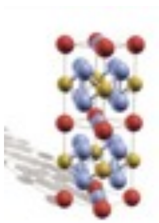
Complex correlated materials from the Dynamical Mean Field Perspective.

RUTGERS
THE STATE UNIVERSITY OF NEW JERSEY

Kristjan Haule

Support:



Tallahassee, 2012

Thanks To

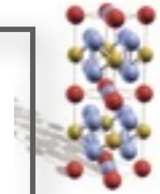
Collaborators:

Gabriel Kotliar, Zhiping Yin, Hyowon Park, Chuck-Hou Yee, Jan Tomczak, Ronald Cohen






Motivation



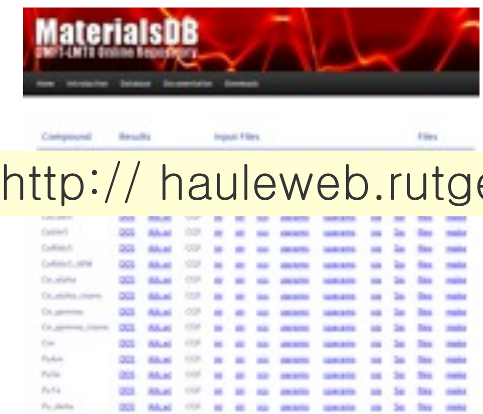
Motivation: Testing our ability to understand the electronic structure of complex correlated materials.

The driving force:
Experimental probes
Optics,APRES,STM,
...

interplay

Computational tool
is (DFT,DMFT)

Developing DMFT into an electronic structure tool, understanding qualitatively universal and system specific aspects.



http:// hauleweb.rutgers.edu

Wien2K+DMFT
multiorbital CTQMC, full potential basis, charge self-consistent.

Computational tools allow to identify system specific fingerprints which give us confidence in our understanding of correlated electron materials

Thermoelectricity in FeSi as Hunds semiconductors

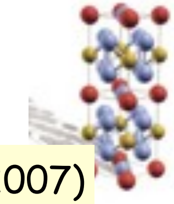
J.Tomczak, KH, G. Kotliar, PNAS (2012)

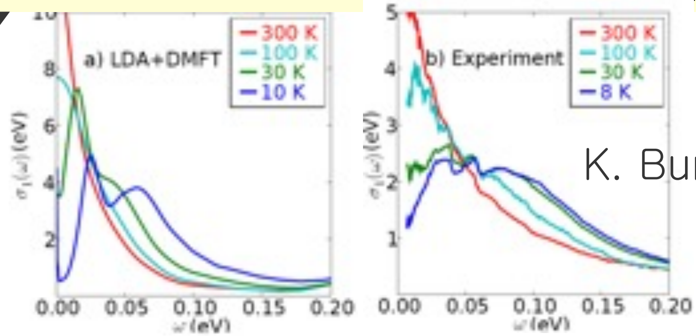
MIT in FeO

K. Ohta, R. Cohen, KH, PRL (2012)

Protracted screening and multiple hybridization Gaps in Ce115's.

J.H.Shim, KH, G.Kotliar,Science 318, 1615 (2007)

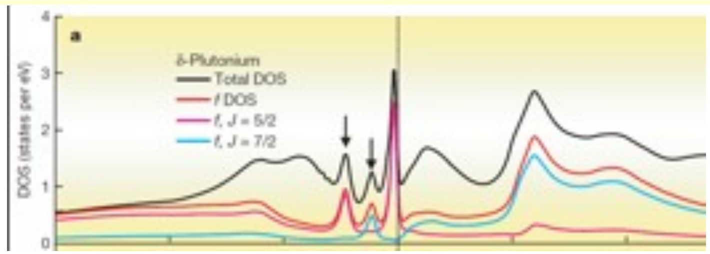




K. Burch et.al.

Quasiparticle multiplets in Plutonium and its Compounds.

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



Strength of correlations in e and h doped cuprates.

C Weber, KH, G. Kotliar, Nature Physics 10, 1038 (2010)

Hidden Order in URu2Si2, Kondo effect and hexadecapole order.

KH, G. Kotliar, Nature Physics 5, 796 - 799 (2009).

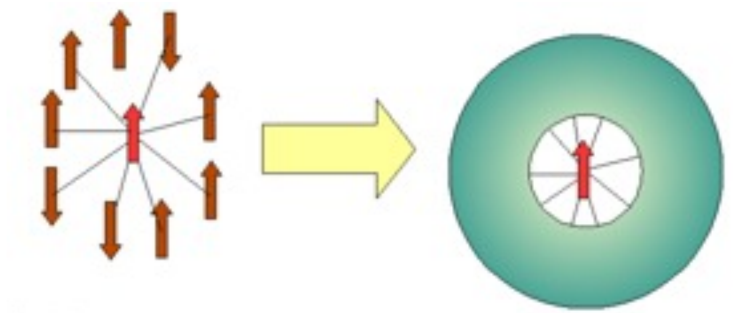
Magnetism and Charge Dynamics in Iron Pnictides.

Z. P. Yin, KH, G. Kotliar, Nature Physics (2011)

Z. P. Yin, KH, G. Kotliar, Nature Materials (2011)

Bright Future:Dynamical Mean Field

Weiss mean field theory for spin systems
Exact in the limit of large z



$$\sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j$$

$$\sum_{i} \mathbf{B}_i\mathbf{S}_i$$

$$\mathbf{B}_i = \sum_{j\neq i} J_{ij}\langle \mathbf{S}_j \rangle$$

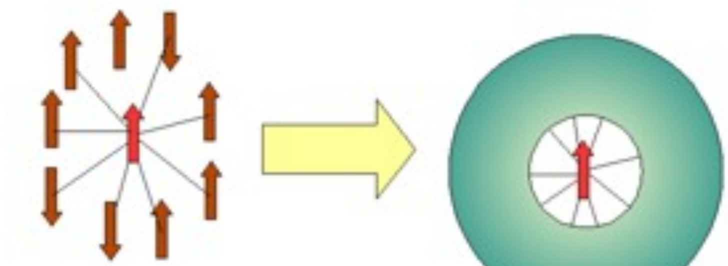
Classical problem of spin in
a magnetic field

Bright Future:Dynamical Mean Field

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

Weiss mean field theory for spin systems
Exact in the limit of large z

Dynamical mean field theory (DMFT)
for the electronic problem
exact in the limit of large z

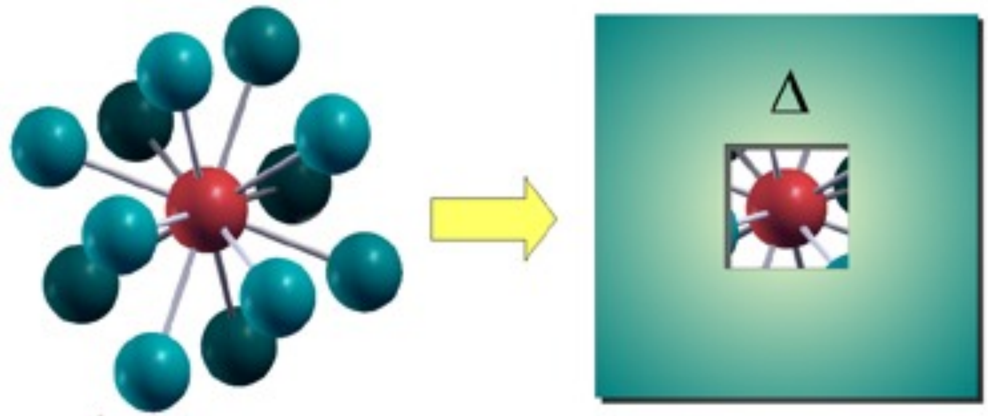


$$\sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j$$

$$\sum_i \mathbf{B}_i\mathbf{S}_i$$

$$\mathbf{B}_i = \sum_{j\neq i} J_{ij}\langle\mathbf{S}_j\rangle$$

Classical problem of spin in
a magnetic field



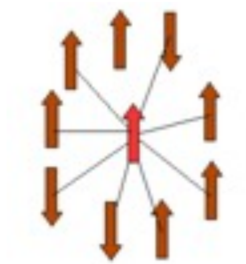
$$Z = \int \mathcal{D}[\psi^\dagger\psi] e^{-\sum_i S_{atom}(i) - \sum_{ij}\int d\tau \psi_i^\dagger(\tau)\hat{H}_{ij}\psi_j(\tau)}$$

$$Z = \int \mathcal{D}[\psi^\dagger\psi] e^{-\sum_i S_{atom}(i) - \sum_i \int d\tau d\tau' \psi_i^\dagger(\tau)\hat{\Delta}(\tau,\tau')\psi_i(\tau')}$$

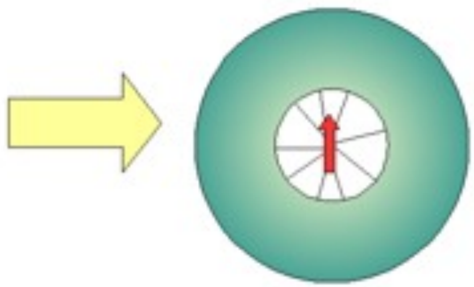
Bright Future:Dynamical Mean Field

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

Weiss mean field theory for spin systems
Exact in the limit of large z



$$\sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j$$

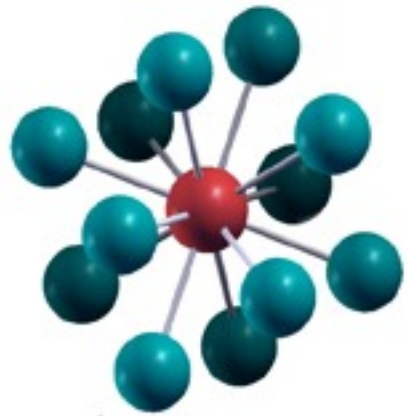


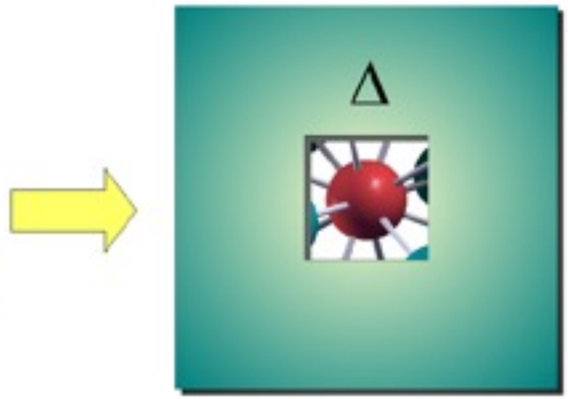
$$\sum_i \mathbf{B}_i\mathbf{S}_i$$

$$\mathbf{B}_i = \sum_{j\neq i} J_{ij}\langle \mathbf{S}_j\rangle$$

Classical problem of spin in
a magnetic field

Dynamical mean field theory (DMFT)
for the electronic problem
exact in the limit of large z





$$Z = \int \mathcal{D}[\psi^\dagger\psi] e^{-\sum_i S_{atom}(i) - \sum_{ij}\int d\tau \psi_i^\dagger(\tau)\hat{H}_{ij}\psi_j(\tau)}$$

$$Z = \int \mathcal{D}[\psi^\dagger\psi] e^{-\sum_i S_{atom}(i) - \sum_i \int d\tau d\tau' \psi_i^\dagger(\tau)\hat{\Delta}(\tau,\tau')\psi_i(\tau')}$$

Problem of a quantum impurity
(atom in a fermionic band)

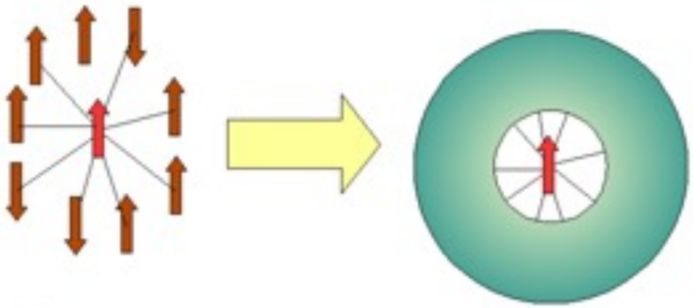
Space fluctuations are ignored,
time fluctuations are treated exactly

Bright Future:Dynamical Mean Field

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

Weiss mean field theory for spin systems
Exact in the limit of large z

Dynamical mean field theory (DMFT)
for the electronic problem
exact in the limit of large z

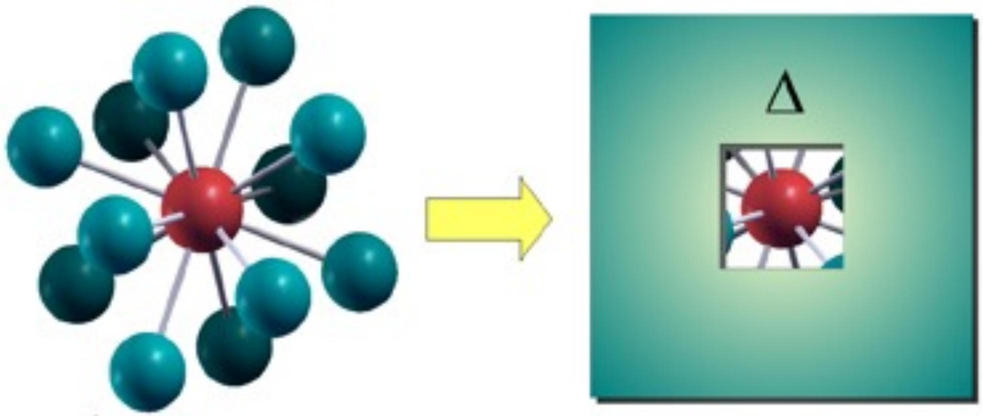


$$\sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j$$

$$\sum_i \mathbf{B}_i\mathbf{S}_i$$

$$\mathbf{B}_i = \sum_{j\neq i} J_{ij}\langle\mathbf{S}_j\rangle$$

Classical problem of spin in
a magnetic field



$$Z = \int \mathcal{D}[\psi^\dagger\psi] e^{-\sum_i S_{atom}(i) - \sum_{ij}\int d\tau \psi_i^\dagger(\tau)\hat{H}_{ij}\psi_j(\tau)}$$

$$Z = \int \mathcal{D}[\psi^\dagger\psi] e^{-\sum_i S_{atom}(i) - \sum_i \int d\tau d\tau' \psi_i^\dagger(\tau)\hat{\Delta}(\tau,\tau')\psi_i(\tau')}$$

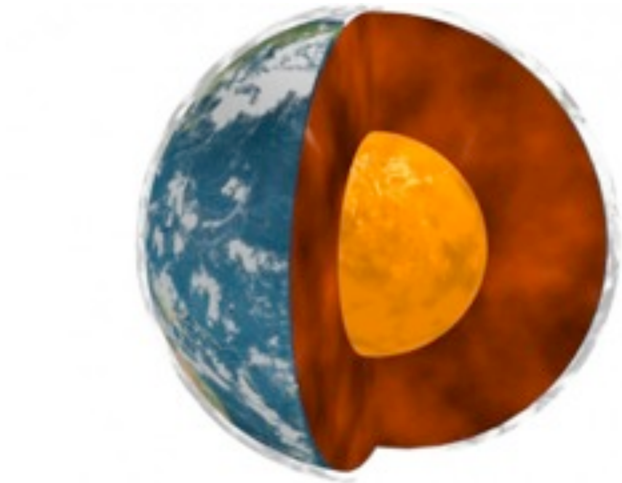
Improvements:
- Impurity solvers (Numerically exact continuous time QMC method)
- Charge SC implementation, avoids construction of low energy models

IRON OXIDE

Very common in life:

Fe^{2+} pigment, in cosmetics & tattoo inks

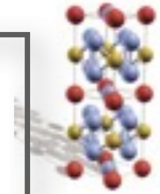
Fe^{3+} corrosion



Wüstite, FeO, is important constituent of the Earth’s lower mantle and possibly in the core

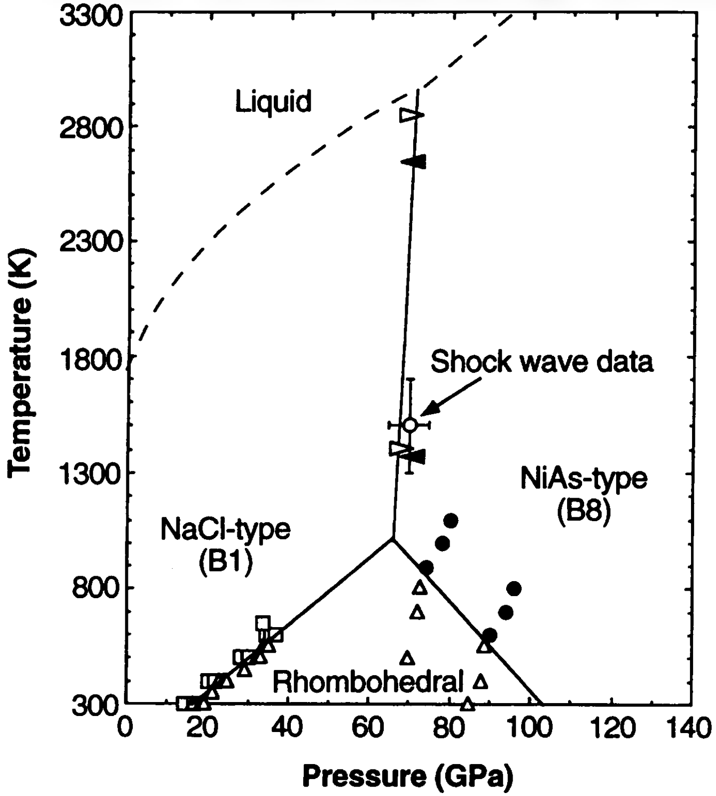
Physical properties under high pressure still poorly understood.
Important for geophysical science : origin of the Earths magnetic field

Is FeO insulating/conducting in the lower mantle under high pressure and high T?
How does B-field (created in the lower mantle) propagate to the surface?
What is magnetomechanical coupling between the Earth’s mantle and core?



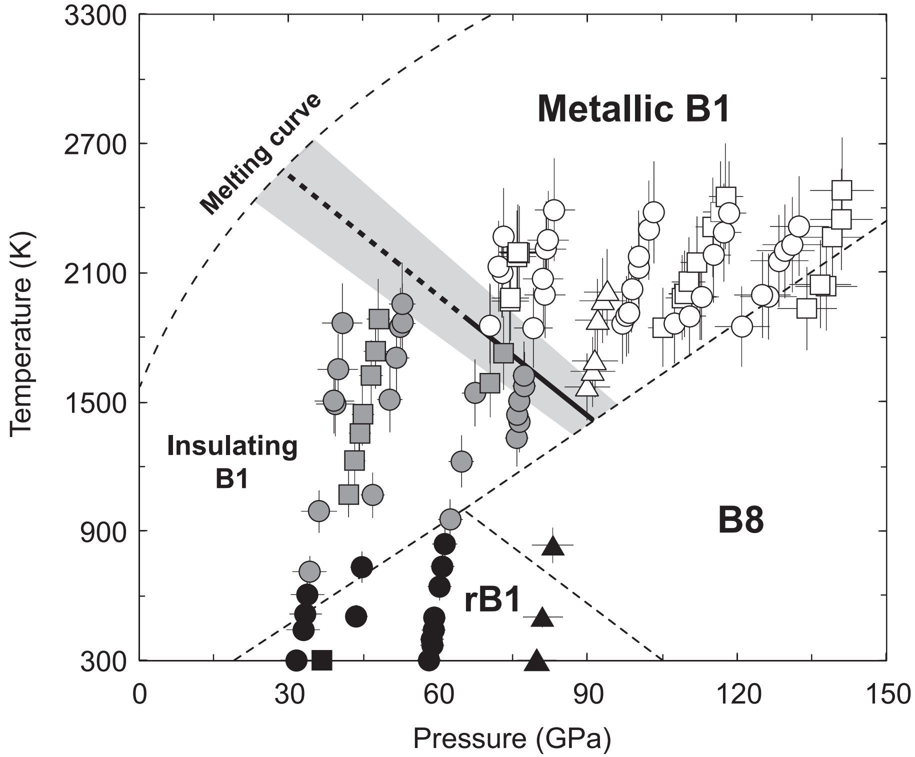
FeO phase diagram

Prior understanding of the PD



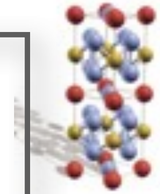
Yingwei Fei and Ho-kwang Mao
Science **266**, 1678 (1994).

New Phase Diagram 2011

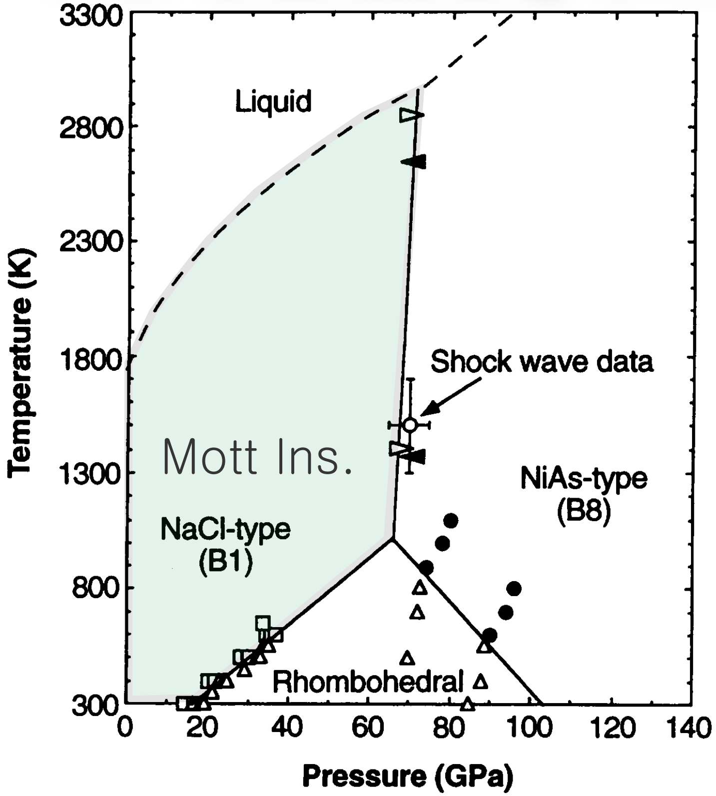


K. Ohta, R.E. Cohen, K. Hirose, K. Haule,
K. Shimizu, Y. Ohishi, PRL 2012

FeO phase diagram

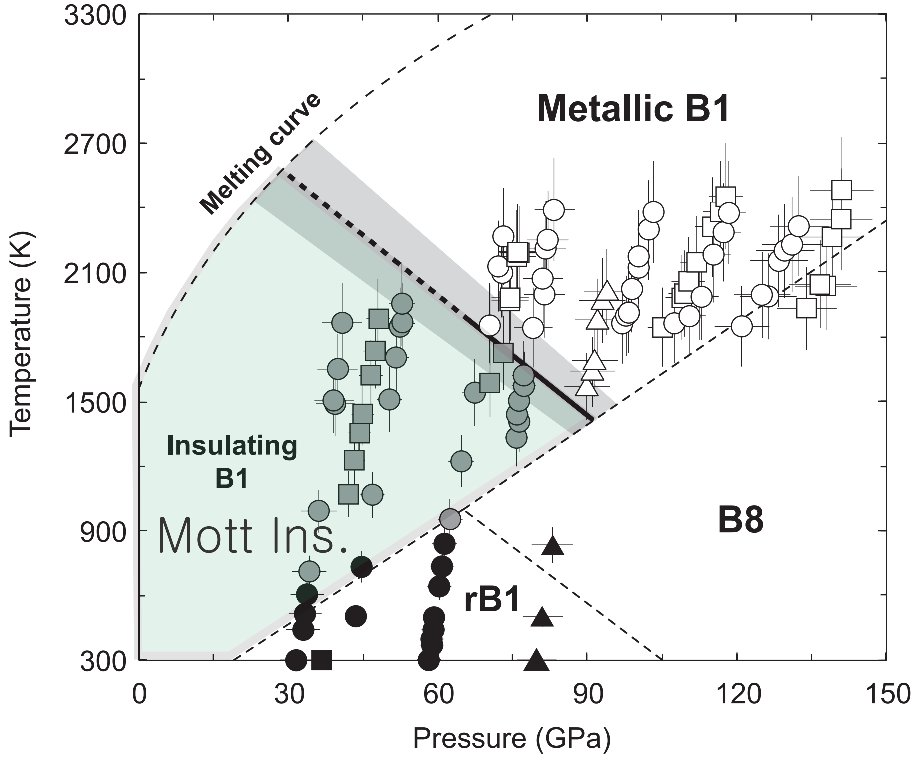


Prior understanding of the PD



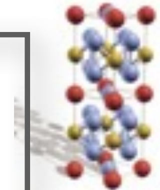
[Yingwei Fei and Ho-kwang Mao](#)
Science **266**, 1678 (1994).

New Phase Diagram 2011

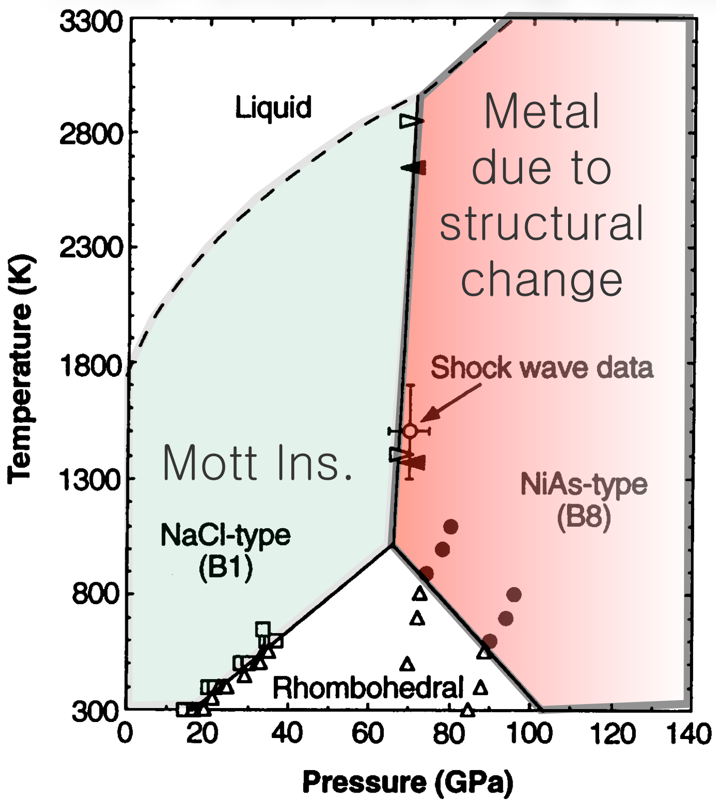


K. Ohta, R.E. Cohen, K. Hirose, K. Haule, K. Shimizu, Y. Ohishi, PRL 2012

FeO phase diagram

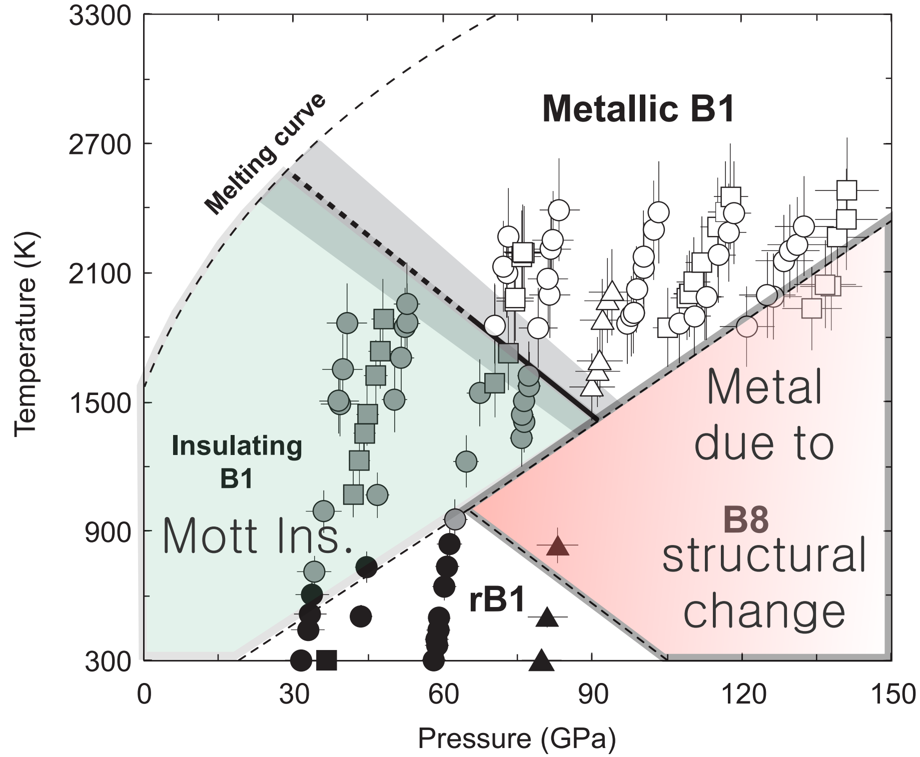


Prior understanding of the PD



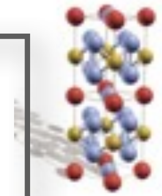
Yingwei Fei and Ho-kwang Mao
Science **266**, 1678 (1994).

