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1957-3

Miniworkshop on Strong Correlations in Materials and Atom Traps

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Band structure of strongly correlated materials from the Dynamical Mean Field perspective.

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Band structure of strongly correlated materials from the Dynamical Mean Field perspective

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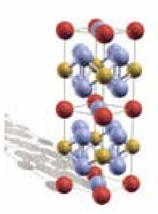
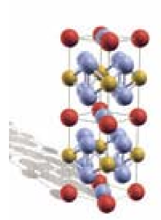
Collaborators: J.H. Shim & G. Kotliar



LT25, 2008

Outline



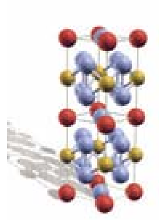
Dynamical Mean Field Theory in combination with band structure

- LDA+DMFT results for 115 materials ($CeIrIn_5$)
- Local Ce 4f - spectra and comparison to AIPES)
- Momentum resolved spectra and comparison to ARPES
- Optical conductivity
- Two hybridization gaps and its connection to optics

References:

•J.H. Shim, KH, and G. Kotliar, Science **318**, 1618 (2007).
•J.H. Shim, KH, and G. Kotliar, Nature **446**, 513 (2007).

Standard theory of solids

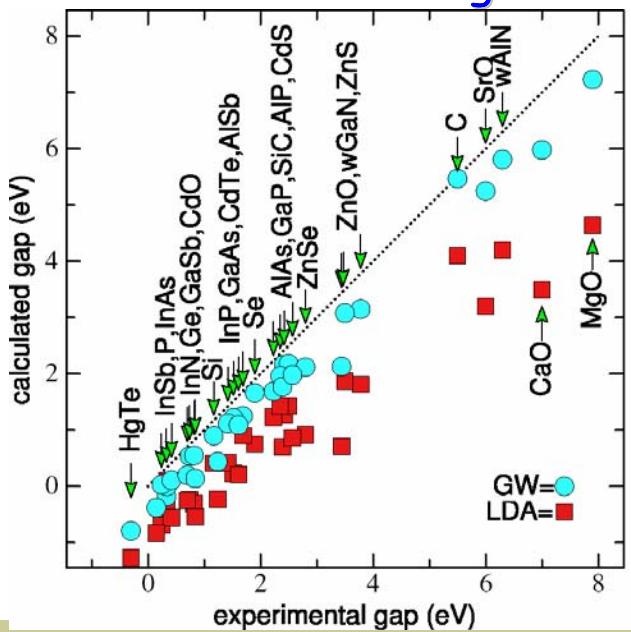


Band Theory: electrons as waves: Rigid band picture: En(k) versus k
Landau Fermi Liquid Theory applicable
Very powerful quantitative tools: LDA,LSDA,GW

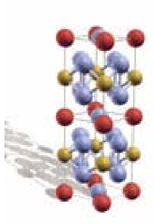
Predictions:

- total energies,
- stability of crystal phases
- optical transitions

M. Van Schilfgarde



Strong correlation – Standard theory fails



- Fermi Liquid Theory *does NOT work*. Need new concepts to replace rigid bands picture!
- Breakdown of the wave picture. Need to incorporate a real space perspective (Mott).
- Non perturbative problem.

Bright future!

Need new concepts, new techniques…

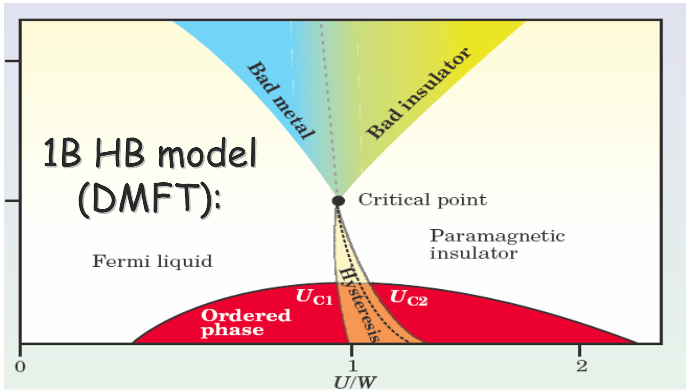
Dynamical Mean Field Theory the simplest approach which can describe the physics of strong correlations

->the spectral weight transfer

->Mott transition

->local moments and itinerant bands, heavy quasiparticles

DMFT can describe Mott transition:



