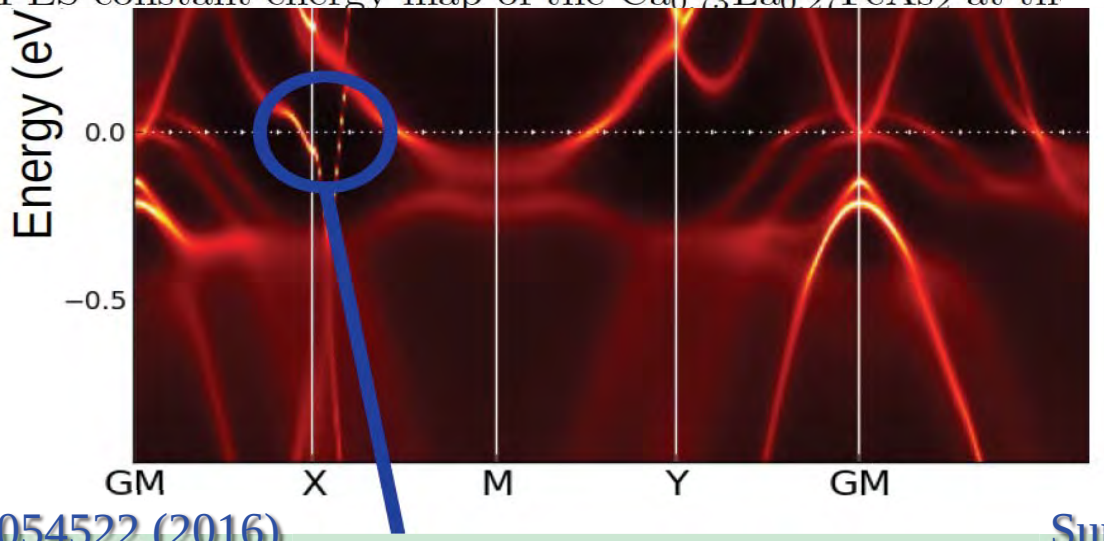
panel: the 2nd der

tical $CaFeAs_2$ and

$Ca_{0.7}La_{0.3}FeAs_2$, fr



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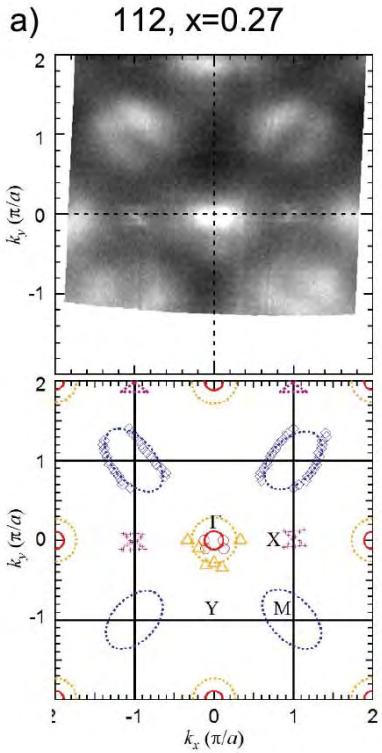
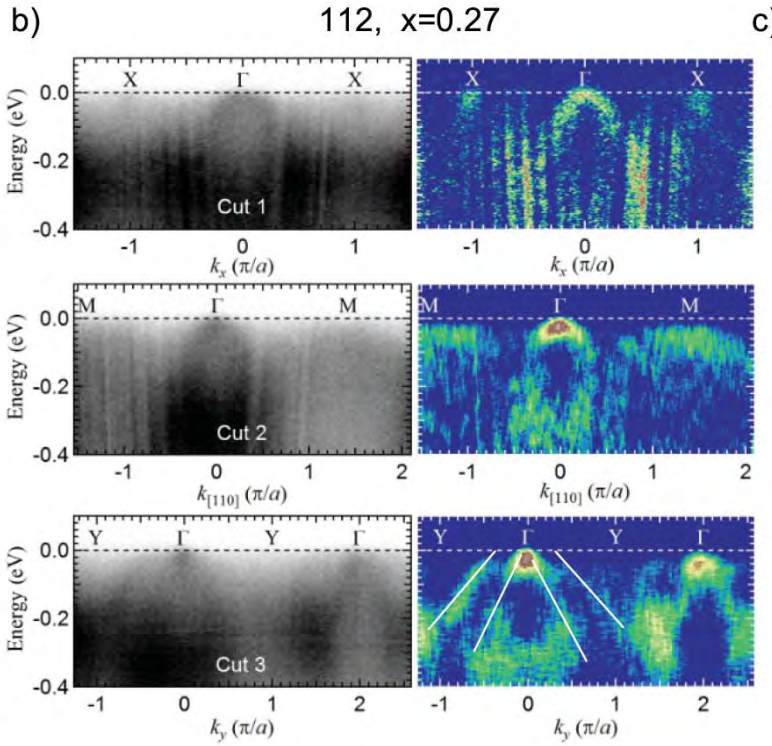
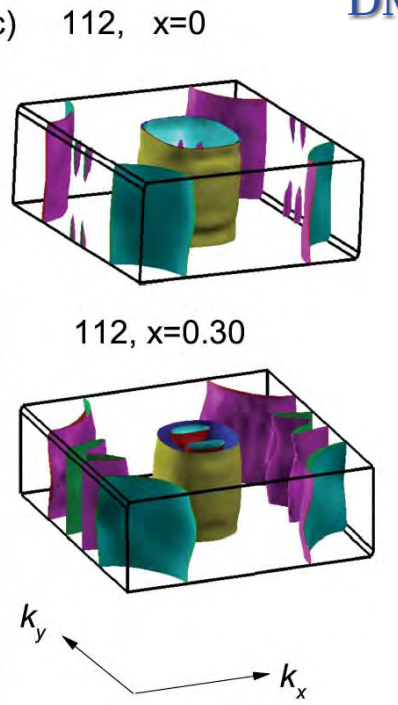
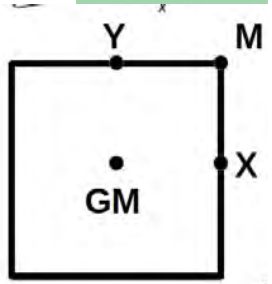
Phys. Rev. B 93, 054522 (2016)

