Introduction to LDA+DMFT

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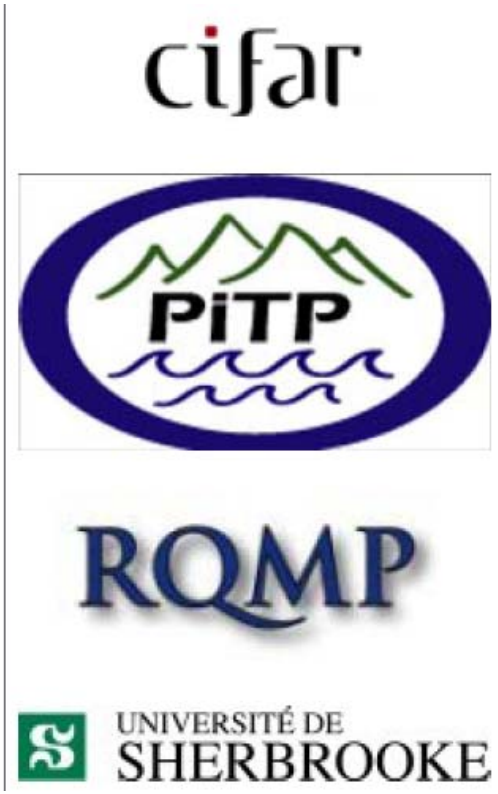

CIFAR-PITP International Summer School on Numerical Methods for Correlated Systems in Condensed Matter
June 1-2 2008

Plan of the lectures

- Motivate the development of a mean field theory of correlated electron materials.
- General formulations of mean field theory: density functional theory, DMFT, spectral density functional, LDA+DMFT.
- Applications to the Mott transition.
- Some applications of LDA+DMFT
- More foundations, extensions, issues of implementation, applications.

Electronic structure calculations with dynamical mean-field theory: *G. Kotliar, S. Savrasov, K. Haule, V. Oudovenko, O. Parcollet, and C. Marianetti*, ***Rev. Mod. Phys. 78, 000865 (2006).***

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Pressure Driven Mott Transition

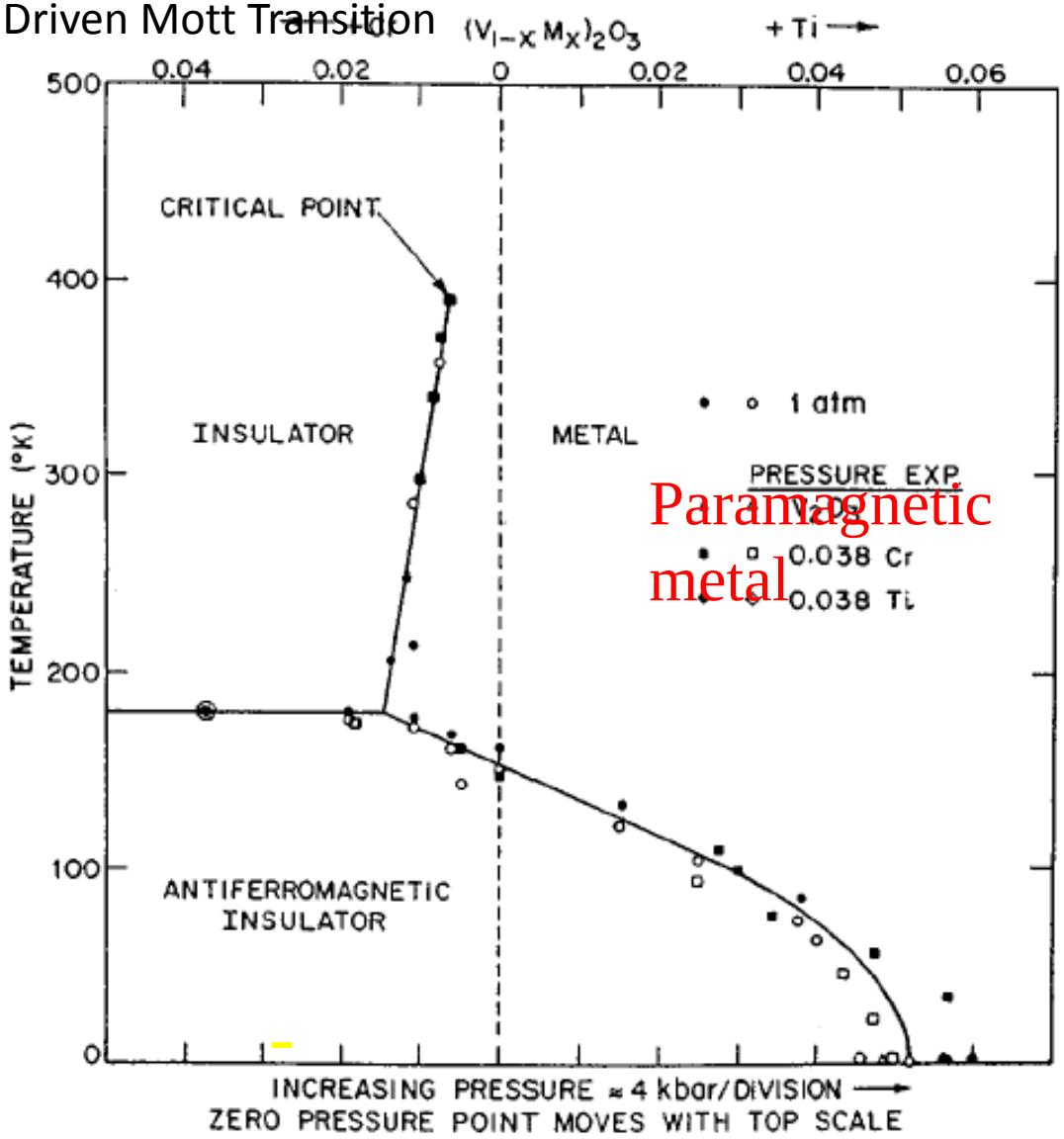
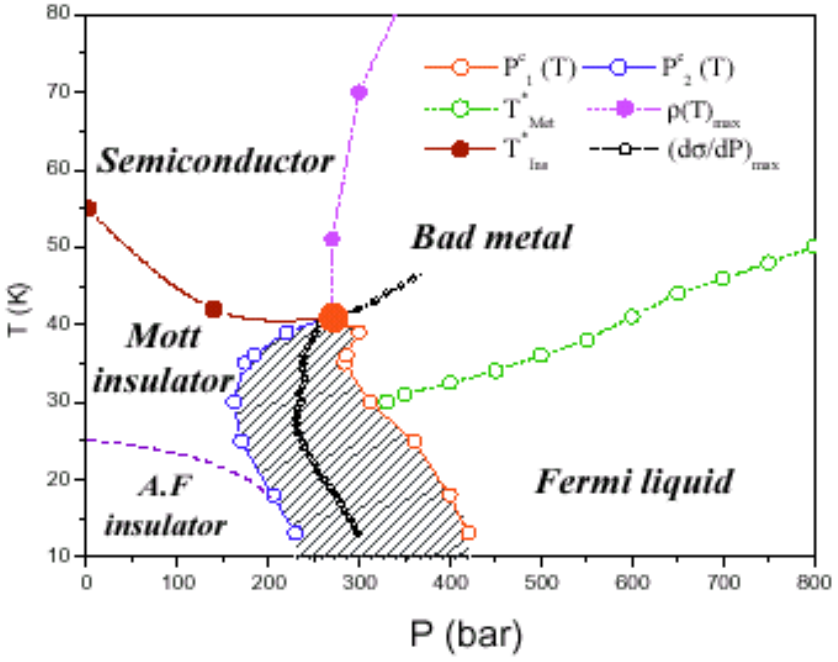


FIG. 70. Phase diagram for doped V_2O_3 systems, $(V_{1-x}Cr_x)_2O_3$ and $(V_{1-x}Ti_x)_2O_3$. From McWhan *et al.*, 1971, 1973.

Mott transition and transport crossovers in the organic compound κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl



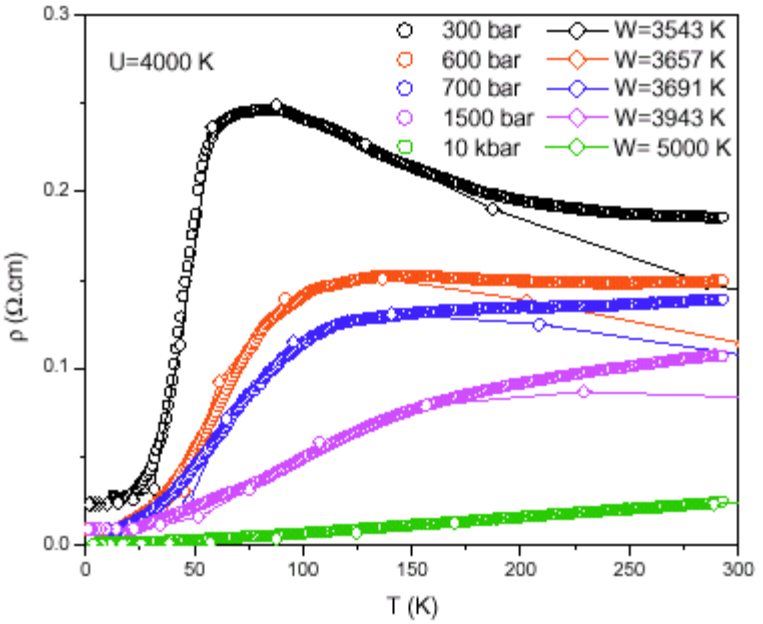


FIG. 6: Temperature-dependence of the resistivity at different pressures. The data (circles) are compared to a DMFT-NRG calculation (diamonds), with a pressure dependence of the bandwidth as indicated. The measured residual resistivity ρ_0 has been added to the theoretical curves.

P. Limelette et al., PRL 91 (2003) 016401

See also:

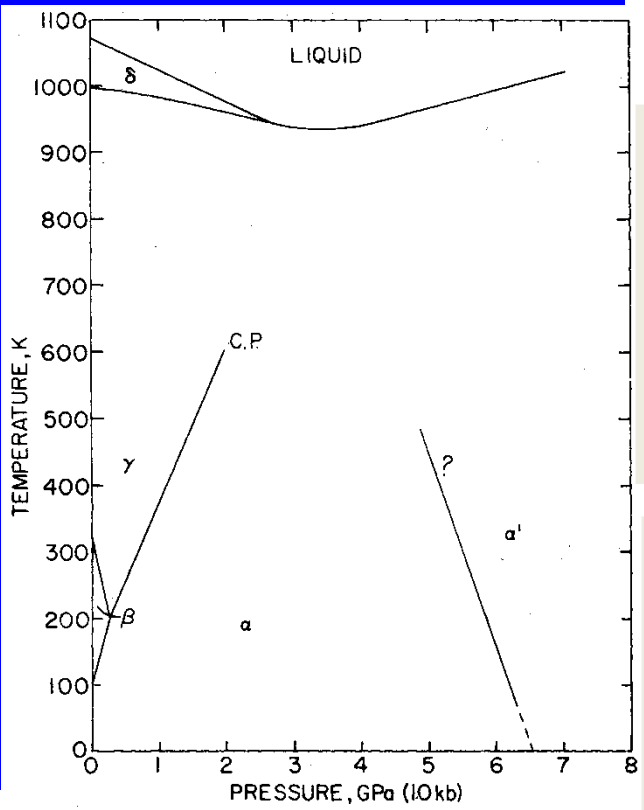
Kagawa et al. cond-mat/0307304

S.Lefebvre et al. :
Phys. Rev. Lett. 85 (2000) p. 5420

Cerium

- Various phases :
  isostructural phase transition (T=298K, P=0.7GPa)
  γ (fcc) phase
  [magnetic moment (Curie-Wiess law)]
  $\rightarrow$ α (fcc) phase
  [loss of magnetic moment (Pauli-para)]

with large volume collapse
$\Delta v/v \approx 15\%$
(γ -phase a $\cong$ 5.16 Å
α-phase a $\cong$ 4.8 Å)



volumes	exp.	LDA	LDA+U
α	28Å^3	24.7Å^3	
γ	34.4Å^3		35.2Å^3

- γ *-phase* (localized):

High T phase
- Curie-Weiss law (localized magnetic moment),
- Large lattice constant
- Tk around 60-80K

- α*-phase* (delocalized:Kondo-physics):

Low T phase
- Loss of Magnetism (Fermi liquid Pauli susceptibility) - completely screened magnetic moment
- smaller lattice constant
- Tk around 1000-2000K

Localization Delocalization in Actinides

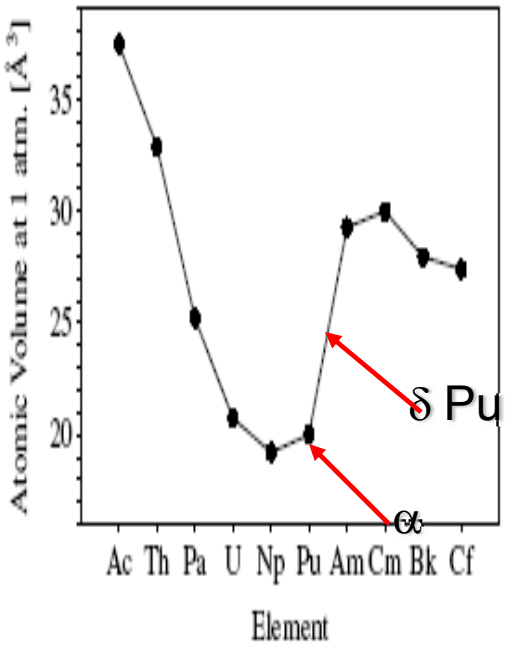
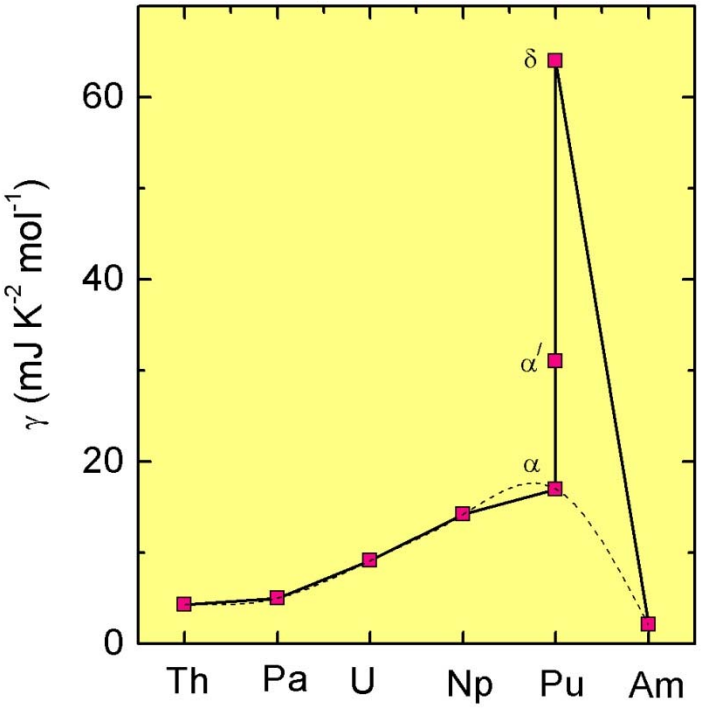


Figure 1. Atomic volumes of actinide metals at atmospheric pressure and 25 °C.



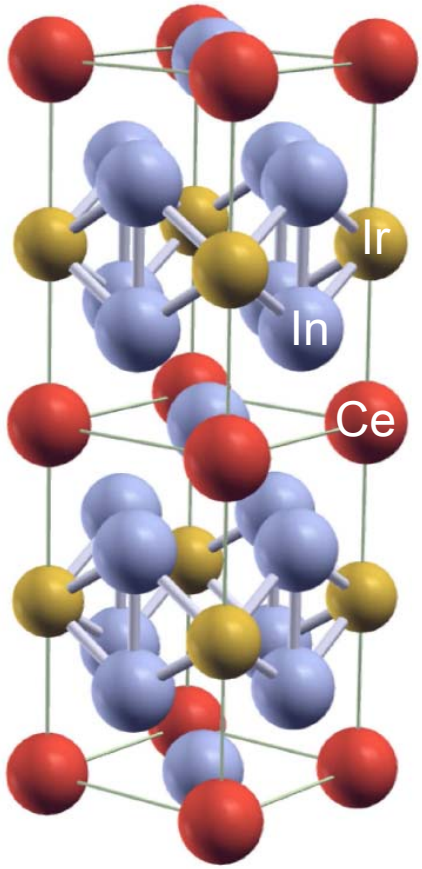
Modern understanding of this phenomena using functional approach toDMFT. K Haule S.Savrasov J Shim

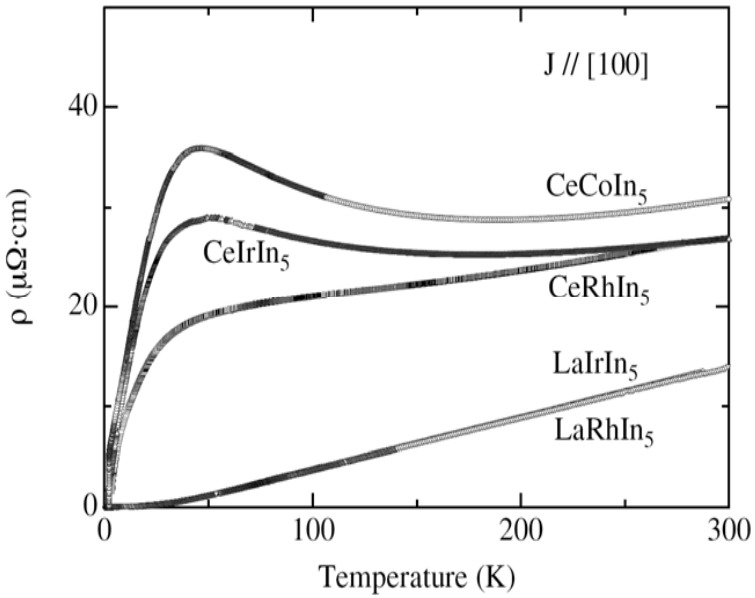
Strongly correlated materials do “big” things Competition of localization and itineracy.