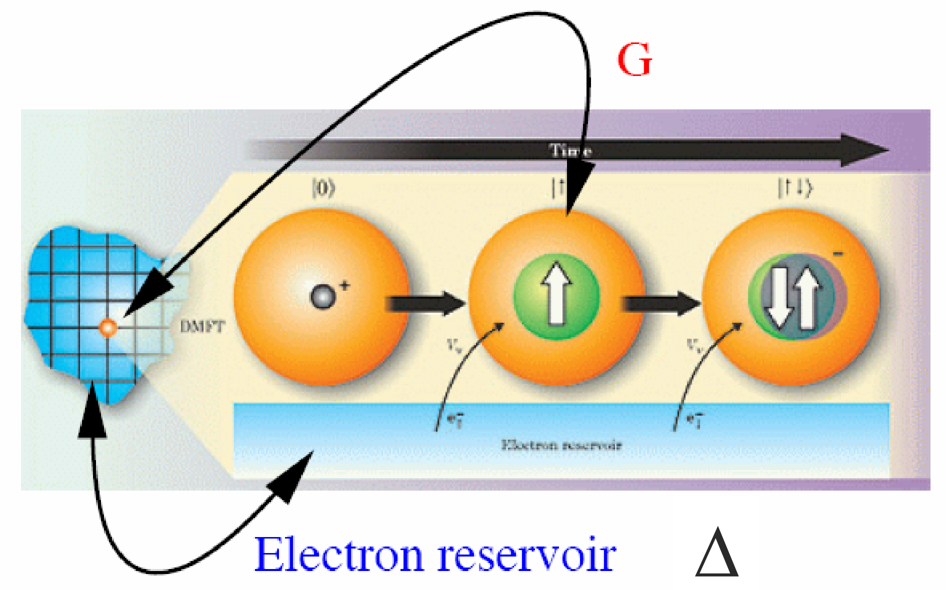
DMFT + electronic structure method

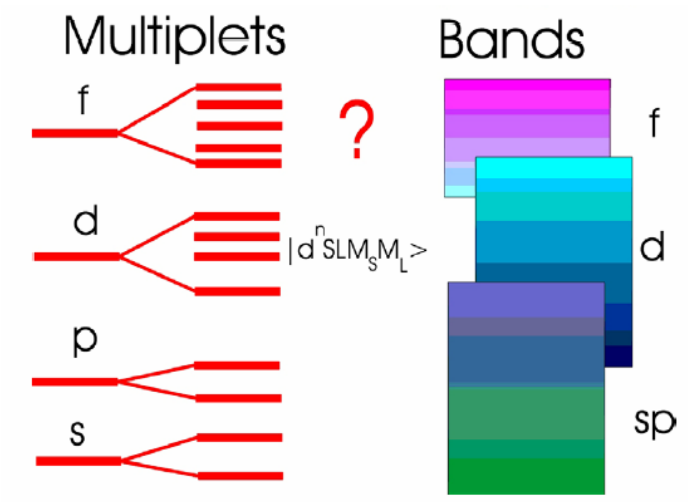
Basic idea of DMFT+electronic structure method (LDA or GW):

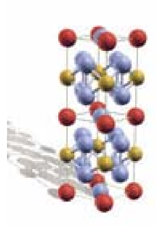
For less correlated bands (s,p): use LDA or GW

For correlated bands (f or d): ***add all local diagrams by solving QIM***

(G. Kotliar S. Savrasov K.H., V. Oudovenko O. Parcollet and C. Marianetti, RMP 2006).



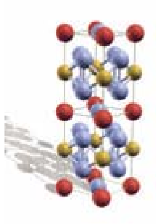




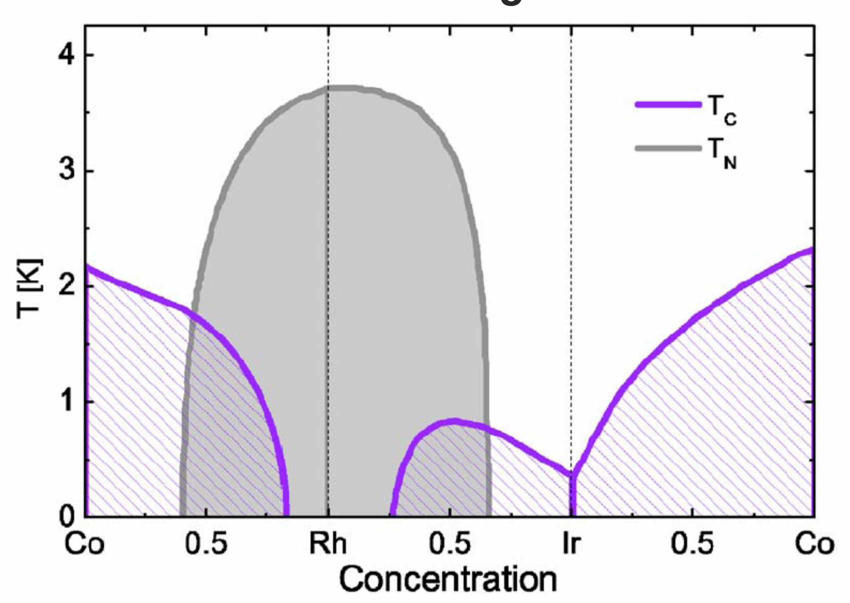
Basic questions to address

- How to compute spectroscopic quantities (single particle spectra, optical conductivity phonon dispersion…) from first principles?
- How to relate various experiments into a unifying picture.
- DMFT maybe simplest approach to meet this challenge for correlated materials

Phase diagram of 115's – heavy fermion systems

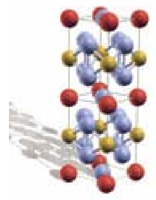


$CeXIn_5$



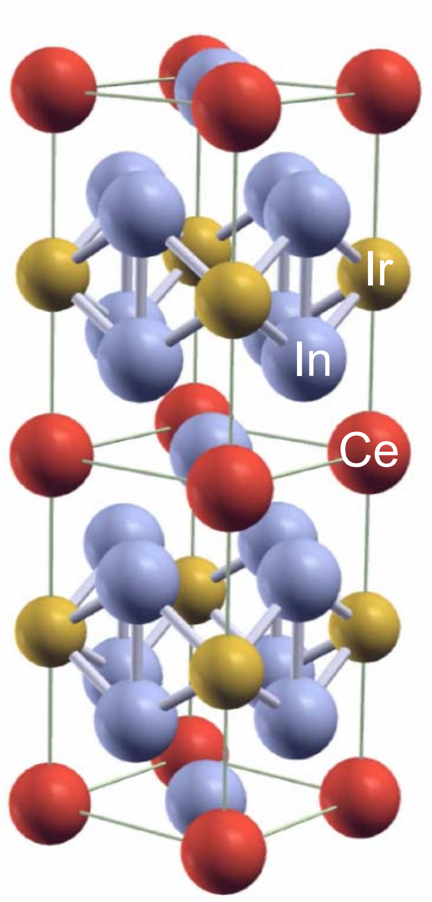
$CeCoIn_5$ $CeRhIn_5$ $CeIrIn_5$ $CeCoIn_5$