New Phase Diagram 2011

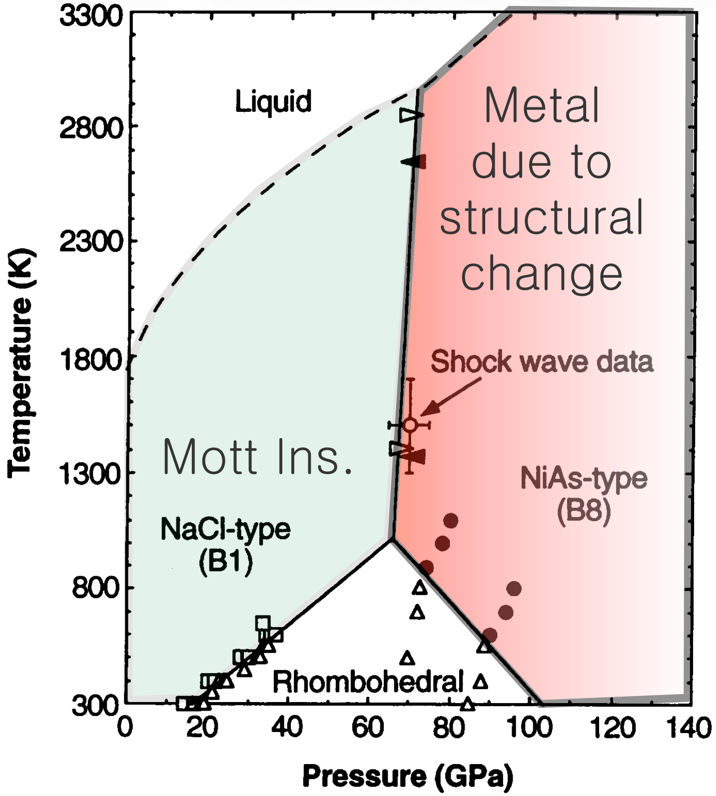


K. Ohta, R.E. Cohen, K. Hirose, K. Haule,
K. Shimizu, Y. Ohishi, PRL 2012

FeO phase diagram

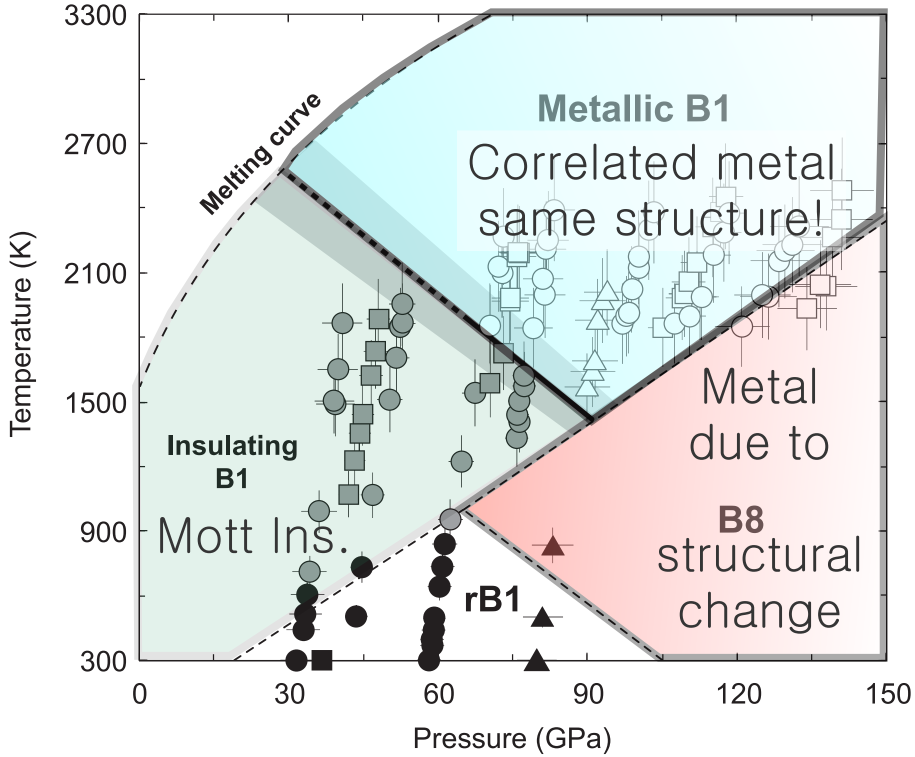


Prior understanding of the PD



Yingwei Fei and Ho-kwang Mao
Science **266**, 1678 (1994).

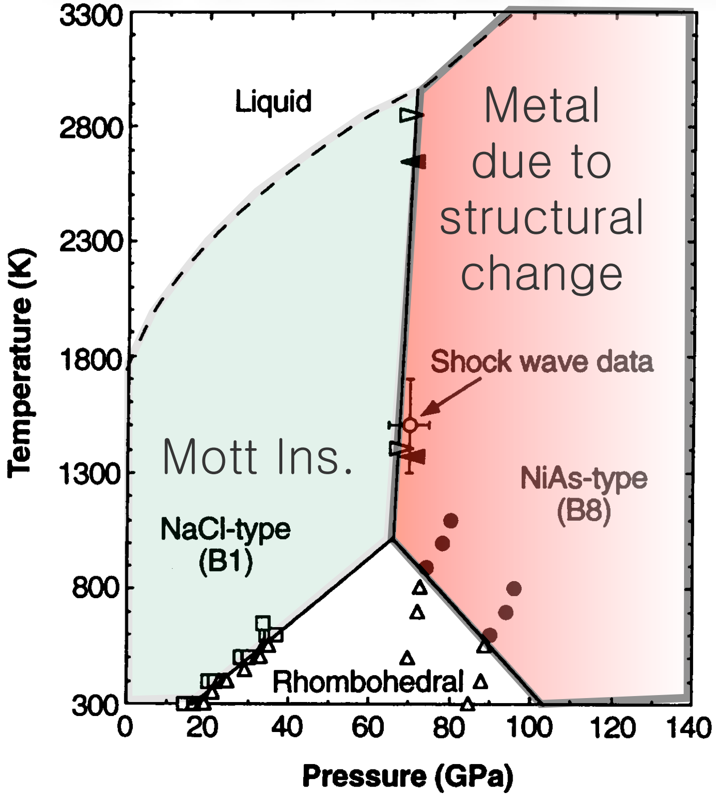
New Phase Diagram 2011



K. Ohta, R.E. Cohen, K. Hirose, K. Haule,
K. Shimizu, Y. Ohishi, PRL 2012

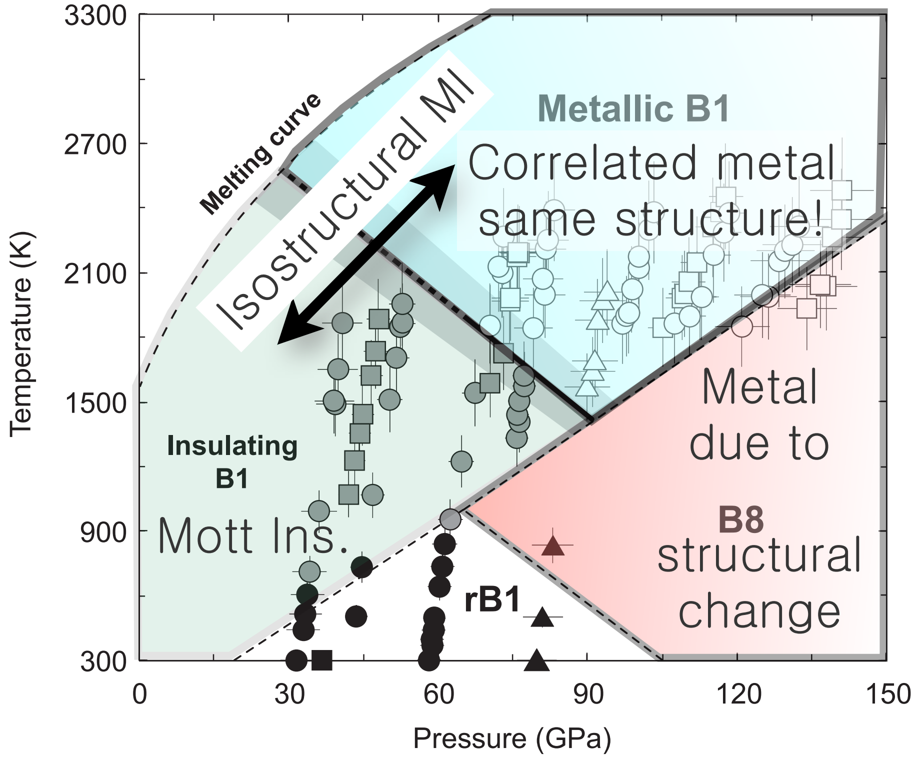
FeO phase diagram

Prior understanding of the PD



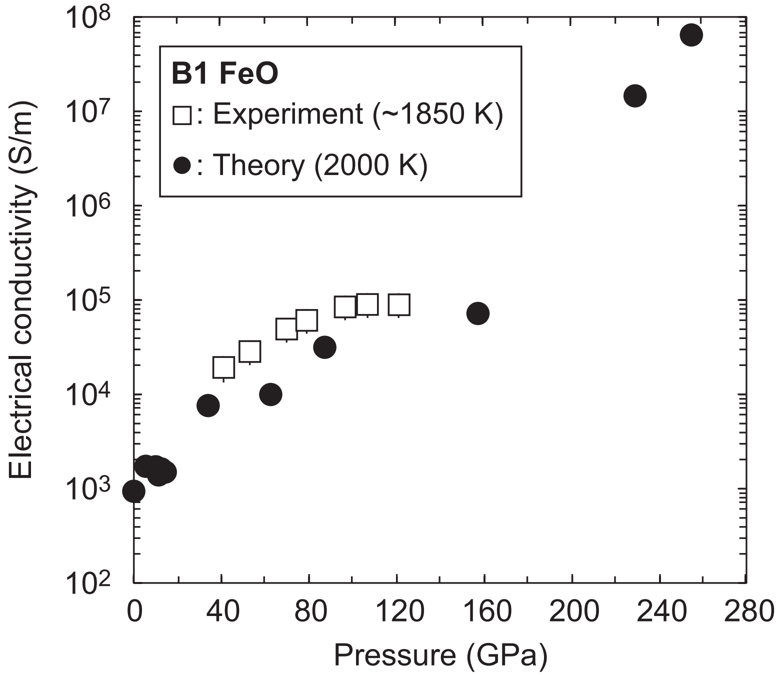
Yingwei Fei and Ho-kwang Mao
Science **266**, 1678 (1994).

New Phase Diagram 2011



K. Ohta, R.E. Cohen, K. Hirose, K. Haule,
K. Shimizu, Y. Ohishi, PRL 2012

FeO conductivity



Mott state in FeO at high temperature unstable

K. Ohta, R.E. Cohen, K. Hirose, K. Haule, K. Shimizu, Y. Ohishi, PRL 2012

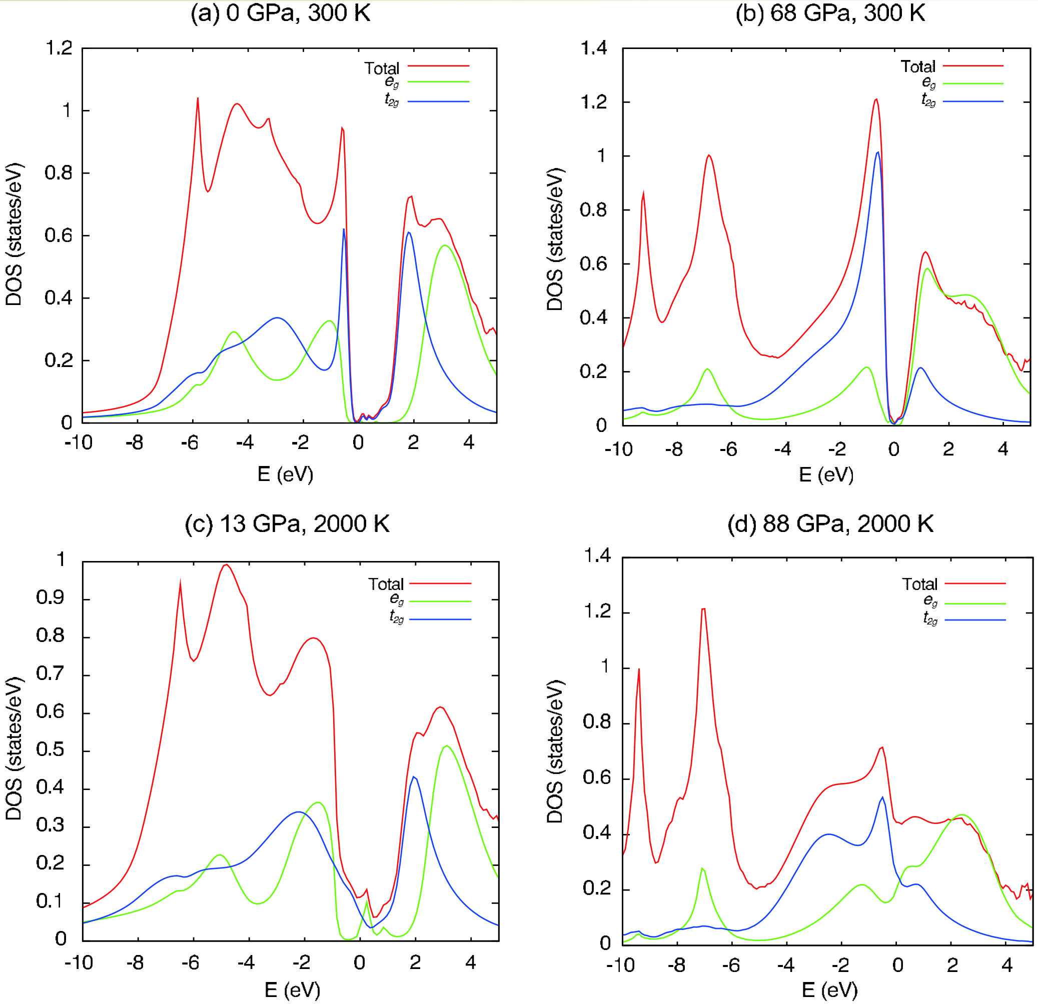
Conductivity increases by orders of magnitude

No sharp phase transition more like crossover

FeO spectra

Low–T insulator
stable under pressure:

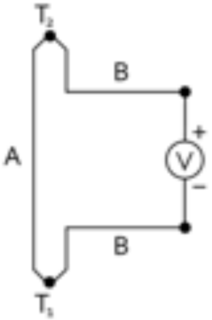
High–T insulator
unstable under pressure:



bad insulator
in high–spin state

bad metal
in low–spin state

Thermoelectricity



Temperature gradient creates electric field

Existing materials only small efficiency
Figure of merit of unity is "good",
"best" is 2–3

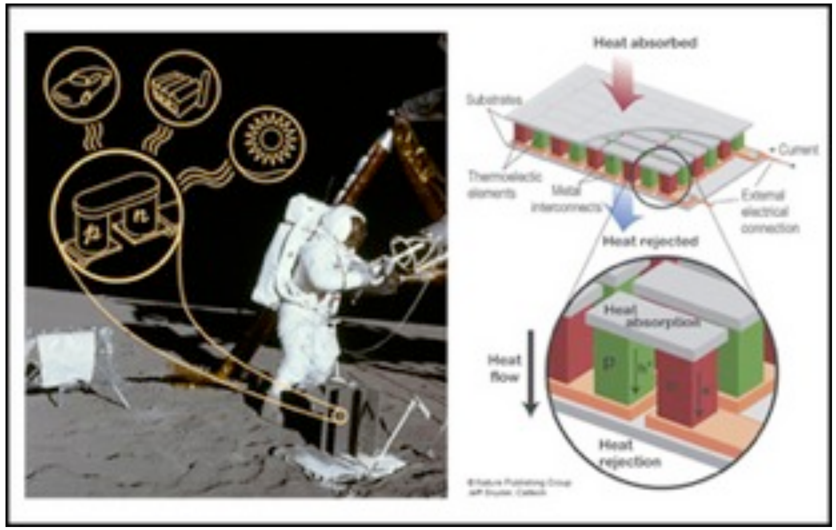
$$ZT = \frac{S^2 \sigma T}{\kappa + \kappa_{phonon}}$$

$L = \kappa/(\sigma T)$ Lorenz number

$$L \approx \frac{\pi^2}{3}(k_B/e)^2 = 2.44 \times 10^{-8} V^2/K^2$$

$$S = \sqrt{ZT \times L} \approx 156 \mu V/K \sqrt{ZT}$$

Volkswagen & BMW have developed
thermoelectric generators
that recover waste heat from a car engine.



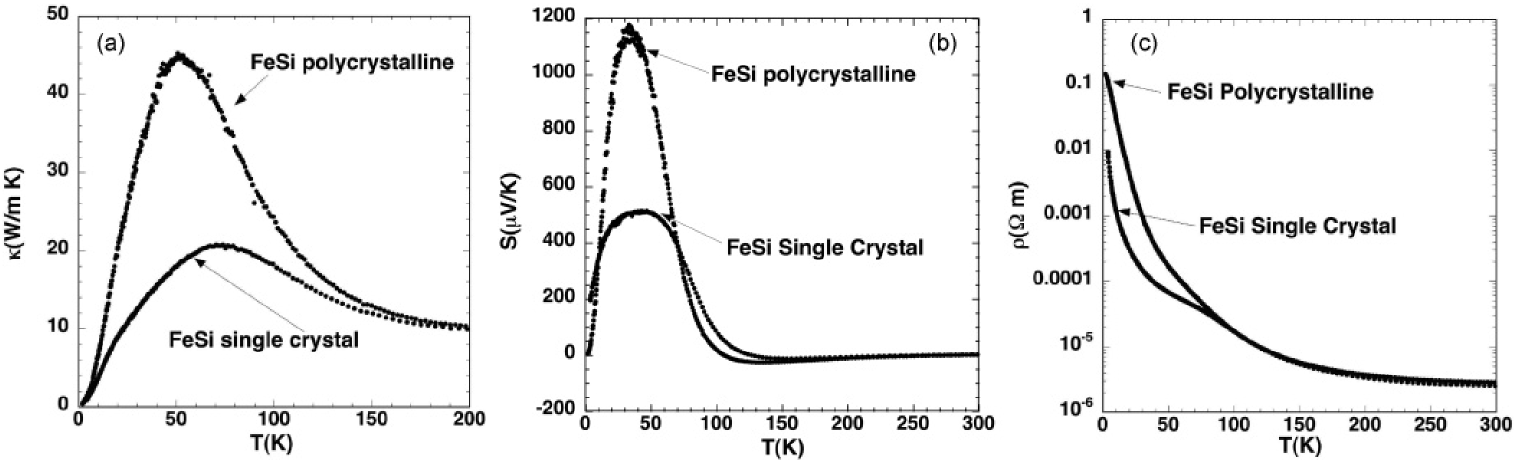
Voyagers 1&2 (10 billion miles beyond Neptune's orbit, 30 years old) still functioning!

Running on thermoelectric generators, converting heat to electricity.

FeSi thermoelectric

Best thermoelectrics are

- lightly doped semiconductors (Bi_2Te_3) or
- correlated semiconductors $FeSb_2$, Na_xCoO_2, FeSi



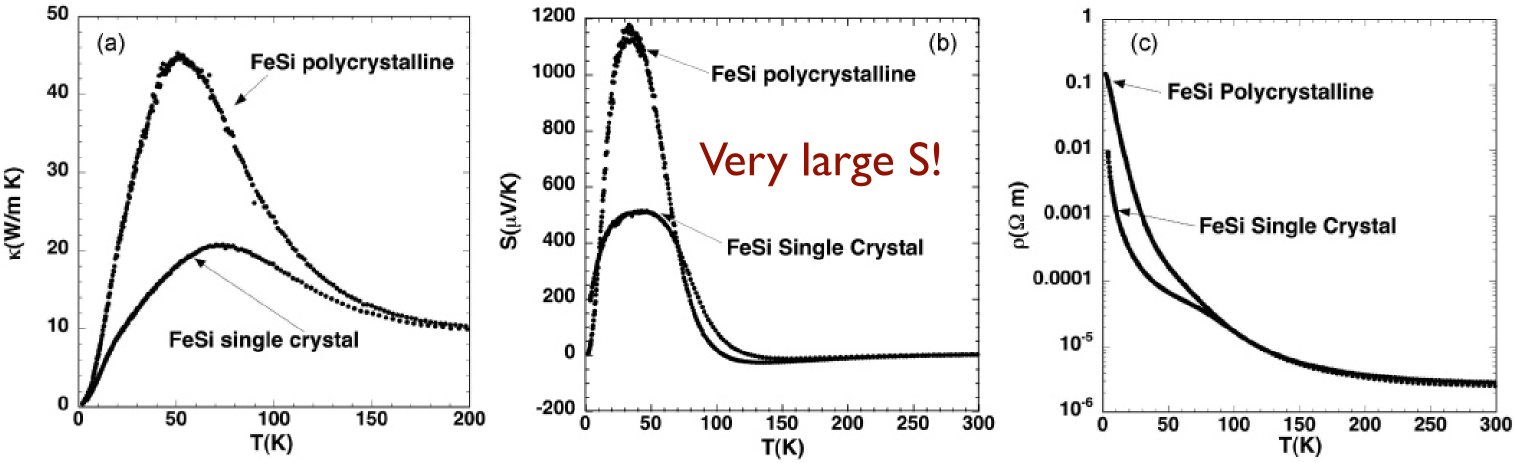
What is the origin? Previous proposals:

- lattice degrees of freedom
- electron-electron correlations due to Hubbard physics
- spin fluctuations
- spin-state transitions : high-spin to low spin
- thermally induced mixed valence

FeSi thermoelectric

Best thermoelectrics are

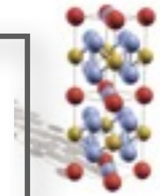
- lightly doped semiconductors (Bi_2Te_3) or
- correlated semiconductors $FeSb_2$, Na_xCoO_2, FeSi

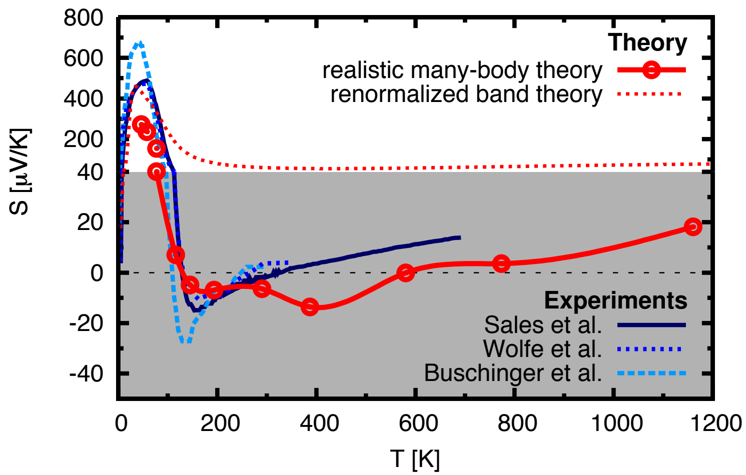


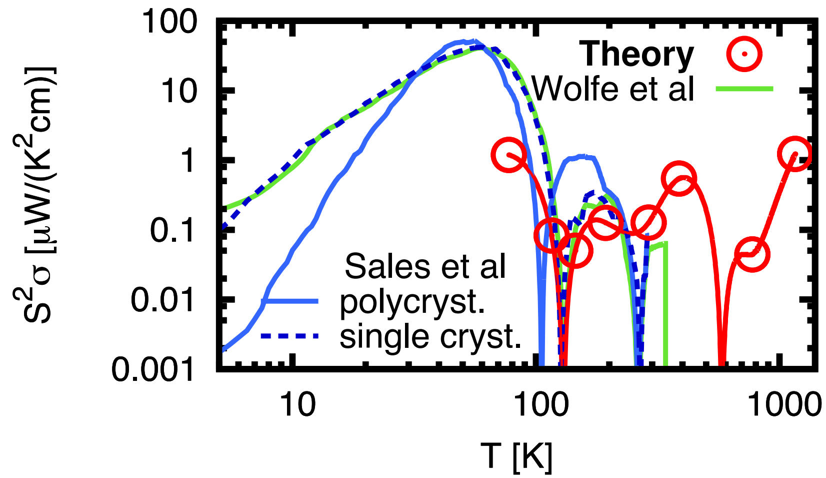
What is the origin? Previous proposals:

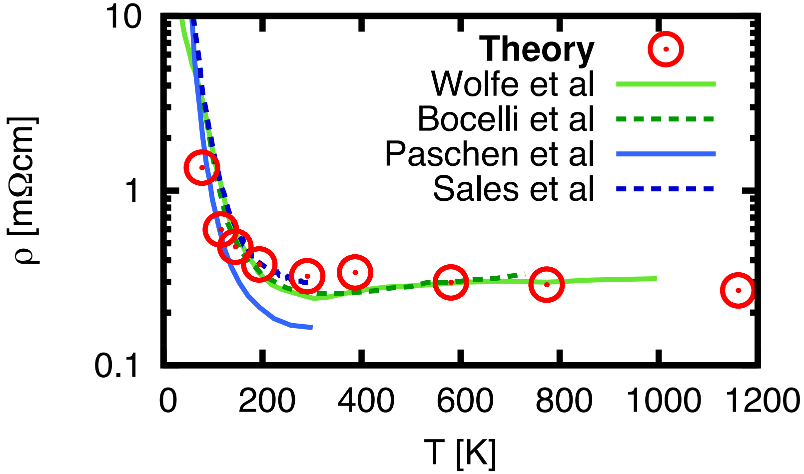
- lattice degrees of freedom
- electron-electron correlations due to Hubbard physics
- spin fluctuations
- spin-state transitions : high-spin to low spin
- thermally induced mixed valence

FeSi by DFT+DMFT







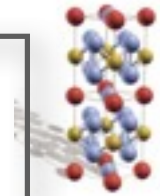


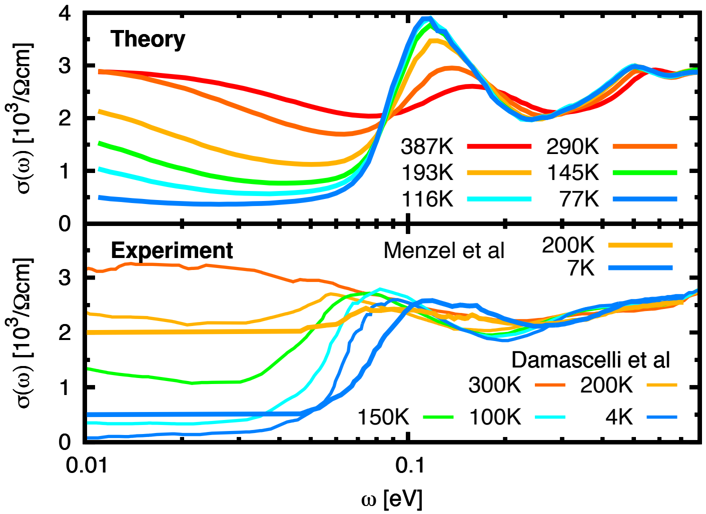
(a)

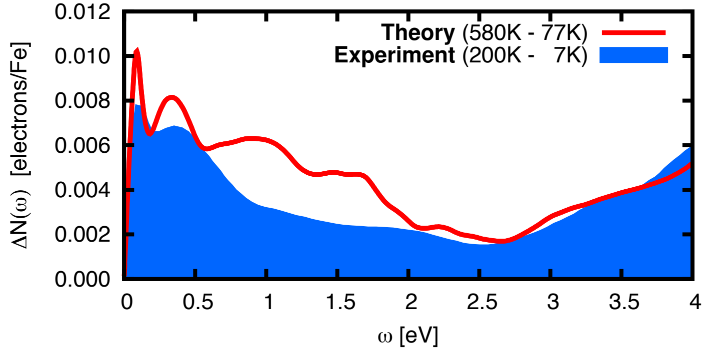
Transport well explained by DFT+DMFT.

J.M.Tomczak, K. Haule, G. Kotliar, Proceedings of the National Academy of Sciences (2012)

Dynamics of FeSi



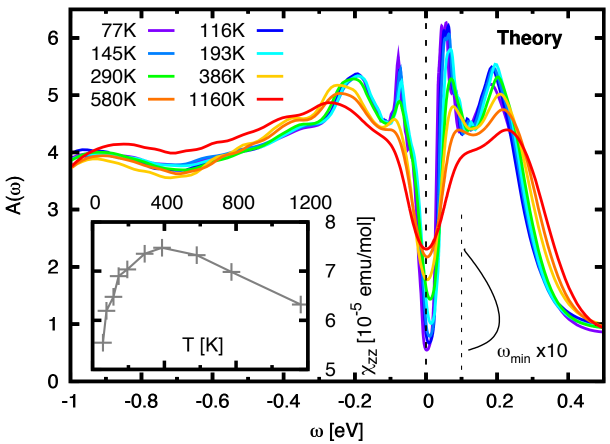




$$N_T(\omega) = \frac{2m_e V}{\pi e^2} \int_0^\omega d\omega' \sigma(\omega', T)$$

$$\Delta N(\omega) = N_{T_1}(\omega) - N_{T_2}(\omega)$$

Even temperature dependent spectral weight transfer well explained by DMFT!



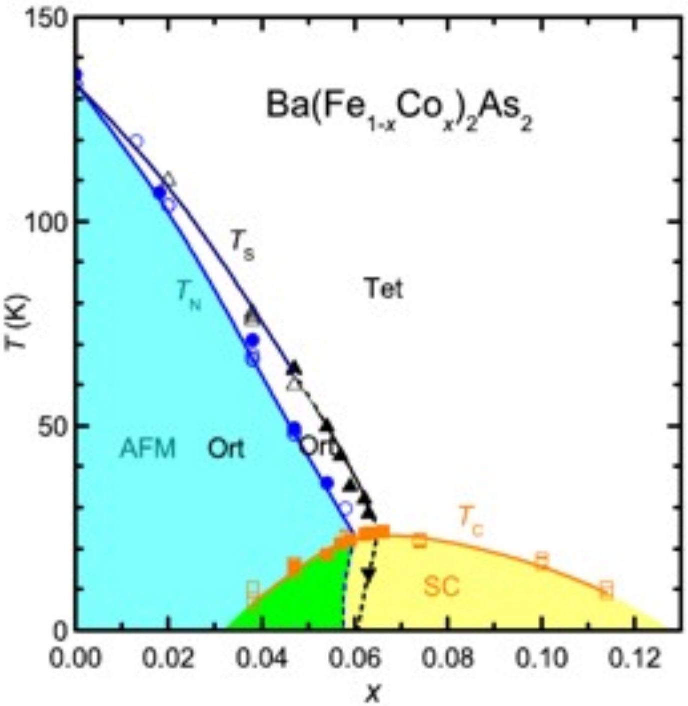
- Closing of the gap is due to incoherence at finite T!
- The origin of strong incoherence is in Hund's coupling

Hund's semiconductor!
(see later for Hund's metals)

J.M. Tomczak, K. Haule, G. Kotliar, Proceedings of the National Academy of Sciences (2012)

Fe pnictides

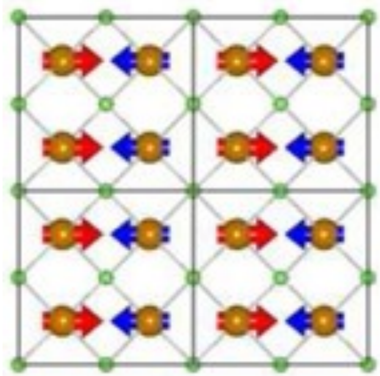
Proximity to magnetic state:
Important to understand nature of SC.
Correlation effects?



Two types of orderings:

SDW

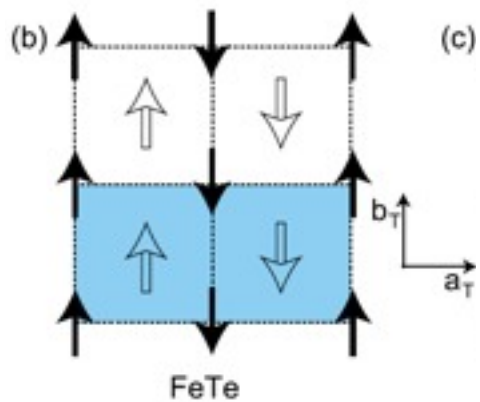
$(\pi, 0, \pi)$



Neutrons by: Clarina de la Cruz et.al, Nature 453, 899 (2008).