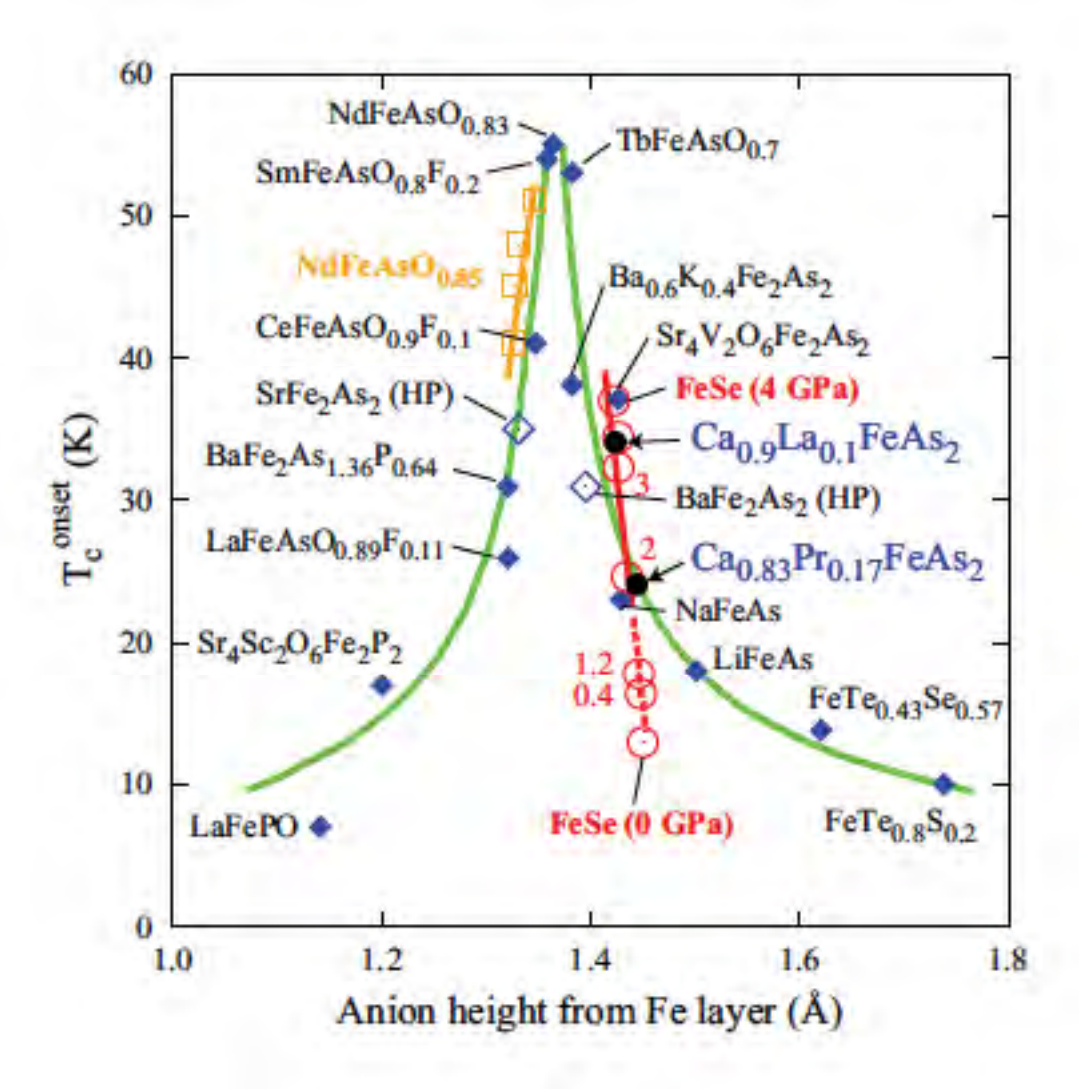
Supported by NSF DMREF











Y. Mizuguchi, Y. Hara, K. Deguchi, S. Tsuda, T. Yamaguchi, K. Takede, H. Kotegawa, H. Tou, and Y. Takano, Supercond. Sci. Technol. 23, 054013 (2010).

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

Local Self-Energy Approach for Electronic Structure Calculations

N. E. Zein,[1,2] S. Y. Savrasov,[2] and G. Kotliar[3,4]
[1]*RRC "Kurchatov Institute", Moscow 123182, Russia*

Validity of the Local Approximation in Iron- Pnictides and Chalcogenides

854, USA

Patrick Sémon, Kristjan Haule, and Gabriel Kotliar
Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854, USA

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 suprisingly local justifying the success of single site DMFT in the iron pnictides and for other Hunds metals

PRL 109, 237010 (2012) PHYSICAL REVIEW LETTERS ng 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]
[1]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*
[2]*Department 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 (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.

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

Outline

- Introduction to correlations in solids. Static and Dynamic Correlations.
- Brief introduction to DMFT + electronic structure.
- Roads to correlations, Mott vs Hund. Vanadium Oxides vs Iron pnictides and chalcogenides.
- Actinides.
- Static correlations, $BaBiO_3$ and their analogs.
- Conclusions.

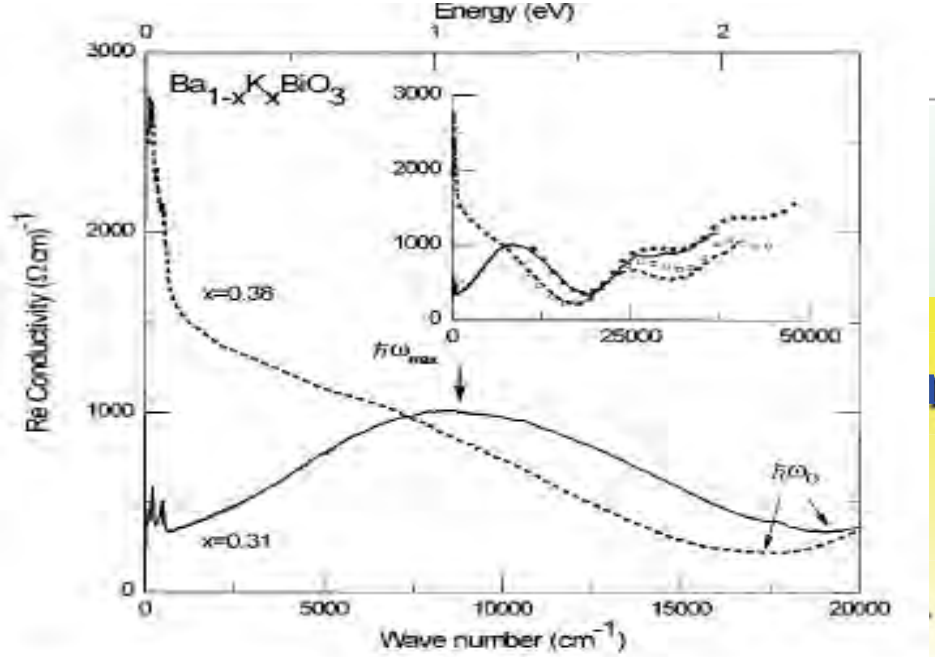
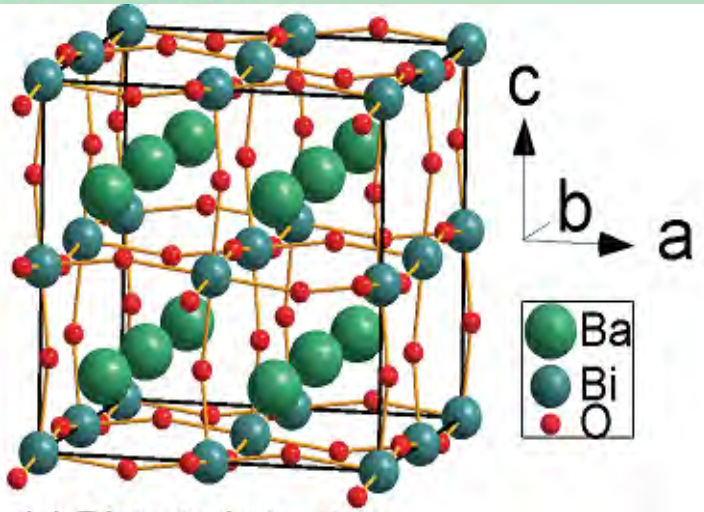


FIG. 1. Theoretical conductivity of $Ba_{1-x}K_xBiO_3$ in the hole-

“Pb4+ =Bi 5+”

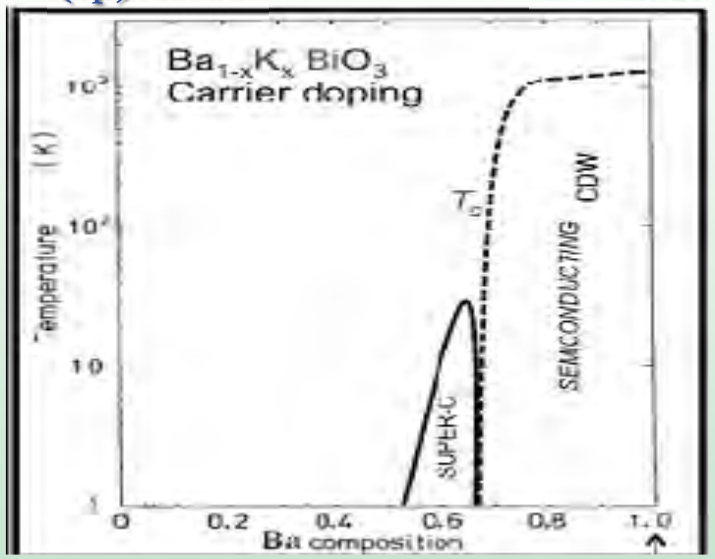
		VA	VIA	VIIA
5 B	6 C	7 N	8 O	9 F
13 Al	14 Si	15 P	16 S	17 Cl
31 Ga	32 Ge	33 As	34 Se	35 Br
49 In	50 Sn	51 Sb	52 Te	53 I
81 Tl	82 Pb	83 Bi	84 Po	85 At