	$CeCoIn_5$	$CeRhIn_5$	$CeIrIn_5$	$PuCoG_5$
Tc[K]	SC 2.3K	N 3.8 K	SC 0.4K	18.3K
$T_{crossover}$	~50K	~50K	~50K	~370K
C_v/T[mJ/molK^2]	300	400	750	100



Crystal structure of 115's

Tetragonal crystal structure



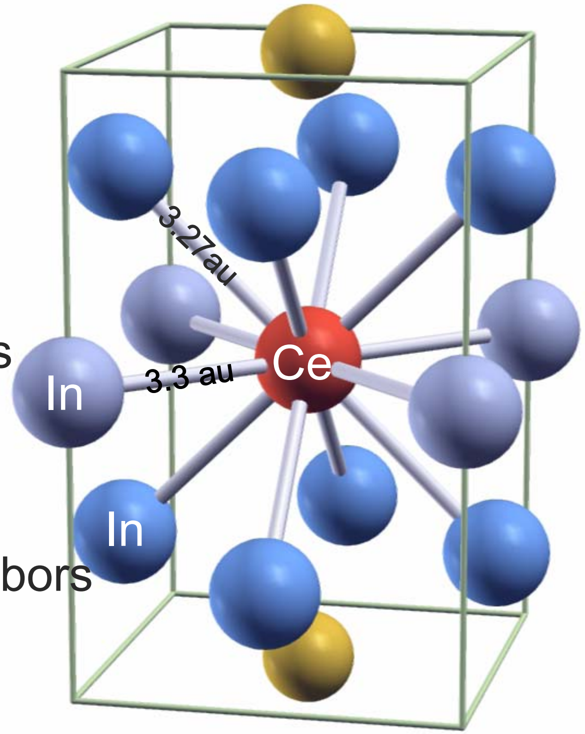
$IrIn_2$ layer

$CeIn_3$ layer

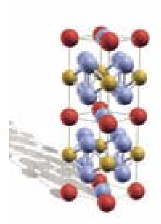
$IrIn_2$ layer

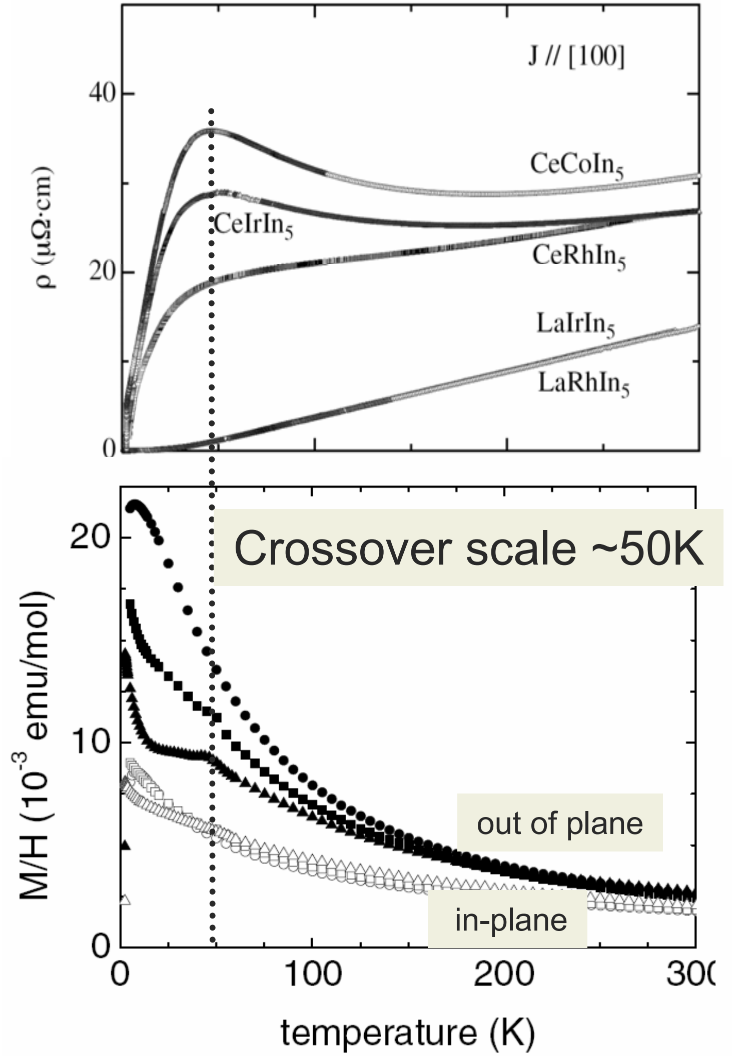
4 in plane In neighbors

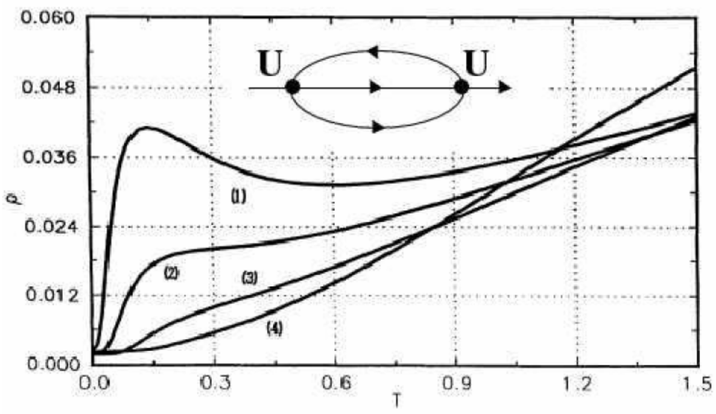
8 out of plane in neighbors



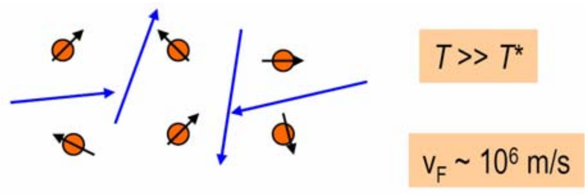
Coherence crossover in experiment