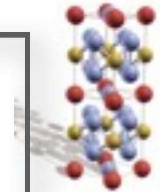
DSDW

$(\pi/2, \pi/2, \pi)$



W. Bao et al., PRL 102, 247001 (2009).

Early DMFT predictions



PRL **100**, 226402 (2008) PHYSICAL REVIEW LETTERS week ending 6 JUNE 2008

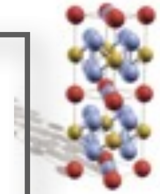
Correlated Electronic Structure of $LaO_{1-x}F_xFeAs$

K. Haule, J. H. Shim, and G. Kotliar
Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA
(Received 9 March 2008; published 2 June 2008)

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

The situation is different in the doped compound [see Fig. 4(b)] where the electron pockets clearly cross the 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.

Early DMFT predictions



PRL **100,** 226402 (2008) PHYSICAL REVIEW LETTERS week ending 6 JUNE 2008

Correlated Electronic Structure of $LaO_{1-x}F_xFeAs$

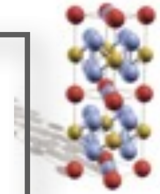
K. Haule, J. H. Shim, and G. Kotliar
Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA
(Received 9 March 2008; published 2 June 2008)

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

Unconventional SC
Phonon Tc<1K

The situation is different in the doped compound [see Fig. 4(b)] where the electron pockets clearly cross the 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.

Early DMFT predictions



PRL **100,** 226402 (2008) PHYSICAL REVIEW LETTERS week ending 6 JUNE 2008

Correlated Electronic Structure of $LaO_{1-x}F_xFeAs$

K. Haule, J. H. Shim, and G. Kotliar
Department of Physics, Rutgers University, Piscataway, New Jersey 08854, USA
(Received 9 March 2008; published 2 June 2008)

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

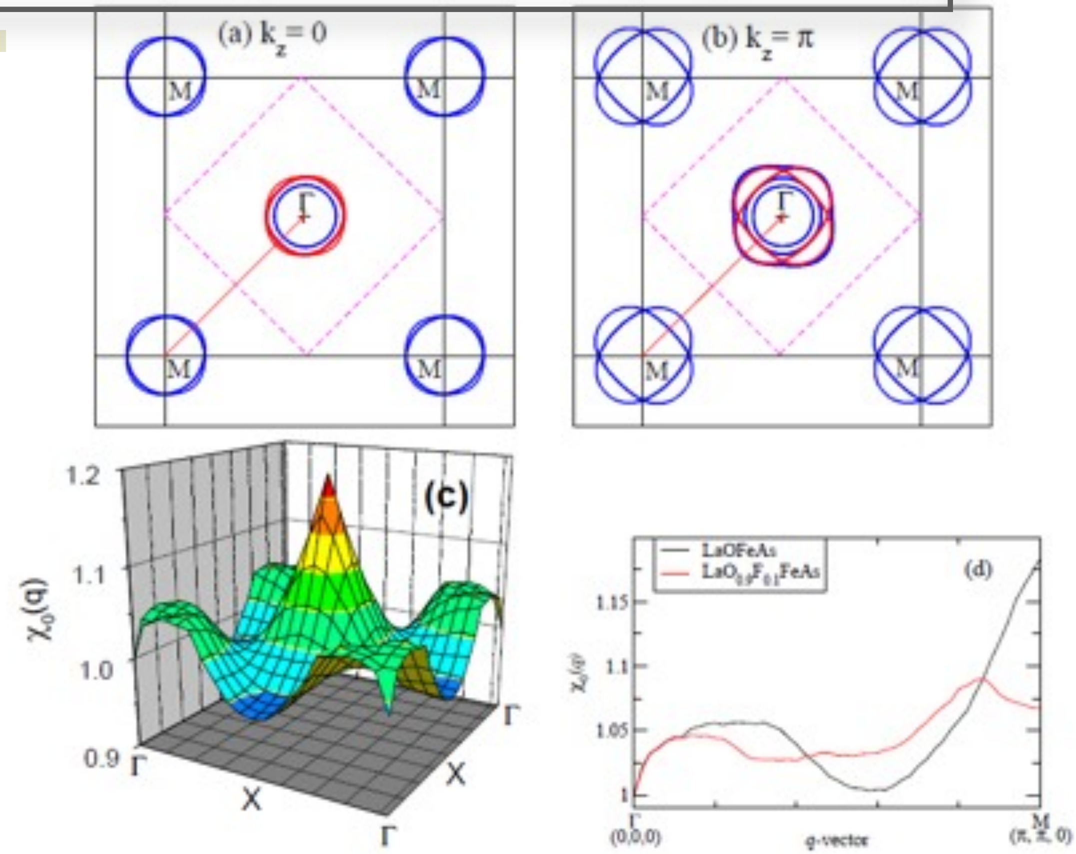
Unconventional SC
Phonon Tc<1K

The situation is different in the doped compound [see Fig. 4(b)] where the electron pockets clearly cross the 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.

Importance of correlations
Mass enhancement 3–5

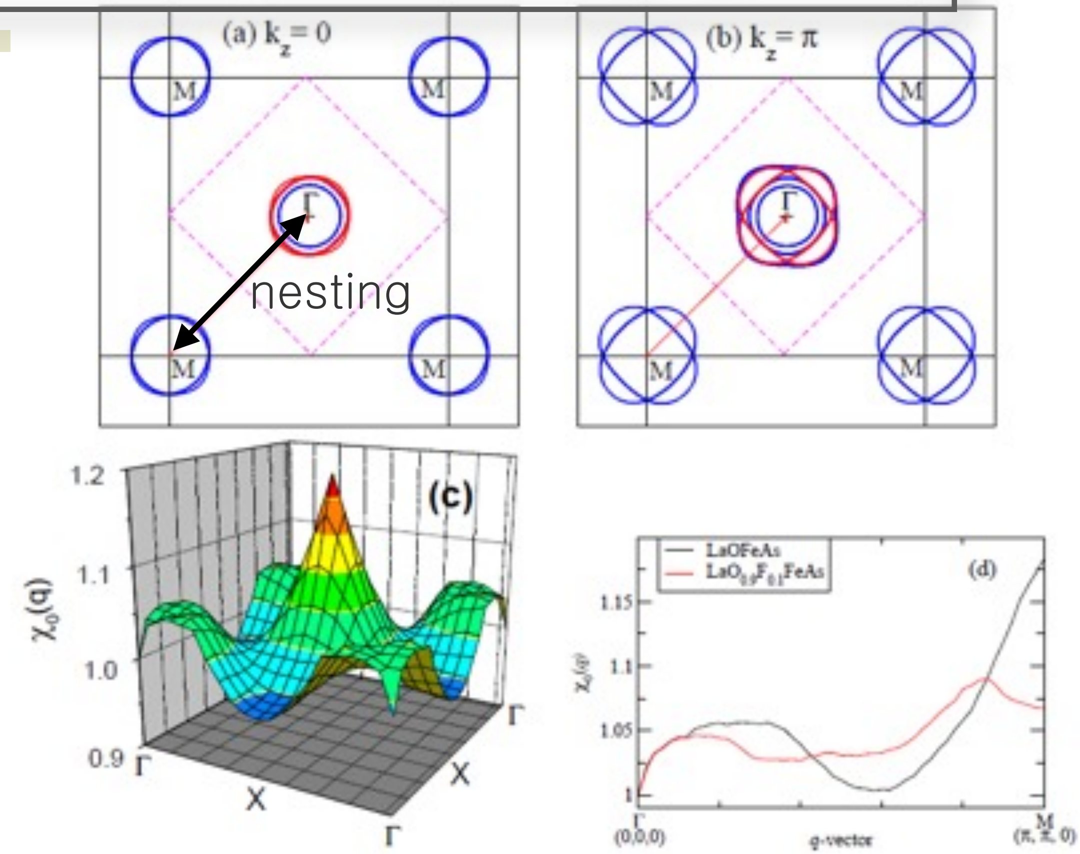
Magnetic state in standard theory (LDA)

Magnetic ordering correctly predicted by LDA, (nesting)



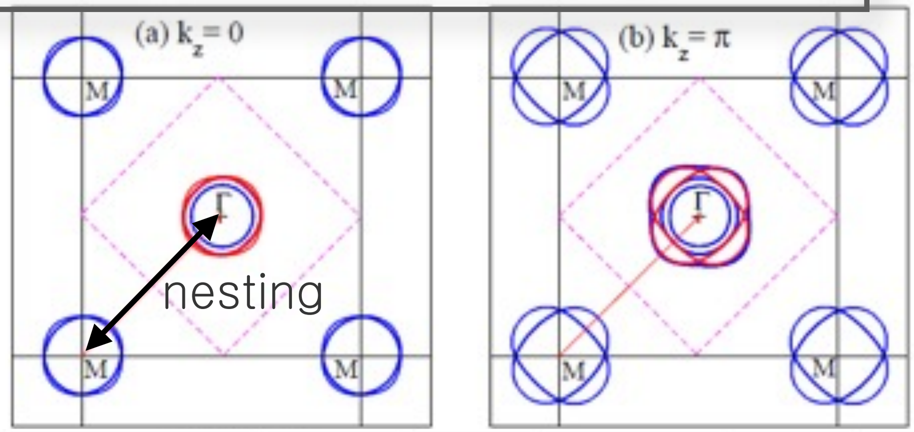
Magnetic state in standard theory (LDA)

Magnetic ordering correctly predicted by LDA, (nesting)



Magnetic state in standard theory (LDA)

Magnetic ordering correctly predicted by LDA, (nesting)



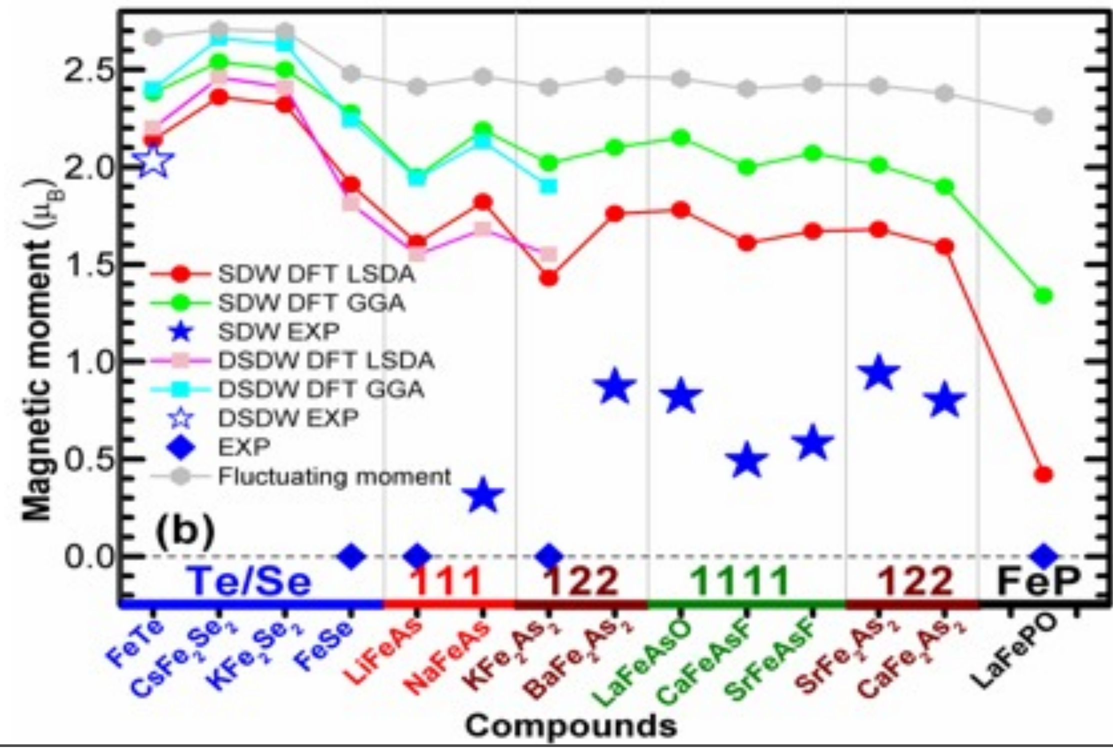
Magnetic moment:

LDA ~2μB ,

exp ~ 0-0.9μB (2 in FeTe)

too large moment!

Wrong trend in the size of the moment across compounds

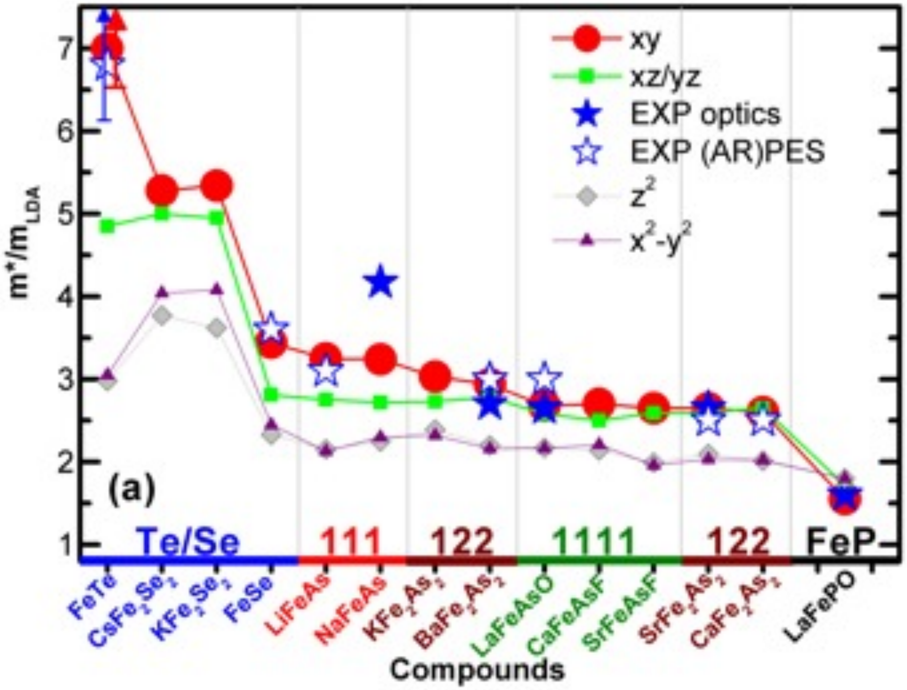


Mass enhancement & Magnetic moment

Mass enhancement & Magnetic moment

Z. P.Yin, KH, G. Kotliar, Nature Materials (2011)

Correlation diagram of Hund's metals

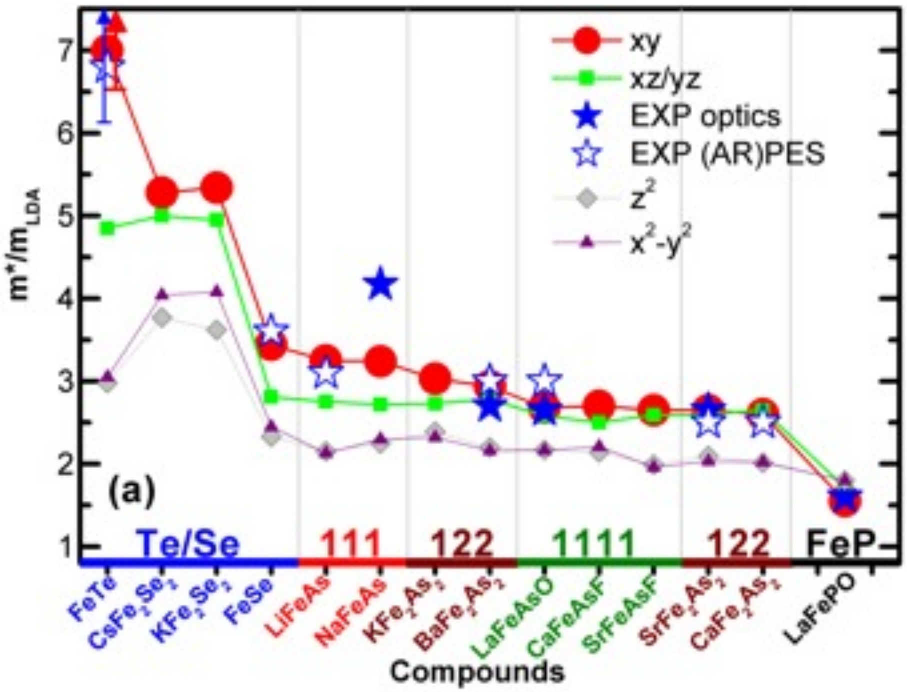


Mass enhancement substantial
Electrons have dual nature

Mass enhancement & Magnetic moment

Z. P. Yin, KH, G. Kotliar, Nature Materials (2011)

Correlation diagram of Hund's metals



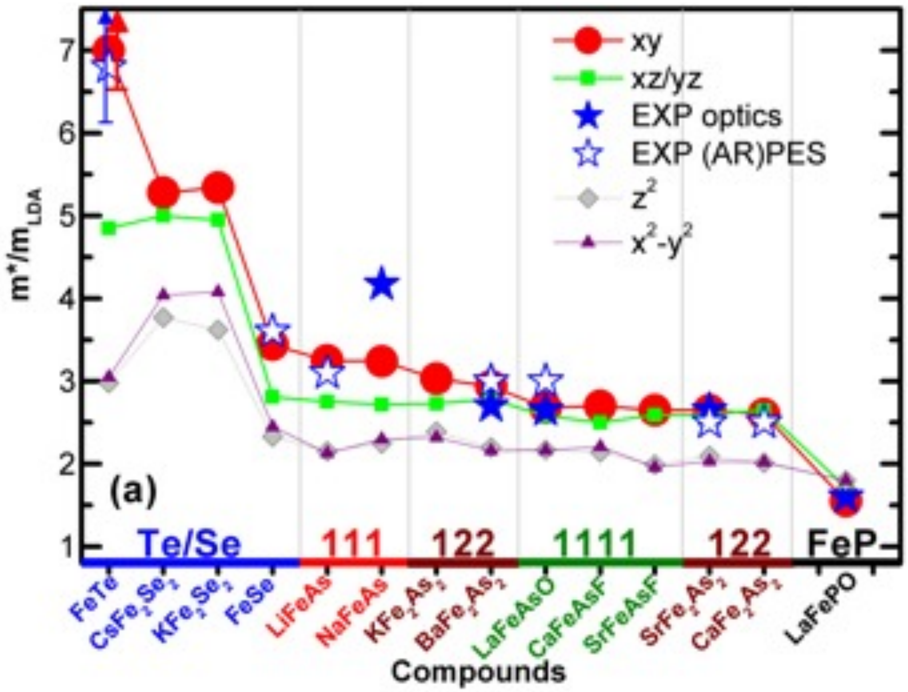
Mass enhancement substantial
Electrons have dual nature

Good agreement with experiment!
We fixed U=5eV and J=0.8eV to our first principles estimates. (PRB 82, 045105 (2010)).

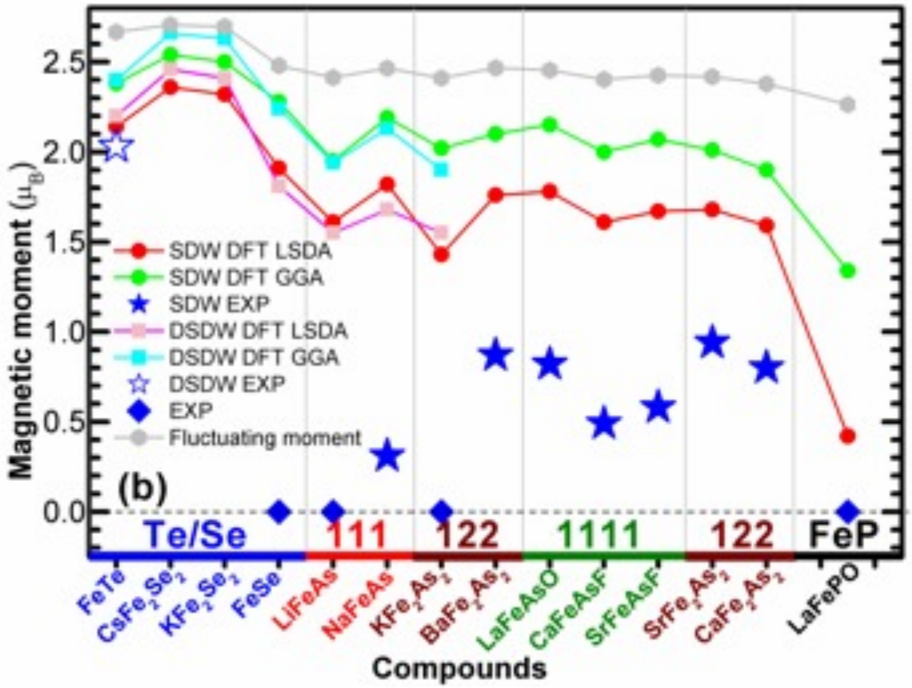
Mass enhancement & Magnetic moment

Z. P.Yin, KH, G. Kotliar, Nature Materials (2011)

Correlation diagram of Hund's metals



Static ordered moment within DFT



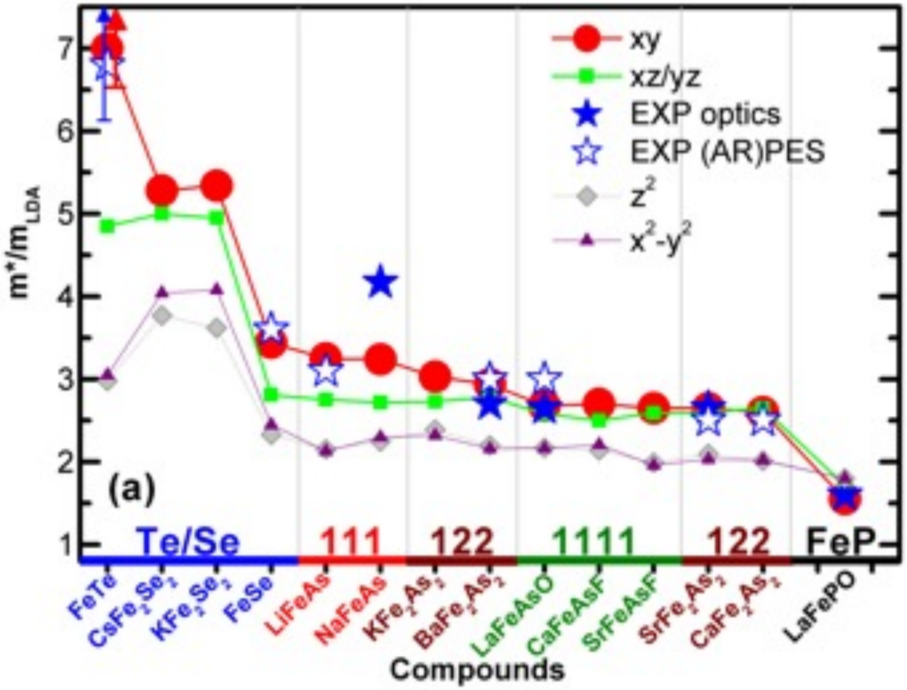
Mass enhancement substantial
Electrons have dual nature

Good agreement with experiment!
We fixed U=5eV and J=0.8eV to
our first principles estimates.
(PRB 82, 045105 (2010)).

Mass enhancement & Magnetic moment

Z. P. Yin, KH, G. Kotliar, Nature Materials (2011)

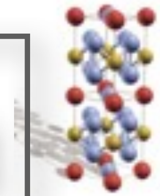
Correlation diagram of Hund's metals



Mass enhancement substantial
Electrons have dual nature

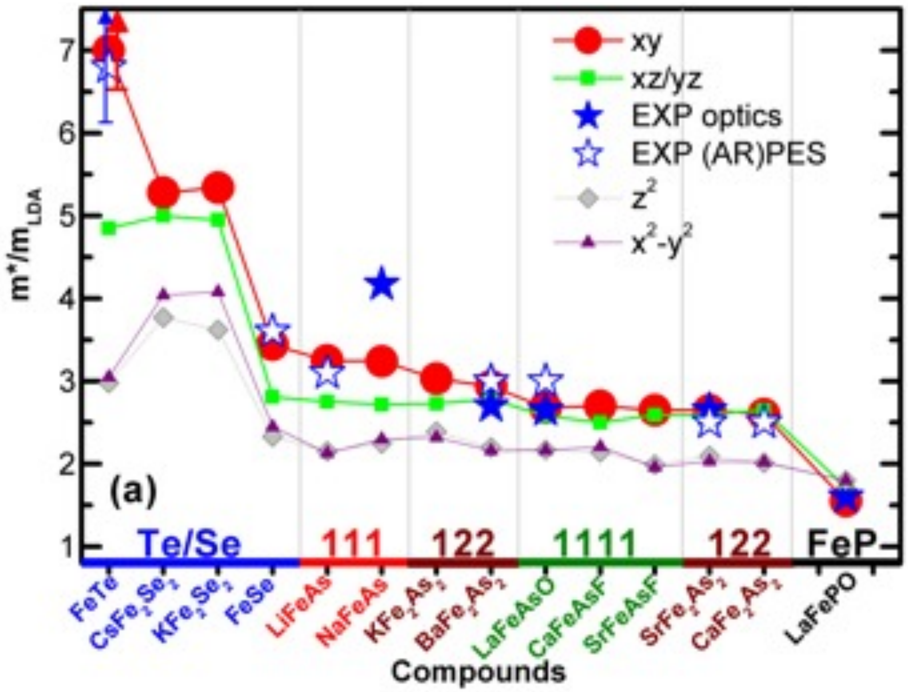
Good agreement with experiment!
We fixed U=5eV and J=0.8eV to
our first principles estimates.
(PRB 82, 045105 (2010)).

Mass enhancement & Magnetic moment



Z. P. Yin, KH, G. Kotliar, Nature Materials (2011)

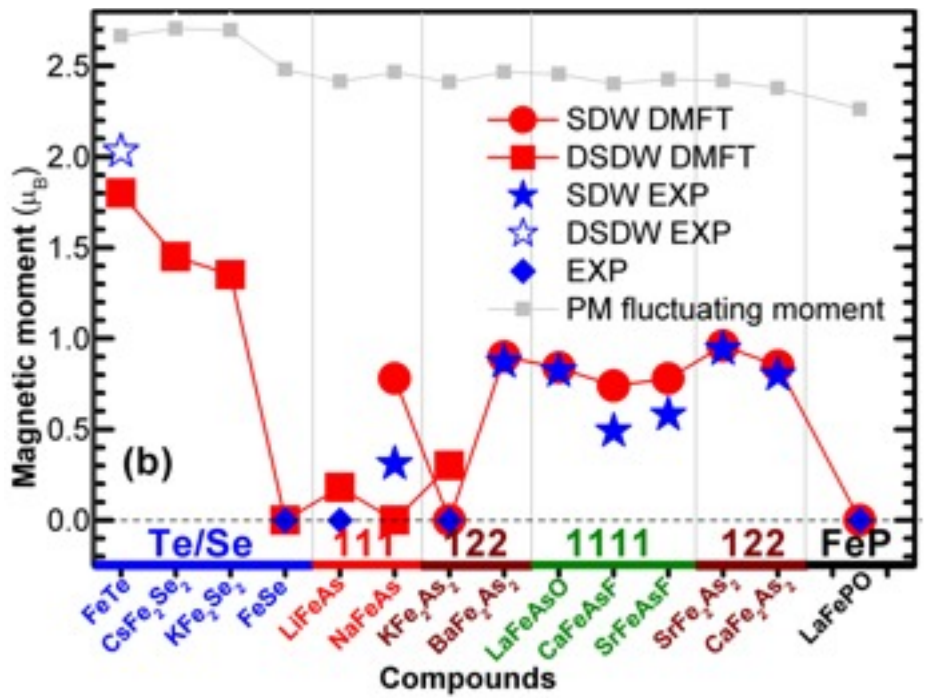
Correlation diagram of Hund's metals



Mass enhancement substantial
Electrons have dual nature

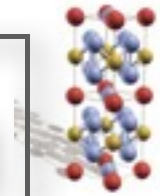
Good agreement with experiment!
We fixed U=5eV and J=0.8eV to our first principles estimates. (PRB 82, 045105 (2010)).

Static ordered moment within LDA+DMFT



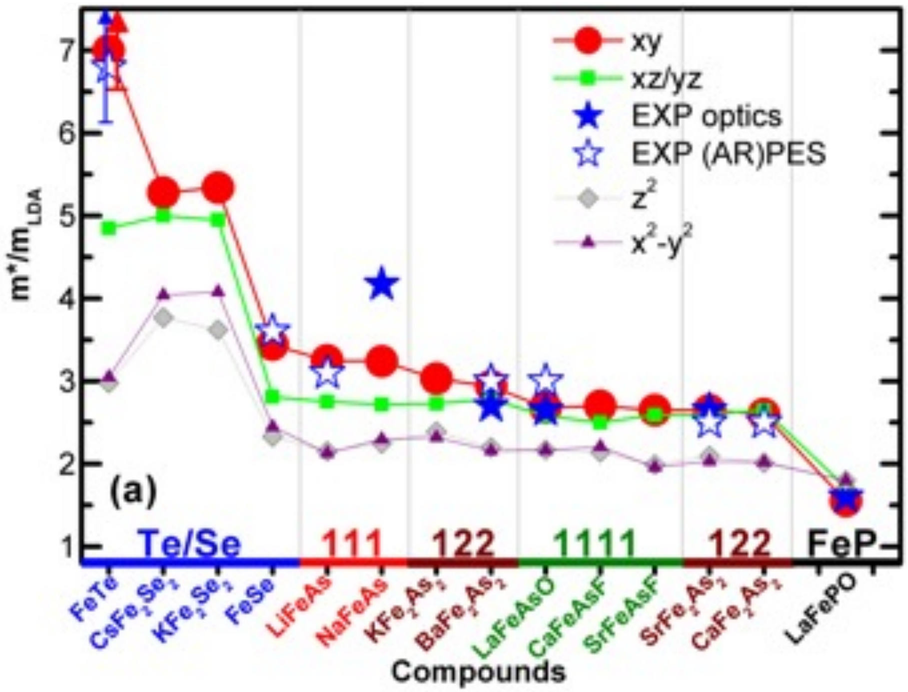
Static ordered moment very small

Mass enhancement & Magnetic moment

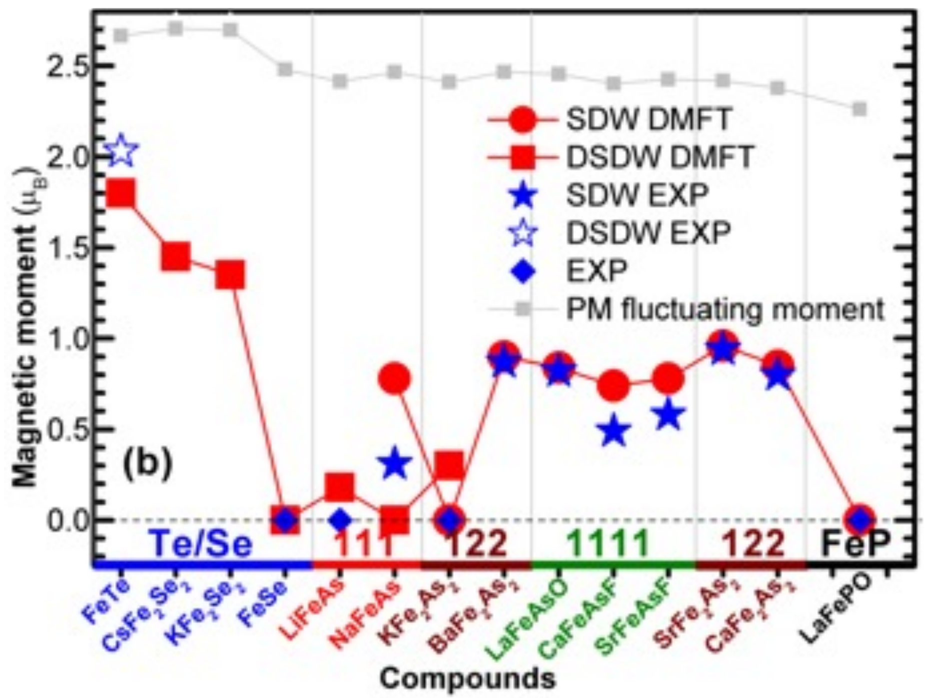


Z. P. Yin, KH, G. Kotliar, Nature Materials (2011)

Correlation diagram of Hund's metals



Static ordered moment within LDA+DMFT



Mass enhancement substantial
Electrons have dual nature

Good agreement with experiment!
We fixed U=5eV and J=0.8eV to our first principles estimates.
(PRB 82, 045105 (2010)).