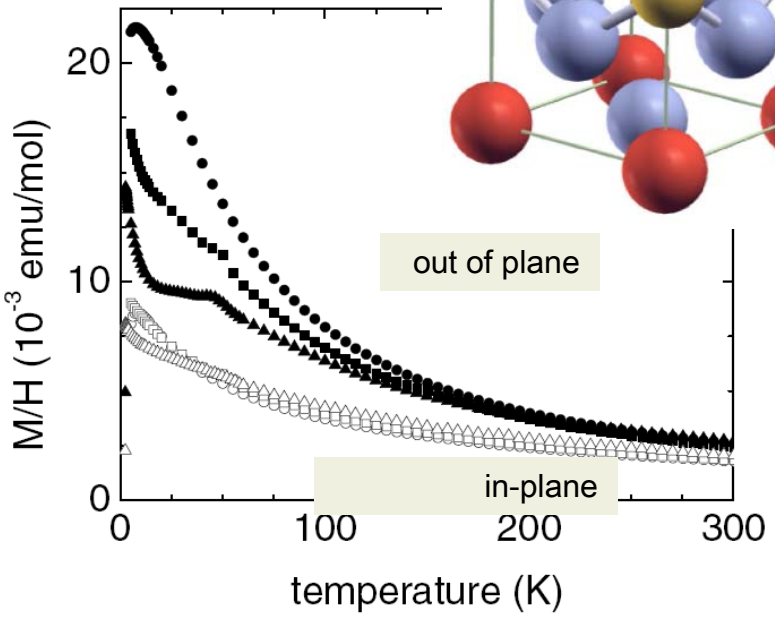
- Huge volume collapses in lanthanides and actindies, eg. Ce , Pu, …….
- Metal insulator transitions as a function of pressure an composition in transition metal oxides, VO2 V2O3
- Quasiparticles with large masses m* =1000 mel in Ce and U based heavy fermions.
- Colossal Magnetoresistance in La1-xSrxMnO3
- High Temperature Superconductivity. 150 K $Ca_2Ba_2Cu_3HgO_8$.
- Large thermoelectric response in $Na_xCo_2O_4$
- 50K superconductivity in SmO1-xFxFeAs
- Many others……

$CeMIn_5$ M=Co, Ir, Rh

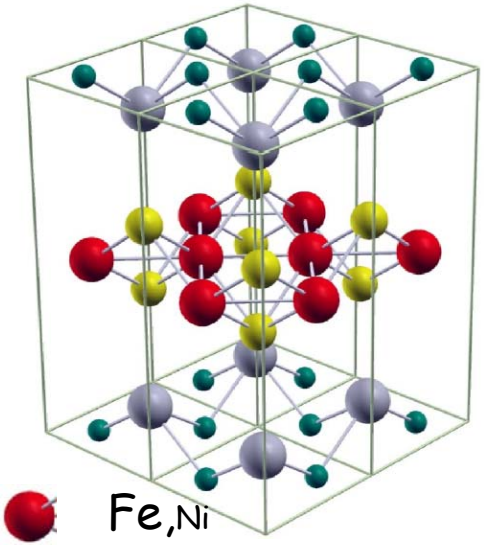
- CeRhIn5: TN=3.8 K; $\gamma \approx 450$ mJ/molK2
- CeCoIn5: Tc=2.3 K; $\gamma \approx$ 1000 mJ/molK2; • CeIrIn5: Tc=0.4 K; $\gamma \approx 750$ mJ/molK2







Iron based high-Tc superconductors



Fe,Ni

As,P

La,Sm,Ce

O

x~5-20%

Smaller c

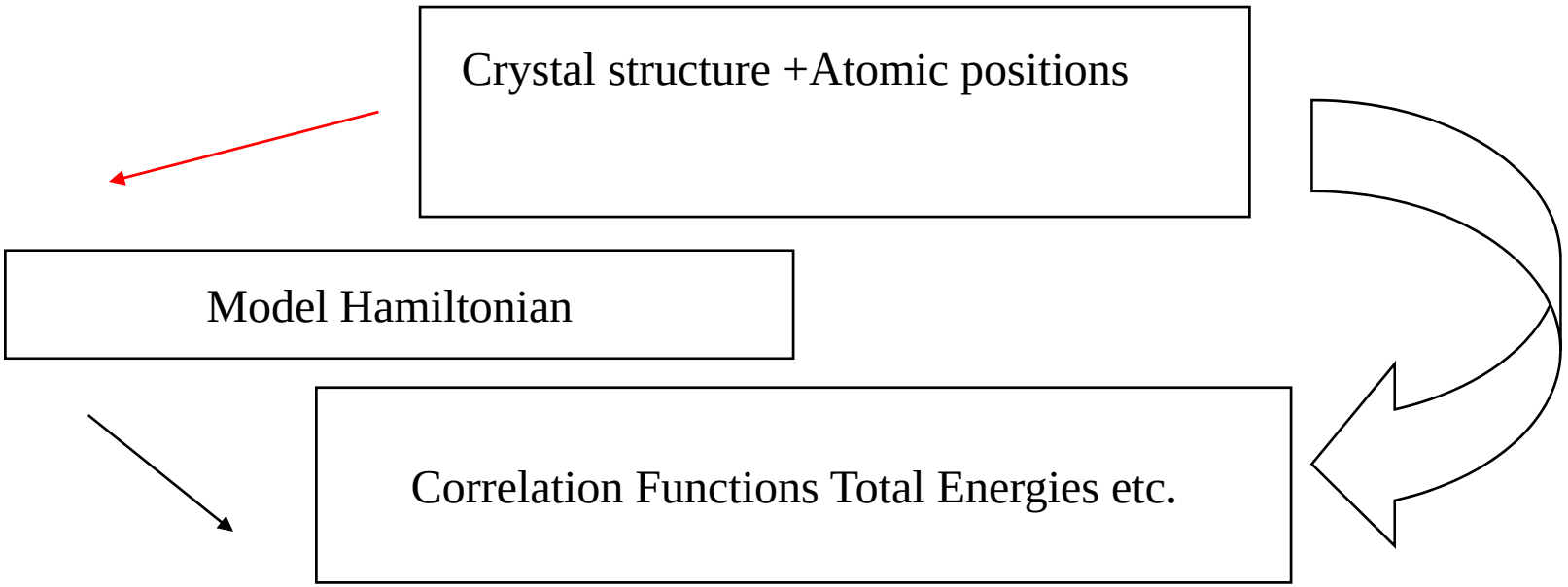
Higher T_c

LaOFeP	**3.2K**, JACS-2006 a=3.964A, **c=8.512A**
$SmF_xO_{1-x}FeAs$ **c)**	**55K**, cm/0803.3603 a=3.940A, **c=8.496A**
$PrF_xO_{1-x}FeAs$ **d)**	**52K**, unpublished a=3.985A, **c=8.595A**
$CeF_xO_{1-x}FeAs$ **b)**	**41 K**, cm/0803.3790 a=3.996A, **c=8.648A**
$LaF_xO_{1-x}FeAs$ **a)**	**26 K**, JACS-2008 a=4.036A, **c=8.739 A**
$La_{1-x}Sr_xOFeAs$	**25K**, cm/0803.3021, a=4.035A, **c = 8.771A**
$LaCa_xO_{1+x}FeAs$	**0 K**
$LaF_xO_{1-x}NiAs$	**2.75K**, cm/0803.2572a =4.119A , **c=8.180A**
$La_{1-x}Sr_xONiAs$	**3.7K**, cm/0803.3978 a=4.045A, **c=8.747A**

a) Y. Kamihara et.al., Tokyo, JACS
b) X.H. Chen, et.al., Beijing, cm/0803.3790
c) G.F. Chen et.al., Beijing, cm/0803.3603
d) Z.A. Ren et.al, Beijing, unpublished

- 2D square lattice of Fe
- Fe - magnetic moment

Two paths for ab-initio calculation of electronic structure of strongly correlated materials



Mean field ideas can be used in both cases.

Mean Field Theory : general construction principles

Spectral density functional. Effective action construction.e.g Fukuda et.al

$$Z = e^{-F[J]} = \int d\psi d\psi^{+} e^{-[S(\psi^{+}\psi)+JA]}$$

$$\frac{\delta F}{\delta J}[J] = < A > = a$$

$$\Gamma[a] = F[J[a]] - aJ[a]$$

$$S = S_0 + \lambda S_{\text{int}}$$

$$J = J_0 + \lambda J_1 + \cdots$$

$$\Gamma[a] = F_0[J_0] - aJ_0 + \lambda\Delta\Gamma[a] + \cdots$$

$$\Delta\Gamma = \Gamma_{hartree} + \Gamma_{xc}$$

$$\Delta\Gamma[a] = \int_0^1 d\lambda < S_{\text{int}} > (\lambda, J(\lambda, a))$$

In practice we need good approximations to the exchange correlation, in DFT LDA. In spectral density functional theory, DMFT. Review: Kotliar et.al. Rev. Mod. Phys. **78**, 865 (2006)

$$\frac{\delta F}{\delta J_0}[J_0] = a \qquad \frac{\delta \Delta\Gamma}{\delta a} = J_0[a]$$

Kohn Sham equations

Remarks:

- Exact functionals of an observable A, $\Gamma_{exact}[a]$
- In practice approx are needed $\Gamma_{mft}[a] \sim \Gamma_{exact}[a]$
- Many a's many theories.

- Introduction of a reference system. Separation into "free part" and exchange+ correlation.
- Formal expression for the correlation part of the exact functional as a coupling constant integration.
- Good approximate functionals obtained by approximating the xc part. [small parameter d helps!]
- While the construction aims to calculate <A>=a, other quantities, e.g. correlation functions, emerge as a byproduct.

Crucial Role of the constraining field

$J_0[a]$

Different reference systems [e.g. band limit or atomic limit] define different constraining fields.

- Different functionals (self energy functional, BK functional, Harris Foulkes functional, etc)

$$\Gamma[a], \Gamma[a, J], \Gamma[a, J_0], \Gamma[J_0]$$

Analogy with spin systems.

Density functional and Kohn Sham reference system

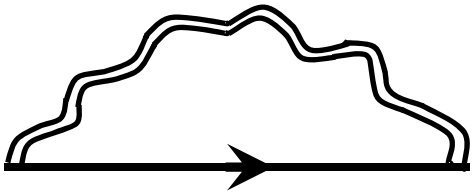
$$-\nabla^2/2 + V_{KS}(r)\,\psi_{kj} = \varepsilon_{kj}\psi_{kj}$$

$$\rho(r) = \sum_{kj} f(\varepsilon_{kj})\,|\psi_{kj}(r)|^2$$

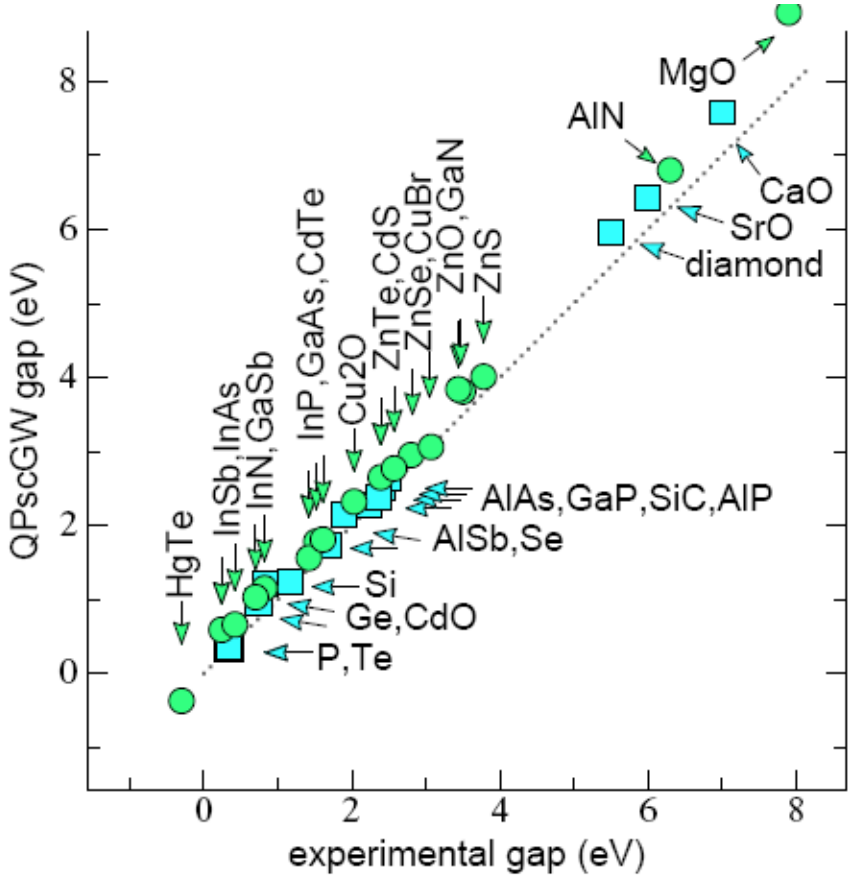
$$V_{KS}(r)[\rho(r)] = V_{ext}(r) + \int \frac{\rho(r')}{|r-r'|}dr' + \frac{\delta E_{xc}}{\delta\rho(r)}[\rho]$$

- Kohn Sham spectra, proved to be an excellent starting point for doing perturbation theory in screened Coulomb interactions GW.

Kohn Sham Eigenvalues and Eigensates: Excellent starting point for perturbation theory in the screened interactions (Hedin 1965)



Self Energy



VanShilfgaarde (2005)

Model Hamiltonians and DMFT

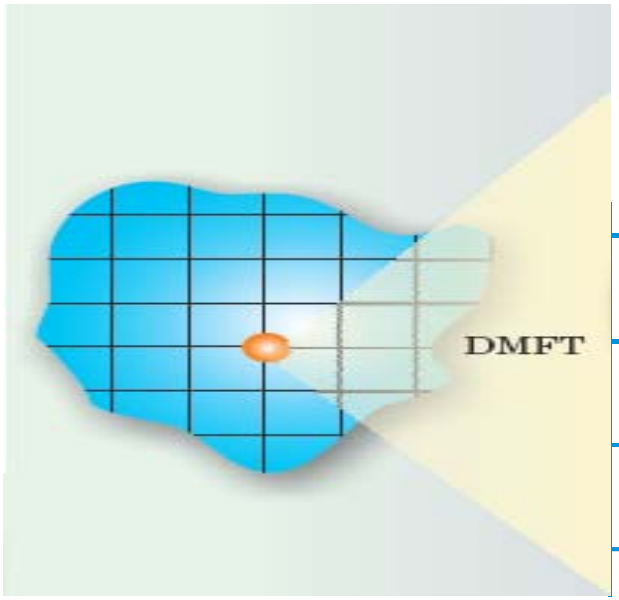
Dynamical Mean Field Theory. Cavity Construction.

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

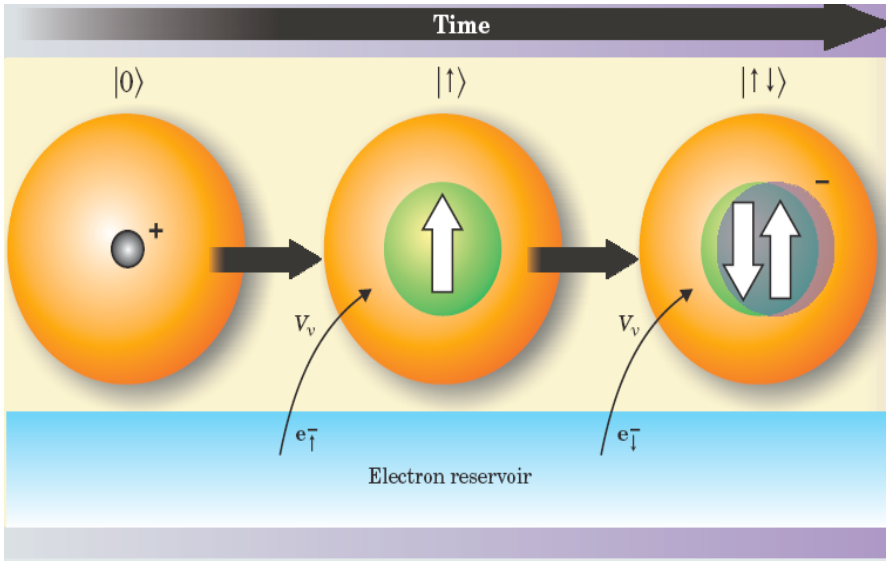
$$-\sum_{i,j} J_{ij} S_i S_j - h\sum_i S_i$$

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

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

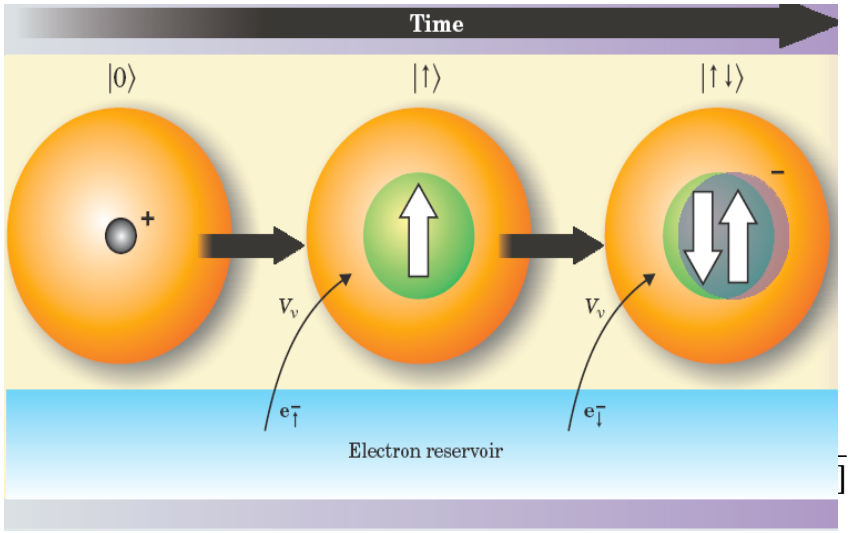


A(ω)



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

$$\int_0^\beta \int_0^\beta c^{\dagger}_{o\sigma}(\tau)[(\frac{\partial}{\partial\tau} + \mu)\delta(\tau - \tau') - \Delta(\tau - \tau')]c_{o\sigma}(\tau') + U\int_0^\beta n_{o\uparrow} n_{o\downarrow}$$



$A(\omega)$ $\Delta(\omega)$

Solving A for given bath, is not easy Impurity solvers; See P. Werner and M Jarrell's talks .