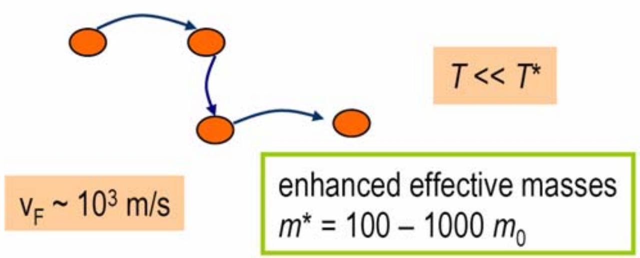




ALM in DMFT Schweitzer& Czycholl,1991

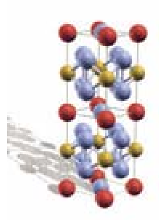


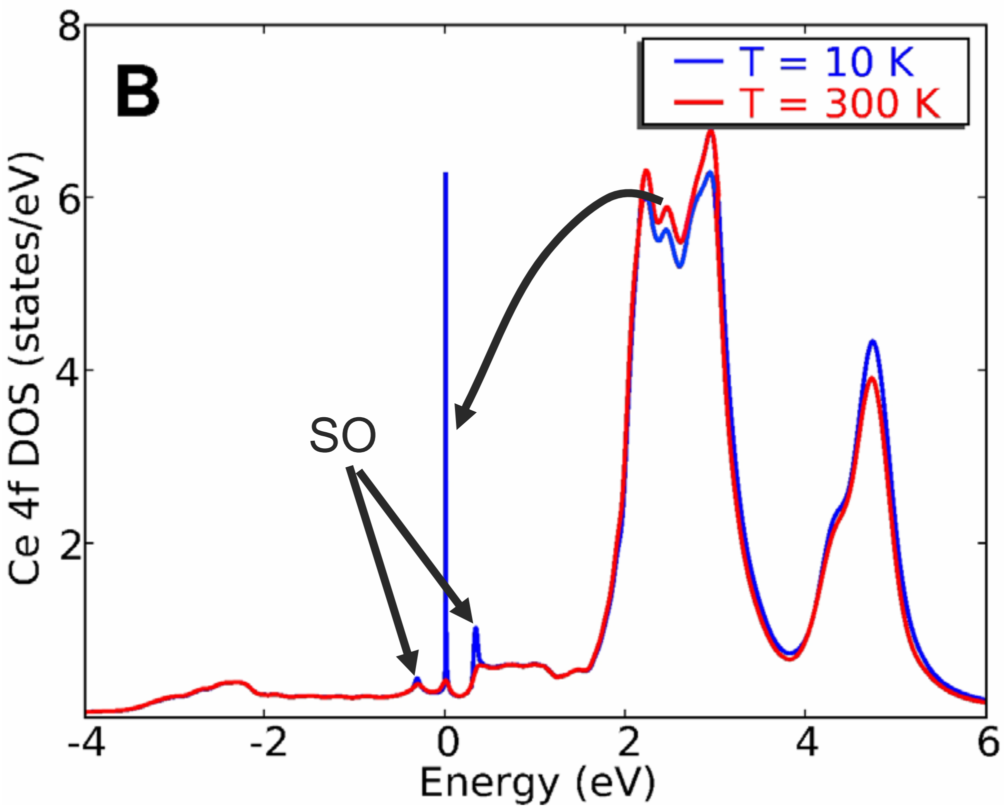
•High temperature Ce-4f local moments



•Low temperature – Itinerant heavy bands

Temperature dependence of the **local Ce-4f** spectra

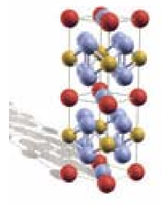




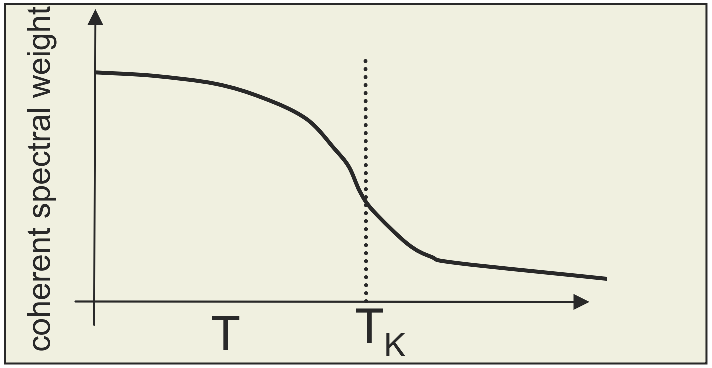
- At 300K, only Hubbard bands
- At low T, very narrow q.p. peak (width ~3meV)
- SO coupling splits q.p.: +-0.28eV
- Redistribution of weight up to very high frequency