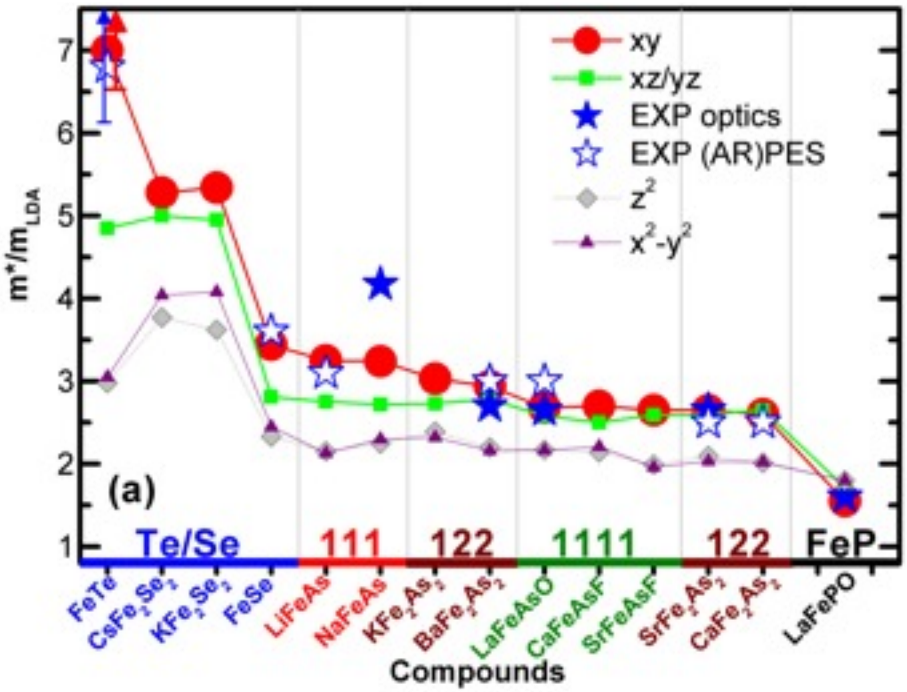
Static ordered moment very small

moment<->mass
Some similarity, but also many differences!

Mass enhancement & Magnetic moment

Z. P.Yin, KH, G. Kotliar, Nature Materials (2011)

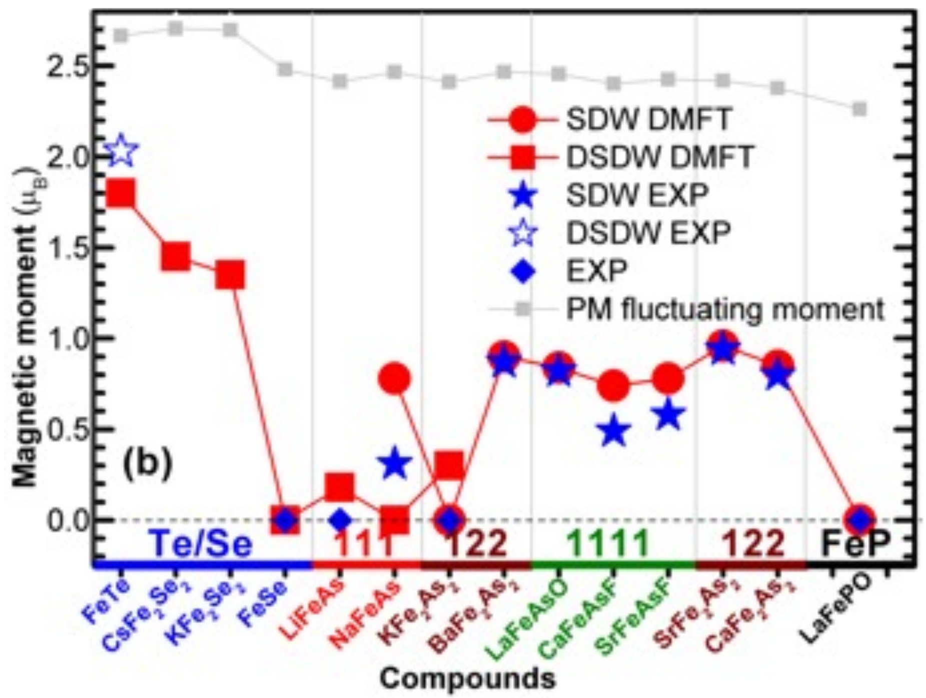
Correlation diagram of Hund's metals



Mass enhancement substantial
Electrons have dual nature

Good agreement with experiment!
We fixed U=5eV and J=0.8eV to our first principles estimates.
(PRB 82, 045105 (2010)).

Static ordered moment within LDA+DMFT



Static ordered moment very small

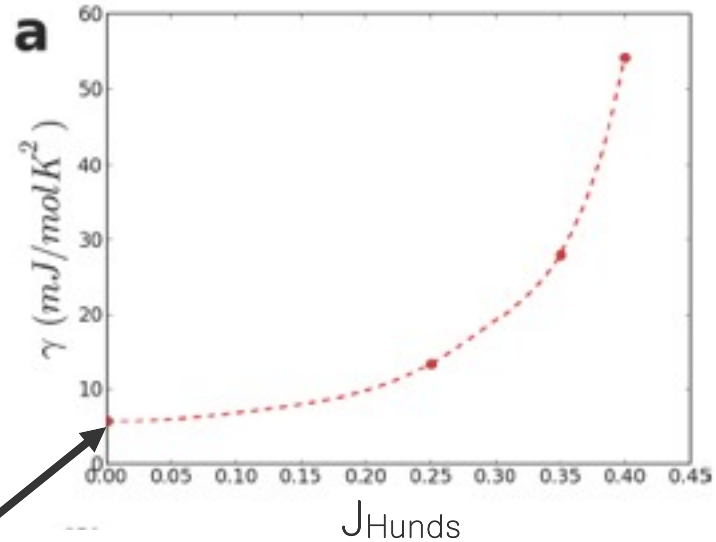
moment<->mass
Some similarity, but also many differences!

NO FITTING PARAMETER

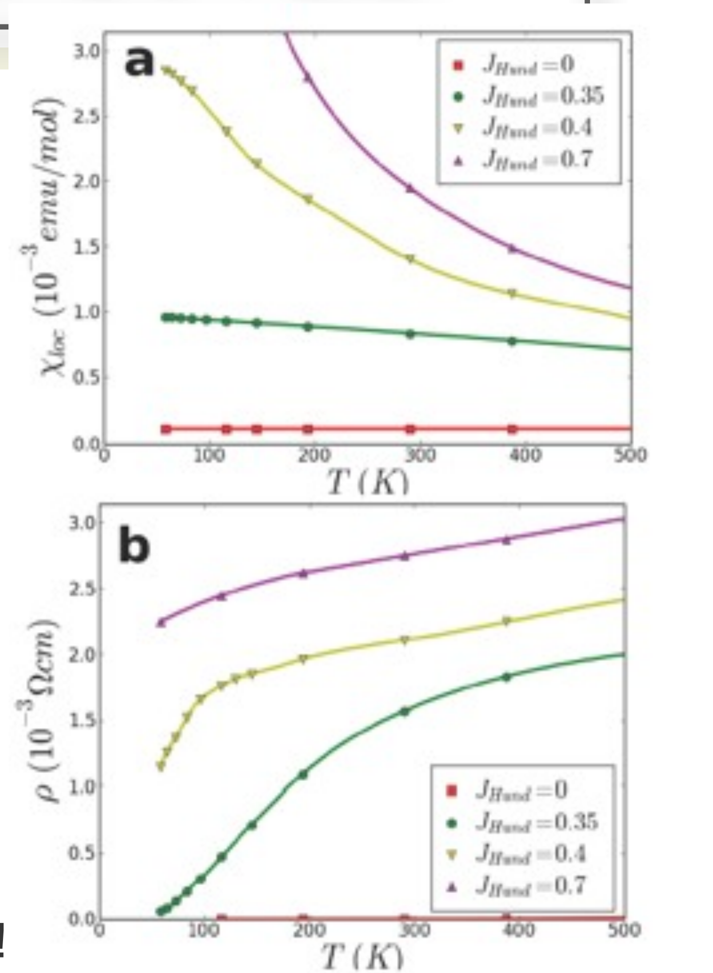
Importance of Hund's rule

Hubbard U is not the "relevant" parameter.

The **Hund's coupling** brings correlations!



LDA value



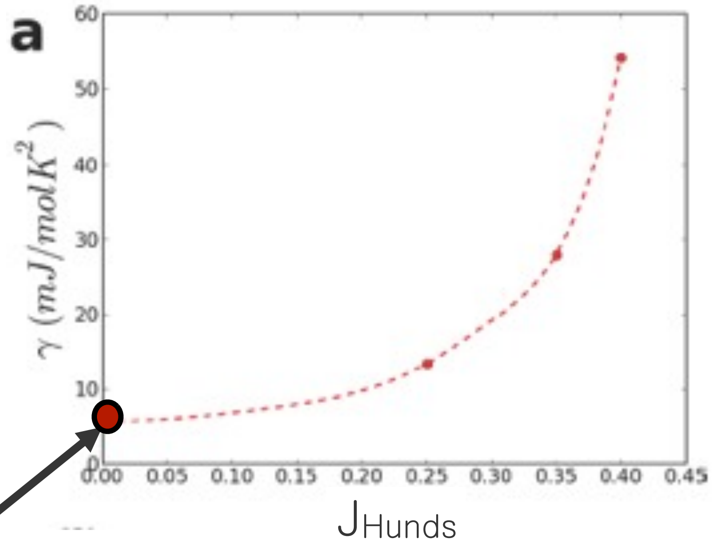
For J=0 there is negligible mass enhancement at U~W!

[New Journal of Physics Volume 11 February 2009]

Importance of Hund's rule

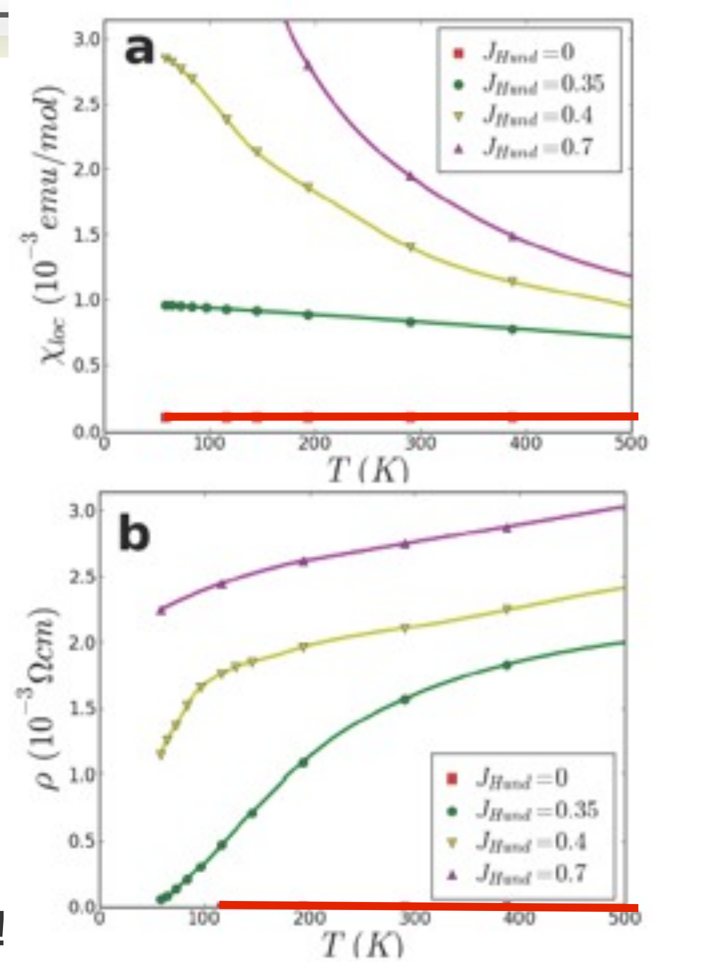
Hubbard U is not the "relevant" parameter.

The **Hund's coupling** brings correlations!



LDA value

J=0



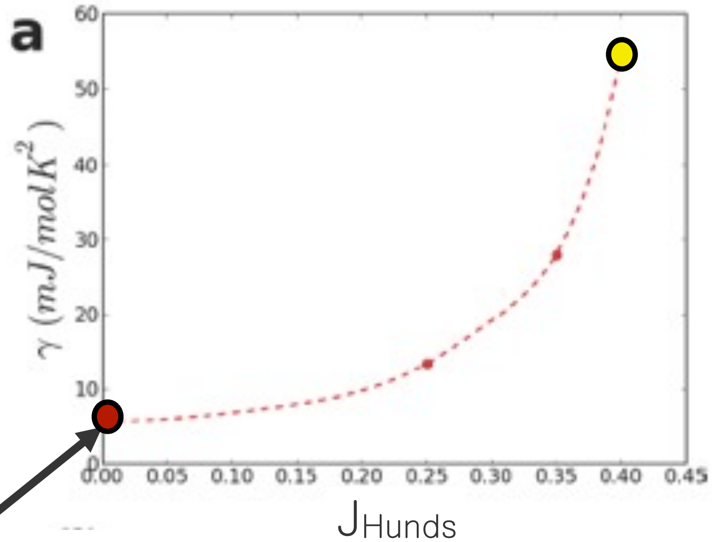
For J=0 there is negligible mass enhancement at U~W!

New Journal of Physics Volume 11 February 2009

Importance of Hund's rule

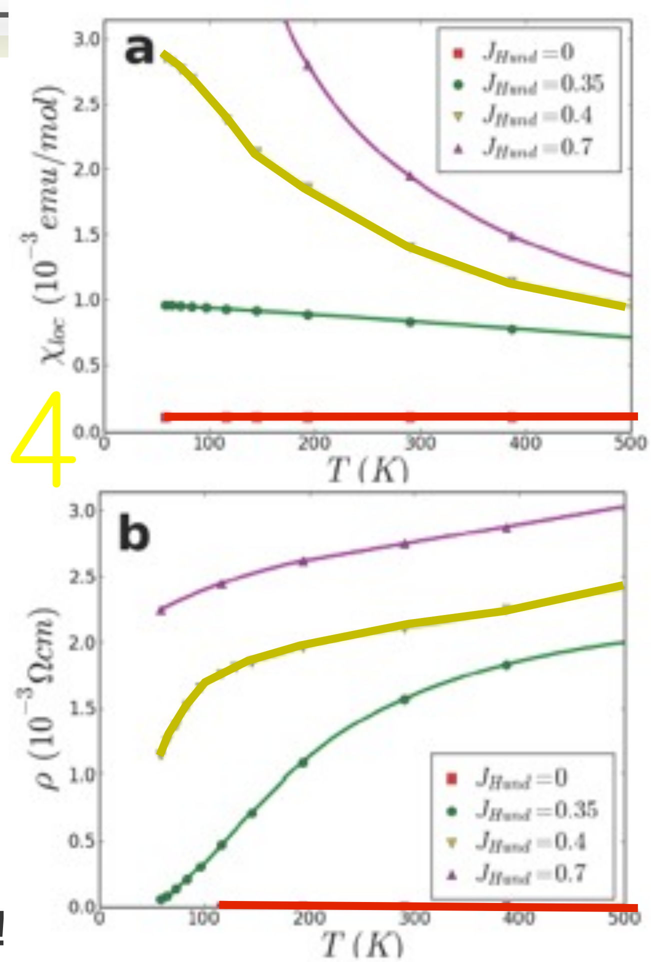
Hubbard U is not the "relevant" parameter.

The **Hund's coupling** brings correlations!



LDA value

J=0.4



For J=0 there is negligible mass enhancement at U~W!

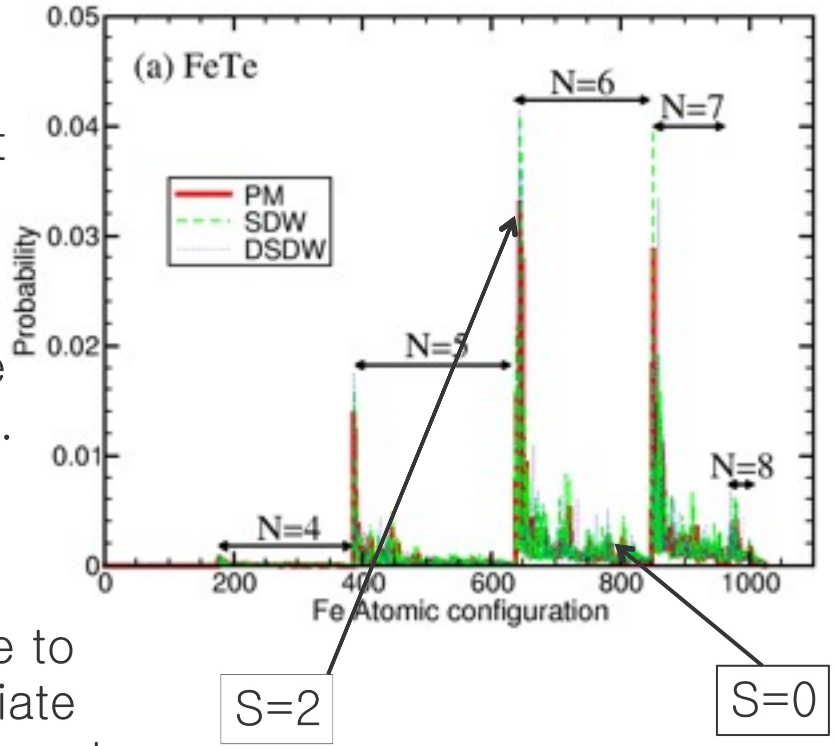
New Journal of Physics Volume 11 February 2009

Histogram of Hunds metals

In oxydes, only a few atomic states (one in each valence) with significant Probability

In pnictides, many states with large probability -> charge fluctuations are not efficiently blocked by Coulomb U. (more itinerant system)

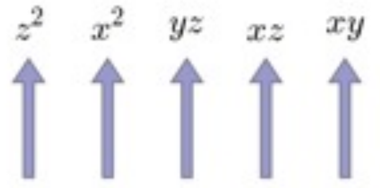
States with high spin more probable than those with low spin -> gives rise to <u>non-Fermi liquid physics</u> at intermediate temperatures, and <u>heavy quasiparticles</u> at Low temperatures.



What reduces Kondo screening?

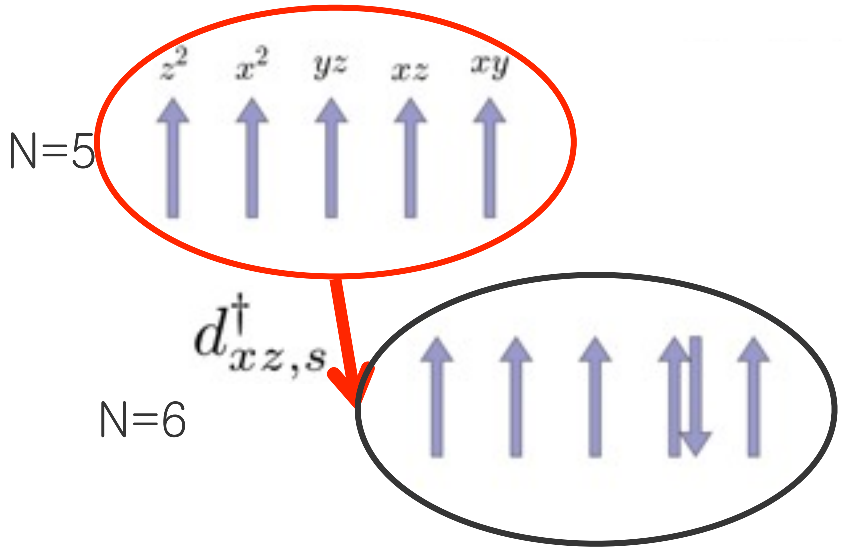
Orbital & spin blocking
due to Hund's coupling

N=5



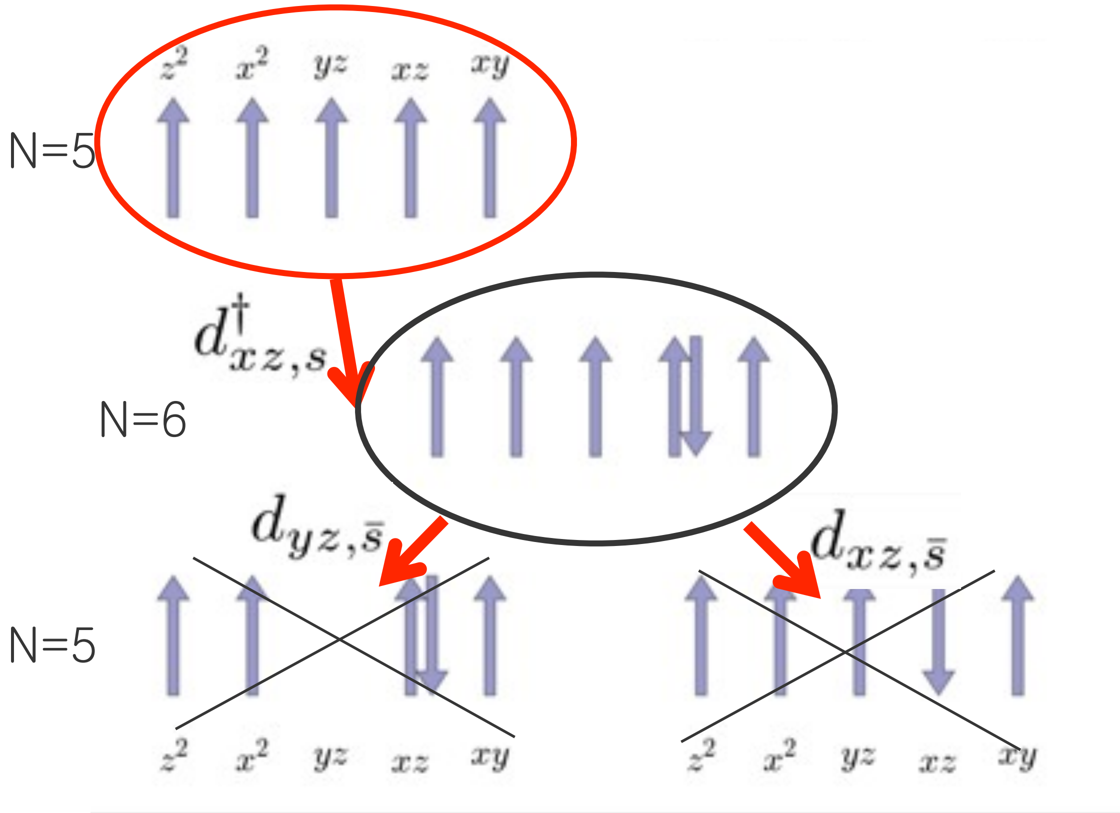
What reduces Kondo screening?

Orbital & spin blocking
due to Hund's coupling



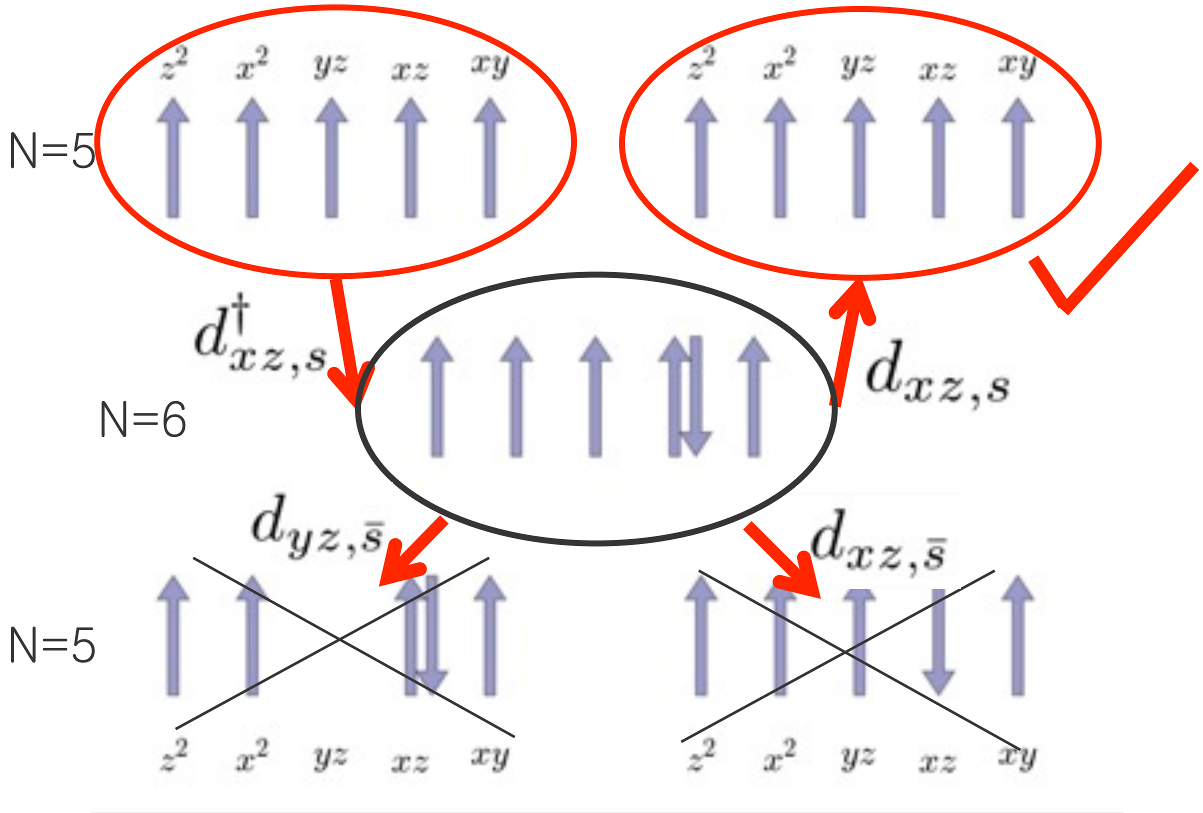
What reduces Kondo screening?

Orbital & spin blocking due to Hund's coupling



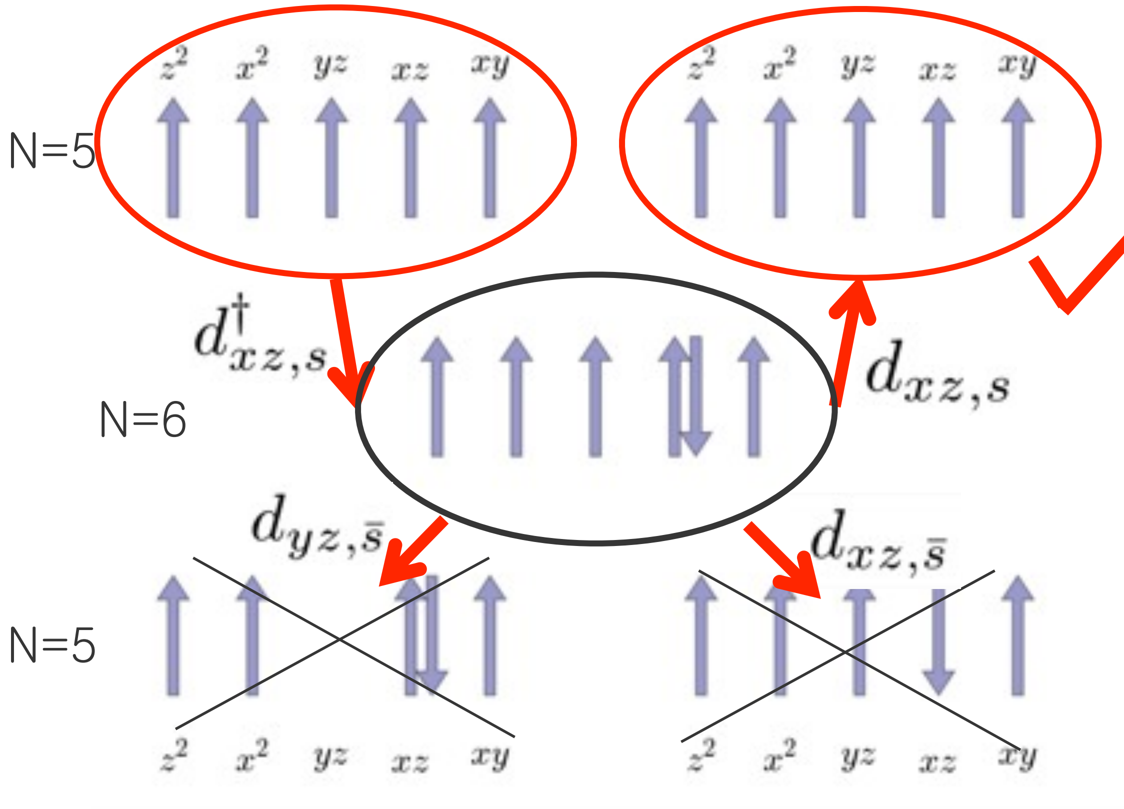
What reduces Kondo screening?

Orbital & spin blocking
due to Hund's coupling



What reduces Kondo screening?