$$m_i = th[\beta \sum_j J_{ij} m_j + h]$$

$$i\omega_n - \Sigma(i\omega_n)[\Delta] \doteq -\Delta(i\omega_n) + \frac{1}{G_{imp}(i\omega_n)[\Delta]}$$

$$i\omega_n - \Sigma(i\omega_n)[\Delta] - t(k) + \mu = \mathrm{G}_{\mathrm{latt}}(i\omega_n, k)^{-1}$$

$$G_{imp}(i\omega_n)[\Delta] = \sum_k \mathrm{G}_{\mathrm{latt}}(i\omega_n, k)[\Delta]$$

DMFT

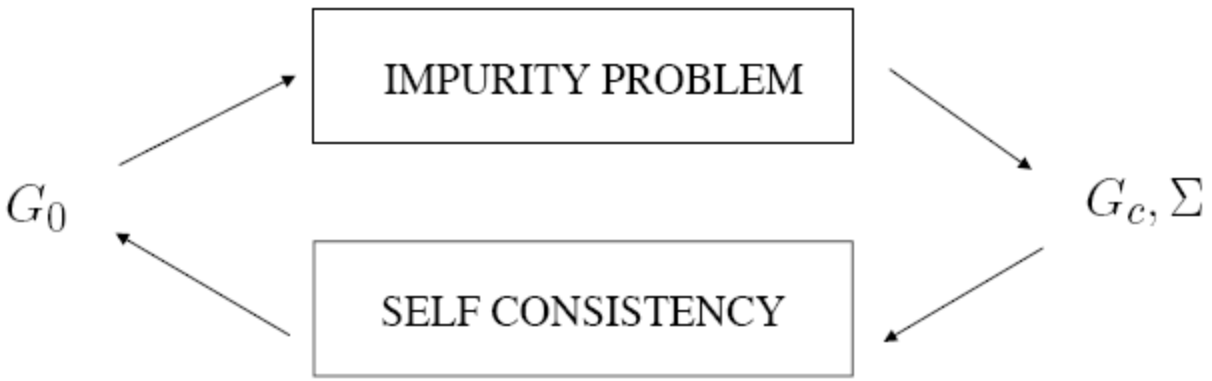
$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}$$

$$G_c(\tau) = -\langle T c(\tau) c^{\dagger}(0) \rangle_{S_{eff}}$$

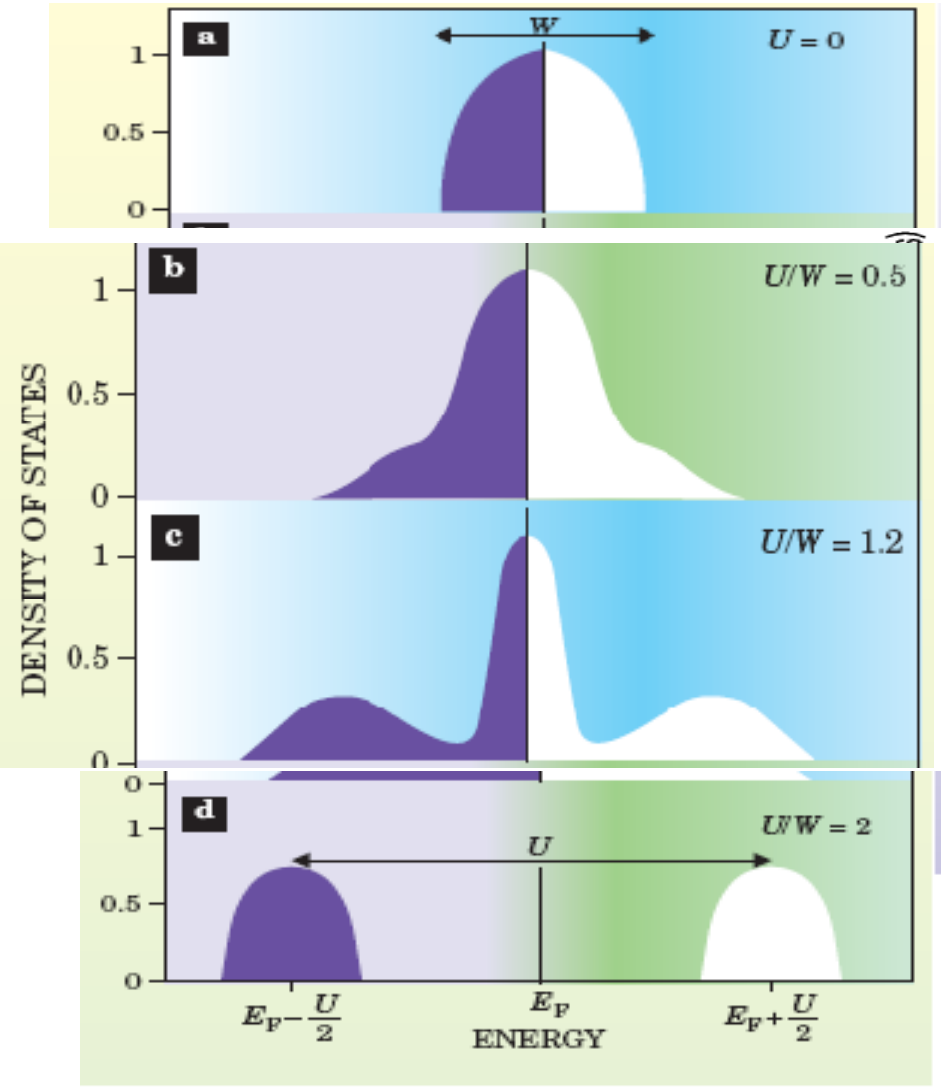
$$S_{\text{eff}} = -\int_0^{\beta} c^{\dagger}_{\sigma}(\tau) G_0^{-1}(\tau - \tau') c_{\sigma}(\tau') + \int_0^{\beta} d\tau U n_{\uparrow}(\tau) n_{\downarrow}(\tau)$$

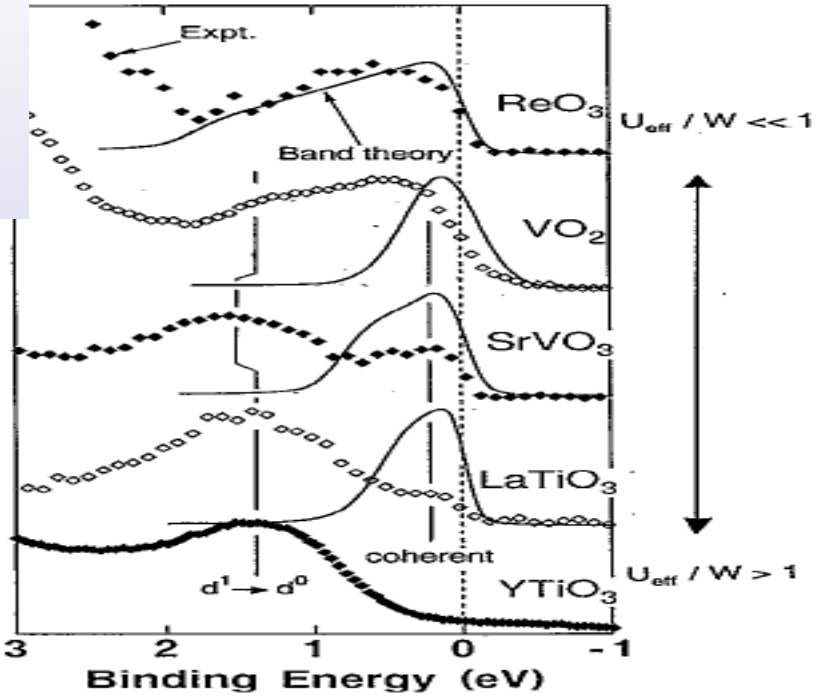
$$\Sigma = G_0^{-1} - G_c^{-1}$$

$$G_0^{-1}(i\omega_n) = \left(\sum_k \frac{1}{i\omega_n + \mu - t(k) - \Sigma(i\omega_n)} \right)^{-1} + \Sigma(i\omega_n)$$



Evolution of the DOS. Theory and experiments



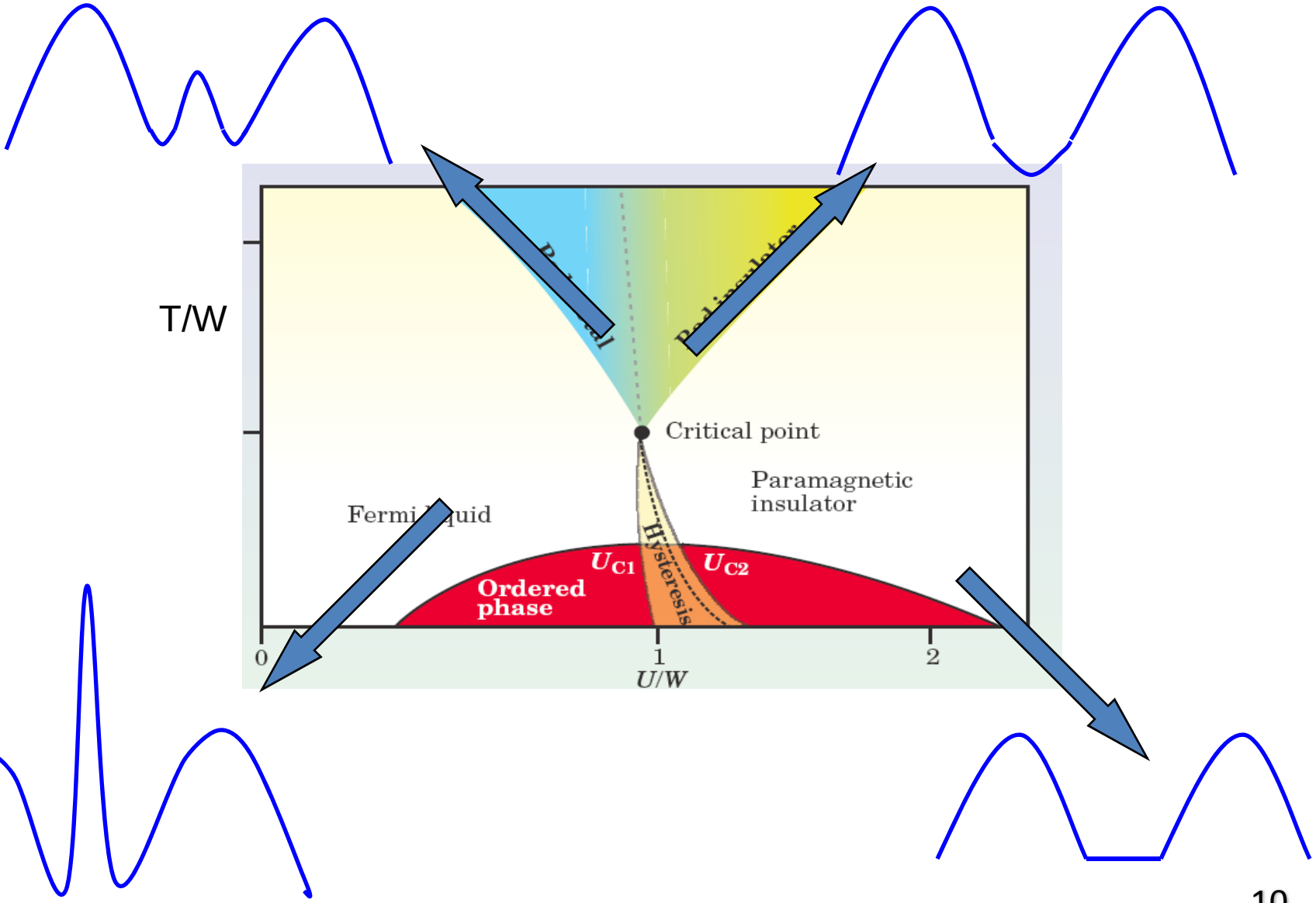


$A(\omega)$

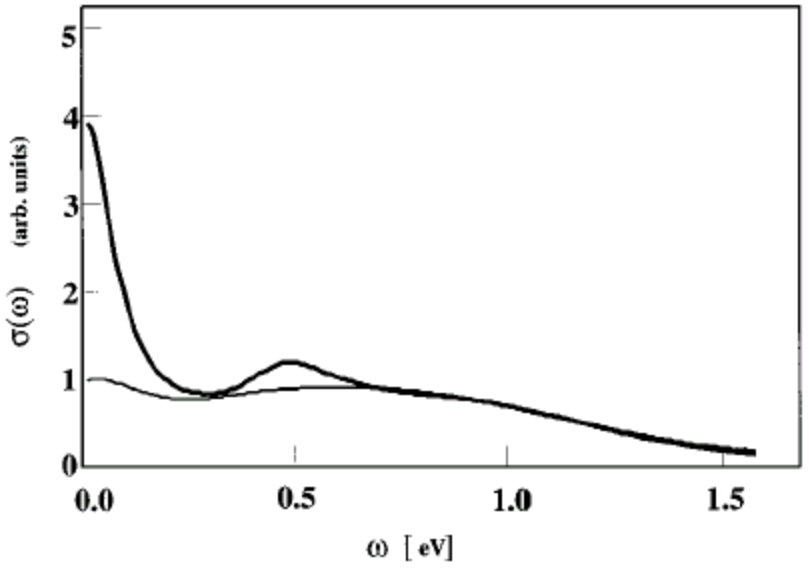
VOLUME 69, NUMBER 12 PHYSICAL REVIEW LETTERS 21 SEPTEMBER 1992

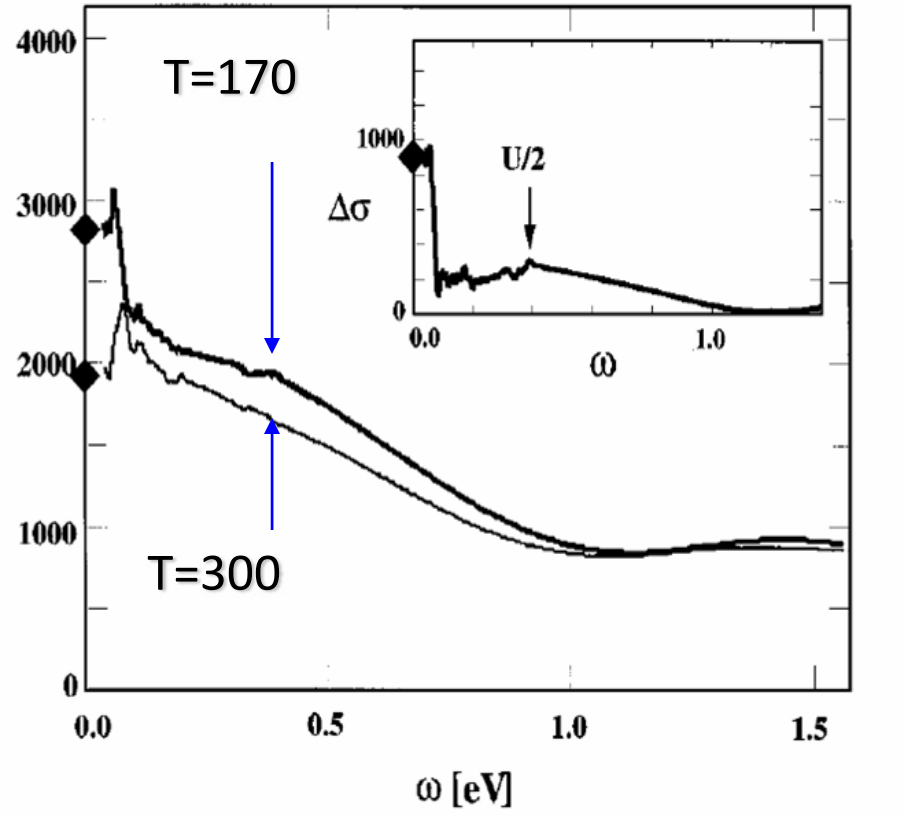
Evolution of the Spectral Function in Mott-Hubbard Systems with d^1 Configuration

Qualitative Phase diagram :frustrated Hubbard model, integer filling *M. Rozenberg et.al. 75, 105 (1995)*



Interaction with Experiments. V2O3:Anomalous transfer of spectral weight

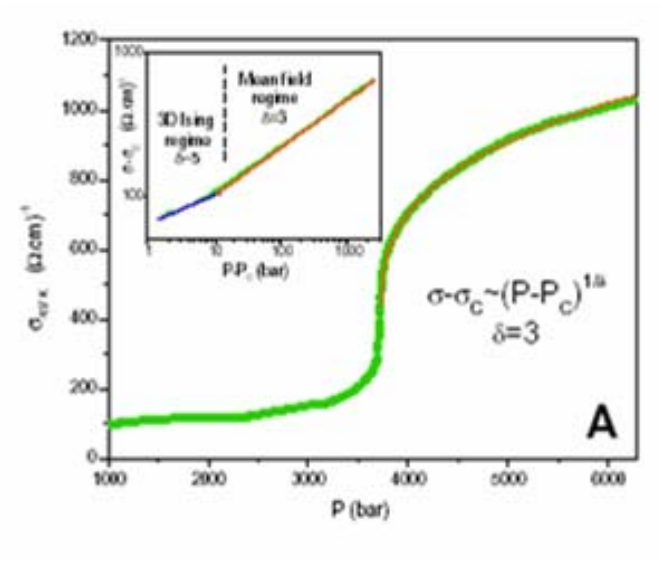


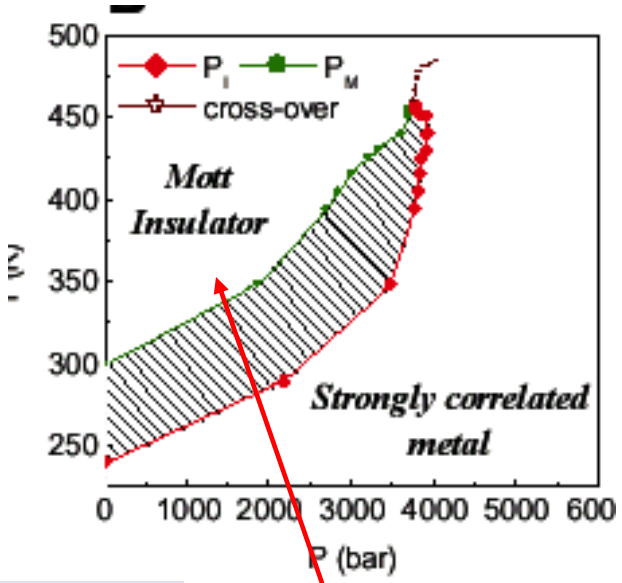


M. Rozenberg G. Kotliar H. Kajueter G Thomas D. Rapkine J Honig and P Metcalf Phys. Rev. Lett. 75, 105 (1995)

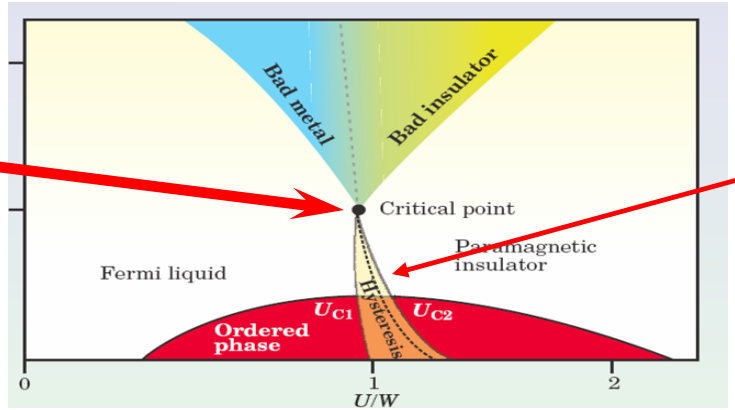
Spinodals and Ising critical endpoint.