J. H. Shim, KH, and G. Kotliar Science 318, 1618 (2007).

Buildup of coherence

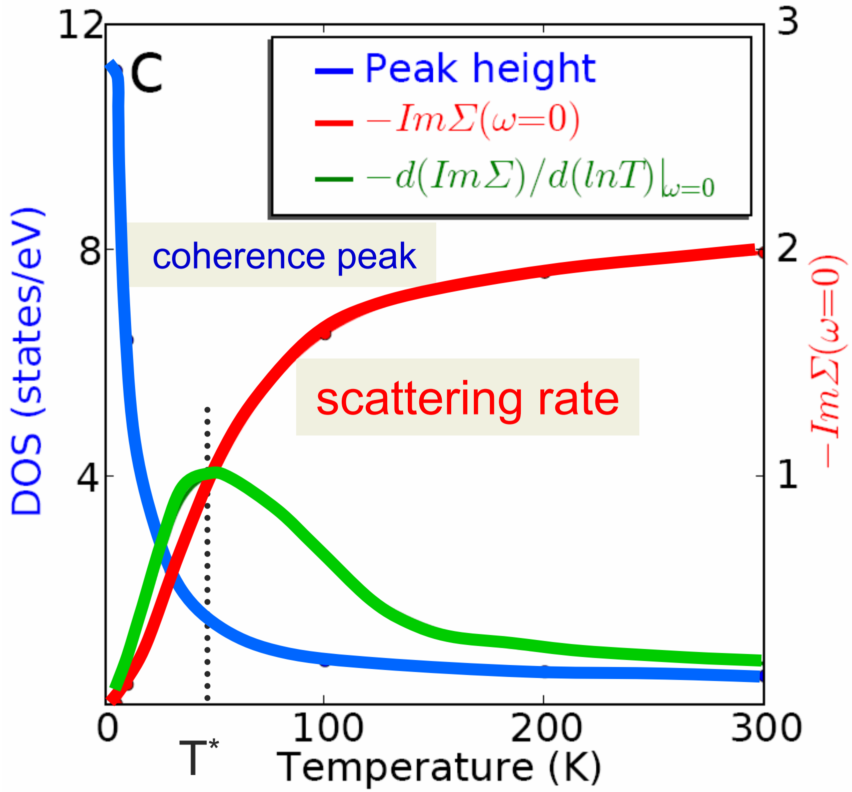


Buildup of coherence in single impurity case



Slow crossover pointed out by NPF 2004

Very slow crossover!



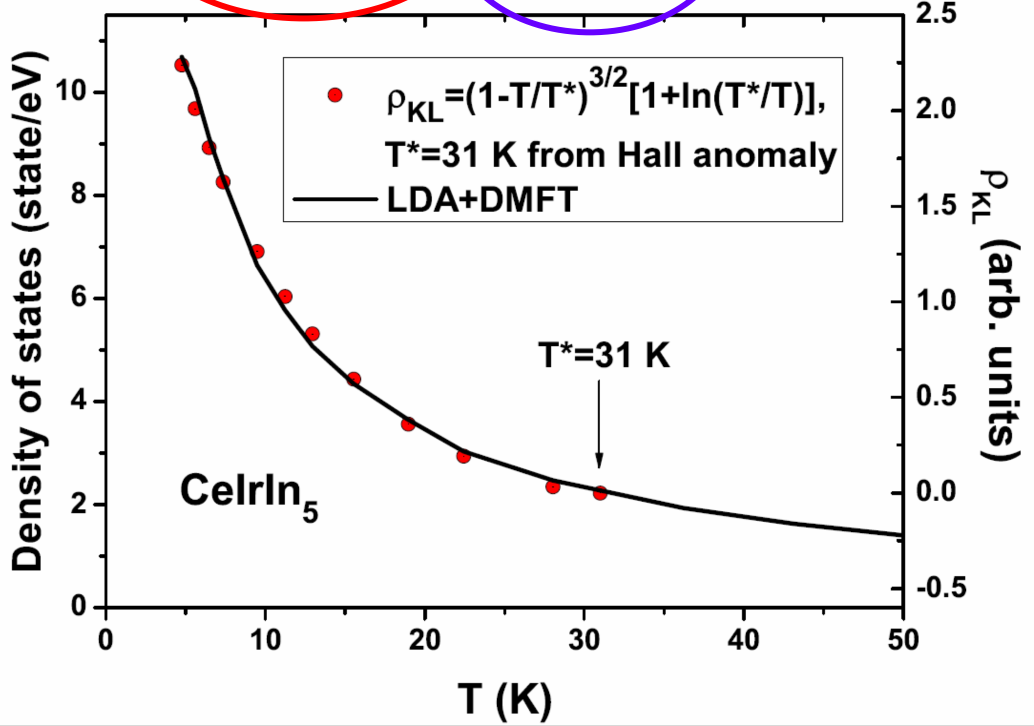
Crossover around 50K

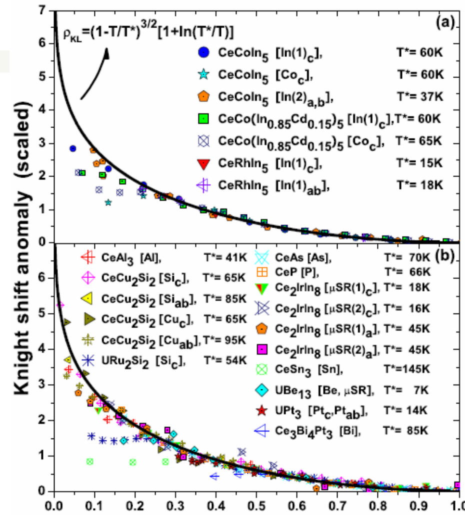
Consistency with the phenomenological approach of NPF