Orbital & spin blocking due to Hund's coupling



Low energy Kondo-like Hamiltonian

$$J_K\, d^\dagger_{\alpha,s} d_{\beta,s'} c^\dagger_{\beta,s'} c_{\alpha,s} = 0$$

unless $\alpha = \beta$

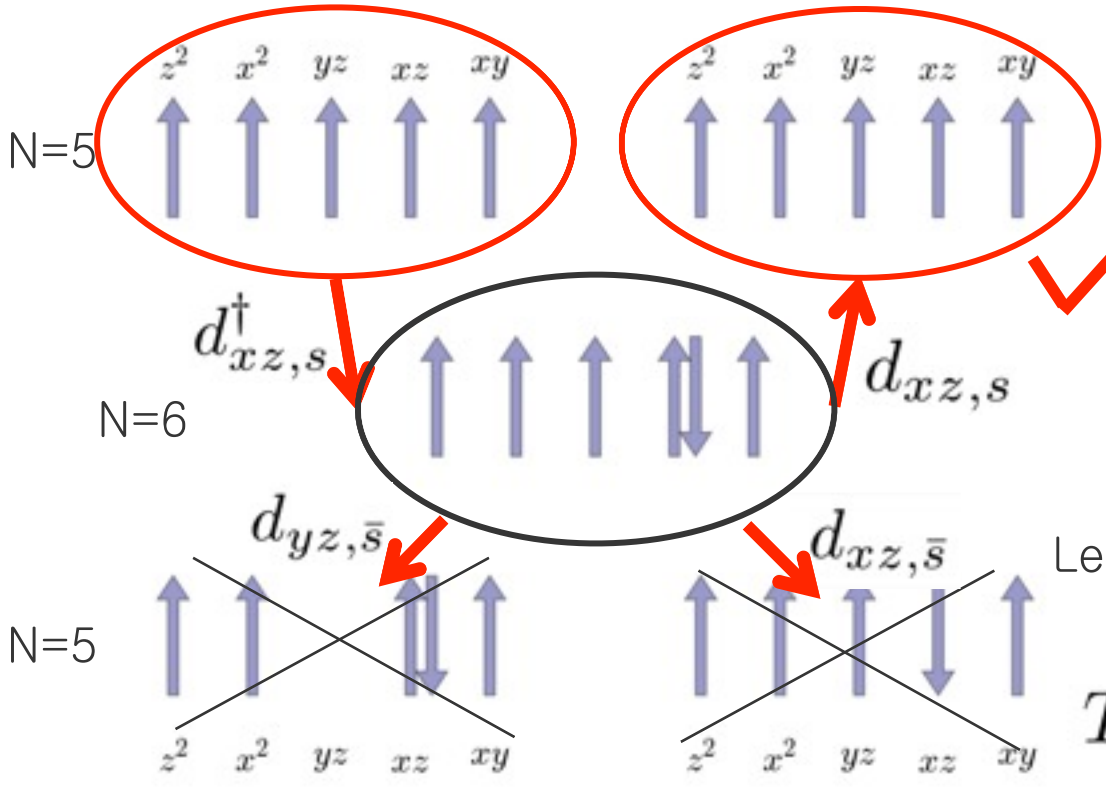
Only diagonal Kondo coupling

$$J_K \vec{S}_\alpha \vec{\sigma}_\alpha$$

+Schrieffer-Wolf tr.

What reduces Kondo screening?

Orbital & spin blocking due to Hund's coupling



I. Okada, K. Yoshida,
Progress of Theoretical Physics 49, 1483 (1973).

Low energy Kondo-like Hamiltonian

$$J_K\, d^\dagger_{\alpha,s} d_{\beta,s'} c^\dagger_{\beta,s'} c_{\alpha,s} = 0$$

unless $\alpha = \beta$

Only diagonal Kondo coupling

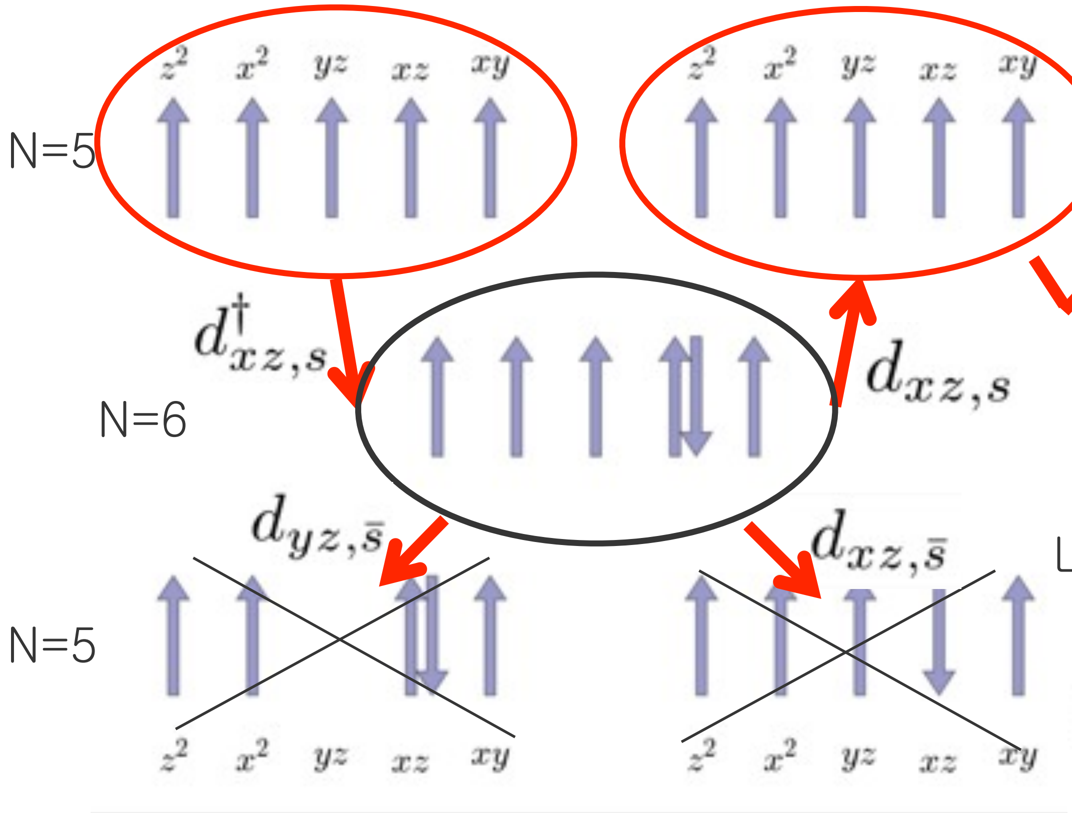
$$J_K \vec{S}_\alpha \vec{\sigma}_\alpha$$

+Schrieffer-Wolf tr.
Leads to coherence temperature:

$$T^* \propto exp\left(-\frac{(2S+1)^2}{\rho J_K}\right)$$

What reduces Kondo screening?

Orbital & spin blocking
due to Hund's coupling



Low energy Kondo-like Hamiltonian

$$J_K\, d^\dagger_{\alpha,s} d_{\beta,s'} c^\dagger_{\beta,s'} c_{\alpha,s} = 0$$

unless $\alpha = \beta$

Only diagonal Kondo coupling

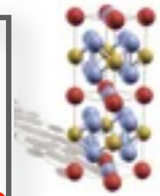
$$J_K \vec{S}_\alpha \vec{\sigma}_\alpha$$

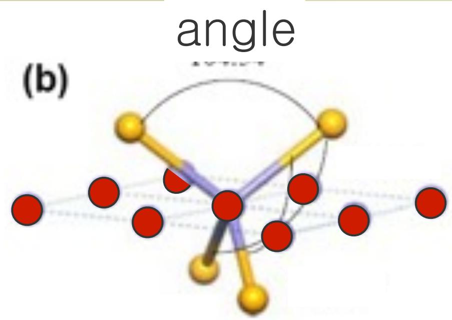
+Schrieffer-Wolf tr.
Leads to coherence temperature:

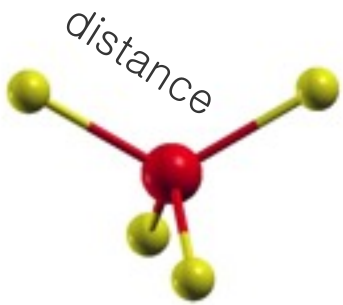
$$T^* \propto exp\left(-\frac{25}{\rho J_K}\right)$$

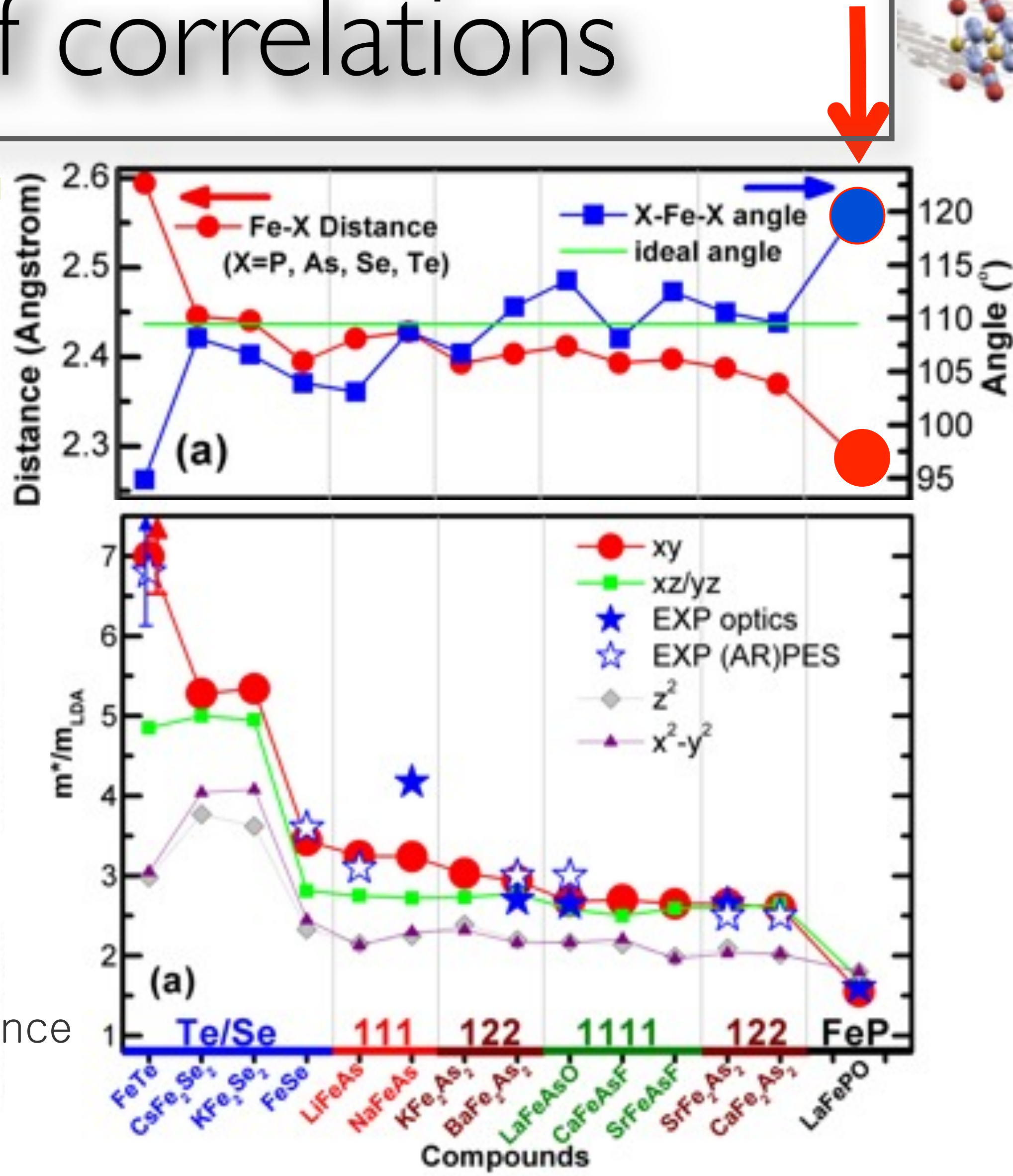
I. Okada, K. Yoshida,
Progress of Theoretical Physics 49, 1483 (1973).

Strength of correlations





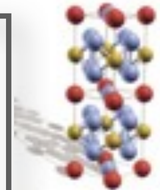




Overal trend consistent with Fe-As distance

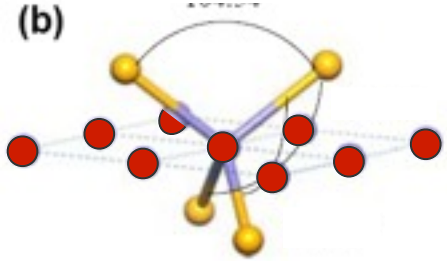
Hybridization with pnictogen

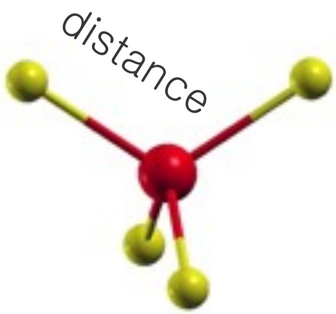
Strength of correlations

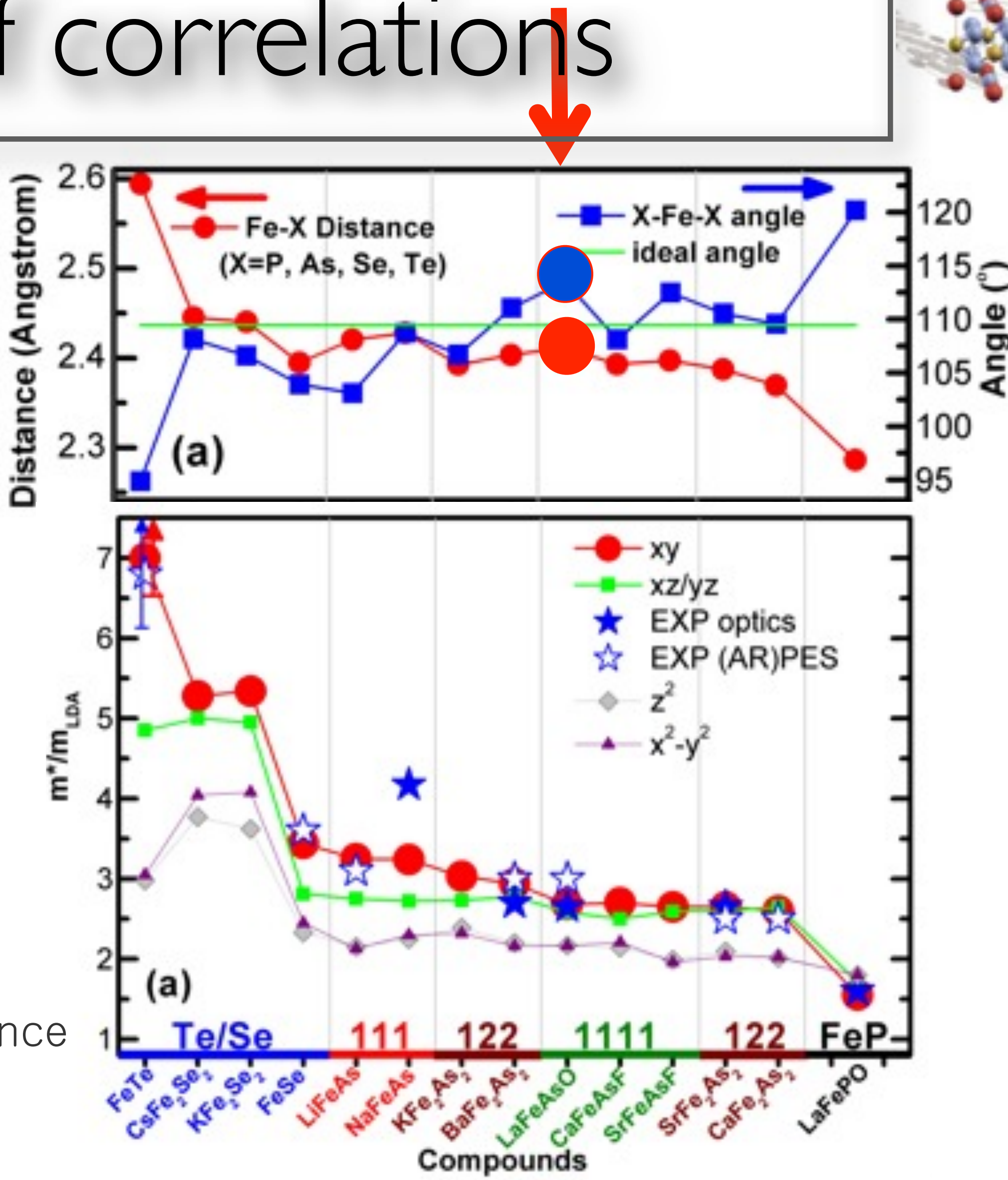


angle

(b)



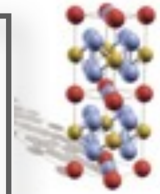


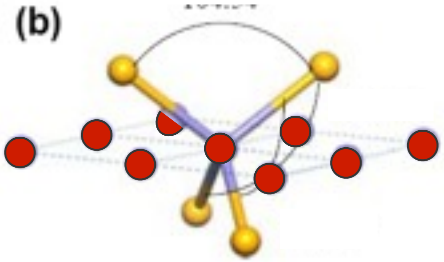


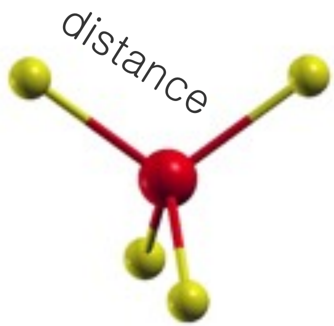
Overal trend consistent with Fe-As distance

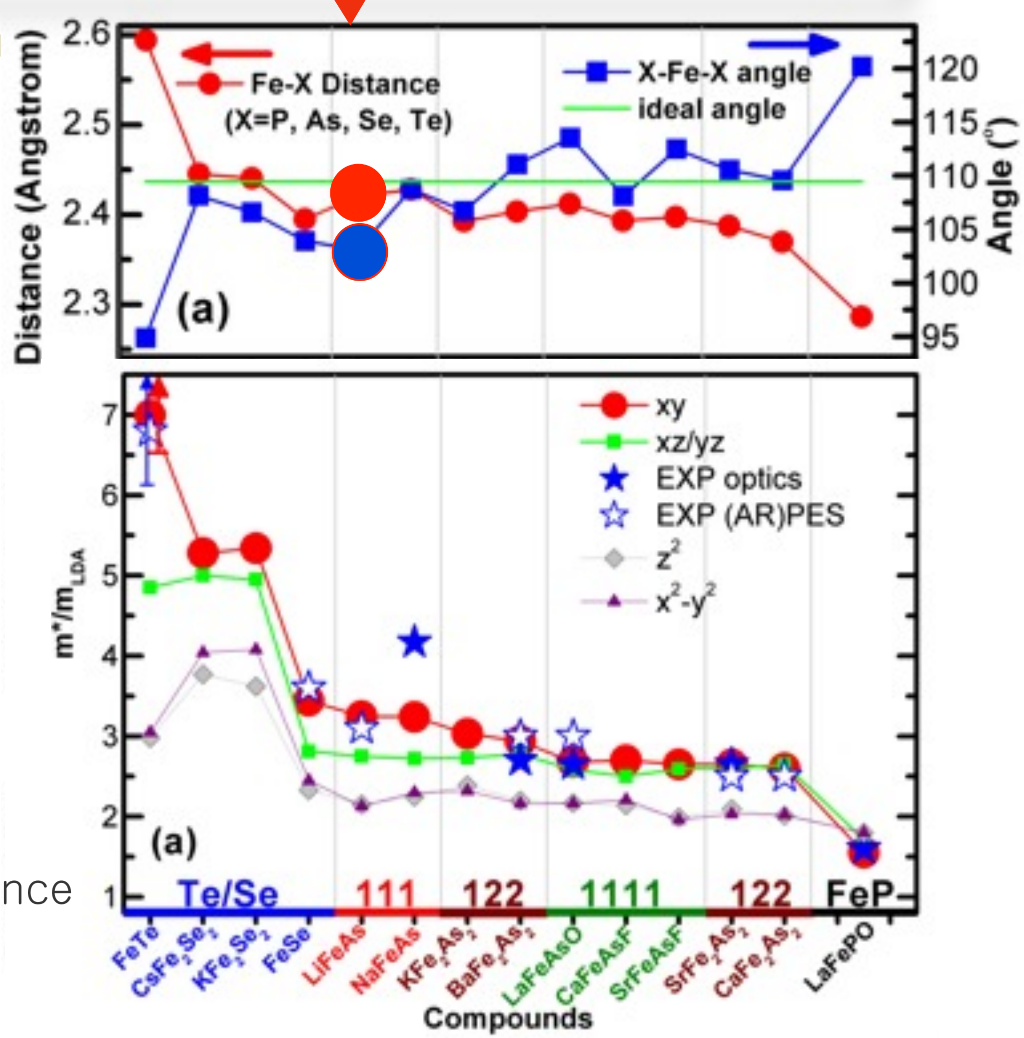
Hybridization with pnictogen

Strength of correlations





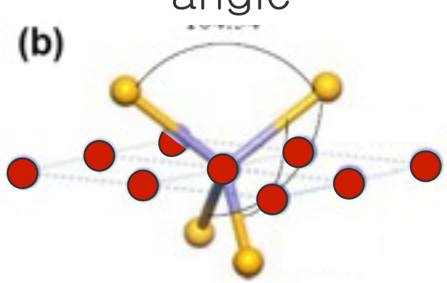


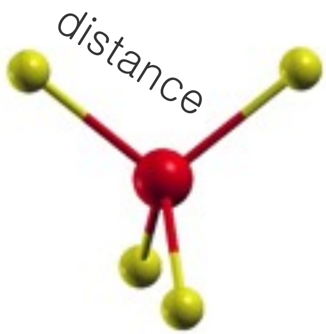


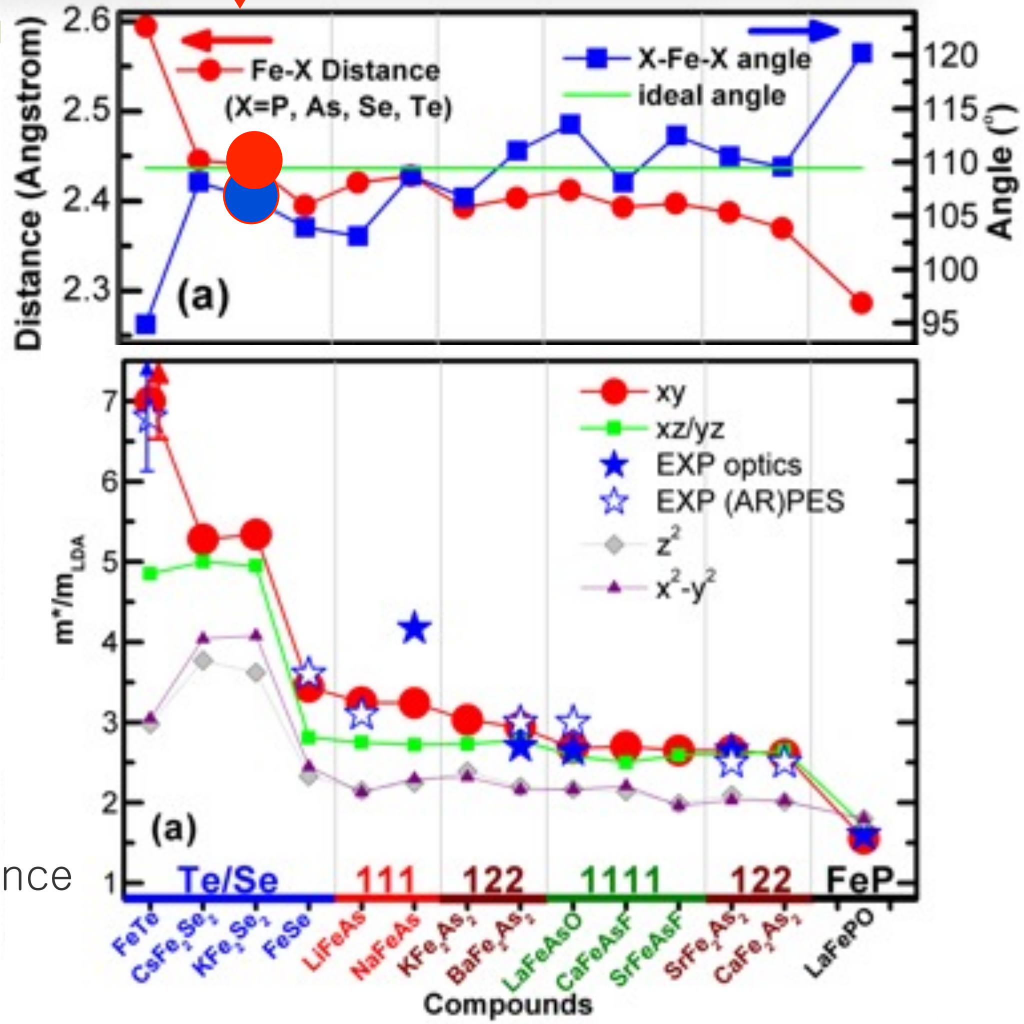
Overal trend consistent with Fe-As distance

Hybridization with pnictogen

Strength of correlations



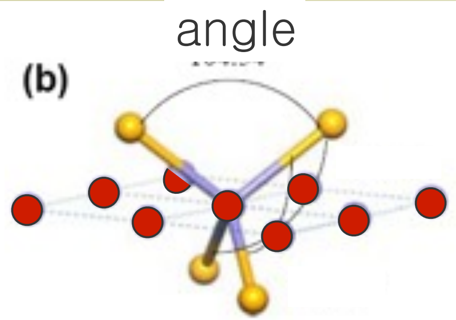


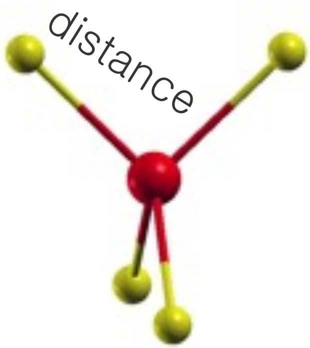


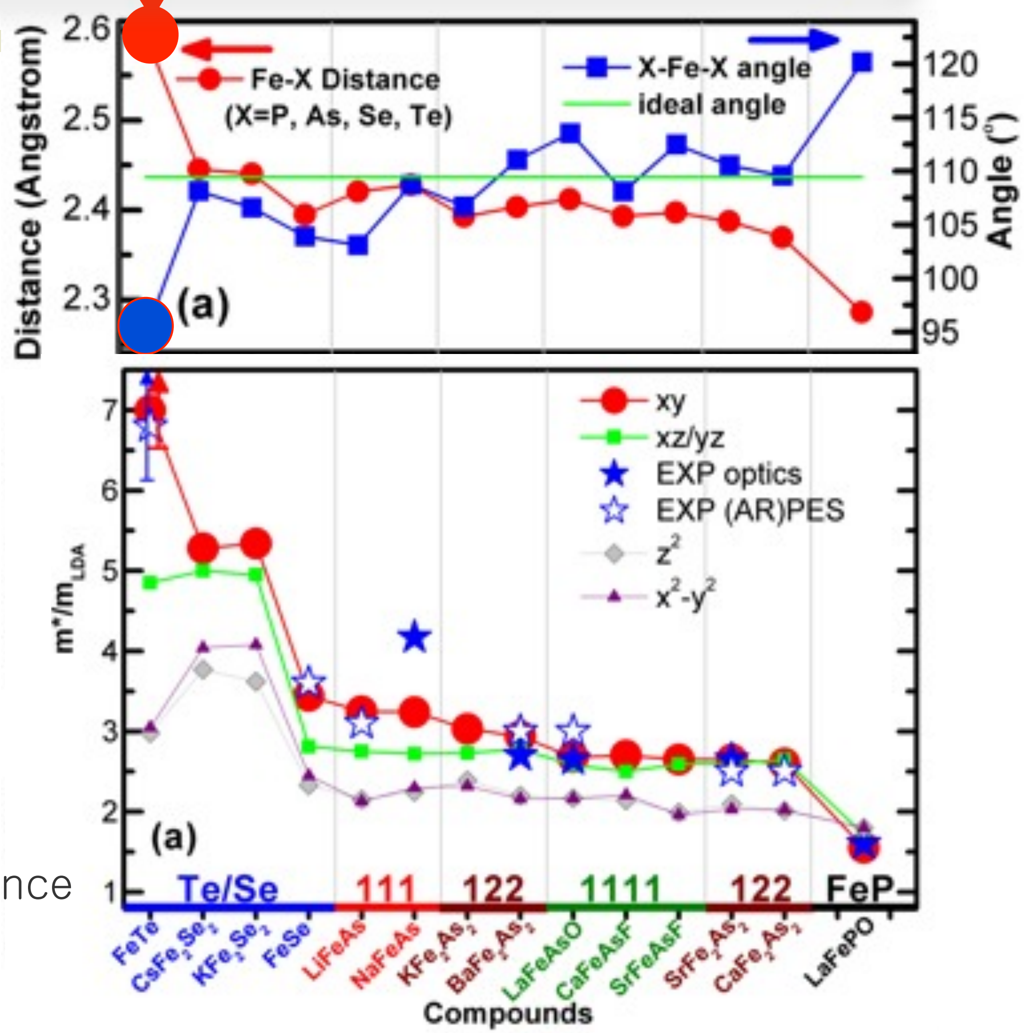
Overal trend consistent with Fe-As distance