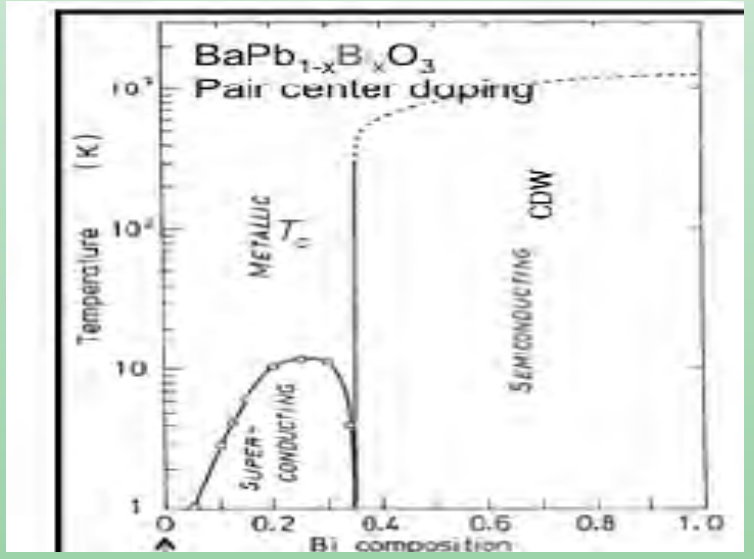


(c) Distorted structure

$(sp)^0$ Bi5+

Bi4+$(sp)^1$





$(sp)^0$

$(sp)^1$

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Current Applied Physics 2 (2002) 425–430
Physics, Chemistry and Materials Sciences
www.elsevier.com/locate/cap

The superconducting bismuth-based mixed oxides ☆

E.V. Antipov [a,*], N.R. Khasanova [a], J.S. Pshirkov [a], S.N. Putilin [a], C. Bougerol [b], O.I. Lebedev [c], G. Van Tendeloo [c], A.N. Baranov [d], Y.W. Park [d]

PHYSICAL REVIEW X 3, 021011 (2013)

Correlation-Enhanced Electron-Phonon Coupling: Applications of *GW* and Screened Hybrid Functional to Bismuthates, Chloronitrides, and Other High-T_c Superconductors

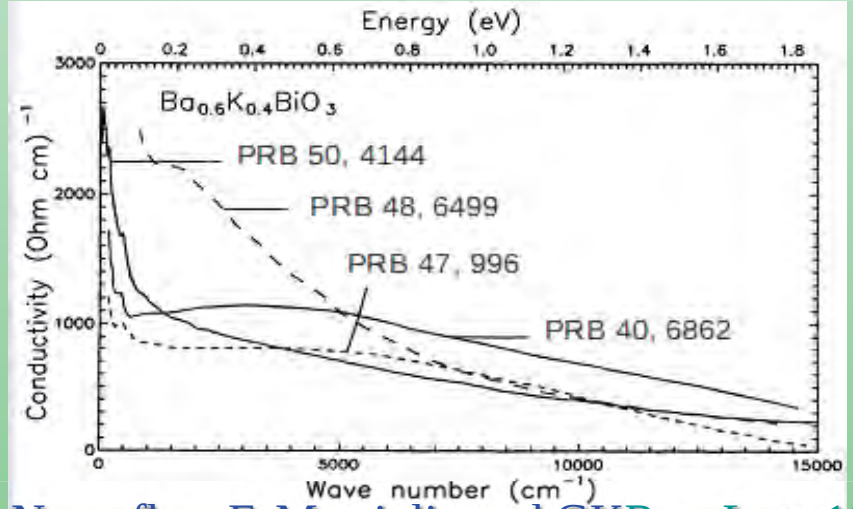
Z. P. Yin,* A. Kutepov, and G. Kotliar

Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, United States

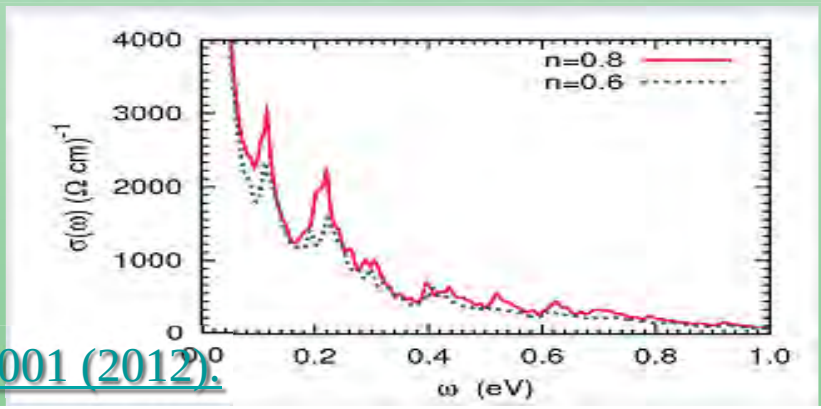
(Received 26 September 2012; revised manuscript received 7 March 2013; published 30 May 2013)

We show that the electron-phonon coupling (EPC) in many materials can be significantly underestimated by the standard density-functional theory (DFT) in the local-density approximation (LDA) due to large nonlocal correlation effects. We present a simple yet efficient methodology to evaluate the realistic EPC, going beyond the LDA by using more advanced and accurate *GW* and screened-hybrid-functional DFT approaches. The corrections that we propose explain the extraordinarily high superconducting temperatures that are observed in two distinct classes of compounds—the bismuthates and the transition-metal chloronitrides—thus solving a 30-year-old puzzle. Our work calls for the critical reevaluation of the EPC of certain phonon modes in many other materials, such as cuprates and iron-based superconductors. The proposed methodology can be used to design new correlation-enhanced high-temperature superconductors and other functional materials that involve electron-phonon interaction.

Our proposal: the correlation enhancement of λ relative to its LDA estimate is responsible for superconductvity in BaKBiO3 ($\lambda \sim .1$) , Occurs in many other systems close to an insulating state. This is what charcaterizes the "Other High Temperature superconductors". HfNCl, Borocarbides, Bucky Balls.



Anomalous optical conductivity in the metallic region can be understood within DMFT $\lambda \sim .1$.



R. Nourafkan F. Marsiglio and GK Rev. Lett. 109, 017001 (2012).

PHYSICAL REVIEW B VOLUME 46, NUMBER 21 1 DECEMBER 1992-I

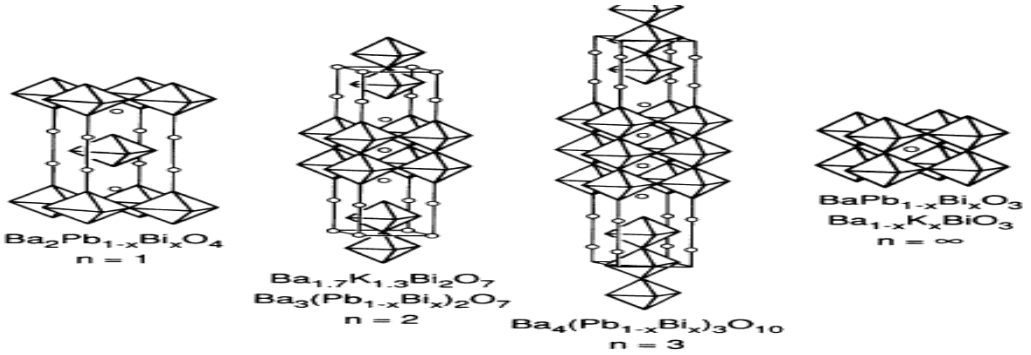
Synthesis and characterization of $Ba_3(Pb_{1-x}Bi_x)_2O_7$

R. J. Cava and H. Takagi
AT&T Bell Laboratories, Murray Hill, New Jersey 07974

H. W. Zandbergen
National Centre for High Resolution Electron Microscopy, Technical University, Delft, The Netherlands

B. Hessen, J. J. Krajewski, and W. F. Peck, Jr.
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
(Received 18 June 1992)

The synthesis and initial characterization of a layered perovskite-based lead-bismuth oxide are reported. The phase, $Ba_3(Pb_{1-x}Bi_x)_2O_7$, for $0 \le x \le 0.5$, is the $n=2$ member of the Ruddlesden-Popper series $A_{n+1}B_nO_{3n+1}$. It can be synthesized only under very narrowly defined conditions. Despite the analogy to the well-known three-dimensional perovskite superconductor $BaPb_{0.75}Bi_{0.25}O_3$, layered $Ba_3Pb_2O_7$ does not become superconducting (down to 1.8 K) on doping with Bi.