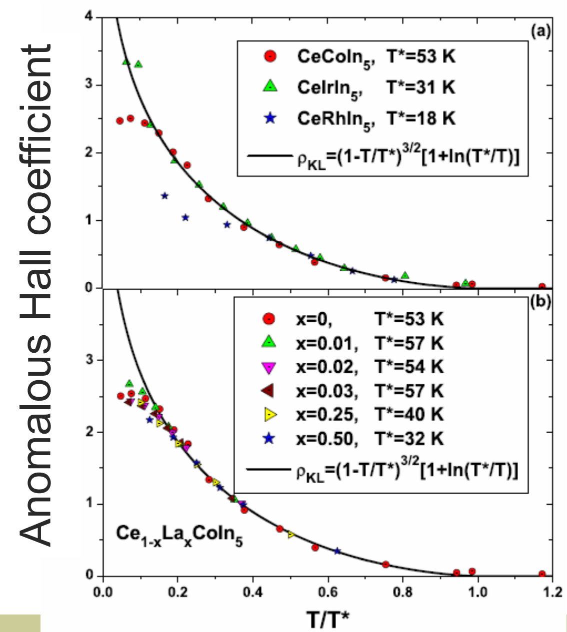
Fraction of itinerant heavy fluid

$$\rho_{KL} = \left(1 - \frac{T}{T^*}\right)^{3/2}\left(1 + \ln\frac{T^*}{T}\right)$$

m* of the heavy fluid

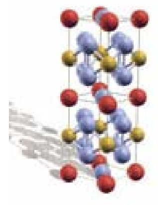


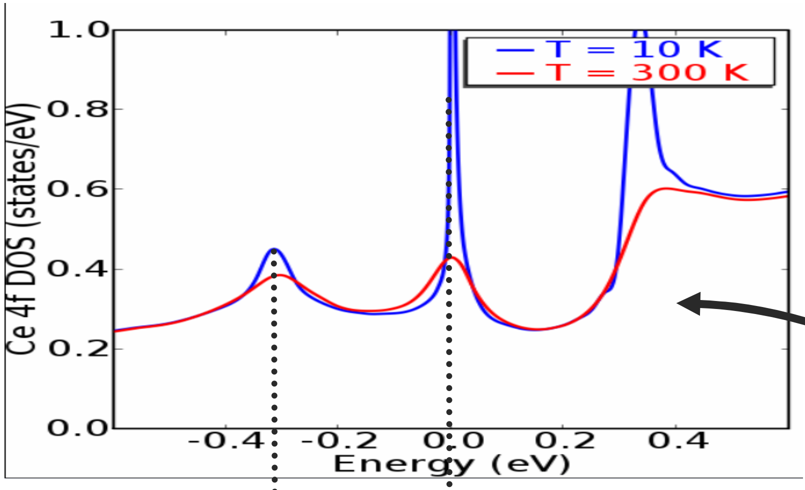


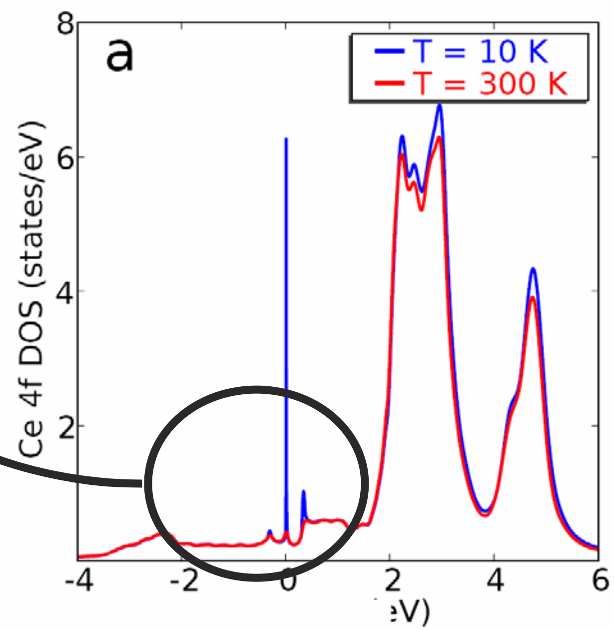


Remarkable agreement with Y. Yang & D. Pines Phys. Rev. Lett. **100**, 096404 (2008).

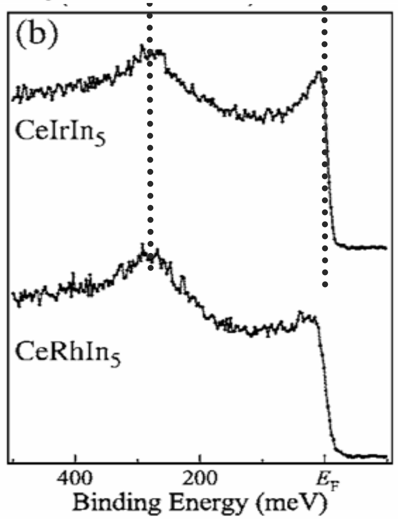
Angle integrated photoemission vs DMFT







4d-4f on-resonance (hν=122 eV)