Hybridization with pnictogen

Strength of correlations



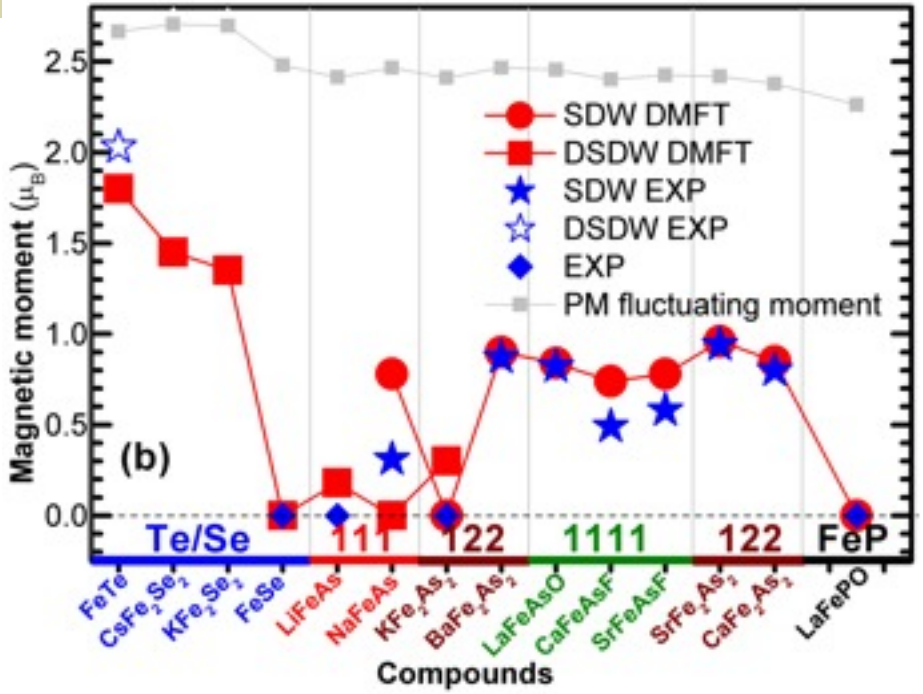




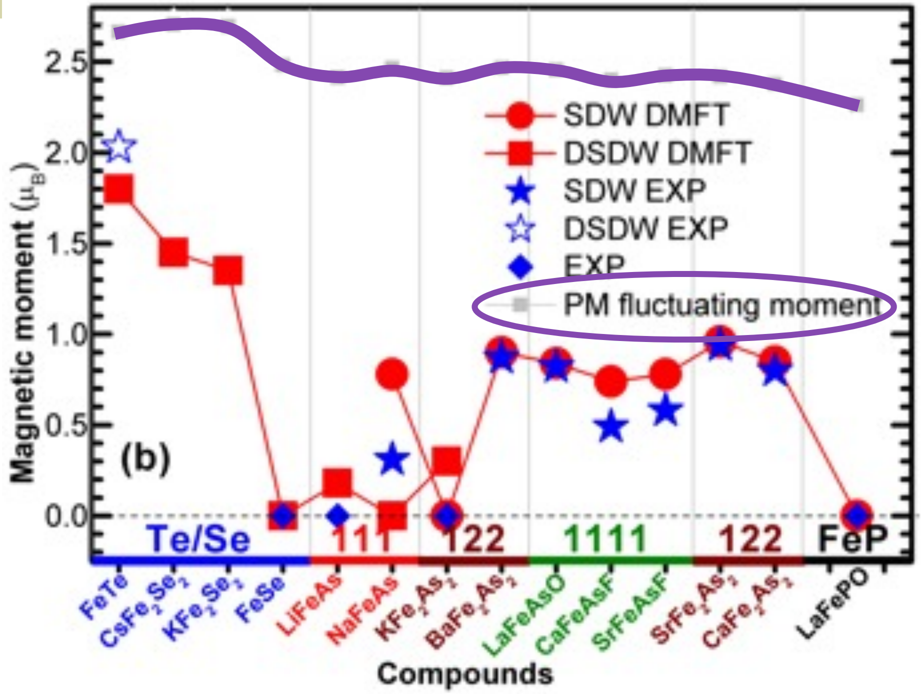
Overal trend consistent with Fe-As distance

Hybridization with pnictogen

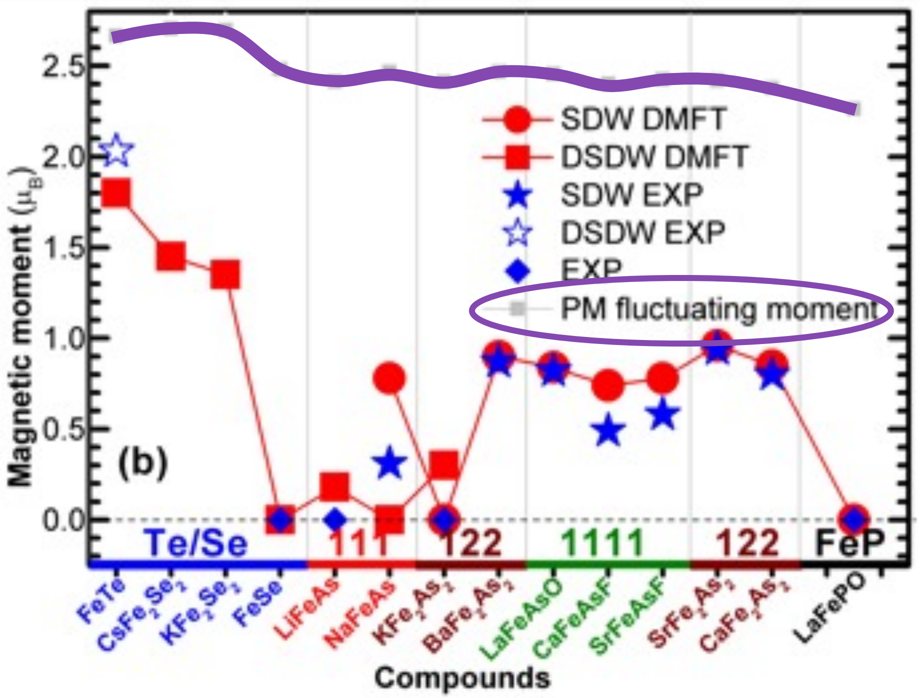
Fluctuating moment



Fluctuating moment



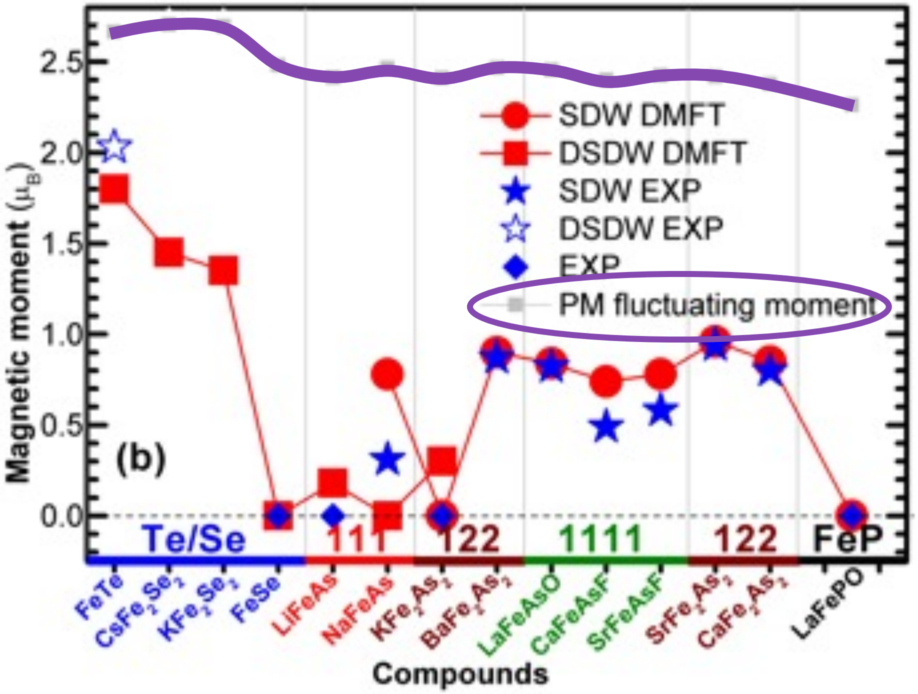
Fluctuating moment



High spin states gain weight with
Increased correlations,
fluctuating moment larger

Due to itinerancy, fluctuating moment
reduced from $4\mu_B$ to $\sim 2.5\mu_B$!

Fluctuating moment

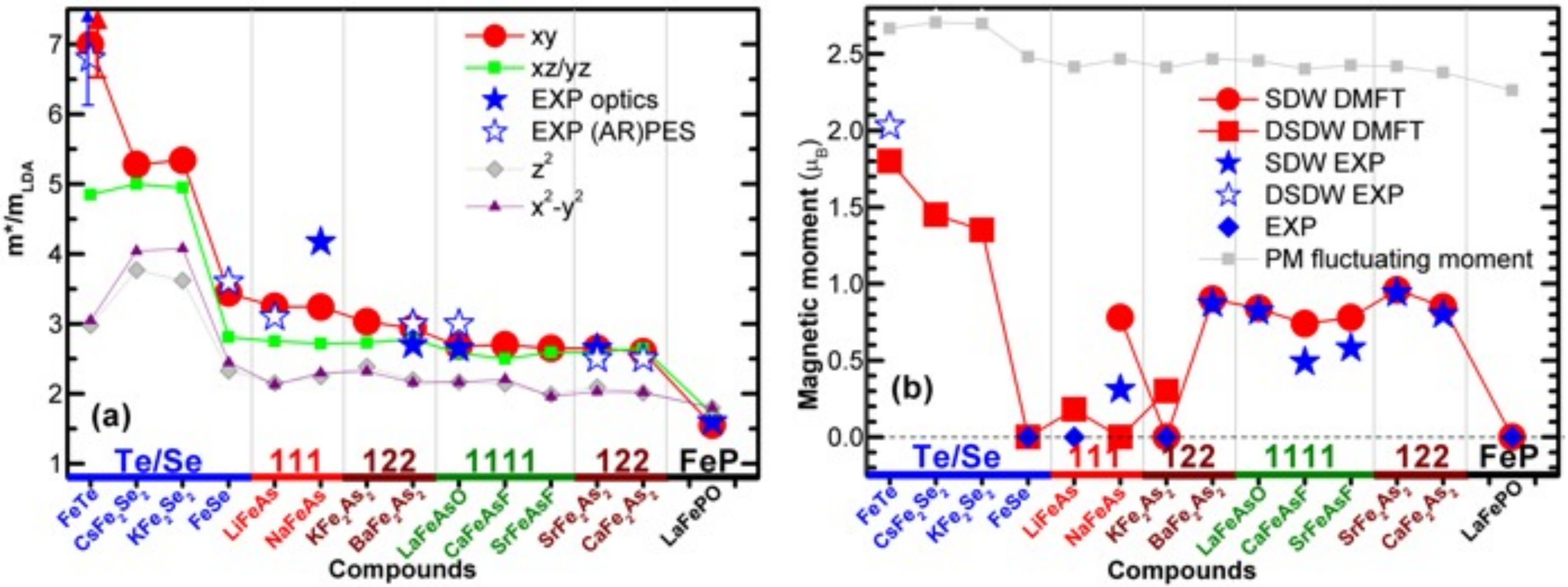


High spin states gain weight with
Increased correlations,
fluctuating moment larger

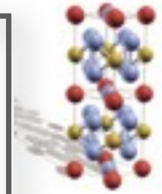
Due to itinerancy, fluctuating moment
reduced from $4\mu_B$ to $\sim 2.5\mu_B$!

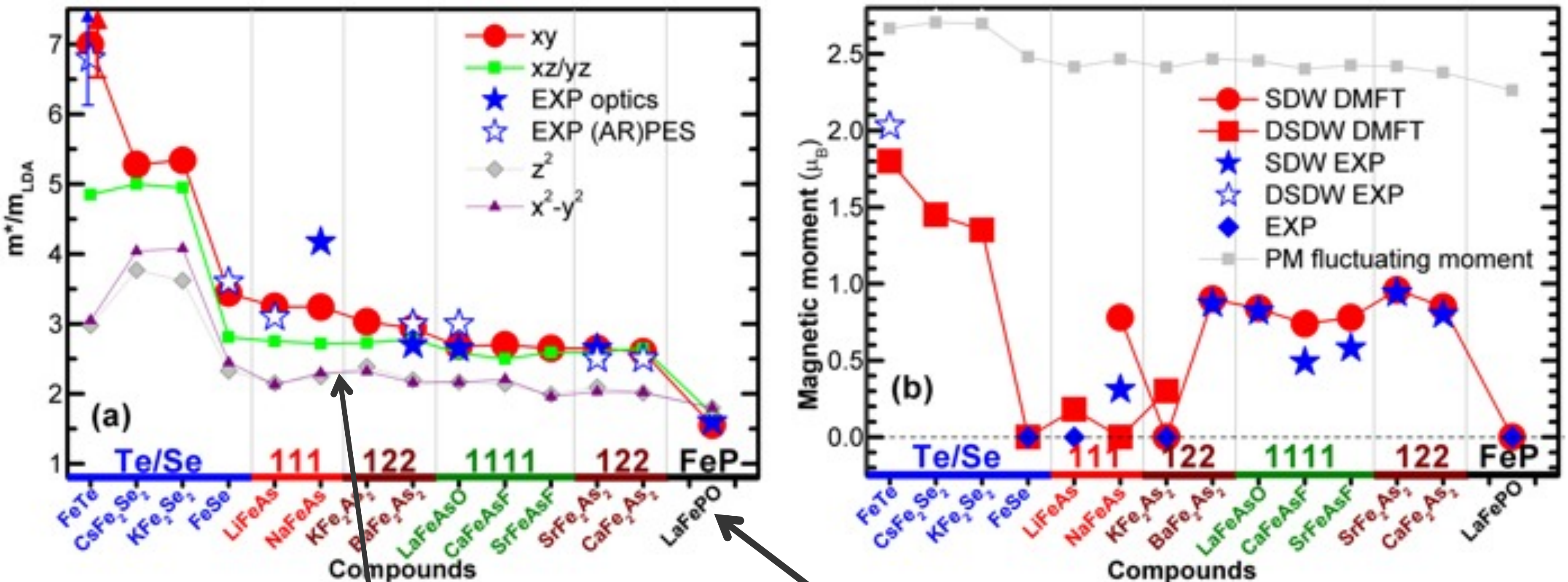
Only small fraction of the fluctuating moment orders!

Orbital differentiation



Orbital differentiation



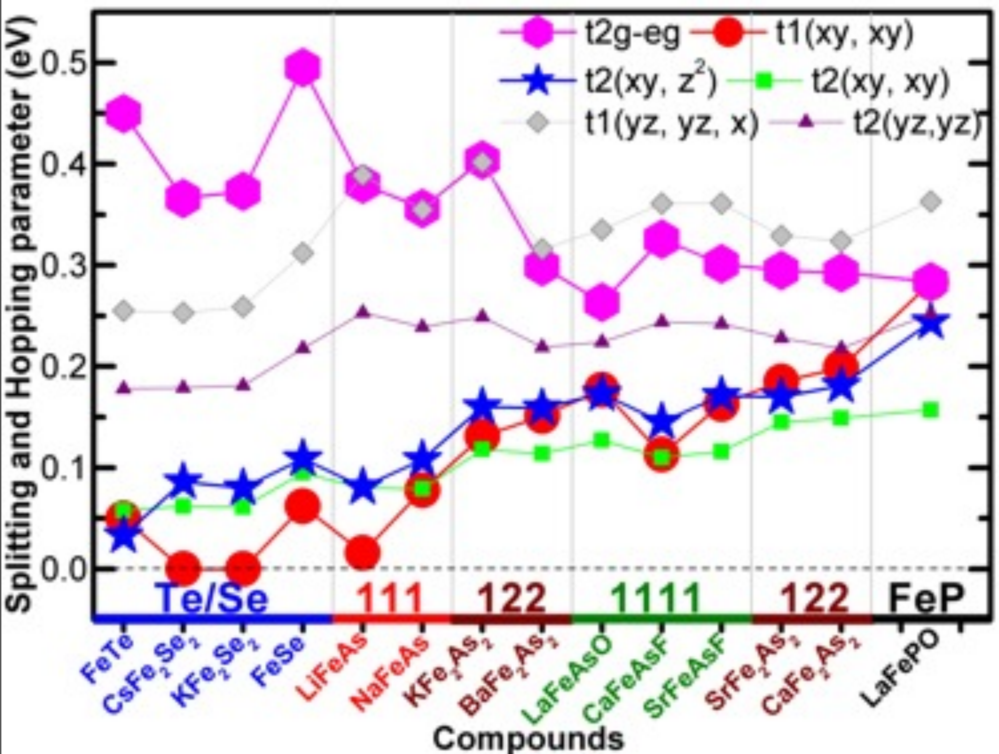


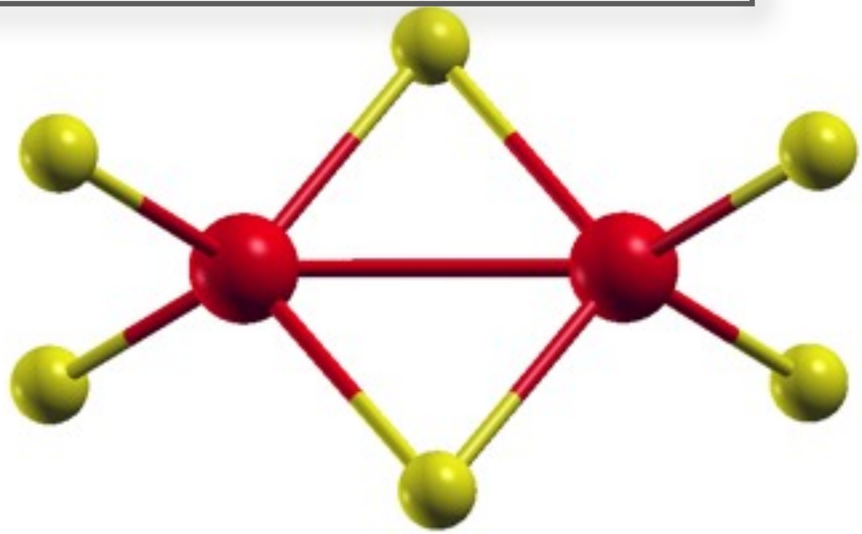
Too itinerant to order
kinetic frustruation large

eg orbitals too itinerant to contribute
to static magnetic order

Kinetic frustration

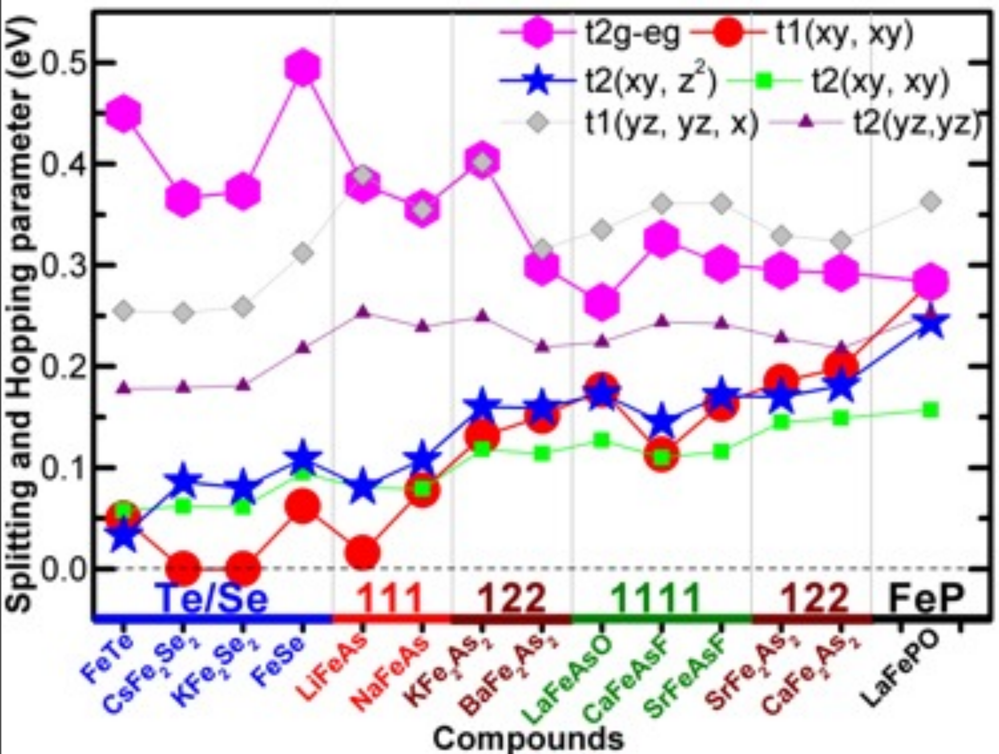
Effective low energy hoppings

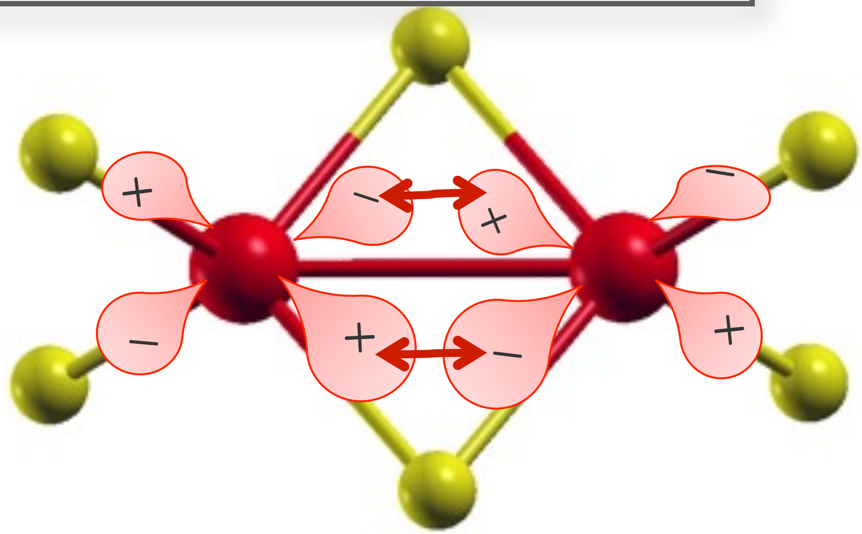




Kinetic frustration

Effective low energy hoppings

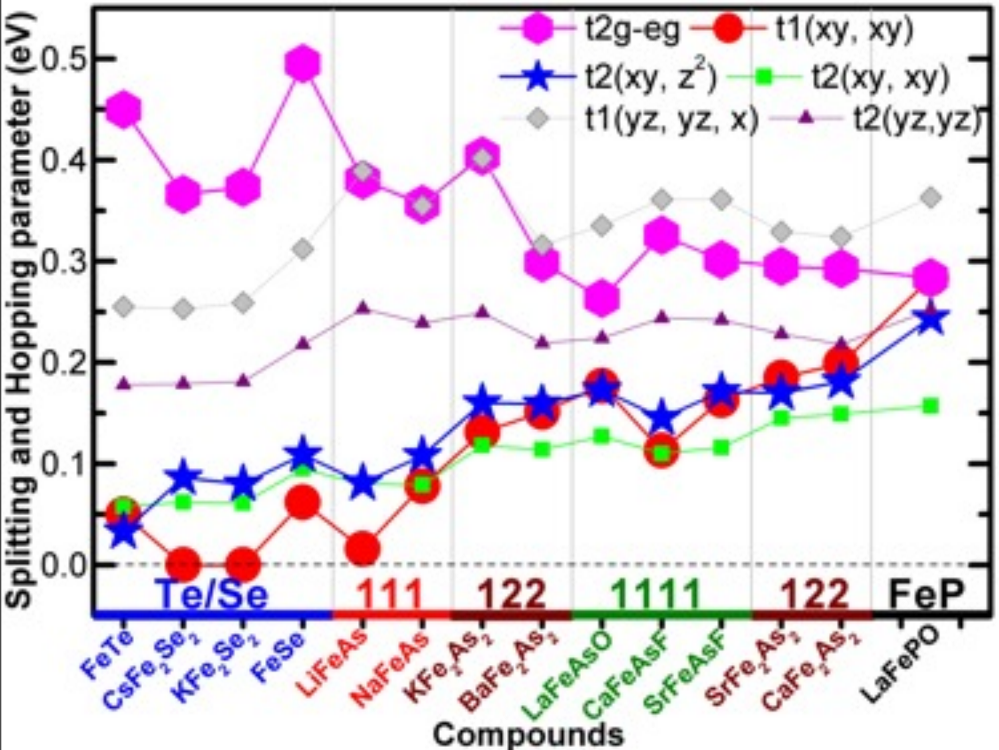


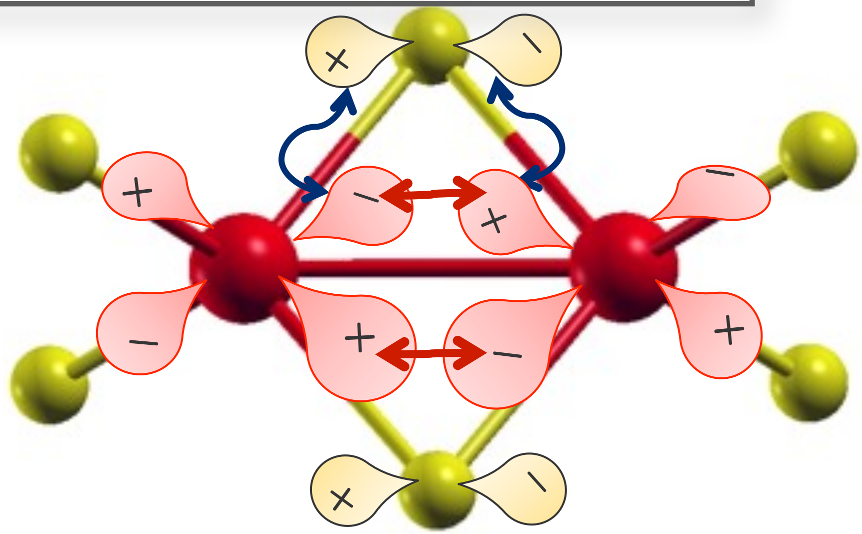


$$t^{direct}_{xy,xy} < 0$$

Kinetic frustration

Effective low energy hoppings

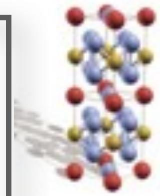




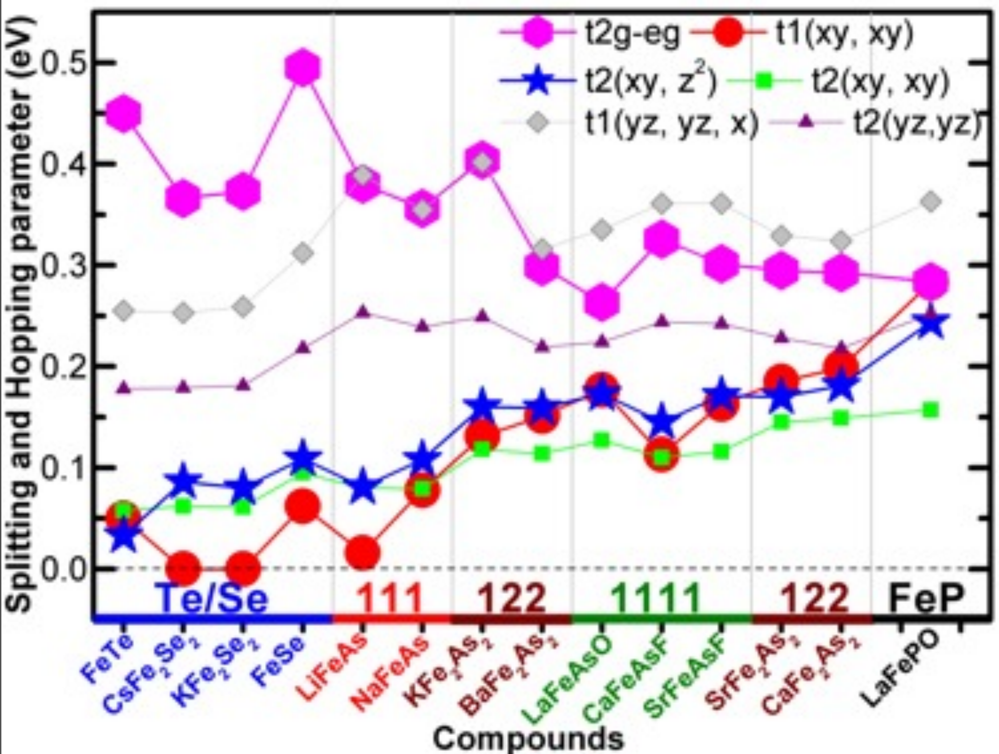
$$t_{xy,xy}^{direct} < 0$$

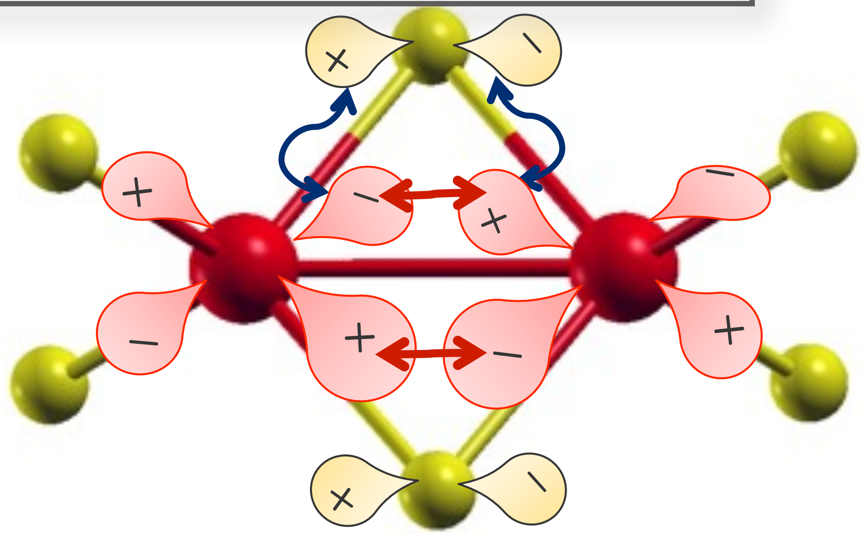
$$t_{xy,xy}^{As} > 0$$

Kinetic frustration



Effective low energy hoppings



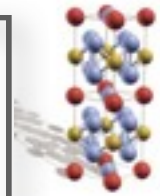


$$t^{direct}_{xy,xy} < 0$$

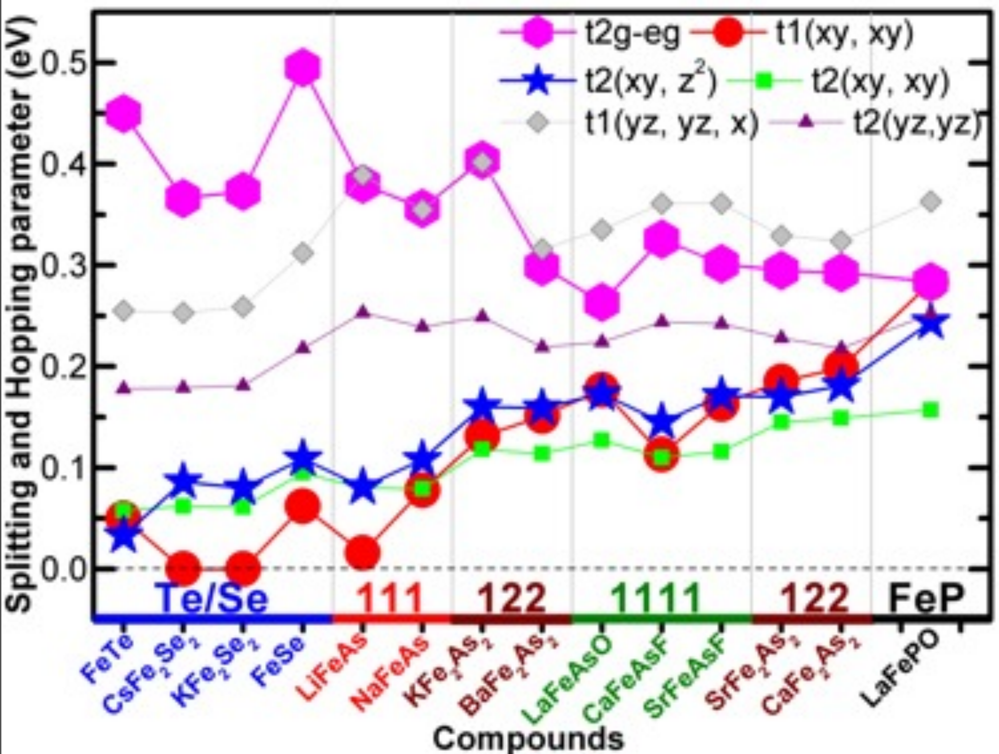
$$t^{As}_{xy,xy} > 0$$

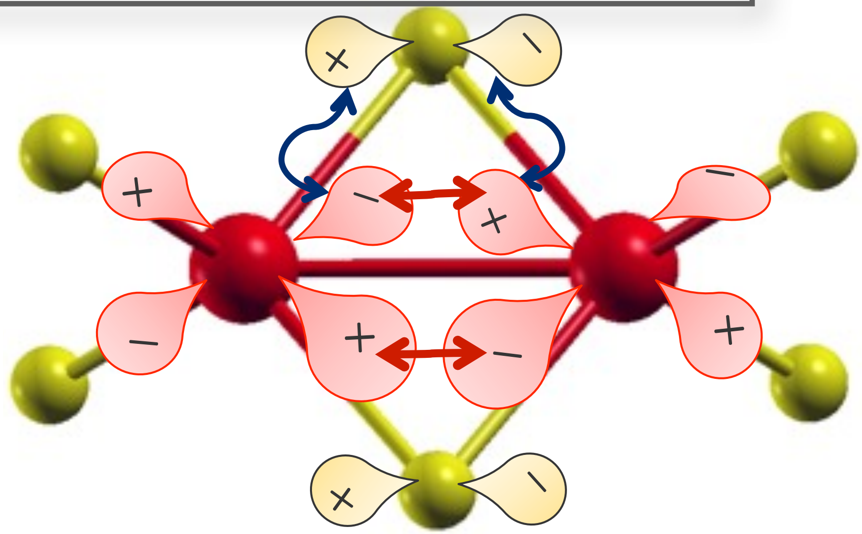
t^{As} usually larger, but not when pnictogen height large!