Observation in V_2O_3 : *P. Limelette et.al. Science 302, 89 (2003)*





Critical endpoint



Spinodal Uc2

LDA+DMFT

LDA+DMFT V. Anisimov, A. Poteryaev, M. Korotin, A. Anokhin and G. Kotliar, J. Phys. Cond. Mat. 35, 7359 (1997). A Lichtenstein and M. Katsnelson PRB 57, 6884 (1988).

- 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.

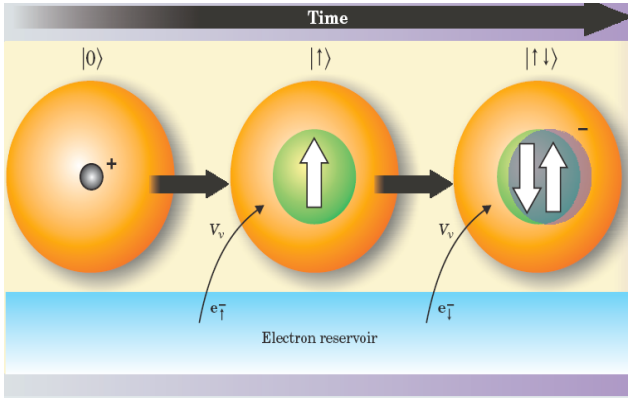
LDA+DMFT. V. Anisimov, A. Poteryaev, M. Korotin, A. Anokhin and G. Kotliar, J. Phys. Cond. Mat. 35, 7359 (1997).

Spectra=- Im G(k,ω)

$$G(k,i\omega) = \frac{1}{i\omega - t(k) - \Sigma(i\omega)}$$

$$U \longrightarrow U_{abcd}$$

$$\Sigma \longrightarrow \begin{pmatrix} 0 & 0 \\ 0 & \Sigma_{ff} \end{pmatrix}$$



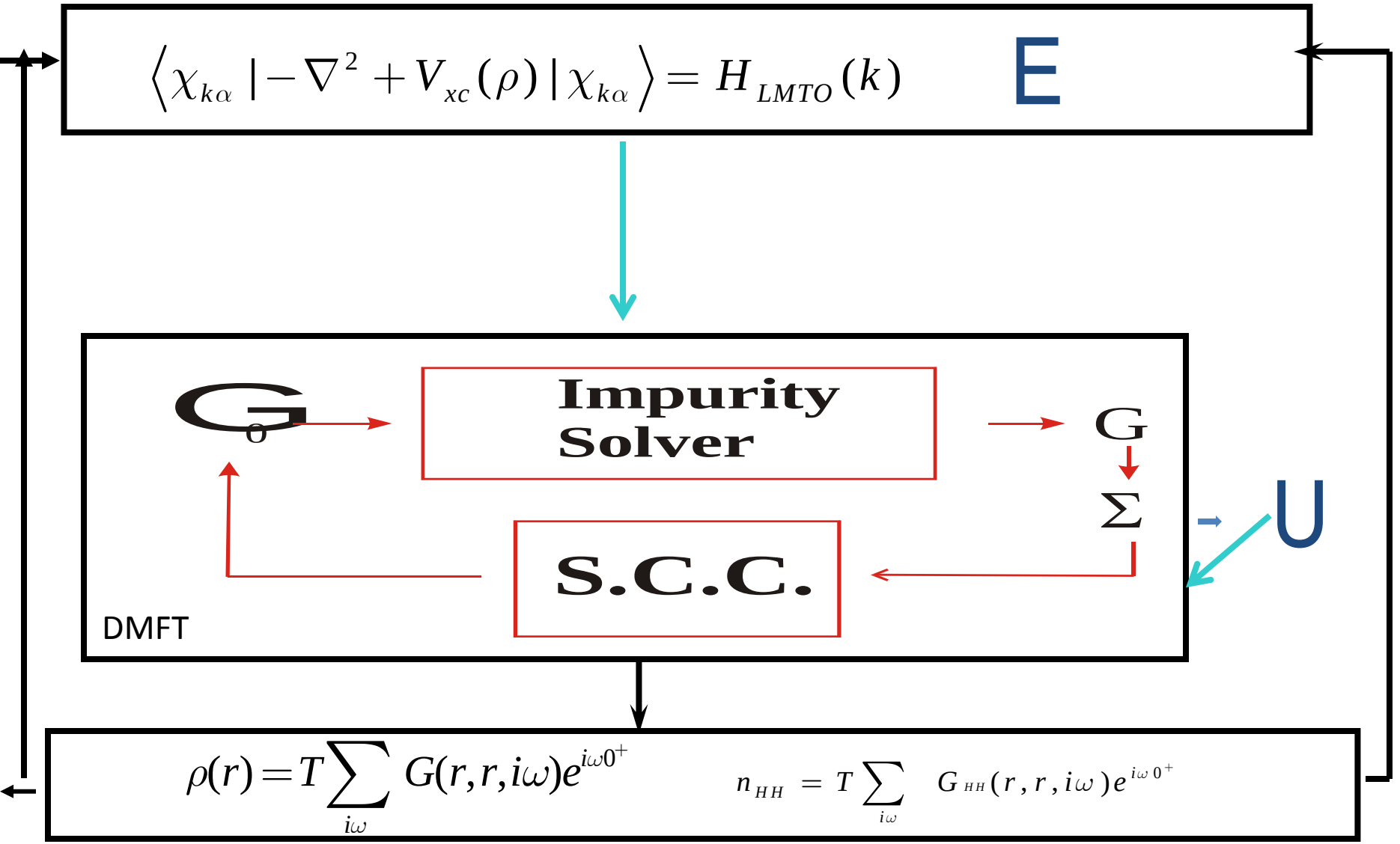
$$t(k) \longrightarrow \begin{pmatrix} H[k]_{spd,sps} & H[k]_{spd,f} \\ H[k]_{f,spd} & H[k]_{ff} \end{pmatrix}$$

$$|0>,|\uparrow>,|\downarrow>,|\uparrow\downarrow> \longrightarrow |LSJM_J\gamma...>$$

Determine energy and and Σ self consistently from extremizing a functional Chitra and Kotliar (2001) . Savrasov and Kotliar (2001) Full self consistent implementation

$$\Gamma_{dft}[\rho] \longrightarrow \Gamma_{lda+dmft}[G_{loc}, \rho, U]$$

LDA+DMFT Self-Consistency loop



LDA+DMFT functional

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

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

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

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

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

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

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

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

Embedding

$$\Sigma_{HH} \rightarrow \hat{\Sigma}$$

$$\Sigma_{HH} = \begin{bmatrix} \Sigma_{22} & 0 \\ 0 & \Sigma_{11} \end{bmatrix} \rightarrow \hat{\Sigma} = \begin{bmatrix} 0 & 0 \\ 0 & \Sigma_{HH} \end{bmatrix} \qquad \hat{H} = \begin{bmatrix} H_{LL} & H_{LH} \\ H_{HL} & H_{HH} \end{bmatrix}$$

Inversion

$$i\omega_n \hat{O}_k - \hat{H}(k) - \hat{E} - \hat{\Sigma}(i\omega_n) \rightarrow \frac{1}{i\omega_n \hat{O}_k - \hat{H}(k) - \hat{E} - \hat{\Sigma}(i\omega_n)}$$

Integrating over BZ

$$\hat{G}_{loc}(i\omega_n) = \sum_k \frac{1}{i\omega_n \hat{O}_k - \hat{H}(k) - \hat{E} - \hat{\Sigma}(i\omega_n)}$$

Truncation

$$\hat{G}_{loc} = \begin{bmatrix} 0 & 0 \\ 0 & G_{HH} \end{bmatrix} \rightarrow G_{HH}$$

$$G_0^{-1}(i\omega_n) = G_{HH}^{-1} + \Sigma_{HH}(i\omega_n)$$

Inversion in realistic DMFT

$$[(i\omega + \mu)\hat{O}(\mathbf{k}) - \hat{h}^{(0)}(\mathbf{k}) - \mathcal{M}_{\rm int}(i\omega)]^{-1}$$

$$[h^{(0)}_{\alpha\beta}(\mathbf{k}) + \mathcal{M}_{{\rm int},\alpha\beta}(i\omega) - \epsilon_{\mathbf{k}j\omega} O_{\alpha\beta}(\mathbf{k})]\psi^R_{\mathbf{k}j\omega,\beta} = 0$$

$$\mathcal{G}_{\alpha\beta}(\mathbf{k}, i\omega) = \sum_j \frac{\psi^R_{\mathbf{k}j\omega,\alpha}\psi^L_{\mathbf{k}j\omega,\beta}}{i\omega + \mu - \epsilon_{\mathbf{k}j\omega}}.$$

$$\rho(\mathbf{r}) = T\sum_{i\omega}\sum_{\mathbf{k}j} \frac{\psi^R_{\mathbf{k}j\omega}(\mathbf{r})\,\psi^L_{\mathbf{k}j\omega}(\mathbf{r})}{i\omega + \mu - \epsilon_{\mathbf{k}j\omega}} e^{i\omega 0^+}.$$

Generalized Kohn Sham eigenstates

$$\rho(\mathbf{r}) = T\sum_{i\omega}\sum_{\mathbf{k}j}\frac{\psi^{R}_{\mathbf{k}j\omega}(\mathbf{r})\,\psi^{L}_{\mathbf{k}j\omega}(\mathbf{r})}{i\omega+\mu-\epsilon_{\mathbf{k}j\omega}}e^{i\omega 0^{+}}.$$

$$g_{\mathbf{k}j\omega} = \frac{1}{i\omega+\mu-\epsilon_{\mathbf{k}j\omega}}$$

$$\rho(r) = \sum_{kj} f(\varepsilon_{kj})\,|\,\psi_{kj}(r)\,|^{2}$$

Comments on LDA+DMFT

- Static limit of the LDA+DMFT functional , with $\Phi = \Phi_{HF}$ reduces to LDA+U
- Removes inconsistencies and shortcomings of this approach. DMFT retain correlations effects in the absence of orbital ordering.
- Only in the orbitally ordered Hartree Fock limit, the Greens function of the heavy electrons is fully coherent
- Gives the local spectra and the total energy simultaneously, treating QP and H bands on the same footing.

Localization Delocalization in Actinides

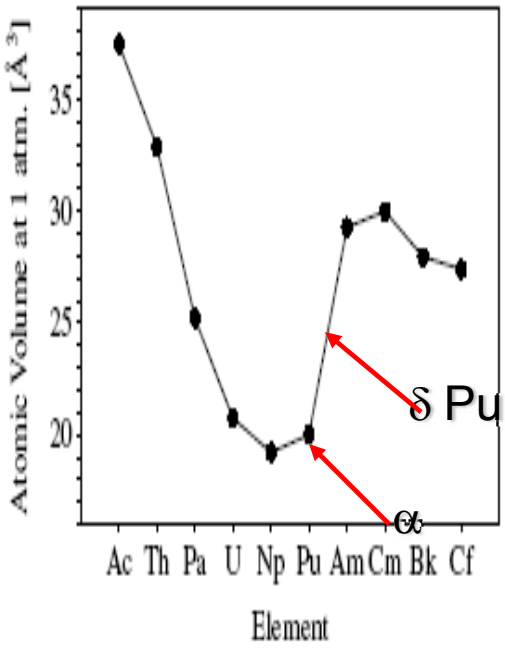
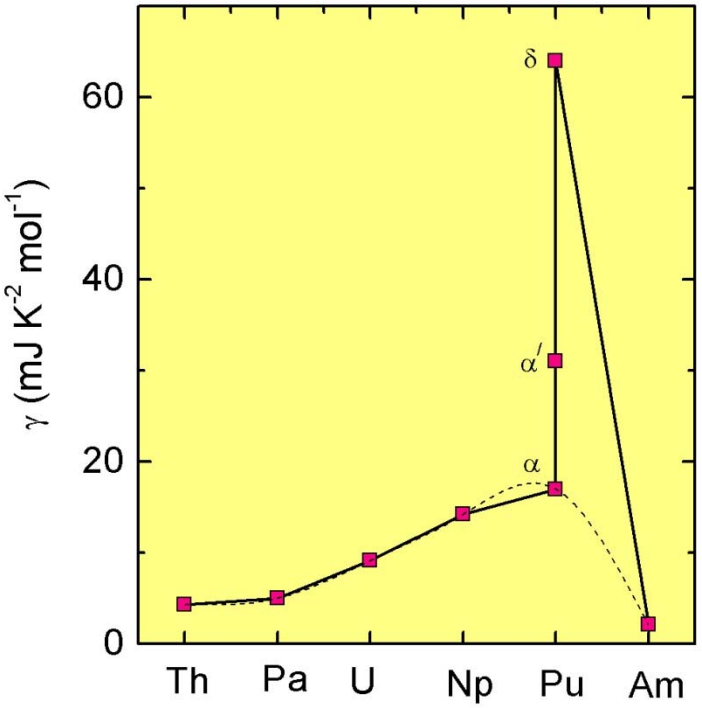
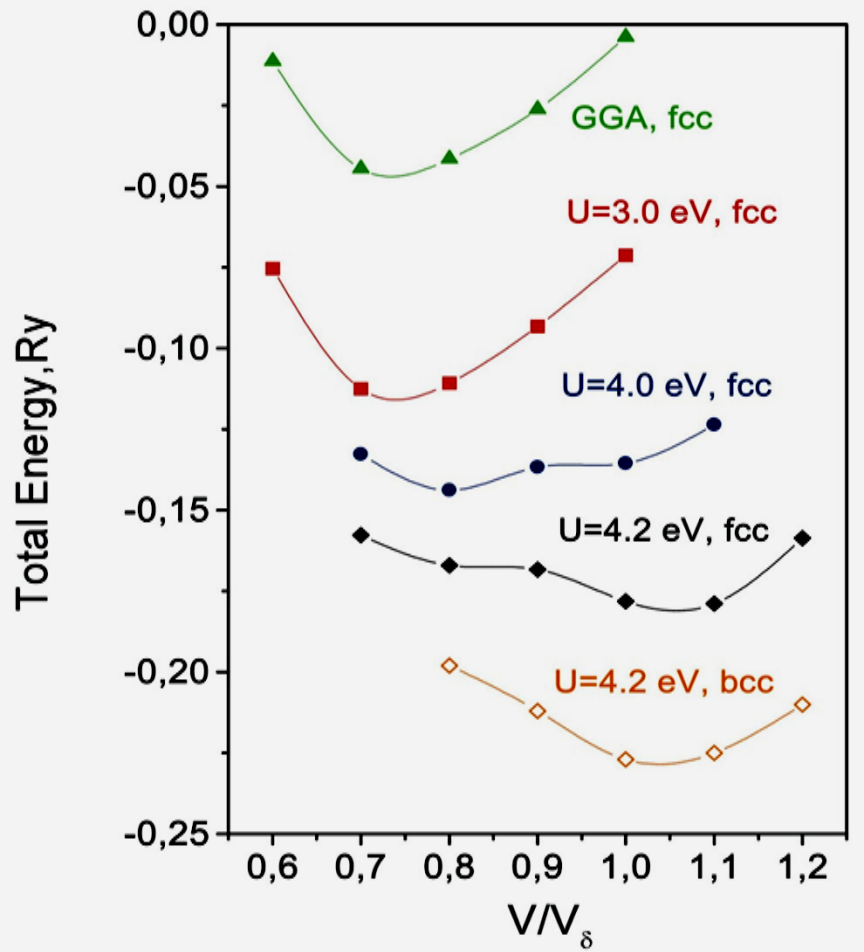


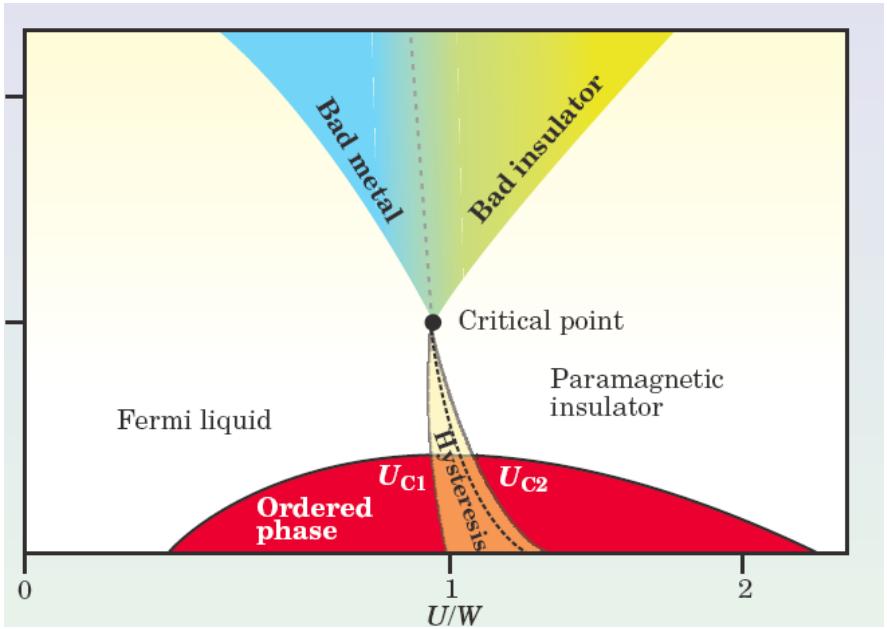
Figure 1. Atomic volumes of actinide metals at atmospheric pressure and 25 °C.