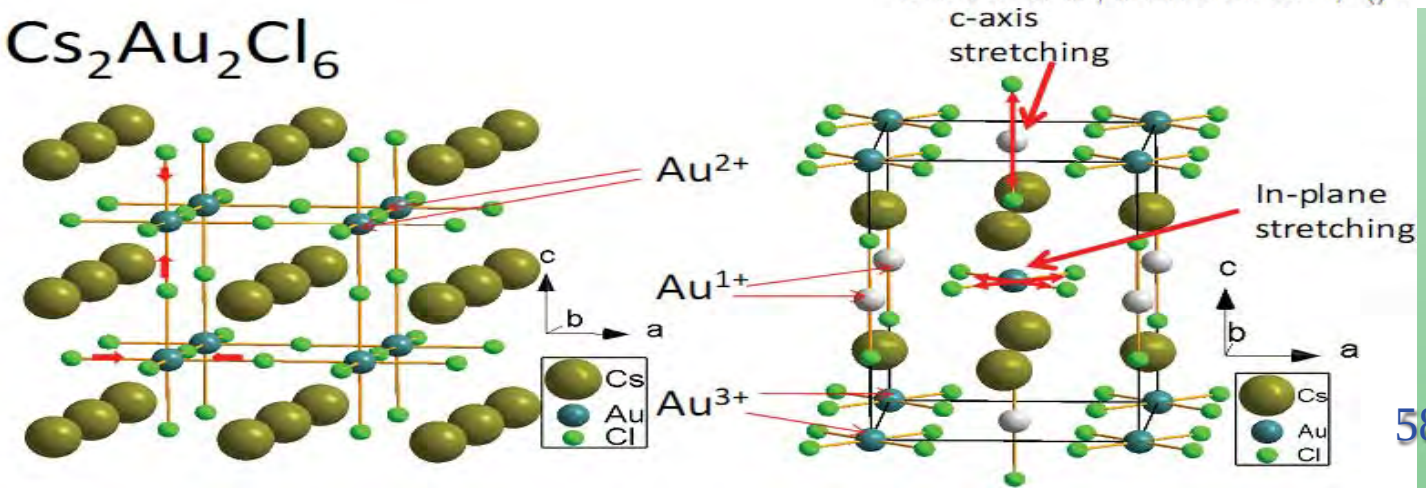


From 3d to 2d

but no Tc

Cs2 Au2Cl6 has been metallized under pressure no SC

KOJIMA N., *Bull. Chem. Soc. Jpn.*, **73** (2000) 1445-1460.
WANG S. *et al.*, *arXiv:1205.1077*, () .



From existing materials to new materials

- Analogous to $BaBiO_3$, same valence electrons

$Ba^{2+}Bi^{3+,5+}O_3^{2-}$

$Cs^{1+}Tl^{1+,3+}Cl_3^{1-}$ → $CsTlCl_3$

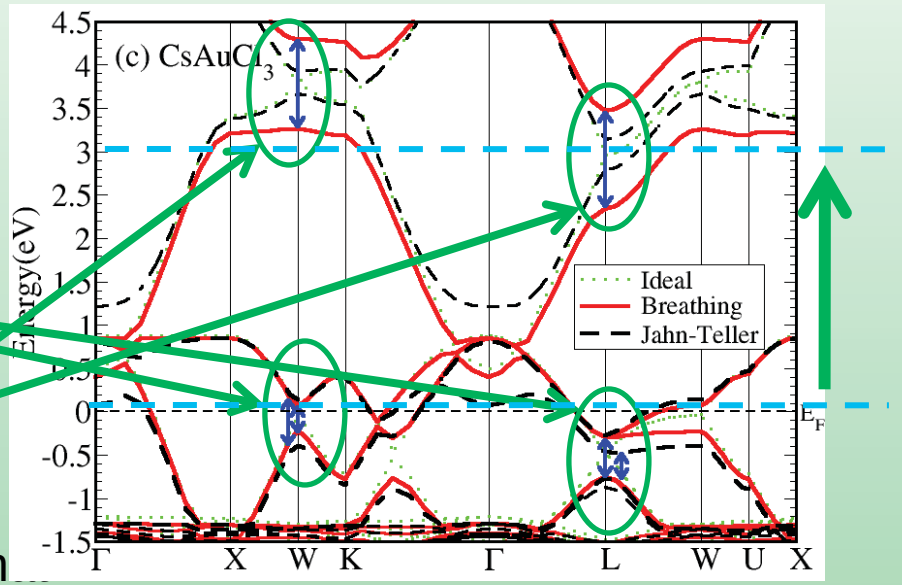
- Starting from $CsAuCl_3$

weak phonon coupled bands near Fermi level

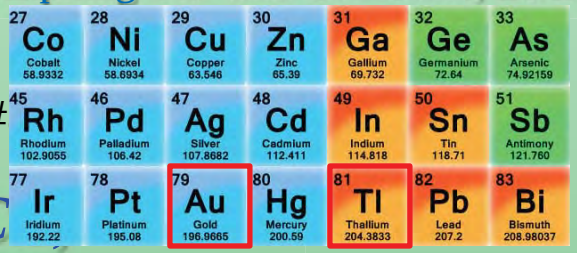
strong phonon coupled bands at about 3 eV above Fermi level

→needs to move Fermi level such th… the strongly phonon coupled bands operating at phonon energies.

2 electrons/f.u. is needed, Au(#79)→ Tl (#…



Ziphing Yin and G. Kotliar, *EPL* **101**,



Candidate materials: *Cs*TlC…

generally $ATlX_3$, where *A*=K, Rb, Cs; *X*=F, Cl, Br

epl A Letters Journal Exploring the Frontiers of Physics

January 2013

EPL, **101** (2013) 27002
doi: 10.1209/0295-5075/101/27002

www.epljournal.org

Rational material design of mixed-valent high-T_c superconductors

Z. P. Yin and G. Kotliar

Department of Physics and Astronomy, Rutgers University - Piscataway, NJ 08854, USA

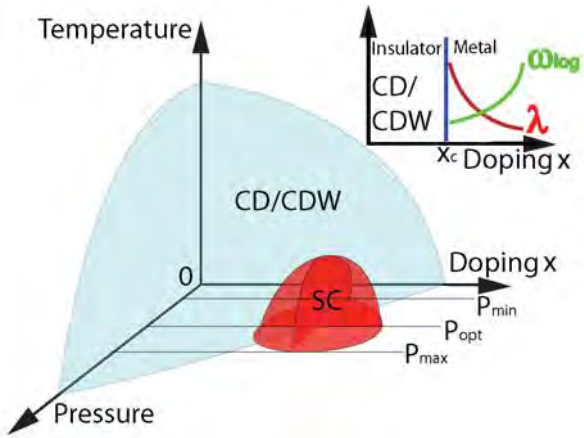
Abstract – We design, from first principles calculations, a novel family of thallium halide-based compounds as candidates for new high temperature superconductors, whose superconductivity is mediated by the recently proposed mechanism of non-local correlation-enhanced strong electron-phonon coupling. Two prototype compounds namely $CsTlF_3$ and $CsTlCl_3$ are studied with various hole doping levels and volumes. The critical superconducting temperature T_c are predicted to be about 30 K and 20 K with ∼0.35/f.u. hole doping and require only modest pressures (∼5 and ∼2 GPa), respectively. Our procedure of designing this class of superconductors is quite general and can be used to search for other "other high temperature superconductors".