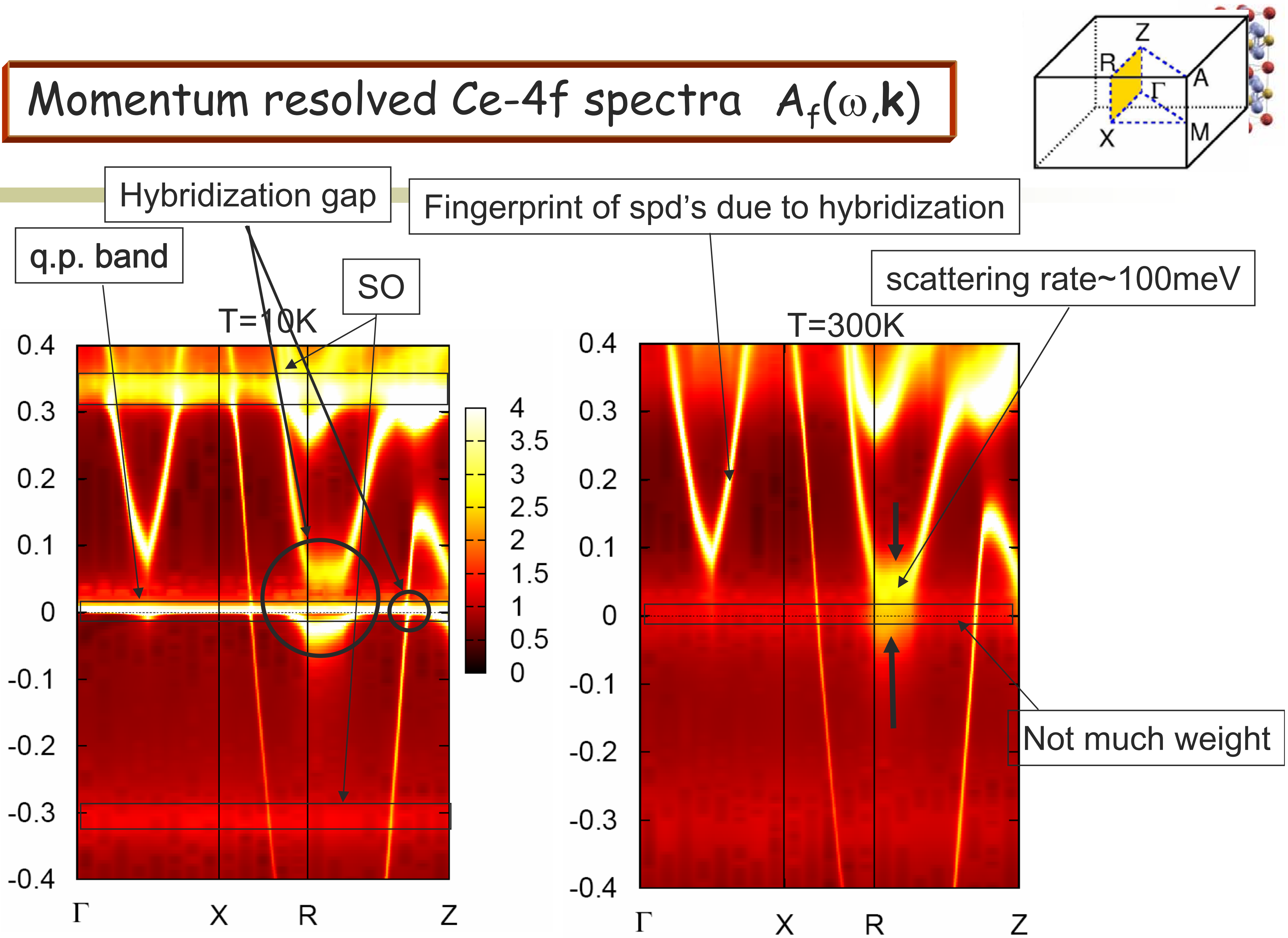


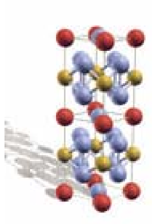
Experiment at T=10K

Maybe surface sensitive at 122eV

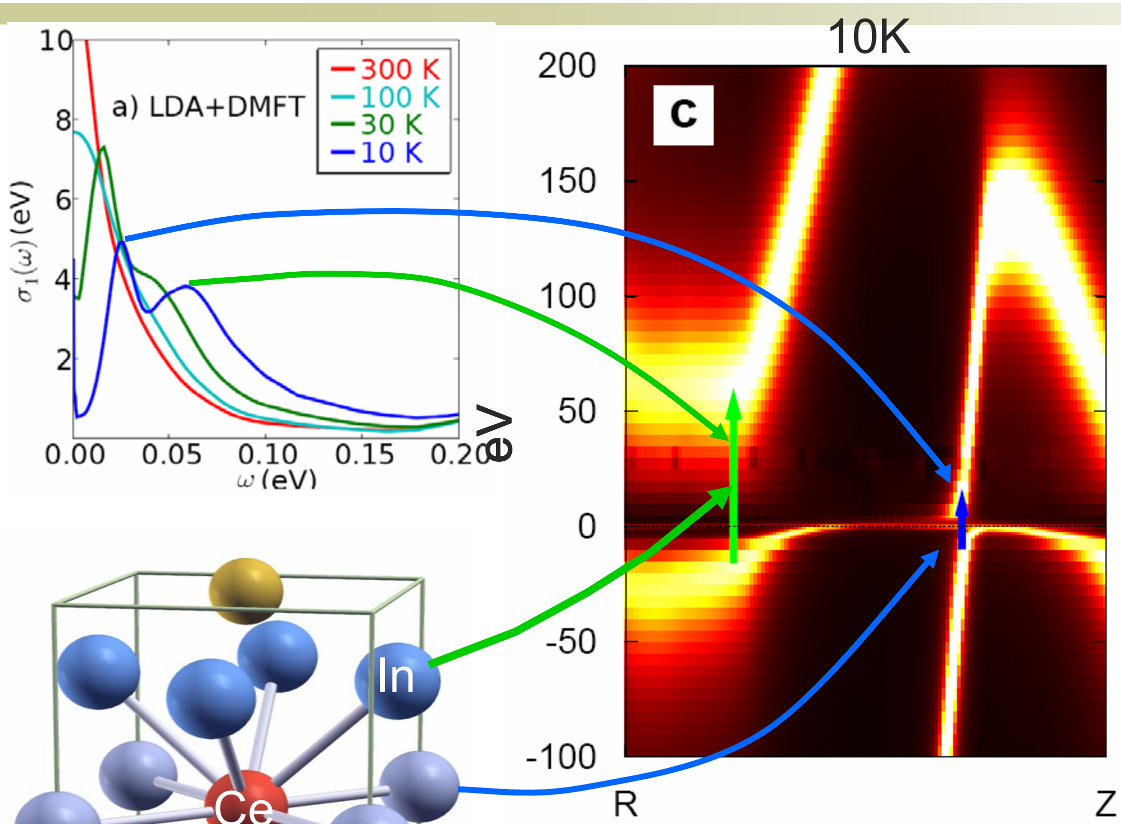
ARPES
Fujimori, 2006

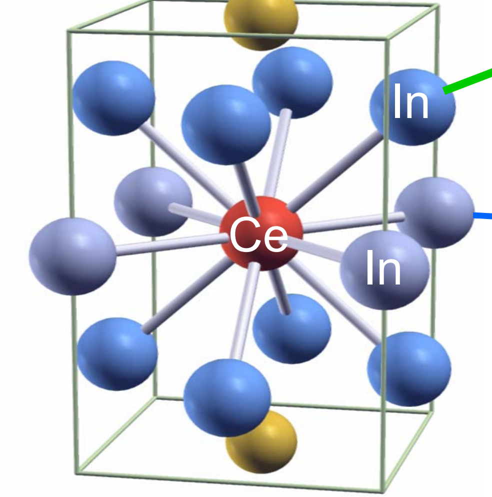
Momentum resolved Ce-4f spectra $A_f(\omega,\mathbf{k})$



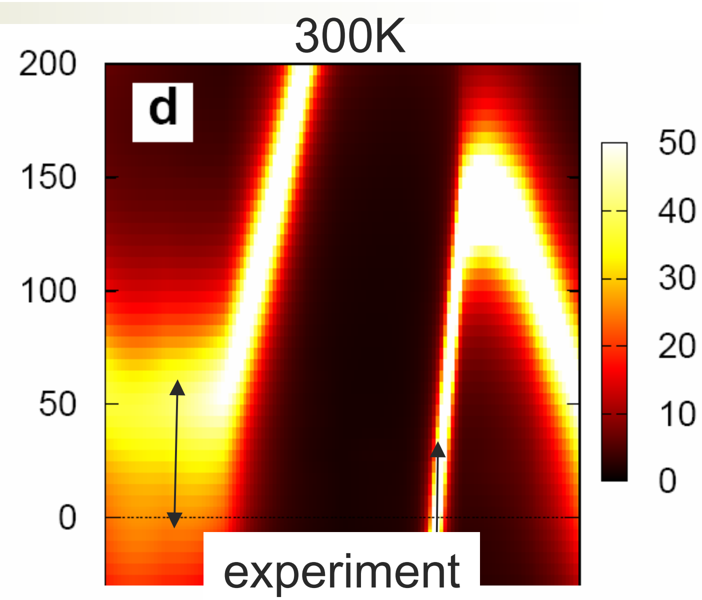


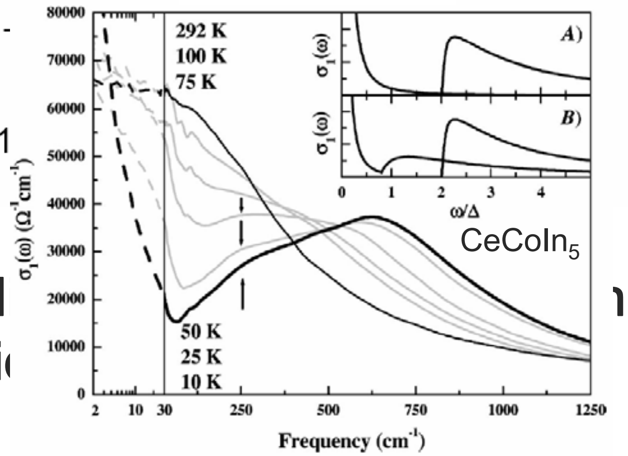
Multiple hybridization gaps





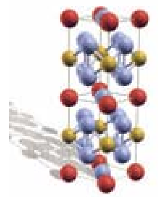
non-f spectra





- Larger gap due to hybrid
- Smaller gap due to hybri

Conclusions



- DMFT can describe crossover from local moment regime to heavy fermion state in heavy fermions. The crossover is very slow.

- Mid-IR peak of the optical conductivity in 115's is split due to pr
esence of two type's of hybridization

- Ce moment is more coupled to out-of-plane In then in-plane In which explains the sensitivity of 115's to substitution of tr
ansition metal ion