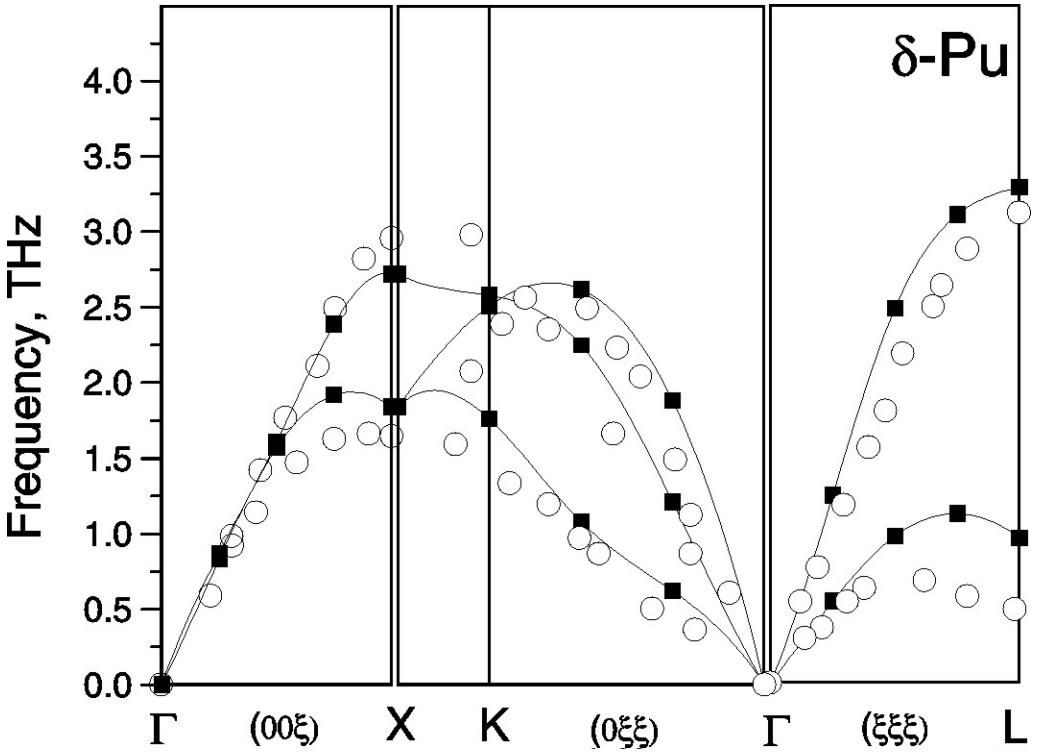
Modern understanding of this phenomena using functional approach toDMFT. K Haule S.Savrasov J Shim

Volume Collapse Transitions: relaxing the lattice positions. Savrasov et. al.





DMFT Phonons in fcc δ-Pu

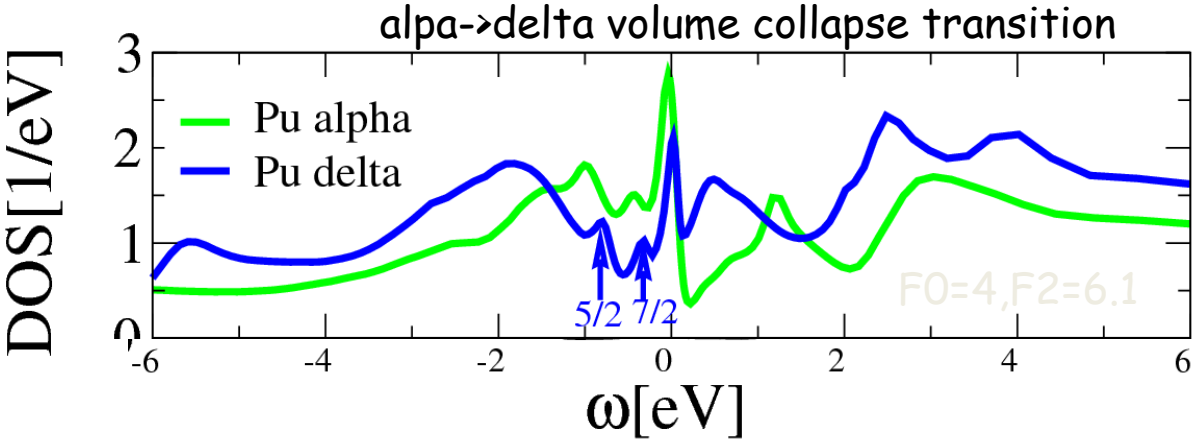


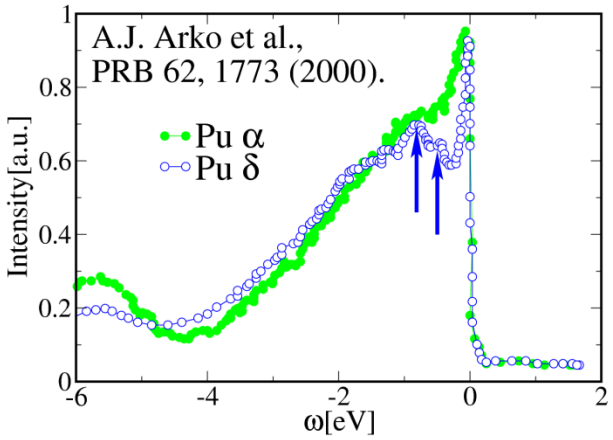
	C_{11} (GPa)	C_{44} (GPa)	C_{12} (GPa)	C'(GPa)
Theory	34.56	33.03	26.81	3.88
Experiment	36.28	33.59	26.73	4.78

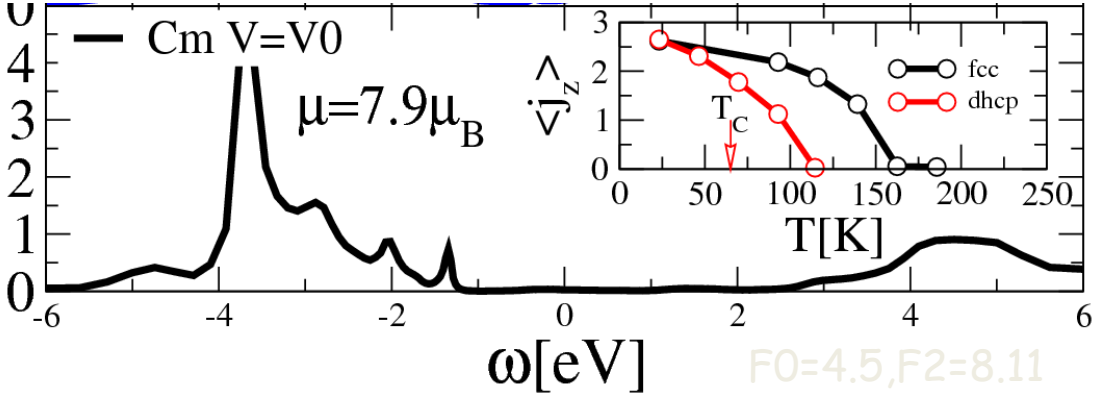
(Dai, Savrasov, Kotliar,Ledbetter, Migliori, Abrahams, Science, 9 May 2003)

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

New Generation of LDA+DMFT tools
K.Haule Nature (2007)

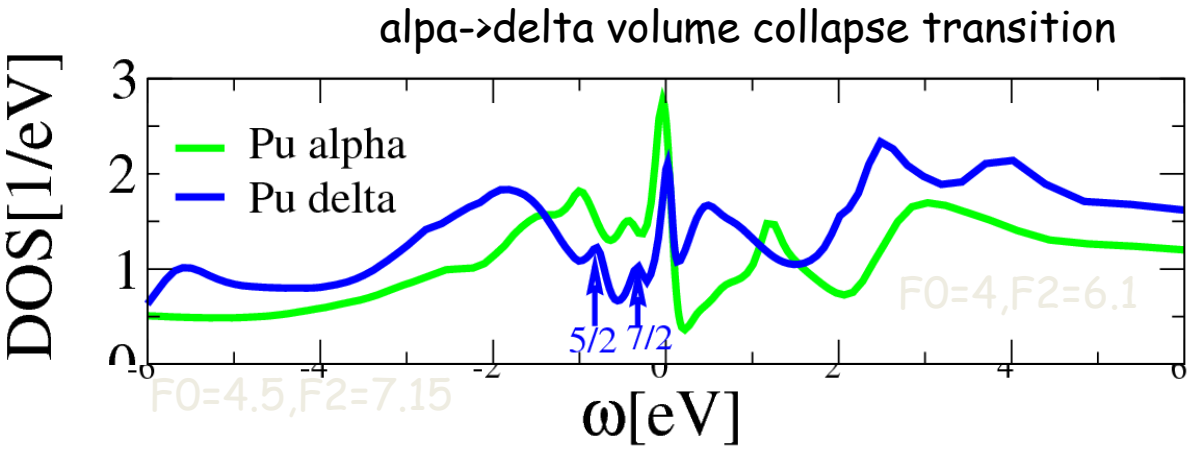


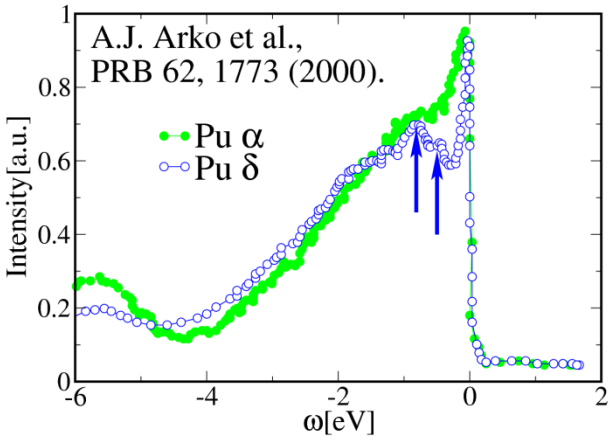


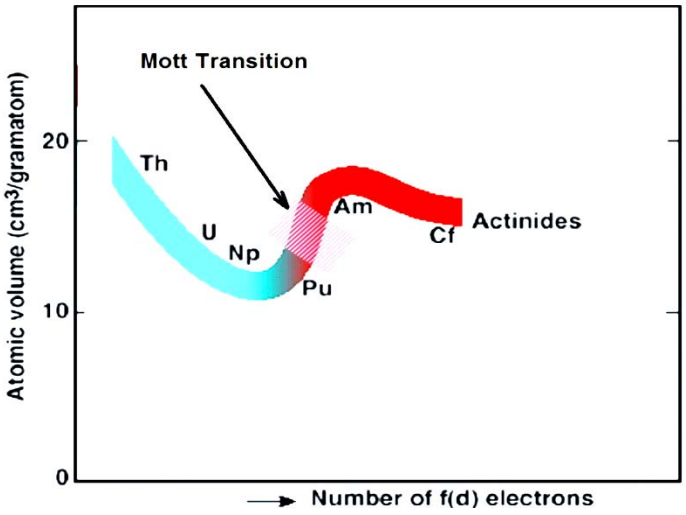


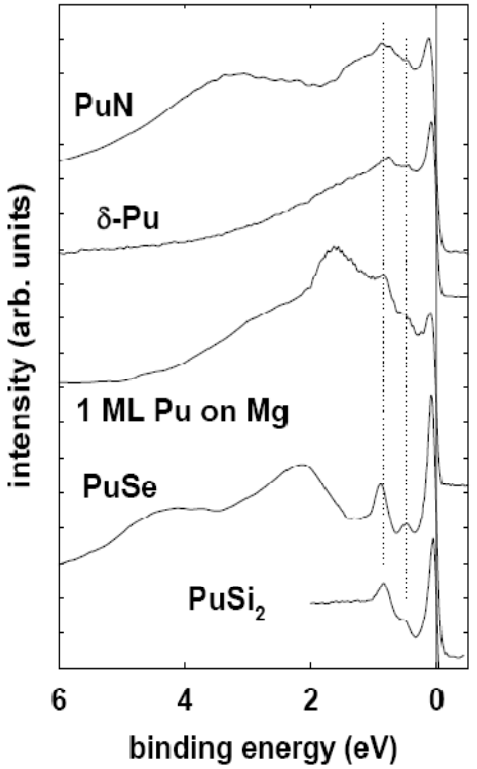
Curium has large magnetic moment and orders antif Pu does is non magnetic.

Volume and Spectra





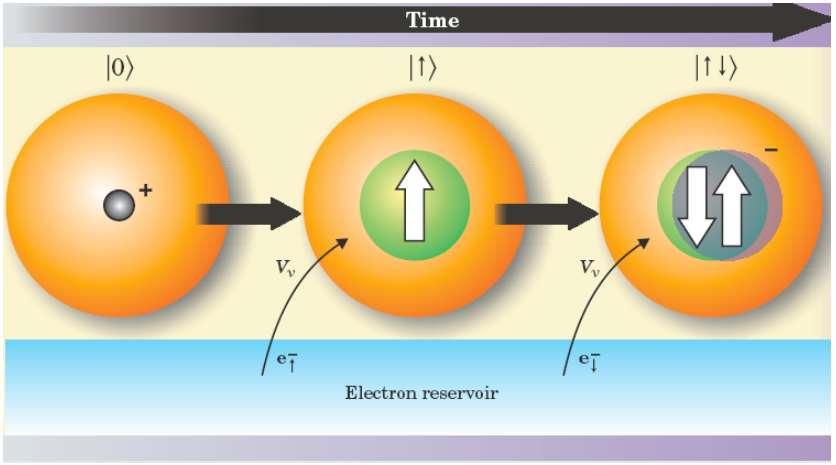


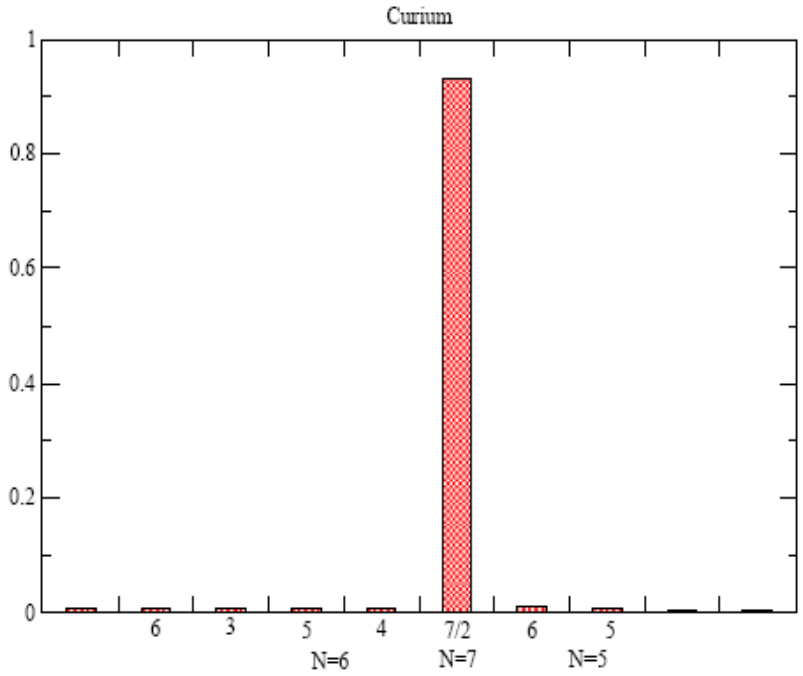


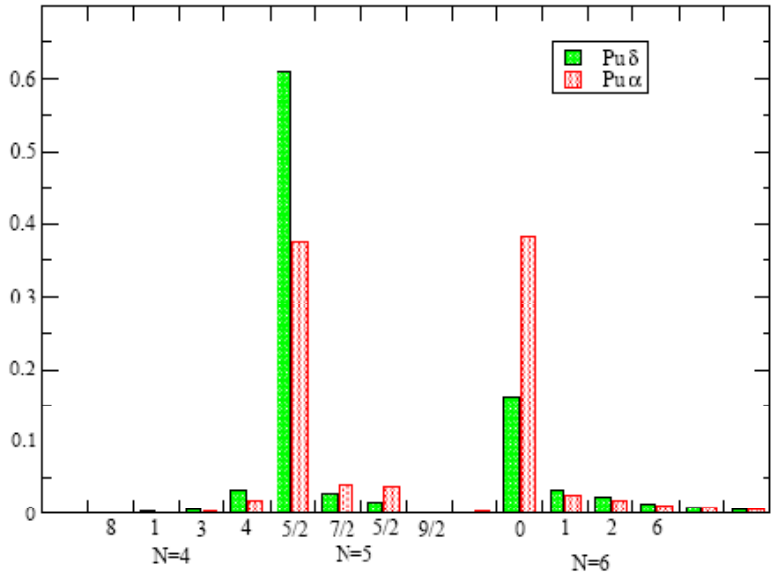
J. H. Shim, K. Haule, G. Kotliar, Nature 446, 513 (2007).

Gouder Havela Lander

The “DMFT-valence” in the late actinides.