To check the energetic stability, we consider here

The materials are not in the ICSD database

The parent compound should be easy to make

It should be hard to dope



currently existing compound Cs_3TlF_6 and a thesis reaction: $3CsF+TlF_3 \rightarrow Cs_3TlF_6+Q$. actually absorbs about 1.7 eV energy per (164 kJ/mol) according to our DFT-GGA Therefore, $CsTlF_3$ is more energetically favored than the existing Cs_3TlF_6 compound.

Synthesis and properties of charge-ordered thallium halide perovskites, CsTl1+0.5Tl3+0.5X3 (X = F, Cl)- theoretical precursors for superconductivity?

Maria Retuerto , Thomas J Emge , Joke Hadermann , Peter W. Stephens , Man-Rong Li , Zhiping P. Yin , Mark C. Croft , Alexander Ignatov , Si-Jia Zhang , Zhen Yuan , Changqing Jin , Jack W. Simonson , Meigan C. Aronson , Athena Pan , Dimitri N. Basov , Gabriel Kotliar , and Martha Greenblatt

***Chemistry of Materials* 25** (20), 4071 (2013).

Two phases

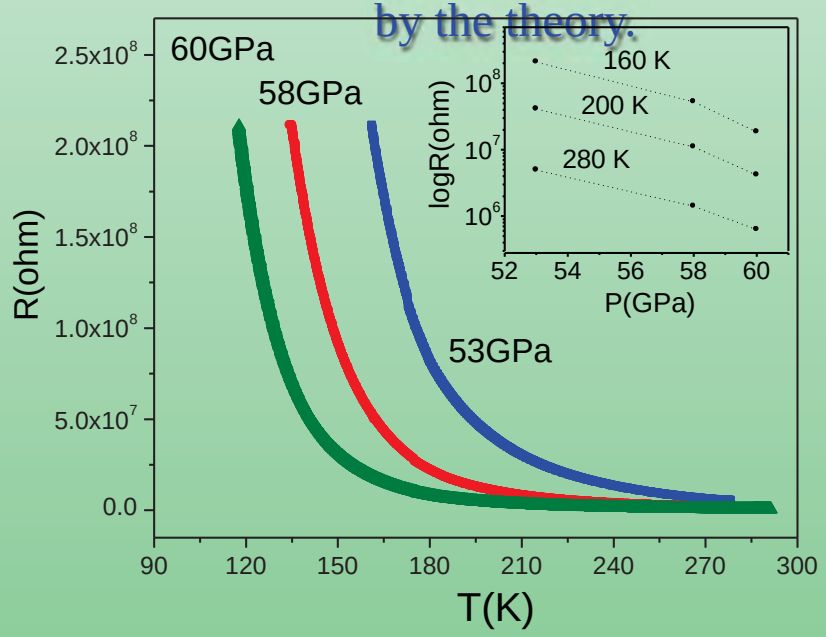
One tetragonal the other cubic

Charge ordered mixed valent Insulator, value of gap~ 2 ev correctly predicted

by the theory.

Attempts to dope were unsuccessful so far…

Good topic for discussion!

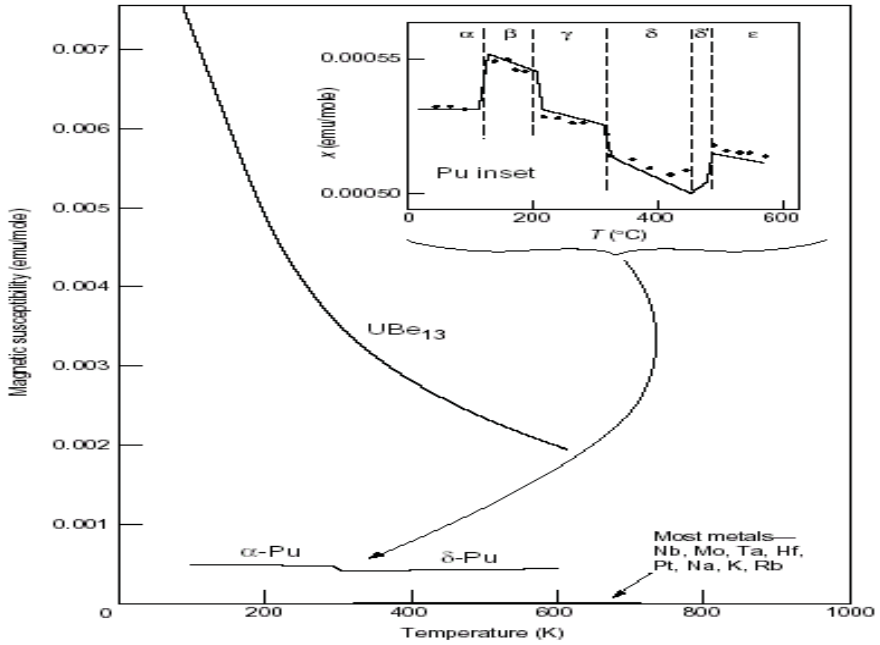


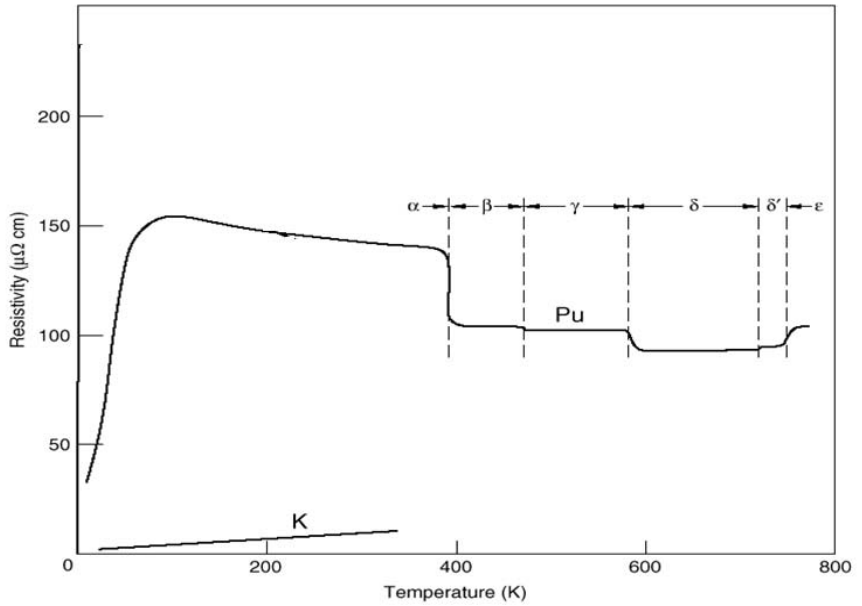
Outline

- Introduction to correlations in solids. Static and Dynamic Correlations.
- Brief introduction to DMFT + electronic structure.
- Roads to correlations, Mott vs Hund. Vanadium Oxides vs Iron pnictides and chalcogenides.
- Actinides.
- Static correlations, $BaBiO_3$ and their analogs.
- Conclusions.