Kinetic frustration



Effective low energy hoppings





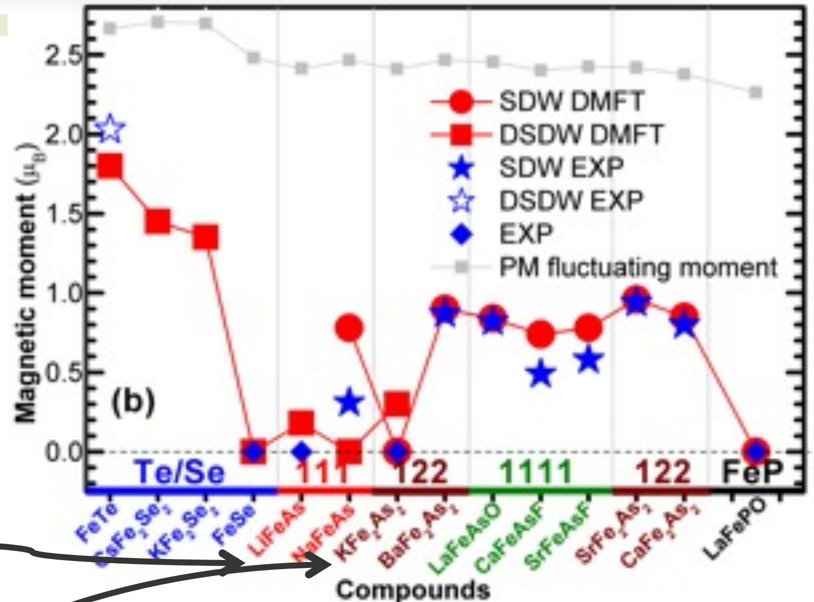
$$t^{direct}_{xy,xy} < 0$$

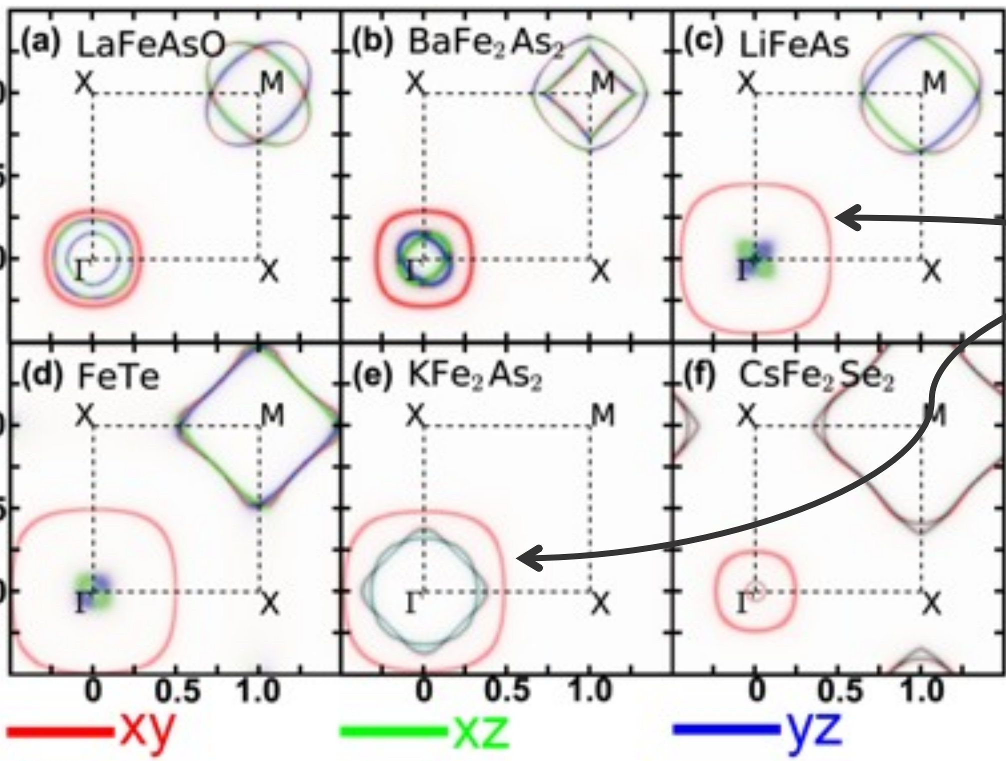
$$t^{As}_{xy,xy} > 0$$

t^{As} usually larger, but not when pnictogen height large!

Destructive interference leads to kinetic frustration!

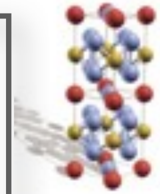
Fermi surface

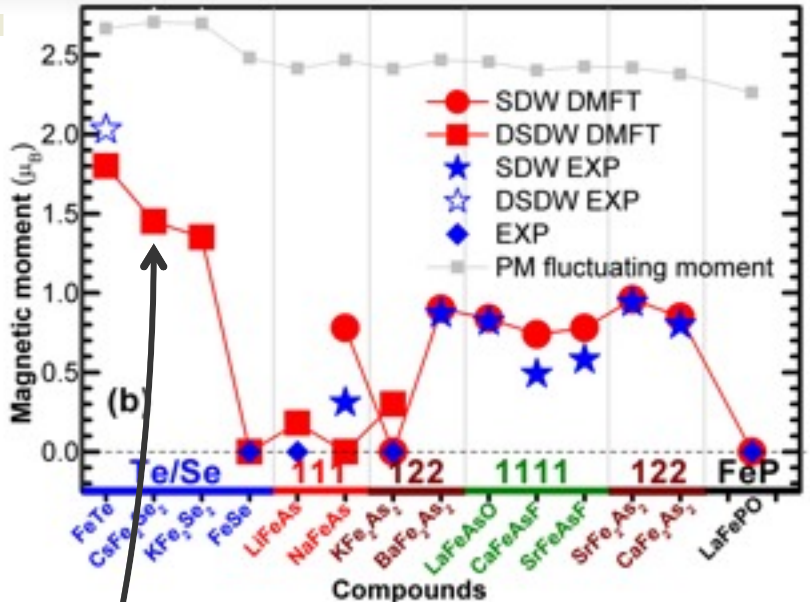




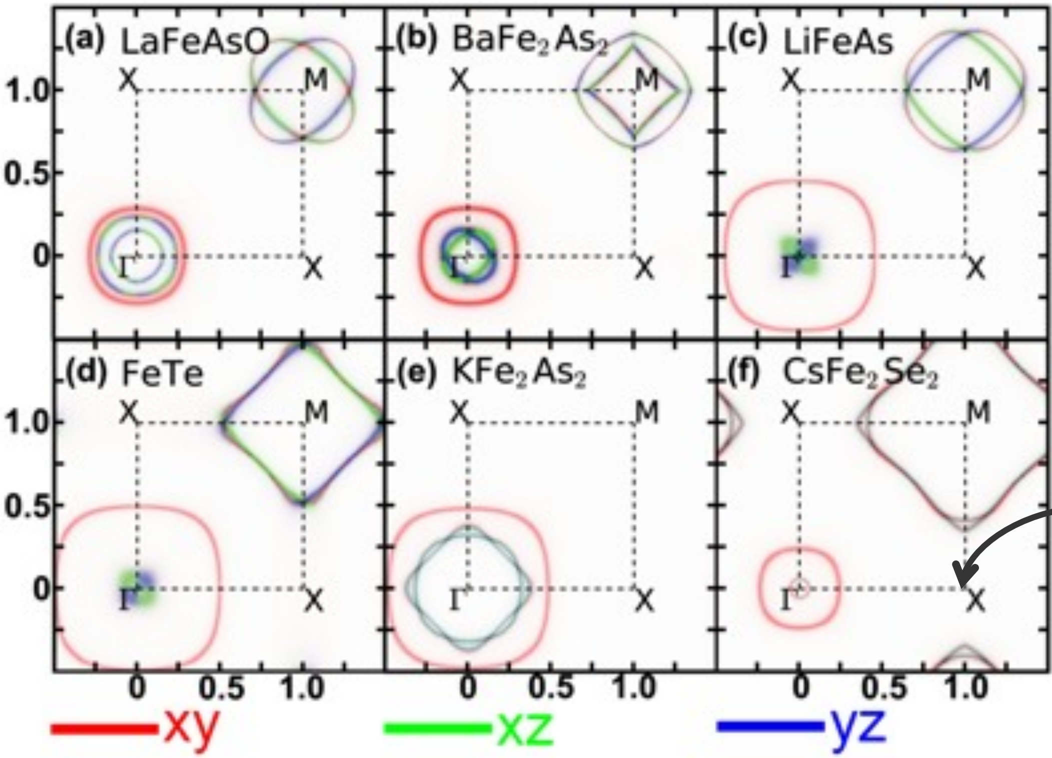
Fermi surface horrible for ordering!

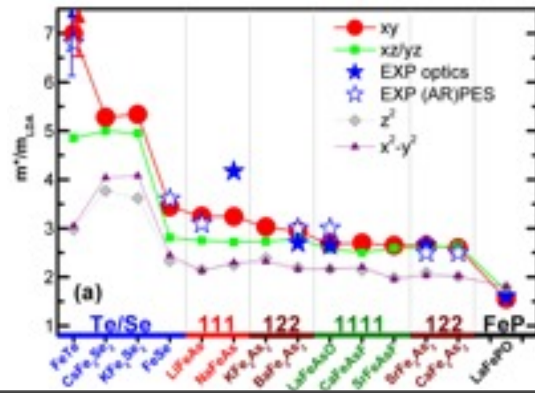
Fermi surface



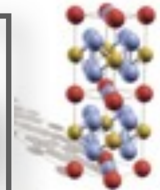


No need for nesting in very Correlated compound CsFe2Se2!

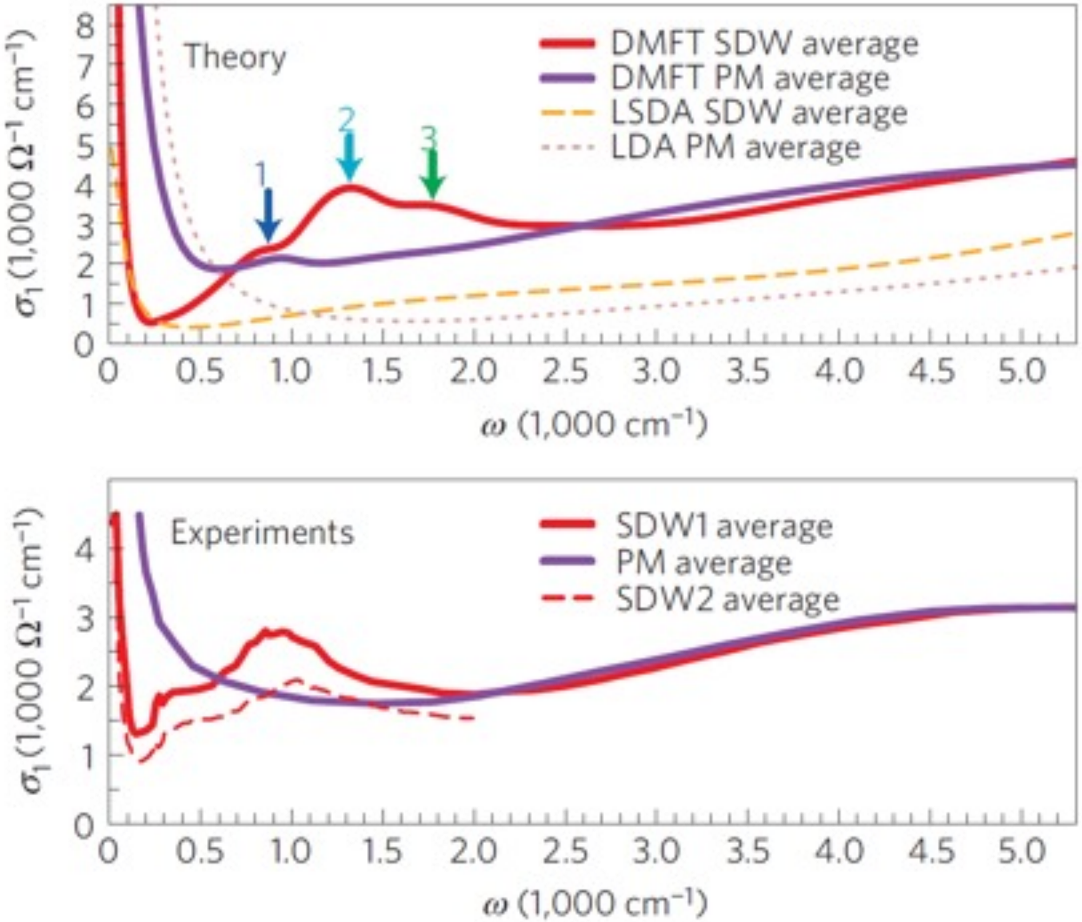




Optics by DFT+DMFT ($BaFe_2As_2$)



Z. Yin, KH, G Kotliar, Nature Physics (2011).



Good agreement with experiment!

Correct plasma ω_{p}:

DMFT ~ 1.6eV
Exp ~ 1.6eV
LDA ~ 2.6eV

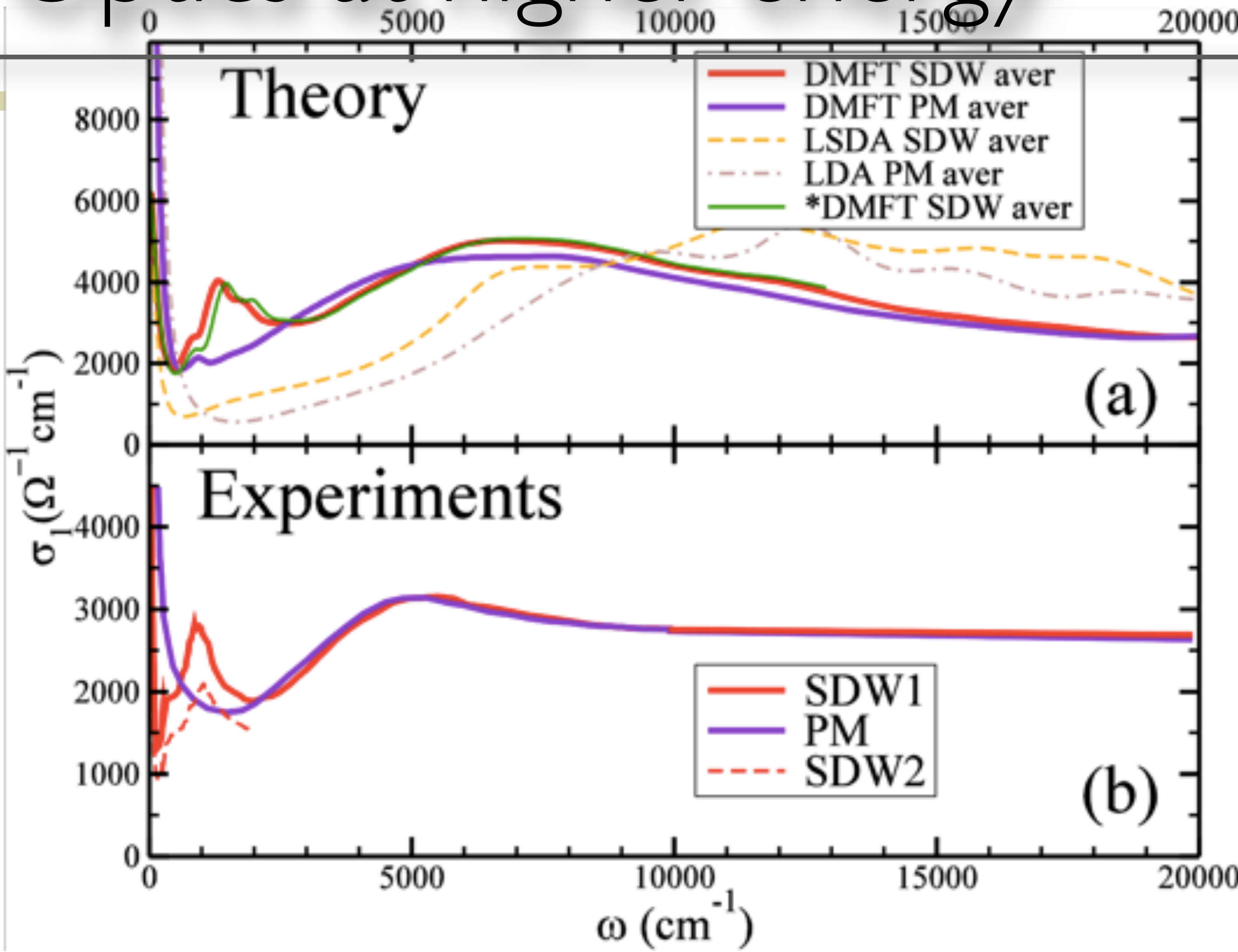
3 peak structure beyond SDW gap

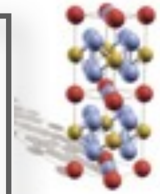
Good agreement at high energy

Experiment: W. Z. Hu, et al, PRL 101, 257005 (2008).
Nakajima, M. et al. Phys. Rev. B 81, 104528 (2010).

Optics at higher energy

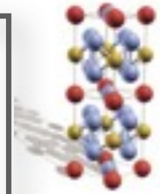
Optics at higher energy

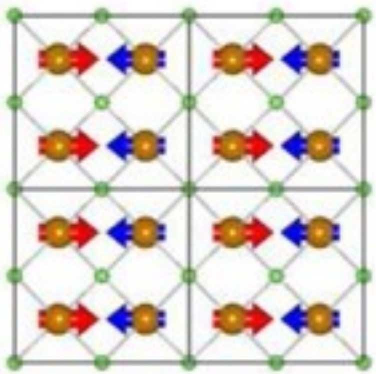


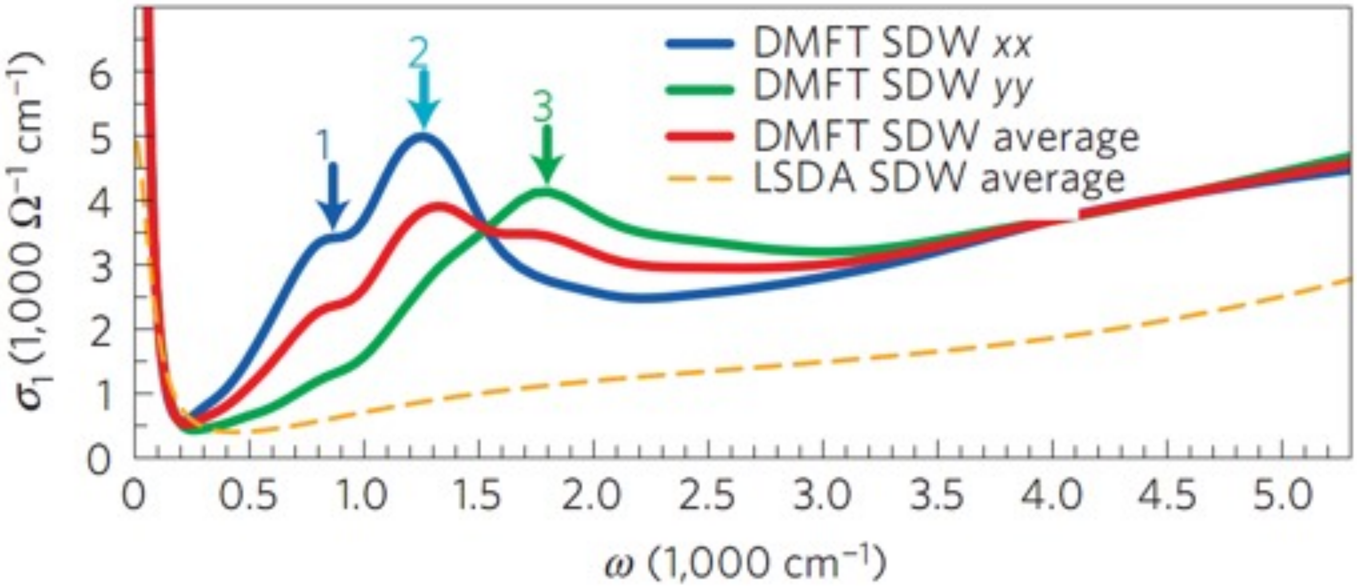


Very good agreement between LDA+DMFT and experiment
In the entire frequency range.

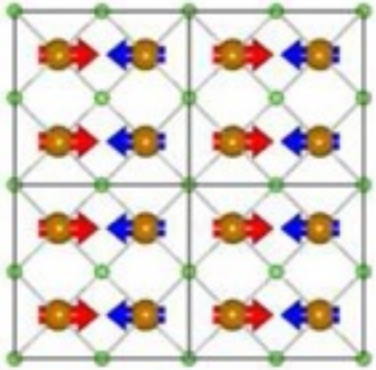
Optical anisotropy predicted

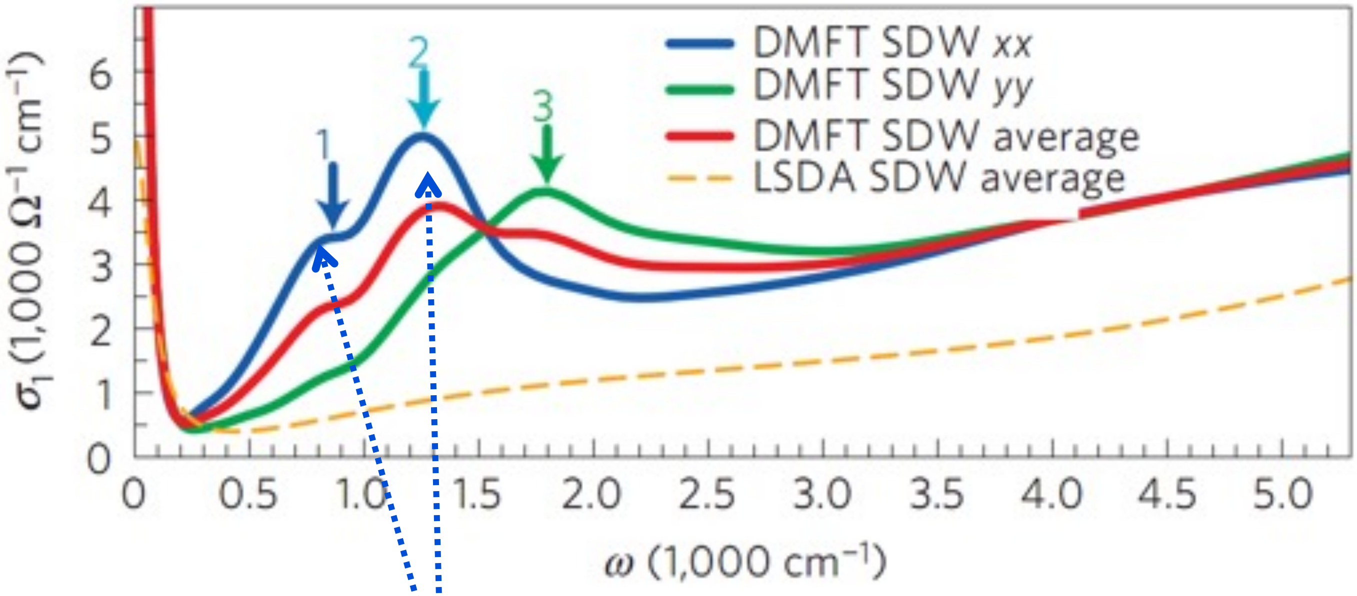






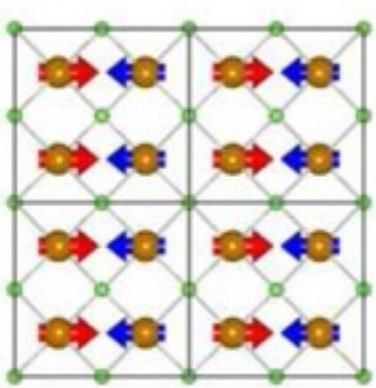
Optical anisotropy predicted

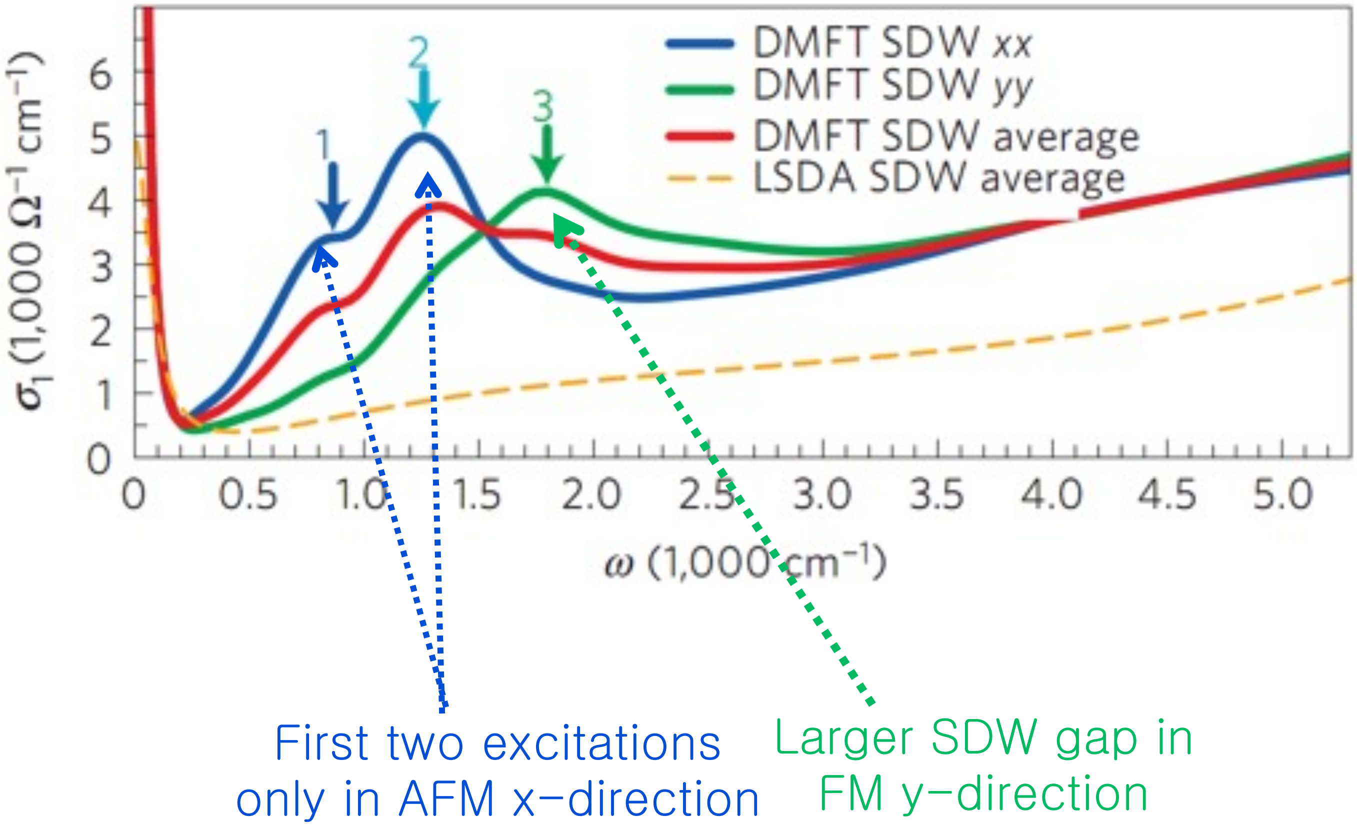




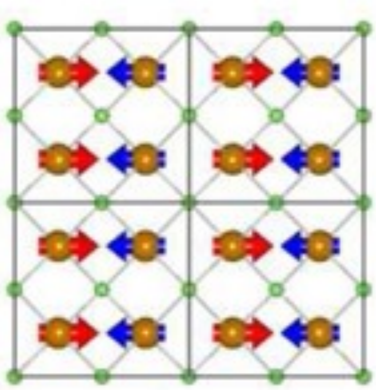
First two excitations
only in AFM x-direction