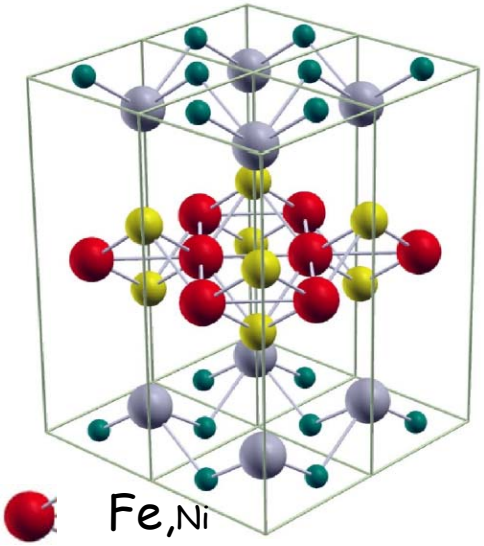






Time scale of the fluctuations. Ef*

Iron based high-Tc superconductors



Fe,Ni

As,P

La,Sm,Ce

O

x~5-20%

Smaller c

Higher T_c

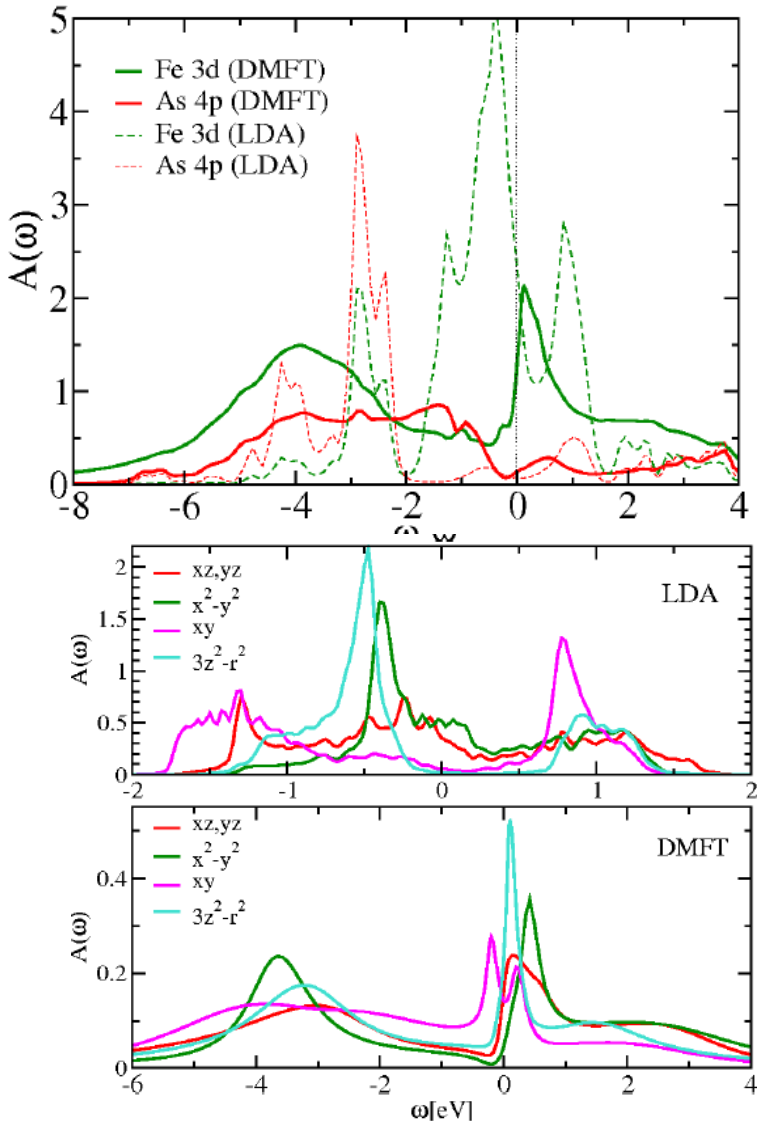
LaOFeP	**3.2K**, JACS-2006 a=3.964A, **c=8.512A**
$SmF_xO_{1-x}FeAs$ **c)**	**55K**, cm/0803.3603 a=3.940A, **c=8.496A**
$PrF_xO_{1-x}FeAs$ **d)**	**52K**, unpublished a=3.985A, **c=8.595A**
$CeF_xO_{1-x}FeAs$ **b)**	**41 K**, cm/0803.3790 a=3.996A, **c=8.648A**
$LaF_xO_{1-x}FeAs$ **a)**	**26 K**, JACS-2008 a=4.036A, **c=8.739 A**
$La_{1-x}Sr_xOFeAs$	**25K**, cm/0803.3021, a=4.035A, **c = 8.771A**
$LaCa_xO_{1+x}FeAs$	**0 K**
$LaF_xO_{1-x}NiAs$	**2.75K**, cm/0803.2572a =4.119A , **c=8.180A**
$La_{1-x}Sr_xONiAs$	**3.7K**, cm/0803.3978 a=4.045A, **c=8.747A**

a) Y. Kamihara et.al., Tokyo, JACS
b) X.H. Chen, et.al., Beijing, cm/0803.3790
c) G.F. Chen et.al., Beijing, cm/0803.3603
d) Z.A. Ren et.al, Beijing, unpublished

- 2D square lattice of Fe
- Fe - magnetic moment

DMFT for $LaF_xO_{1-x}FeAs$

LDA+DMFT: LaOFeAs is at the verge
of the metal-insulator transition
(for realistic U=4eV, J=0.7eV)
For a larger (U=4.5, J=0.7eV) Mott-Slater insulator



Not a one band model: all 5 bands important
(for J>0.3)

K. Haule J. Shim G. Kotliar
arXiv:0803.1279

Iron Pnictides vs Cuprates

- Both are strongly correlated high temperature superconductors.
- In both cases the superconductor is proximate to a Mott insulator and is not well described by Fermi Liquid at high t.

DIFFERENCES

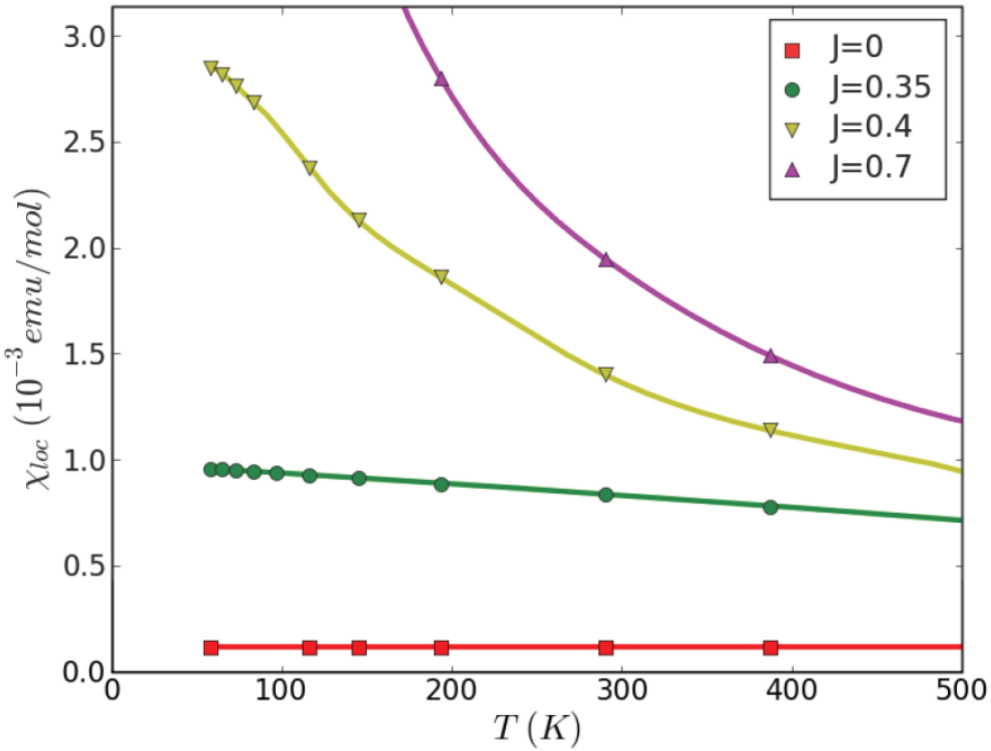
Pnictides

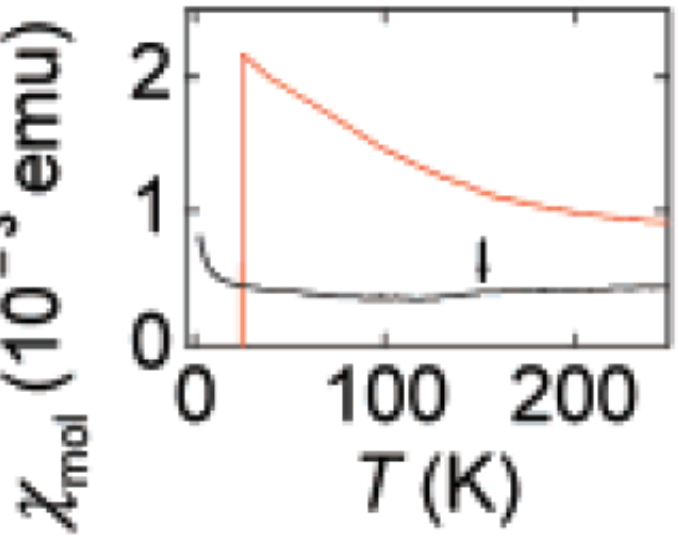
- U< Uc2
- Intrinsically Multiorbital Multiband
- Important role of Jhunds
- Frustrated Magnetism
- Single Site DMFT ?

Cuprates

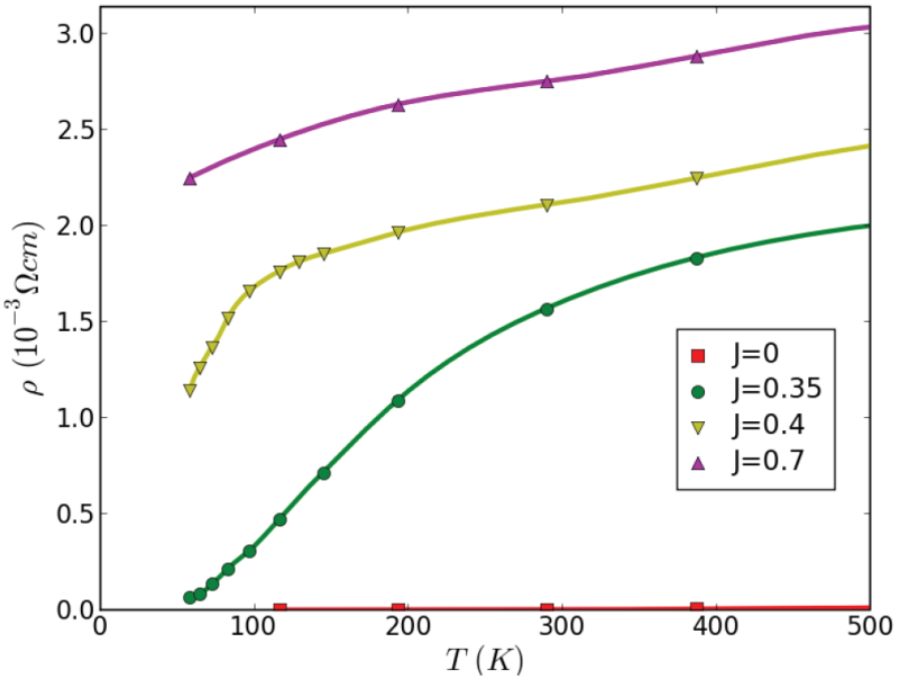
- U> Uc2 , doped Mott insulator
- One band model
- Importance of Superexchange
- Non frustrated magnetism
- Cluster DMFT ?

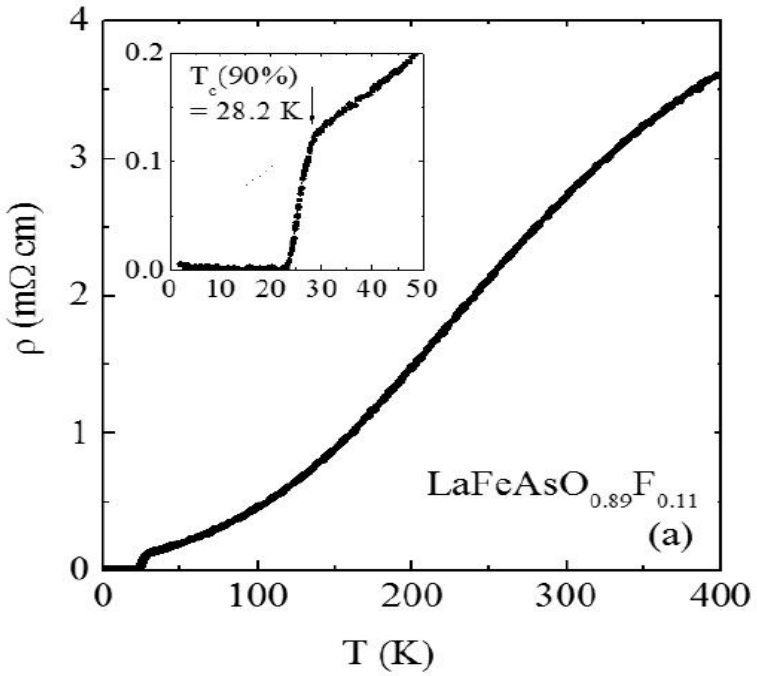
Coherence-incoherence crossover in DMFT : crucial role played by J



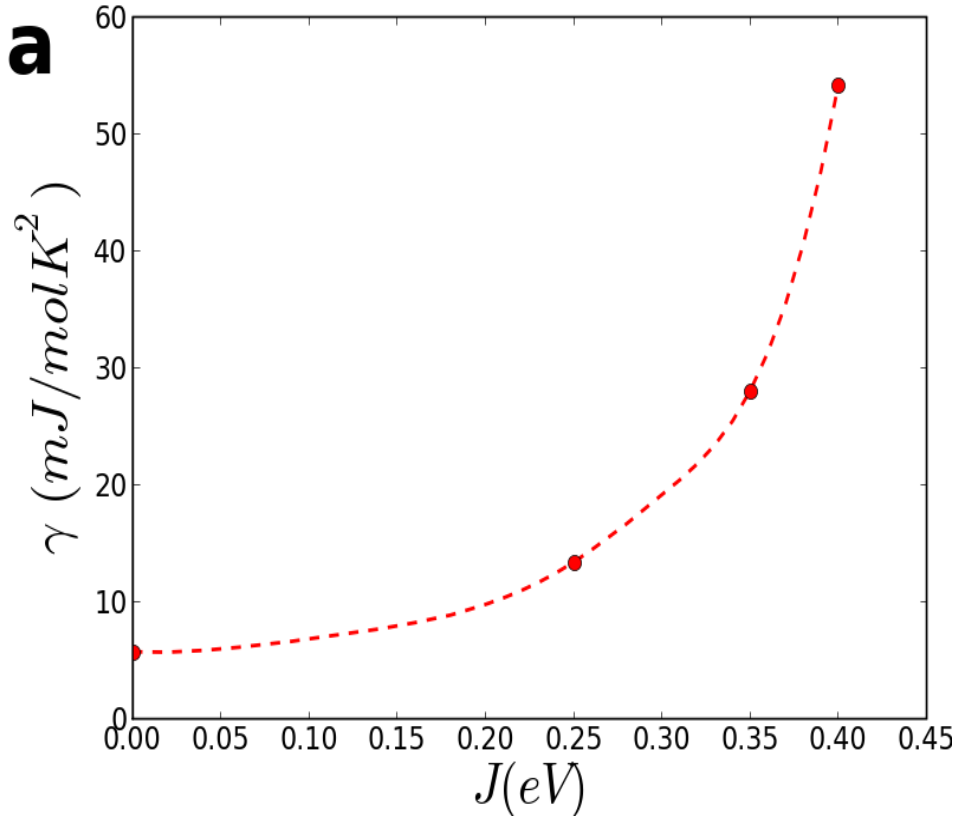


Coherence-incoherence crossover in DMFT : crucial role played by J





Experimental predictions



Functional formulation. Chitra and Kotliar (2001), Ambladah et. al. (1999) Savrasov and Kotliarcond- matt0308053 (2003).

$$S = \int dx\psi^{+}(x)[\partial_\tau - \bigtriangledown^2 + V_{ext}(x)]\psi(x) + \frac{1}{2}\int dxdx'\psi^{+}(x)\psi^{+}(x')v_C(x-x')\psi(x)\psi(x')$$

$$S = \int dx\psi^{+}(x)[\partial_\tau - \bigtriangledown^2 + V_{ext}(x)]\psi(x) + \frac{1}{2}\int\int \phi(x)V_C^{-1}(x,x')\phi(x') + \int i\phi(x)\psi^{\dagger}(x)\psi(x)$$

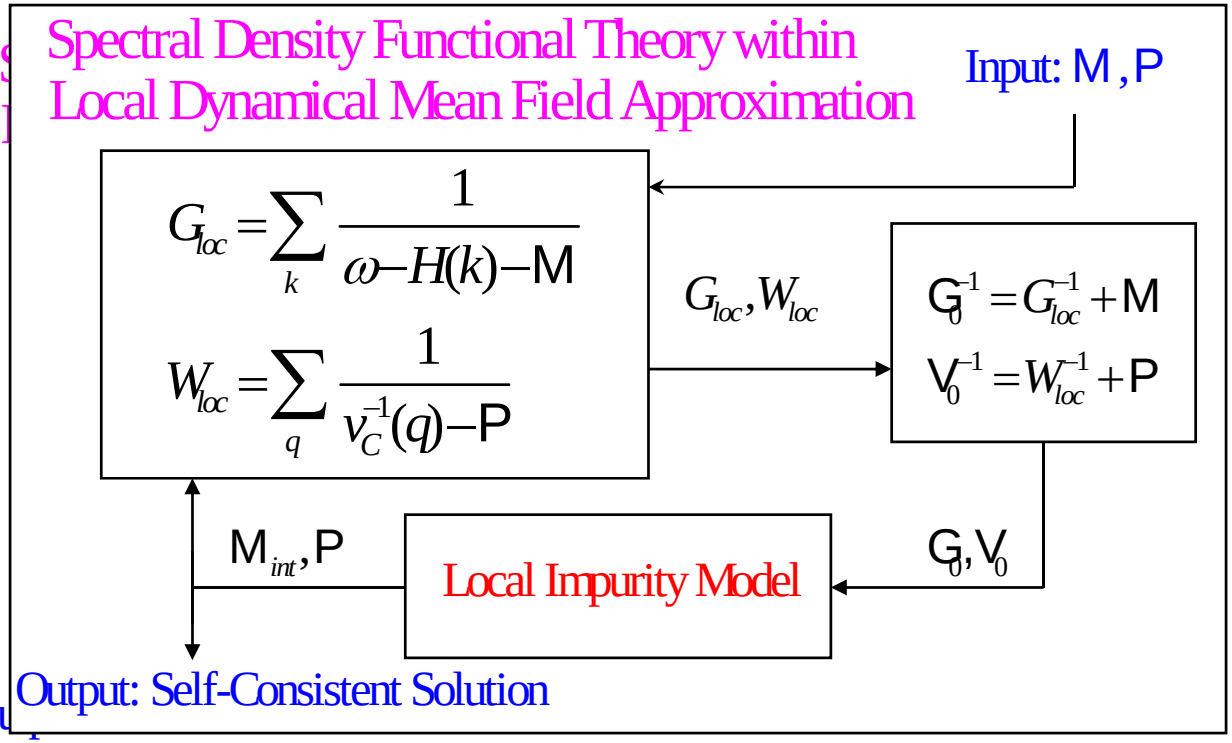
$|r\rangle = |R, \rho\rangle$ $\quad G = -\langle \psi(R\rho')\ \psi^{\dagger}(R\rho')\rangle$ $\quad \langle \phi(R\rho')\phi(R\rho)\rangle - \langle \phi(R\rho')\rangle\langle \phi(R\rho)\rangle = W$

$$\Gamma[G,W] = TrLnG - Tr[G_0^{-1} - G^{-1}]G - \frac{1}{2}TrLnW + \frac{1}{2}Tr[V_C^{-1} - W^{-1}]W + E_{hartree} + \Phi[G,W]$$

$\Phi[G,W] \approx \Phi_{EDMFT}[G_{loc}, W_{loc}, G_{nonloc} = 0, W_{nonloc} = 0]$

Double loop in *Gloc and Wloc*

EDMFT loop G. Kotliar and S. Savrasov in New Theoretical Approaches to Strongly Correlated G Systems, A. M. Tsvelik Ed. 2001 Kluwer Academic Publishers. 259-301 . cond-mat/0208241 *S. Y. Savrasov, G. Kotliar,* Phys. Rev. B **69**, 245101 (2004)



- Full implementation in the context of a a one orbital model. P Sun and G. Kotliar Phys. Rev. B 66, 85120 (2002).