Plutonium Metal

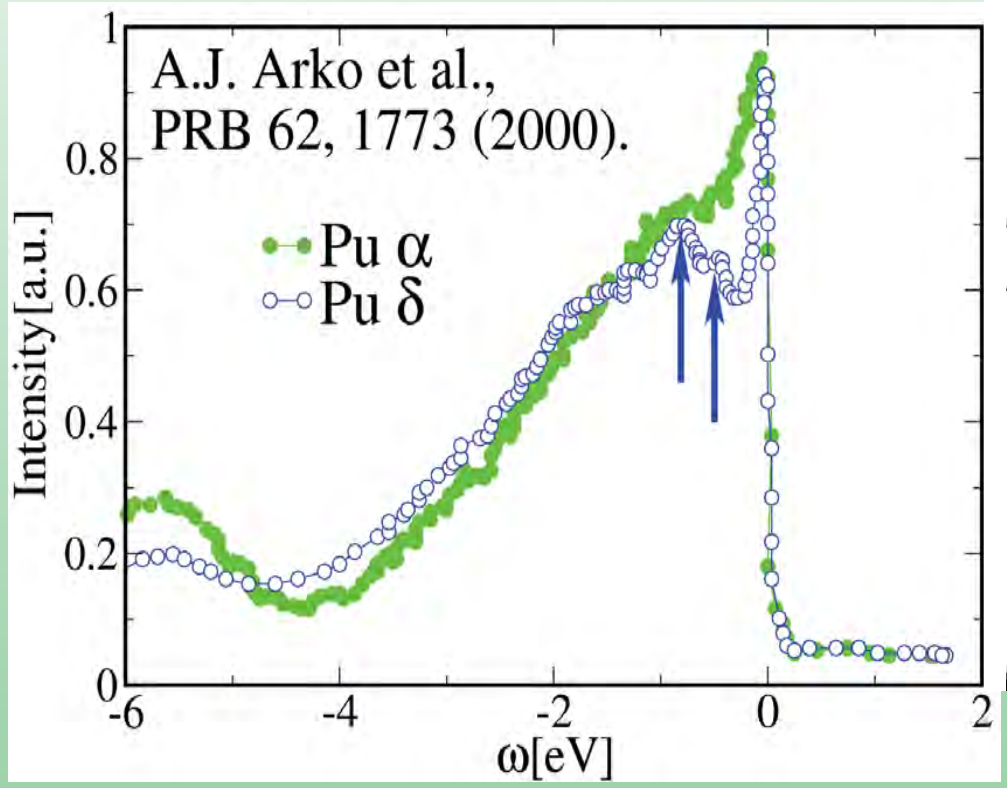
- Multitude of phases, many elastic anomalies
- Thermodynamic and transport and spectroscopic anomalies .DMFT approach, *(Savrasov, Kotliar, Abrahams, Nature (2001).* delta Pu

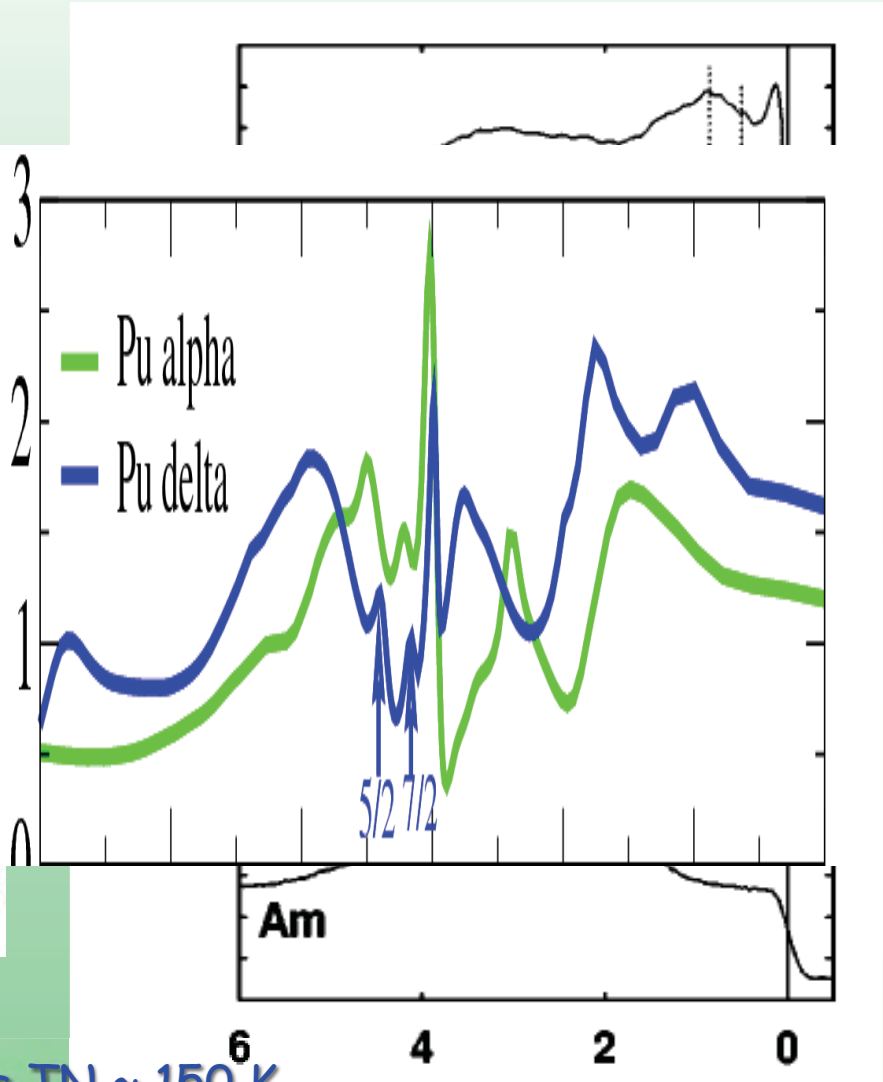




Photoemision Magnetism

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



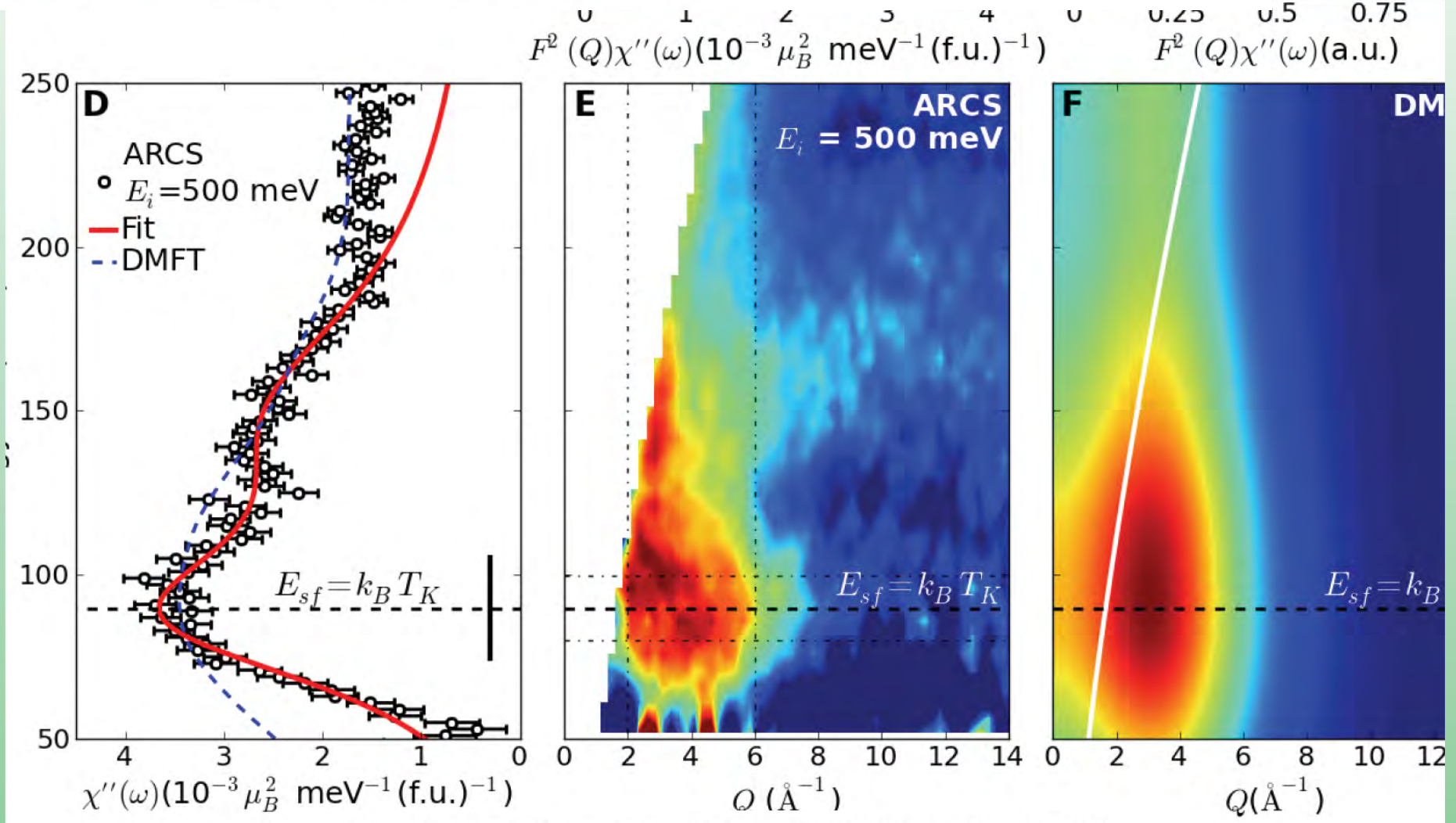


Pu is non magnetic – Cm is magnetic TN ~ 150 K.