- After finishing the loop treat the graphs involving Gnonloc Wnonloc in perturbation theory. P.Sun and GK PRL (2004). Related work, Biermann Aersetiwan and Georges PRL 90,086402 (2003**) .**

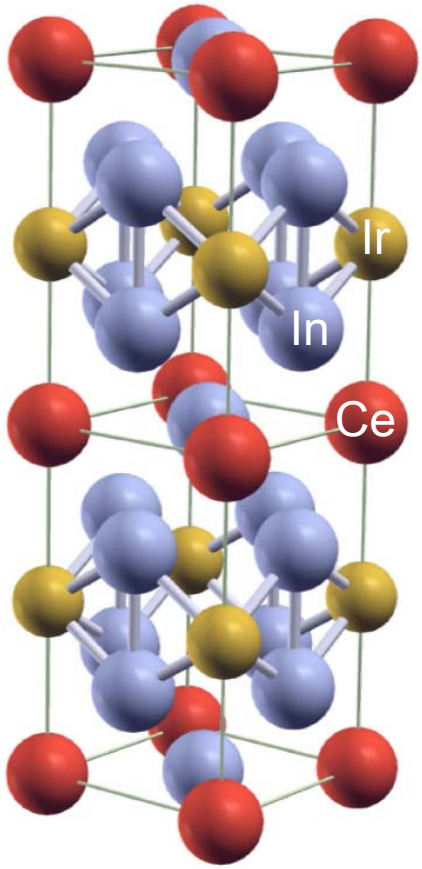
THE END
Thanks for your attention!!!!!

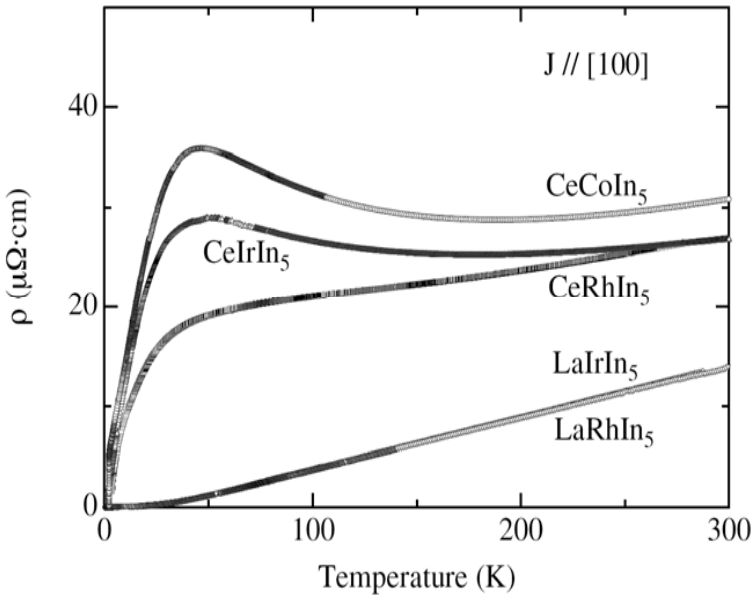
Hope it raised your interest and you want to contribute so that we can have a predictive theory of correlated materials in the very near future…….

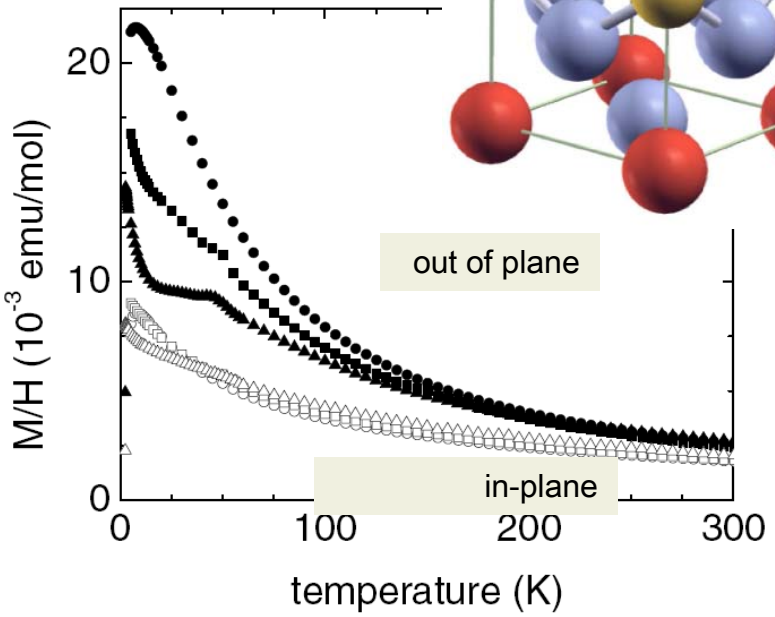
kotliar@physics.rutgers.edu

$CeMIn_5$ M=Co, Ir, Rh

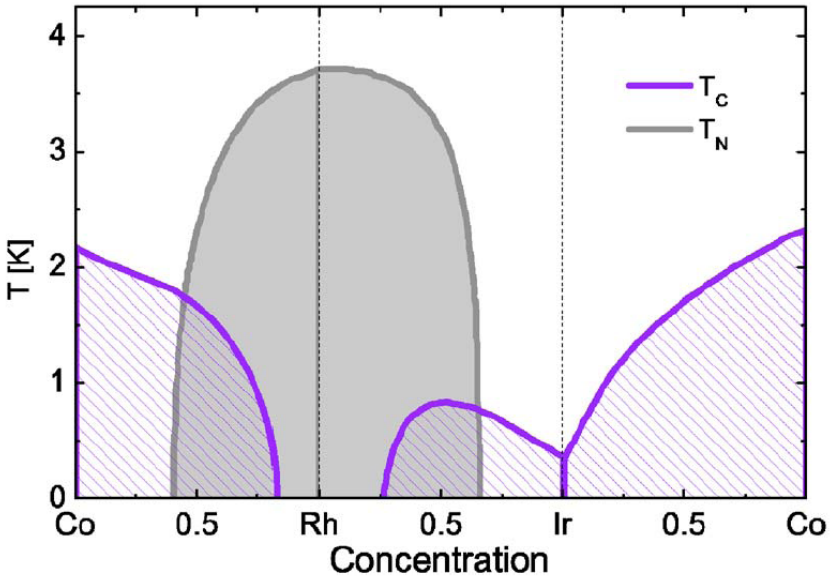
- CeRhIn5: TN=3.8 K; $\gamma \approx 450$ mJ/molK2
- CeCoIn5: Tc=2.3 K; $\gamma \approx$ 1000 mJ/molK2; • CeIrIn5: Tc=0.4 K; $\gamma \approx 750$ mJ/molK2





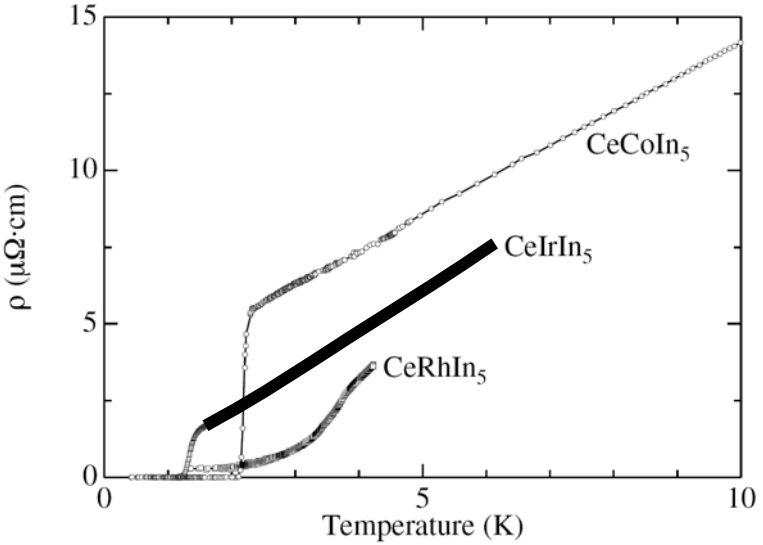


Phase diagram of 115's



Why $CeIrIn_5$?

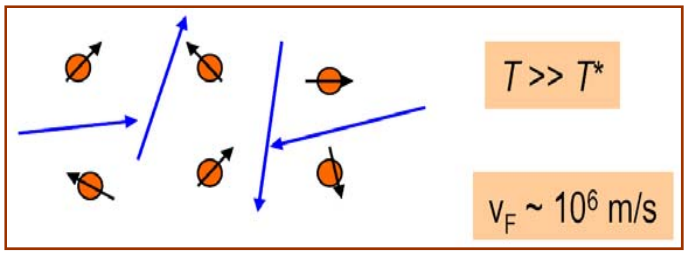
- Ir atom is less correlated than Co or Rh (5d / 3d or 4d)
- $CeIrIn_5$ is more itinerant(coherent) than Co (further away from QCP)



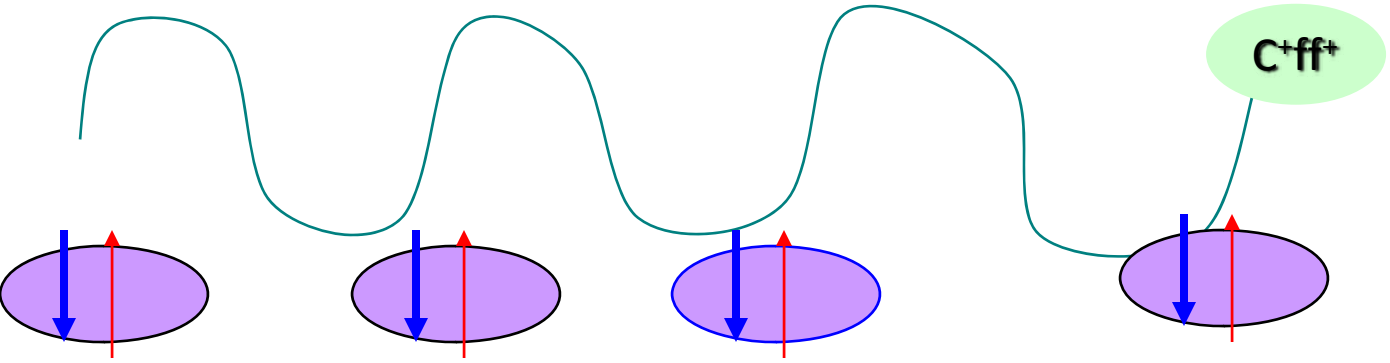
Generalized Anderson Lattice Model

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

$$+ \sum_{<i,j>,\sigma} V_{ij} f_{i\sigma}^{\dagger} c_{j\sigma} + c.c. = H_{ALM}$$



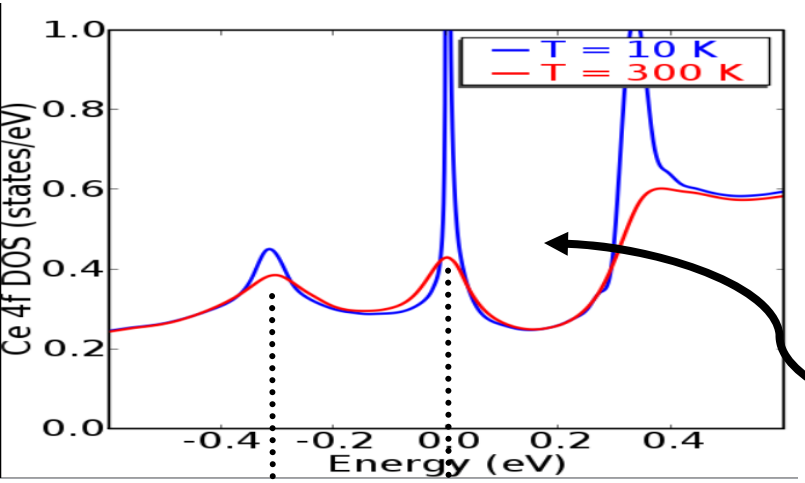
•High temperature
Ce-4f local moments

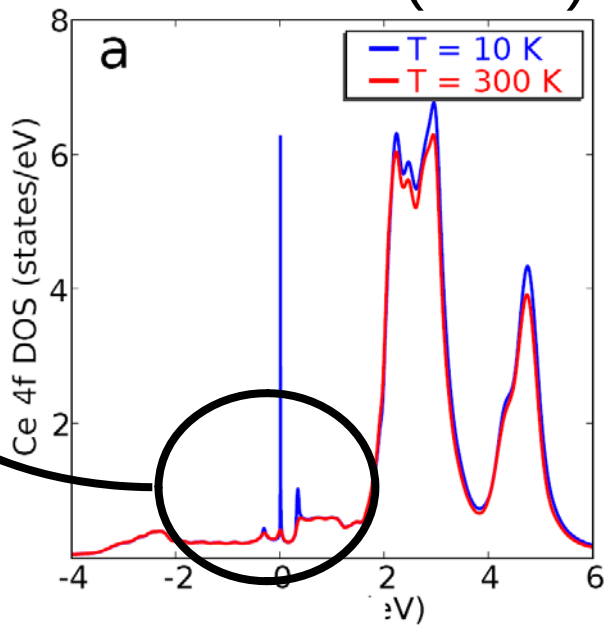


•Low temperature –
Itinerant heavy bands

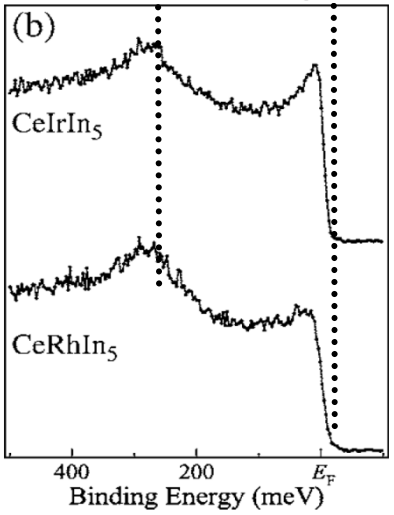
Angle integrated photoemission

Expt Fujimori *et al.*, *PRB* **73**, 224517 (2006) *P.R B* **67**, 144507 (2003).





4*d*-4*f* on-resonance ($h\nu$=122 eV)

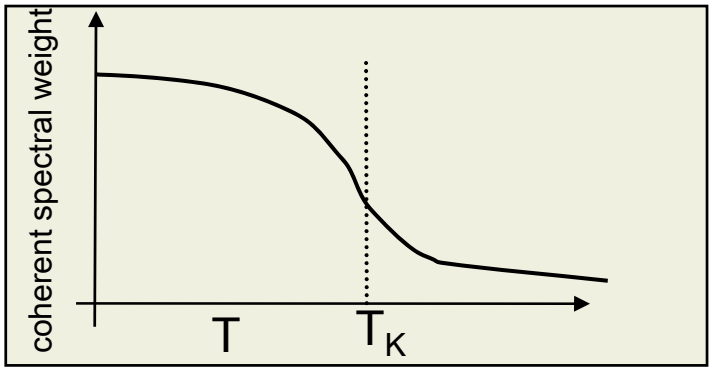


Experimental resolution ~30meV
Surface sensitivity at 122 ev ,
theory predicts 3meV broad band

Theory: LDA+DMFT, impurity solvers SUNCA and CTQMC Shim Haule and GK (2007)

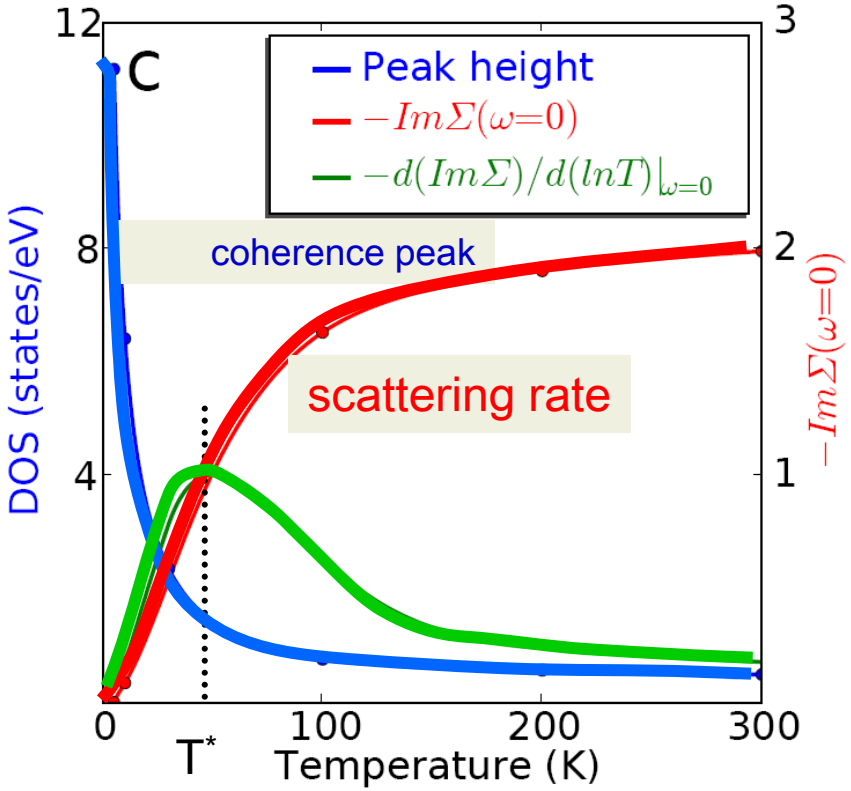
Buildup of coherence

Buildup of coherence in single impurity case



Slow crossover pointed out by NPF 2004

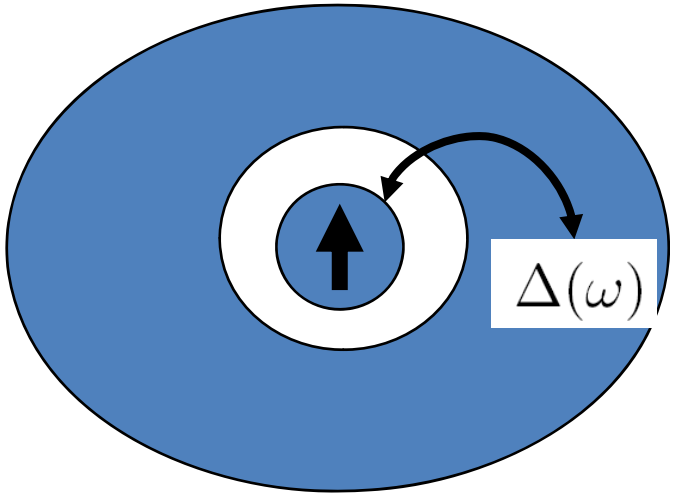
Very slow crossover!



Crossover around 50K

DMFT is not a single impurity calculation

Auxiliary impurity problem:



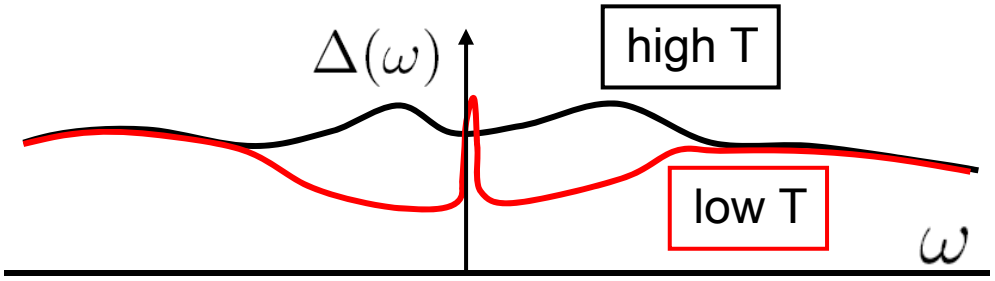
Weiss field $\Delta(\omega)$ temperature dependent:

High-temperature Δ given mostly by LDA

low T: Impurity hybridization affected by the emerging coherence of the lattice (collective phenomena)

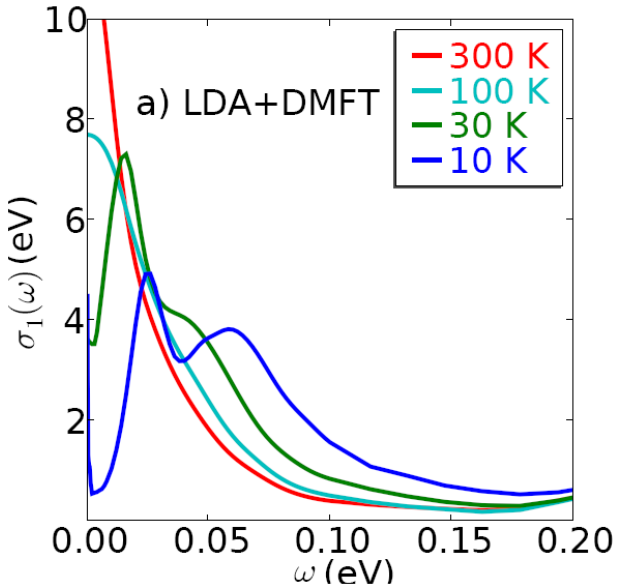
DMFT SCC:

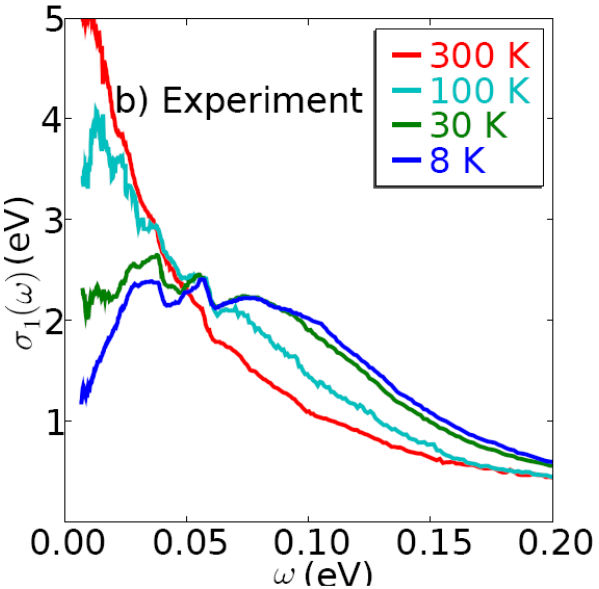
$$\Delta(\omega) = \omega - E_{imp} - \Sigma_\omega - \left(\sum_{\mathbf{k}} \left(\frac{1}{\omega + \mu - H_{\mathbf{k}}^{ff} - H_{\mathbf{k}}^{fc} \frac{1}{\omega + \mu - H_{\mathbf{k}}^{cc}} H_{\mathbf{k}}^{cf} - \Sigma_f(\omega)} \right)^{-1} \right)^{-1}$$



Feedback effect on Δ makes the crossover from incoherent to coherent state very slow!

Optical conductivity in LDA+DMFT



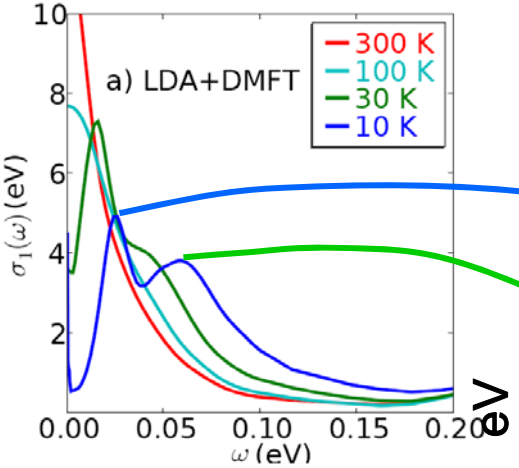


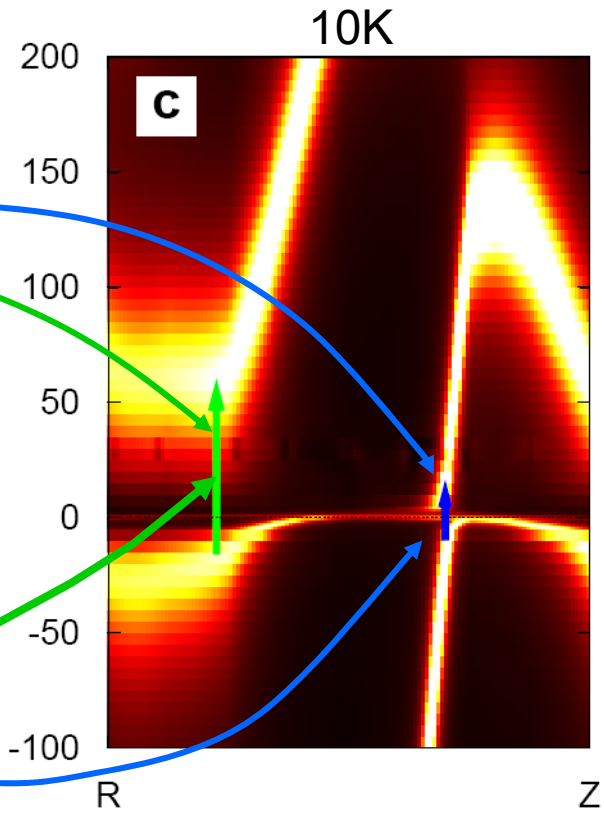
Expts: F. P. Mena, D. van der Marel, J. L. Sarrao, *PRB* **72**, 045119 (2005).
16. K. S. Burch *et al.*, *PRB* **75**, 054523 (2007).
17. E. J. Singley, D. N. Basov, E. D. Bauer, M. B. Maple, *PRB* **65**, 161101(R) (2002).

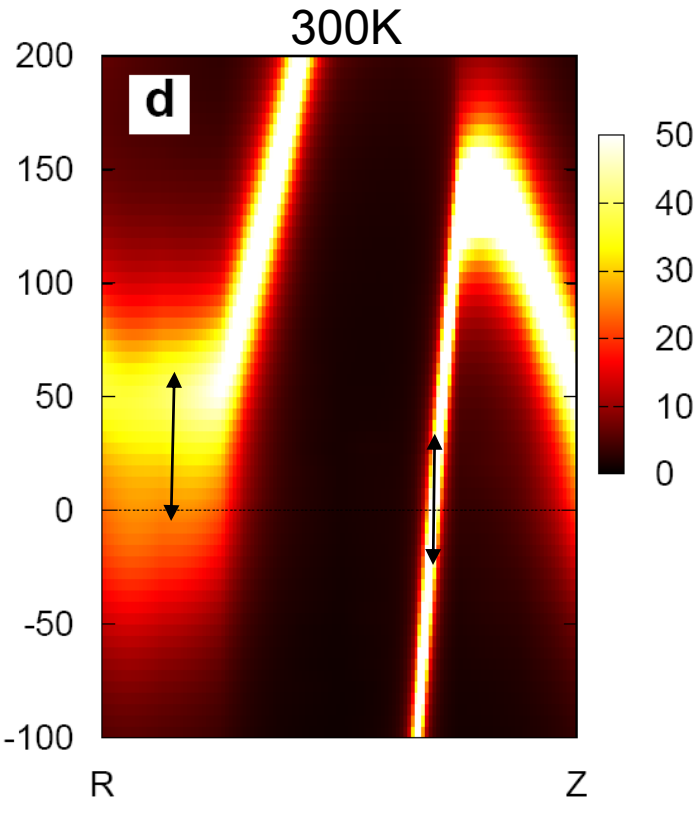
- At 300K very broad Drude peak (e-e scattering, spd lifetime~0.1eV)
- At 10K:
  - very narrow Drude peak
  - First MI peak at 0.03eV~250cm^{-1}
  - Second MI peak at 0.07eV~600cm^{-1}

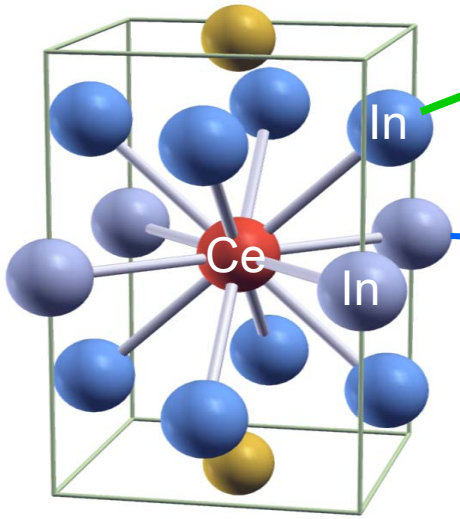
Multiple hybridization gaps

non-f spectra



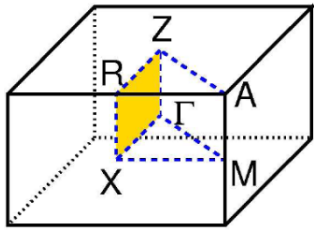






- Larger gap due to hybridization with out of plane In
- Smaller gap due to hybridization with in-plane In

DMFT -Momentum resolved Ce-4f spectra $A_f(\omega,k)$



Hybridization gap

Fingerprint of spd's due to hybridization

q.p. band

SO

scattering rate~100meV

T=10K

T=300K

0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4

4
3.5
3
2.5
2
1.5
1
0.5
0

Γ X R Z

Not much weight

Momentum resolved total spectra trA(ω,k)

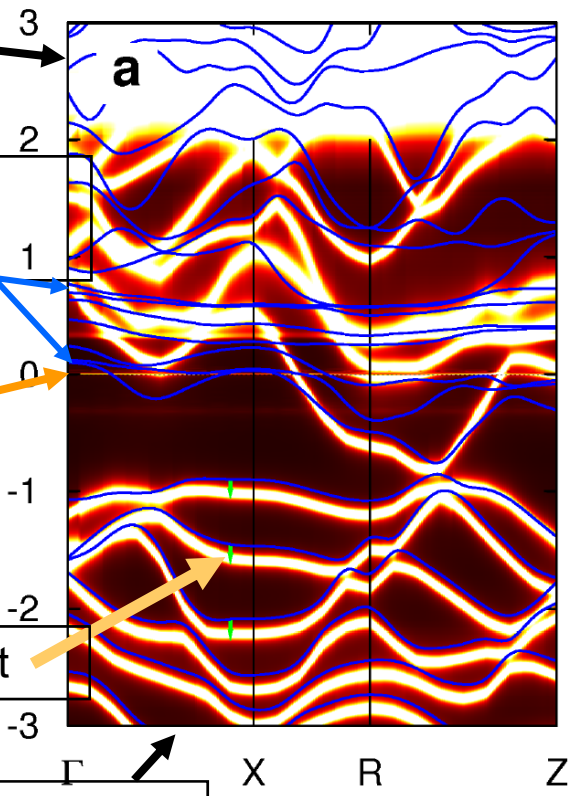
Most of weight transferred into the UHB

LDA *f*-bands [-0.5eV, 0.8eV] almost disappear, only In-p bands remain

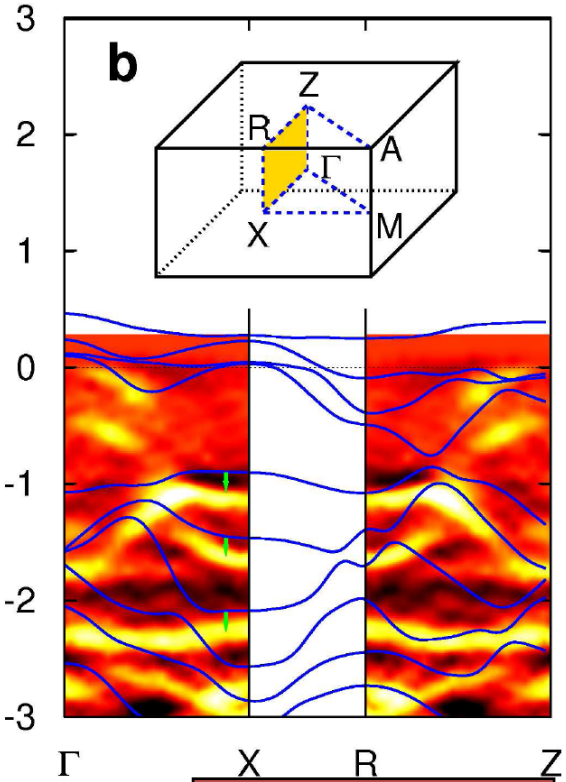
Very heavy qp at Ef, hard to see in total spectra

Below -0.5eV: almost rigid downshift

LDA+DMFT at 10K



ARPES, HE I, 15K

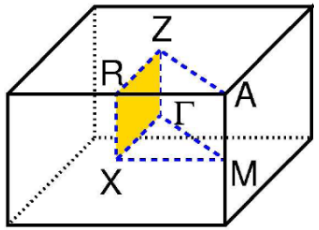


Fujimori, PRB

Unlike in LDA+U, no new band at -2.5eV

Short lifetime of HBs -> similar to LDA(f-core) rather than LDA or LDA+U

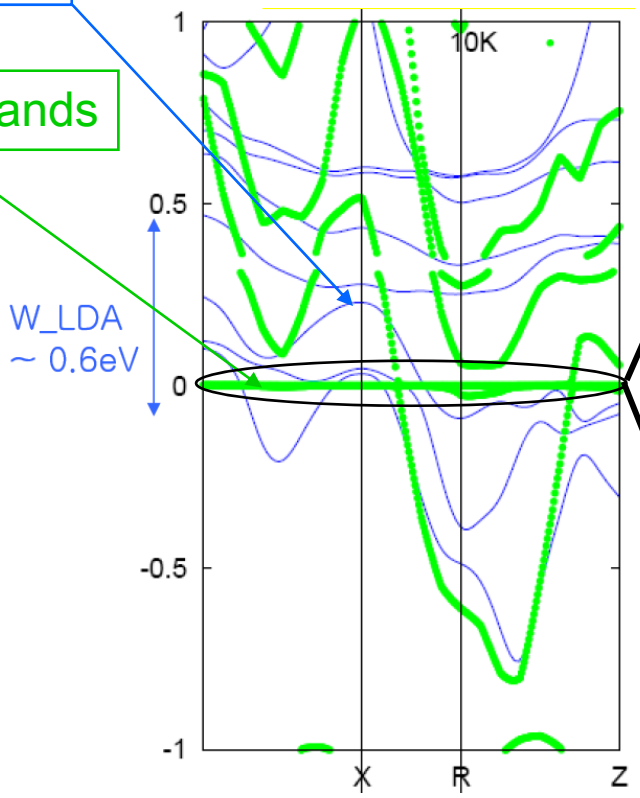
Quasiparticle bands



LDA bands

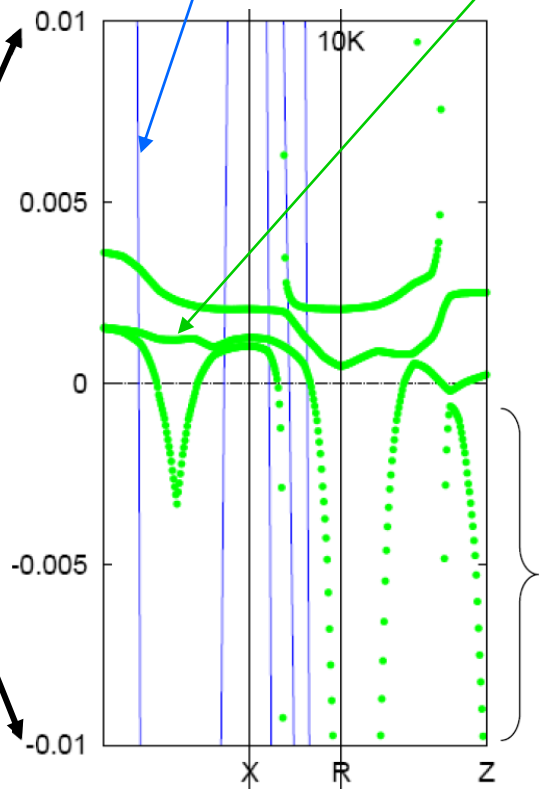
DMFT qp bands

$$\omega = \varepsilon^{(0)}_{\mathbf{k},n} + \Sigma(\omega)$$



LDA bands

DMFT qp bands



three bands, $Z_{j=5/2}$~1/200