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

The valence-fluctuating ground state of plutonium

Marc Janoschek,[1]* Pinaki Das,[1†] Bismayan Chakrabarti,[2] Douglas L. Abernathy,[3] Mark D. Lumsden,[3] John M. Lawrence,[1] Joe D. Thompson,[1] Gerard H. Lander,[4] Jeremy N. Mitchell,[1] Scott Richmond,[1] Mike Ramos,[1] Frans Trouw,[1] Jian-Xin Zhu,[1] Kristjan Haule,[2] Gabriel Kotliar,[2] Eric D. Bauer[1]



Janoschek *et al.* Sci. Adv. 2015;1:e1500188 10 July 2015

Slave Boson Theory of Orbital Differentiation with Crystal Field Effects: Application to UO_2

Nicola Lanatà,[1] Yongxin Yao,[2] Xiaoyu Deng,[3] Vladimir Dobrosavljević,[1] and Gabriel Kotliar[3,4]

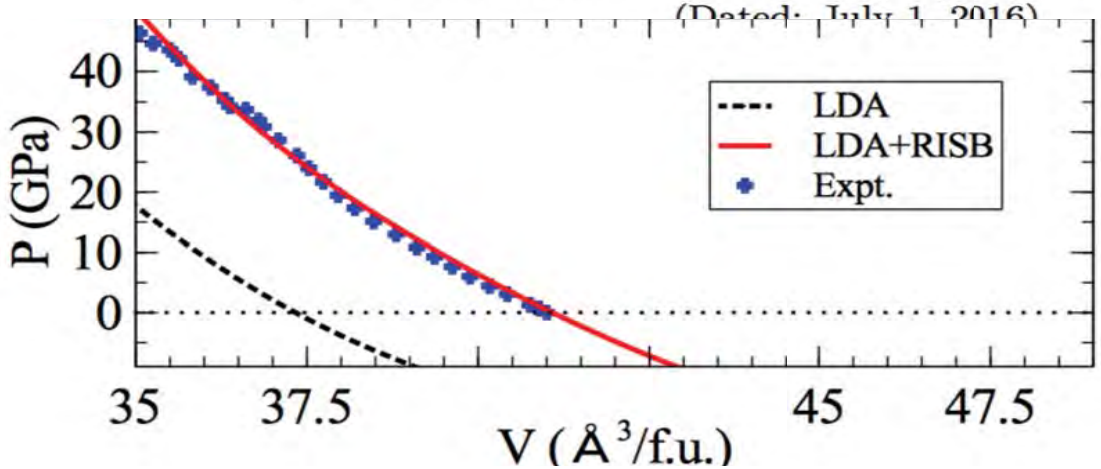
[1] *Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA*

[2] *Ames Laboratory-U.S. DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa IA 50011, USA*

[3] *Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08856-8019, USA*

[4] *Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratories, Upton, NY 11973-5000, USA*

(Dated: July 1, 2016)



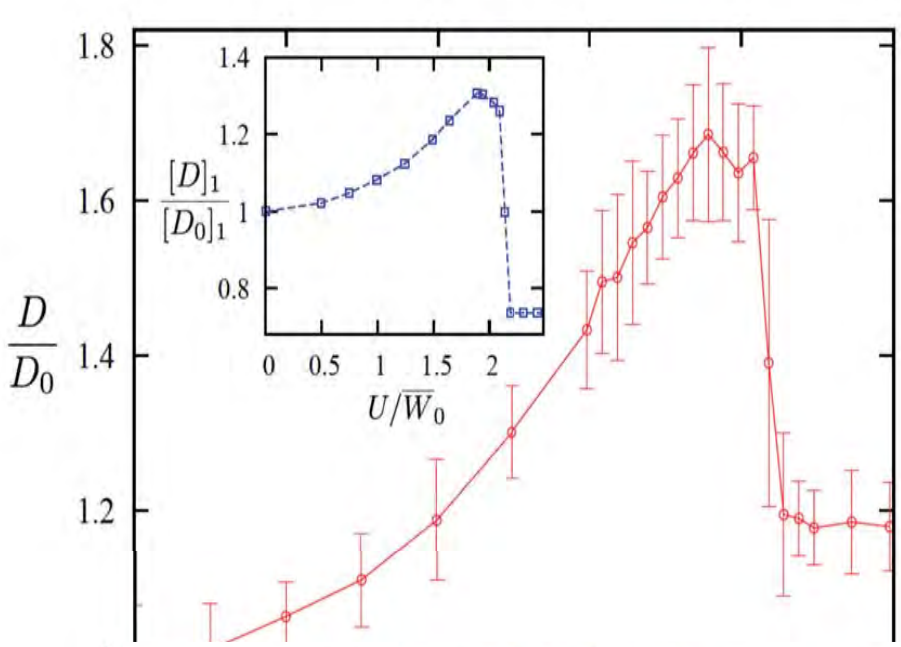
Need to probe excited states with better resolution.

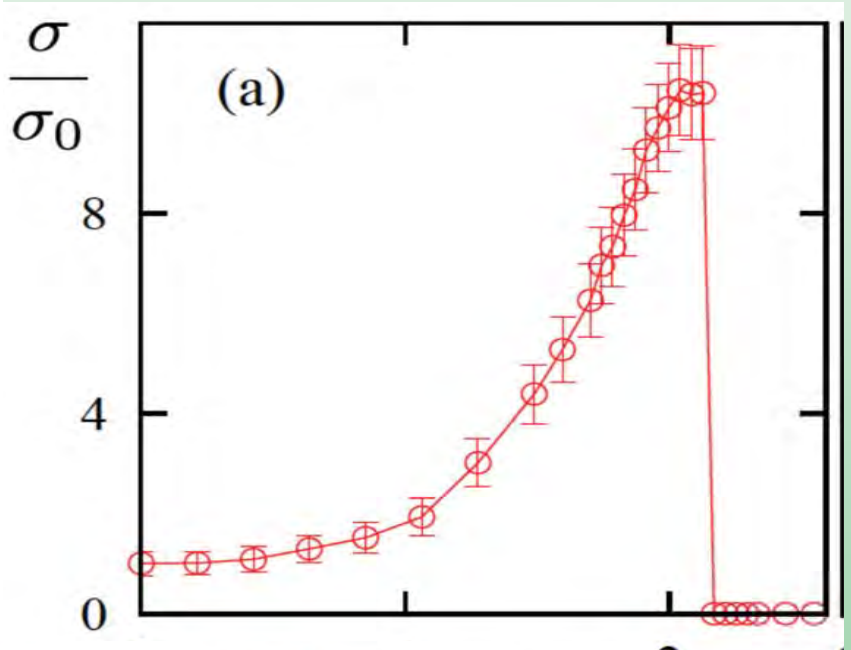
We derive an exact operatorial reformulation of the rotational invariant slave boson method and we apply it to describe the orbital differentiation in strongly correlated electron systems starting from first principles. The approach enables us to treat strong electron correlations, spin-orbit coupling and crystal field splittings on the same footing by exploiting the gauge invariance of the mean-field equations. We apply our theory to the archetypical nuclear fuel UO_2, and show that the ground state of this system displays a pronounced orbital differention within the $5f$ manifold, with Mott localized Γ_8 and extended Γ_7 electrons.

Mott transition in a metallic liquid – Gutzwiller molecular dynamics simulations

Gia-Wei Chern,[1,2,3] Kipton Barros,[1,2] Cristian D. Batista,[1,2] Joel D. Kress,[1] and Gabriel Kotliar[4]

[1] *Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2] *Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[3] *Department of Physics, University of Virginia, Charlottesville, VA 22904, USA*
[4] *Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019, USA*





$$\mathcal{H}_e = \sum_{i\neq j}\sum_{\sigma} t(|\mathbf{r}_i - \mathbf{r}_j|)c^{\dagger}_{i,\sigma}c_{j,\sigma} + U\sum_i n_{i,\uparrow}n_{i,\downarrow}$$
$$+\frac{1}{2}\sum_{i\neq j}\phi(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_i \frac{|\mathbf{p}_i|^2}{2m}.$$

Conclusions

- DMFT self consistent Quantum Impurity Model:

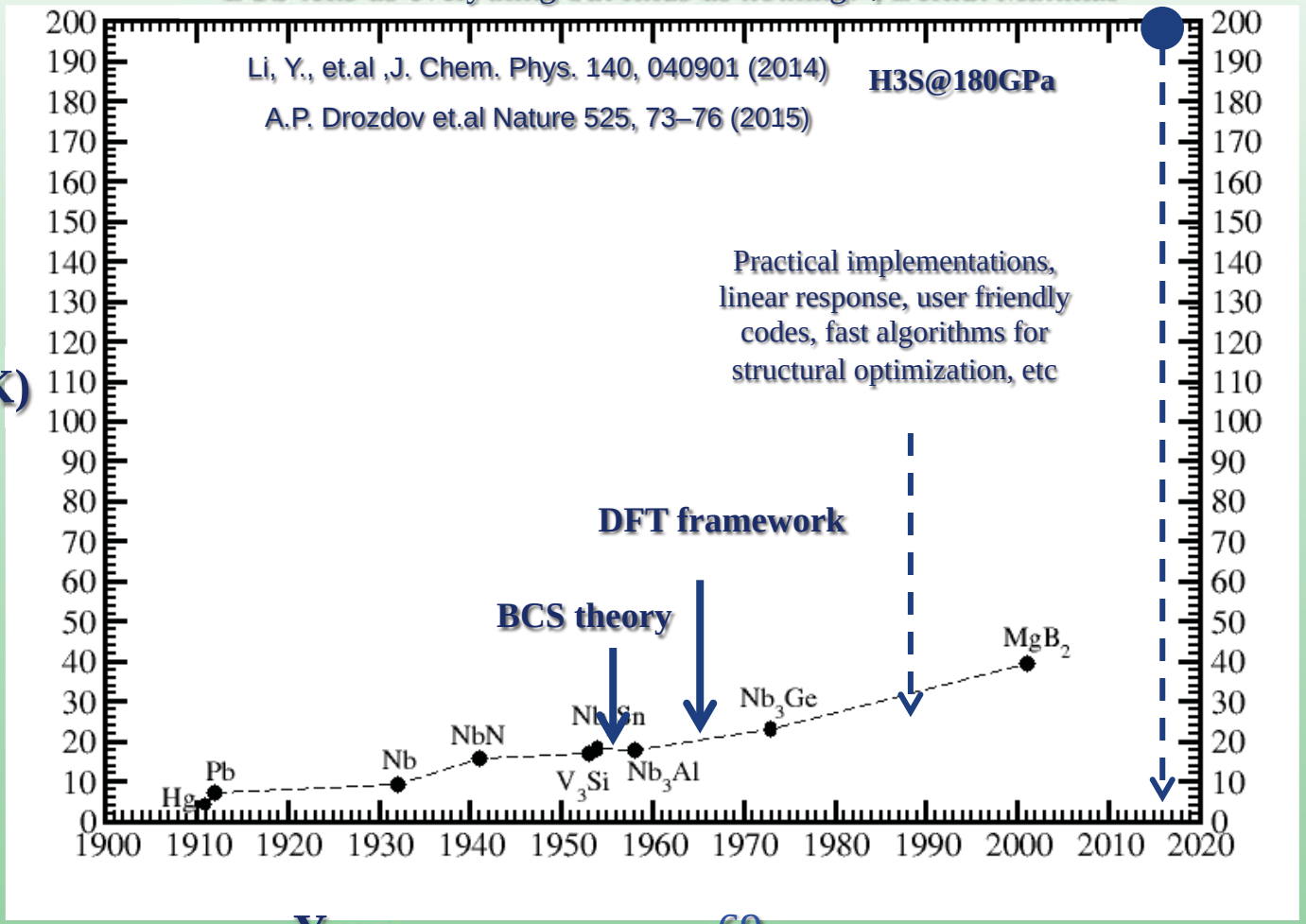
NON GAUSSIAN reference frame.

- (Dynamical) mean field theory gives a zeroth order picture of strongly correlated materials.
- Focused mostly on the normal state.
- Two distinct routes to strong correlations: Mott vs Hunds.
- Temperature dependent electronic structure.
- Reorganization of the degrees of freedom is non local in energy.
- Clear progress in the field of correlated electron systems.

68

Perspective: phonon mediated Tc

"BCS tells us everything but finds us nothing.", Berndt Matthias

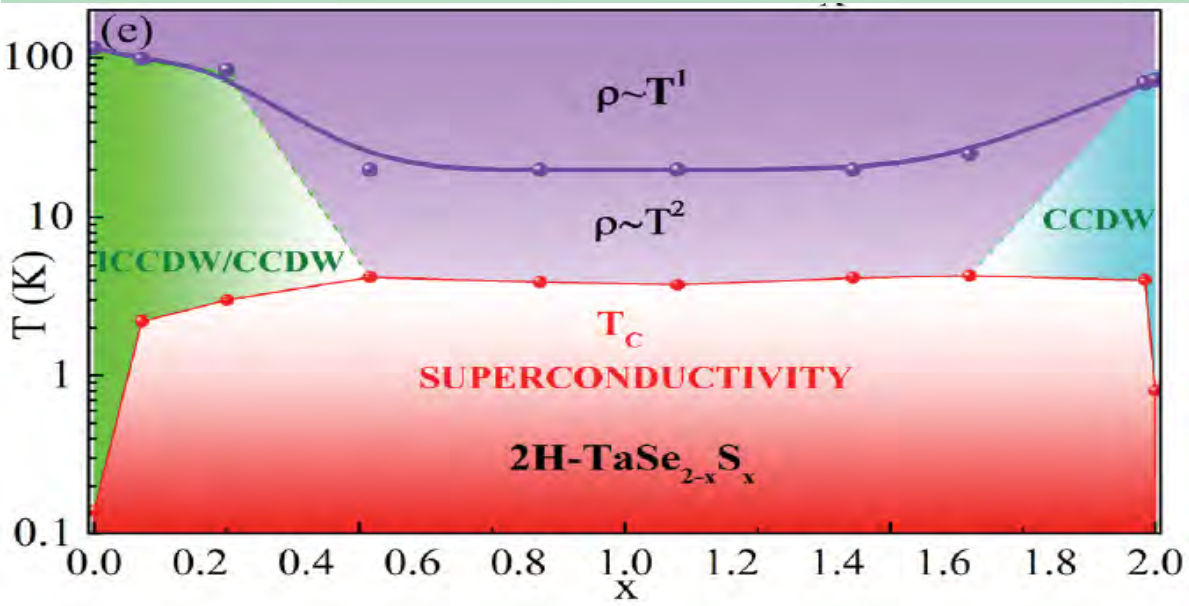


Superconducting Order from Disorder in 2H-$TaSe_{2-x}S_x$

Lijun Li[1,2,†], Xiaoyu Deng[3], Zhen Wang[1], Yu Liu[1], A. M. Milinda Abeykoon[4], E. Dooryhee[4], A. Tomic[5], Yanan Huang[1,*], J. B. Warren[6], E. S. Bozin[1], S. J. L. Billinge[1,5], Y. P. Sun[2,7], Yimei Zhu[1], G. Kotliar[1,3] and C. Petrovic[1,†]

TaSe2 TaS2 archetypical CDW material, low Tc (Tc < .1 K) s Mixing them raises Tc by an order of magnitude to 4K.

T. Smith et. al. *J. Phys. F: Metal Phys.* **5**, 1713 (1975).



Homework:

Find Other Examples using the tools you learn in this school.

Thank you for your attention!!!