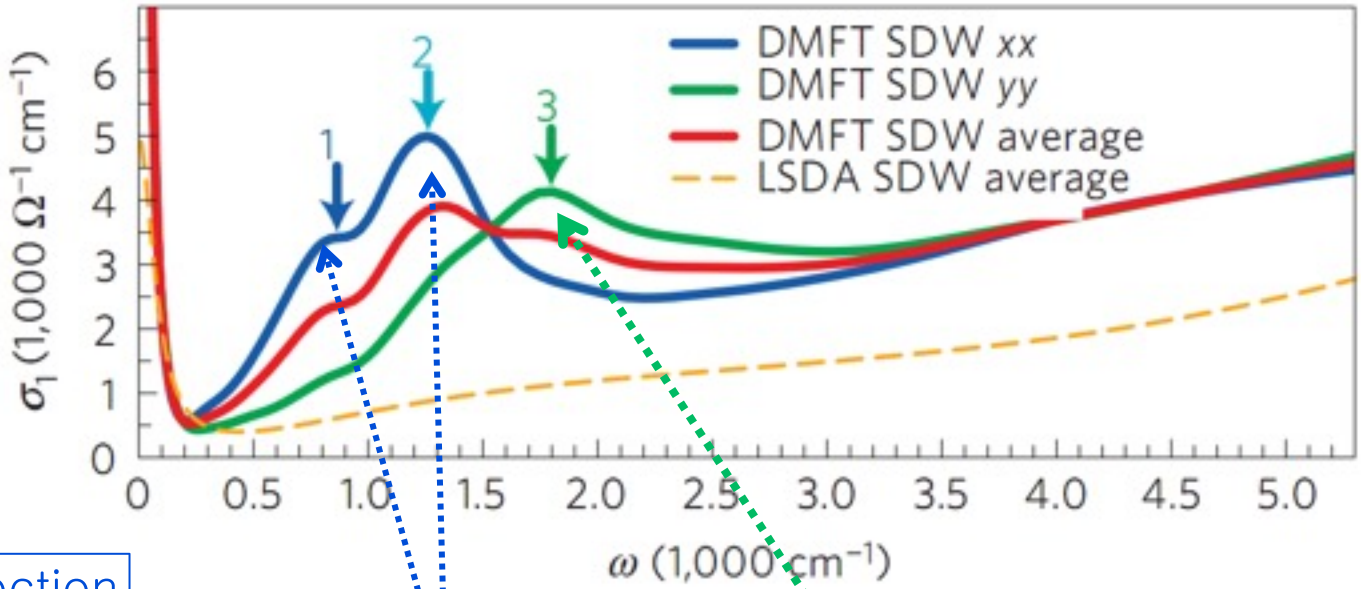
Optical anisotropy predicted





Optical anisotropy predicted





highway in AFM (x) direction

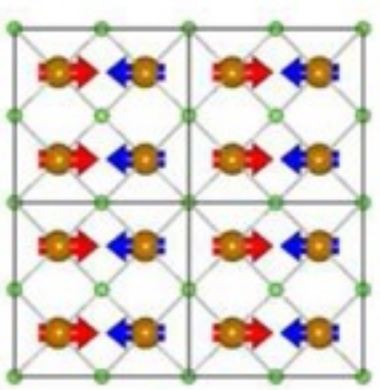
Pauli blocking hinders electron hopping In FM(y) direction

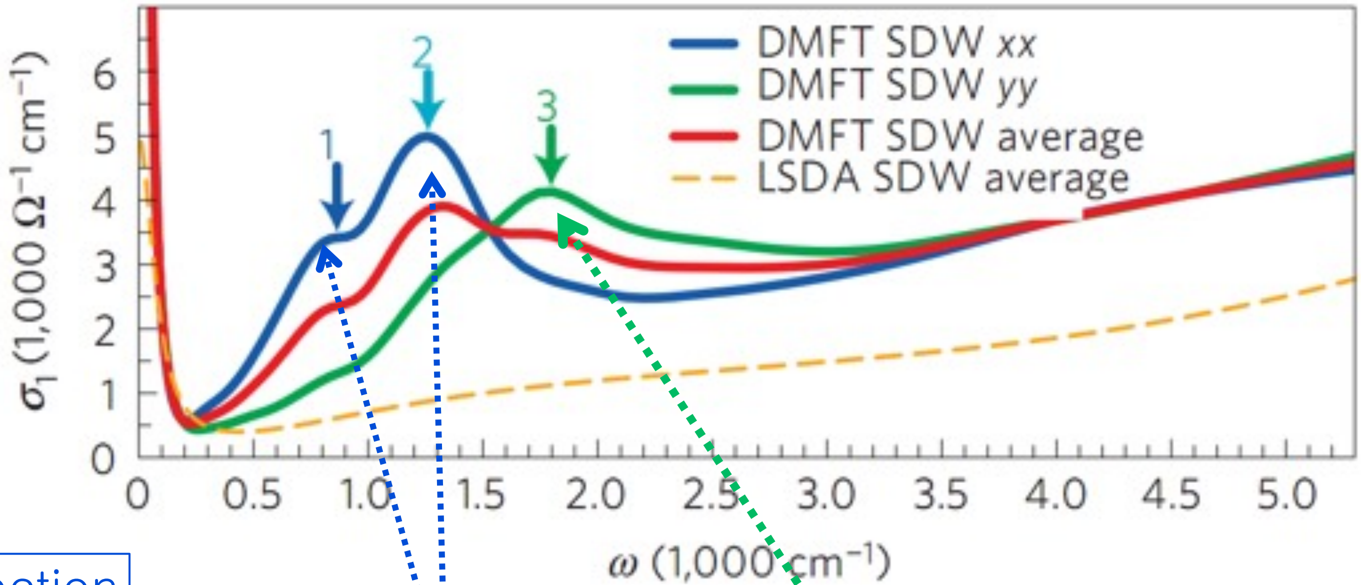
First two excitations only in AFM x-direction

Larger SDW gap in FM y-direction

Z. P. Yin, KH, G. Kotliar, Nature Physics 2011.

Optical anisotropy predicted





highway in AFM (x) direction

Pauli blocking hinders electron hopping In FM(y) direction

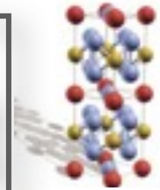
First two excitations only in AFM x-direction

Larger SDW gap in FM y-direction

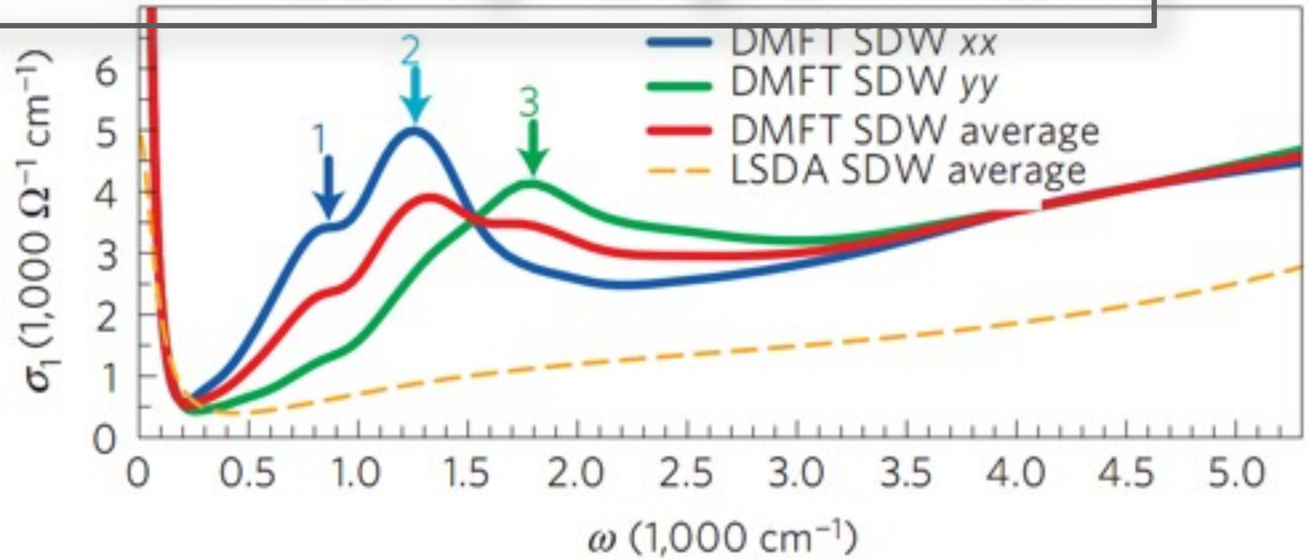
Z. P. Yin, KH, G. Kotliar, Nature Physics 2011.

QP want to decrease their kinetic energy by choosing "best path" → orbital polarization

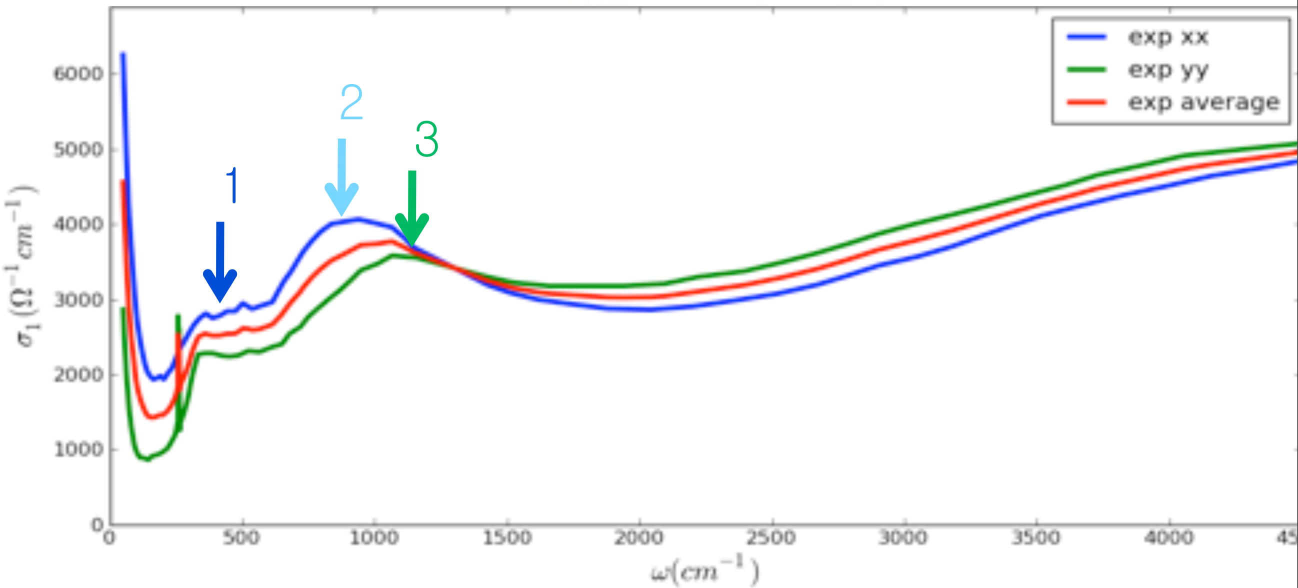
Prediction verified by experiment



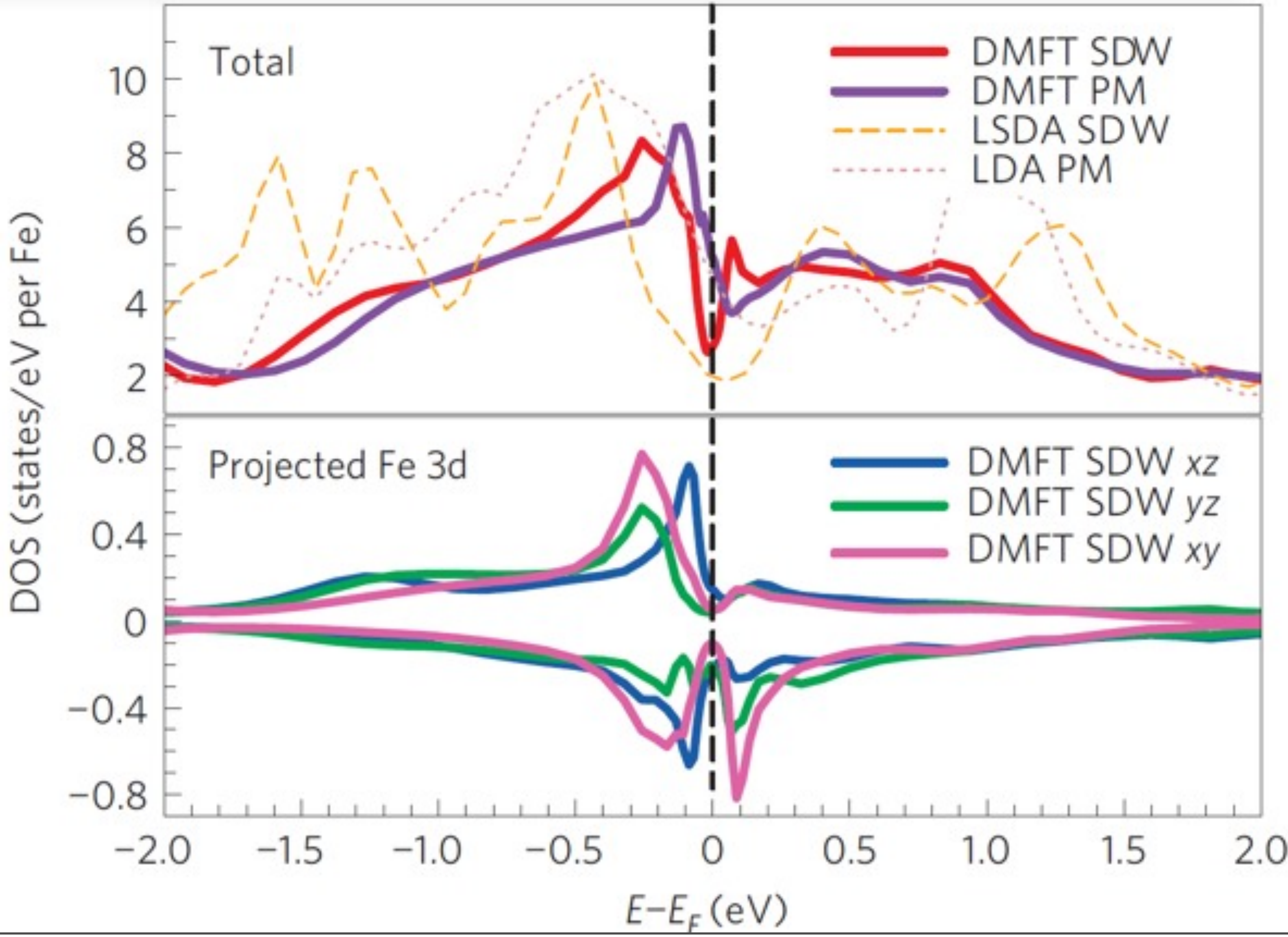
DMFT prediction:
Nature Physics 7, 294 (2011)



Experiment:
M. Nakajima, …,S Uchida,
PNAS 108, 12238 (2011).

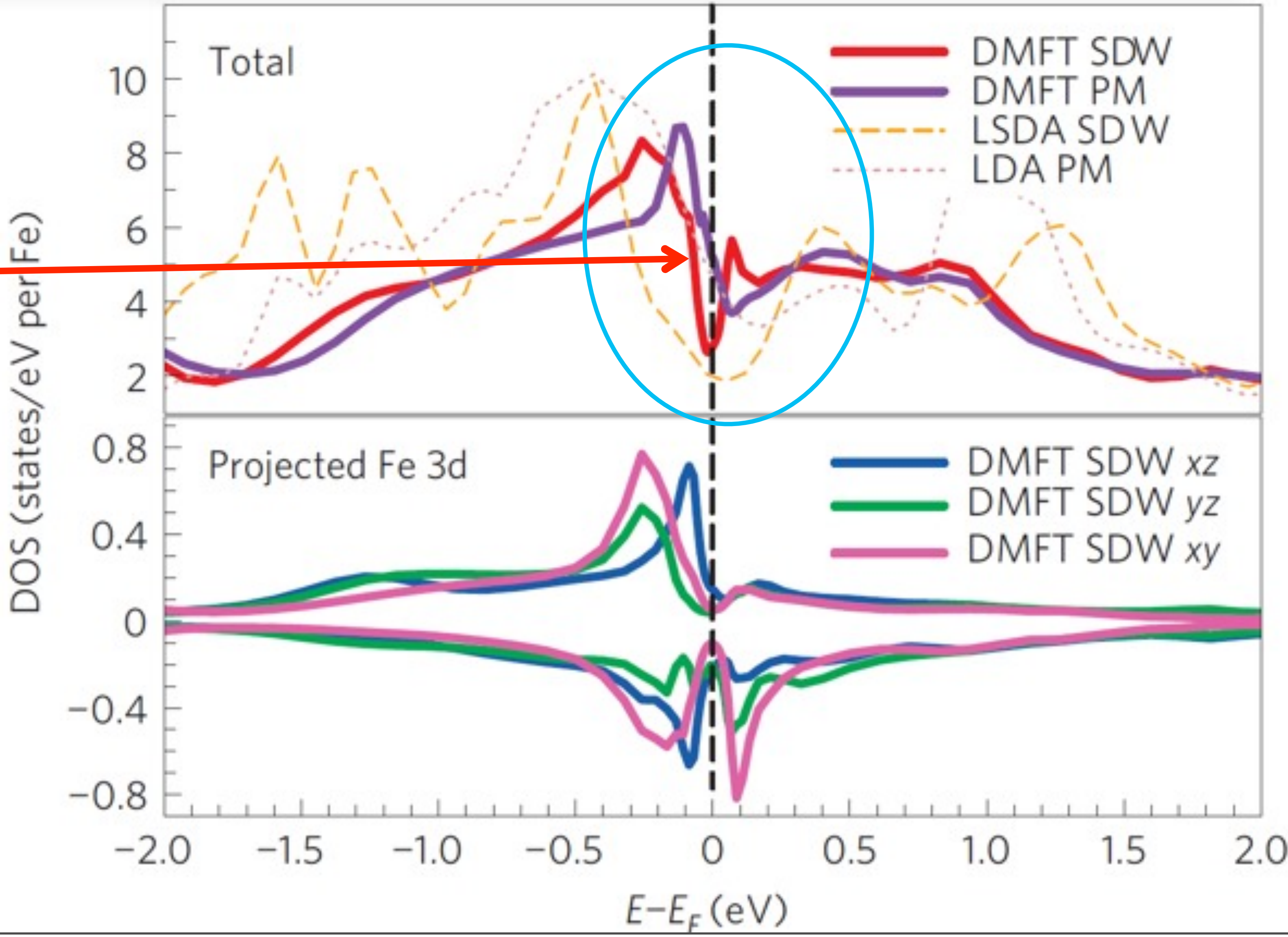


Density of states



Density of states

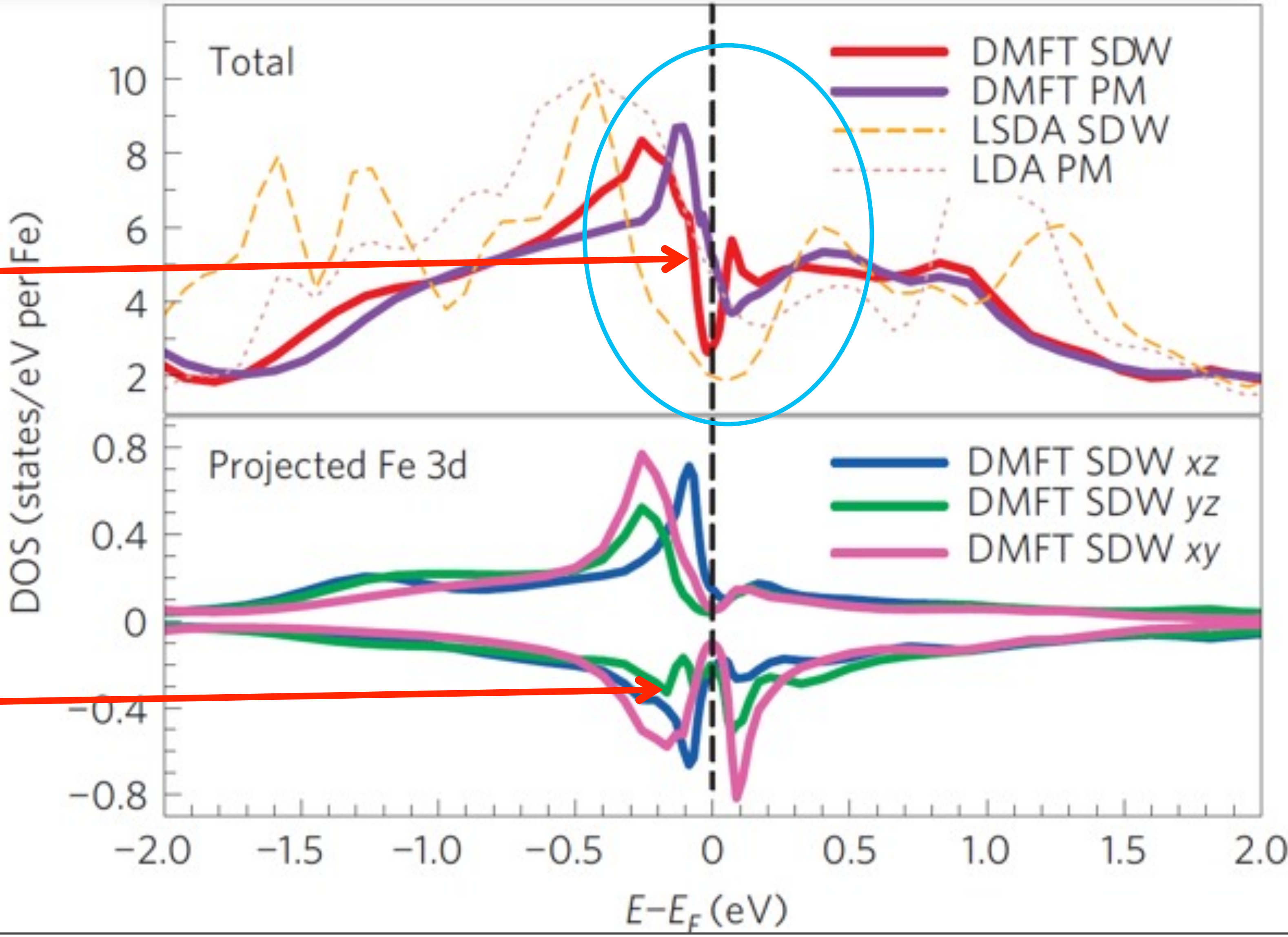
SDW gap
openning



Density of states

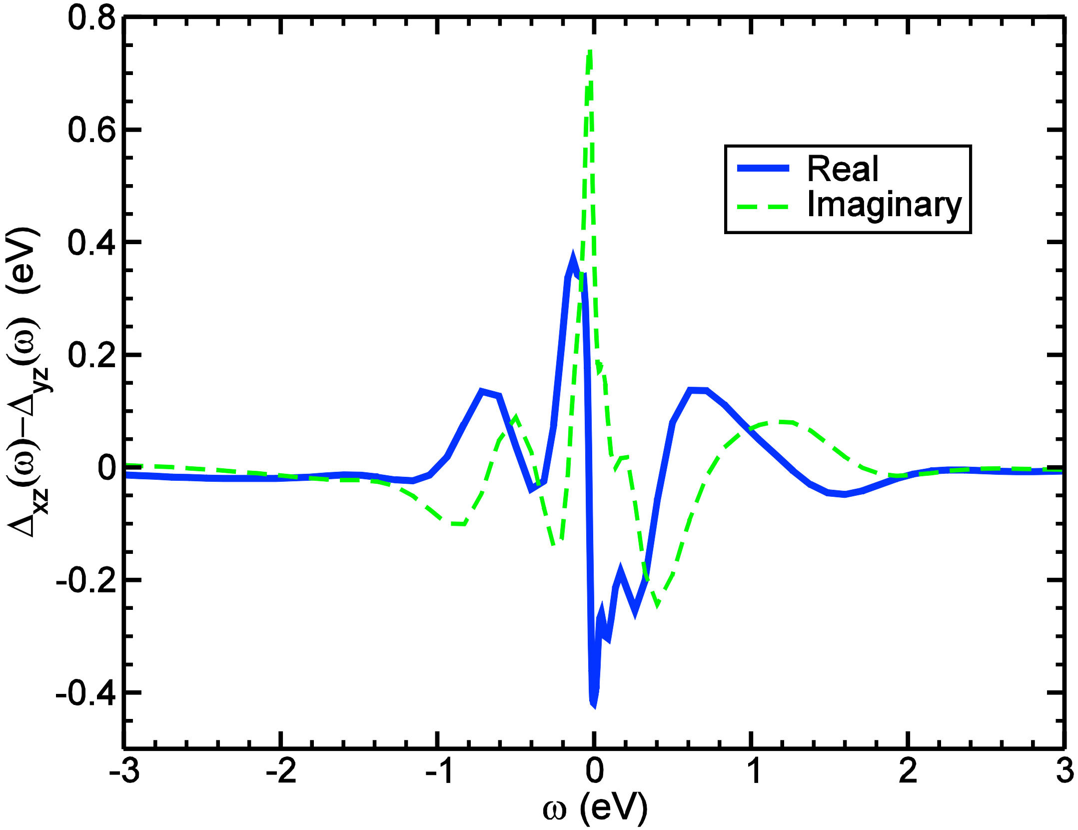
SDW gap openning

Spin and orbital polarization

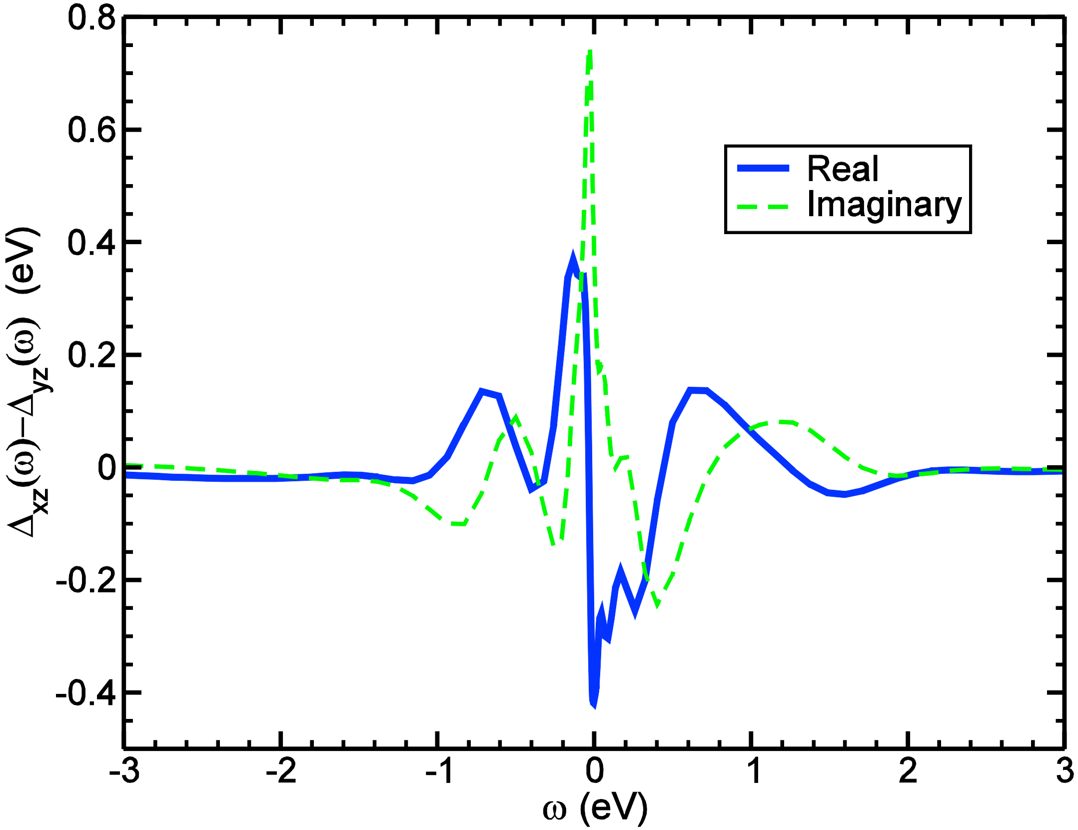


Orbital polarization-low energy phenomena

Orbital polarization-low energy phenomena

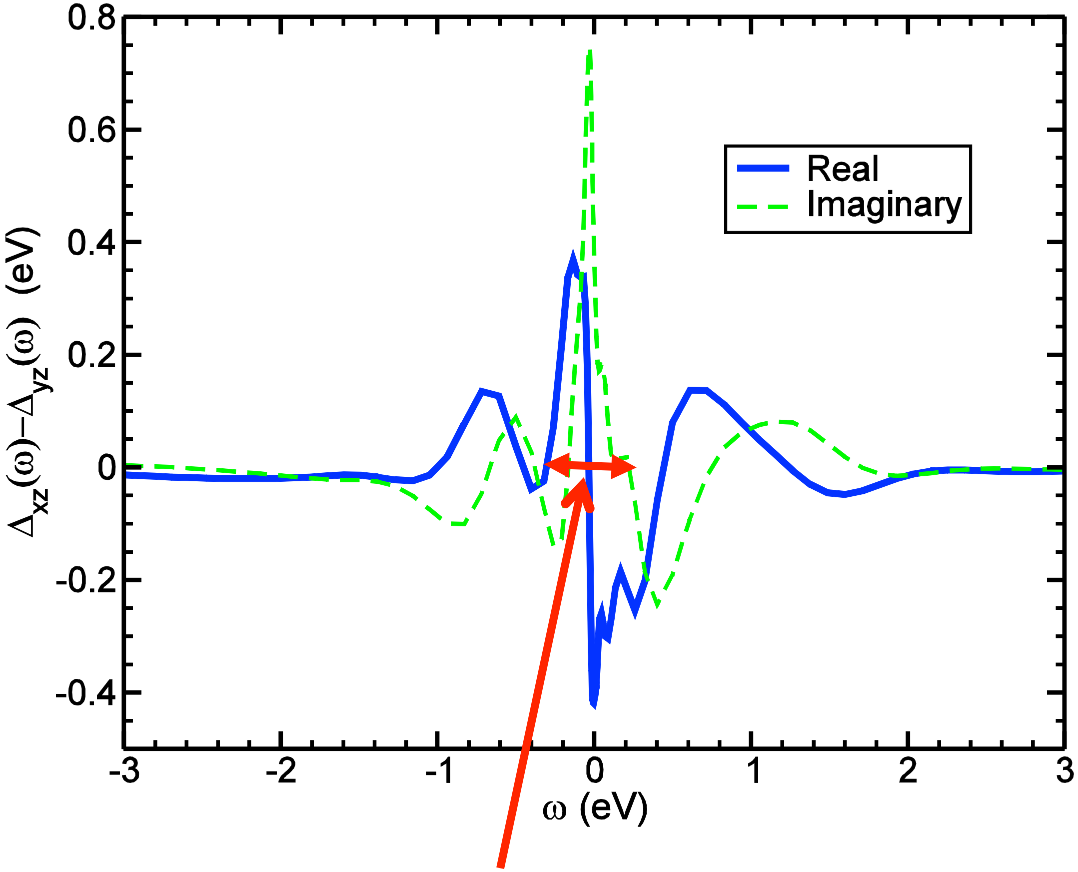


Orbital polarization-low energy phenomena



Orbital polarization large at low energy

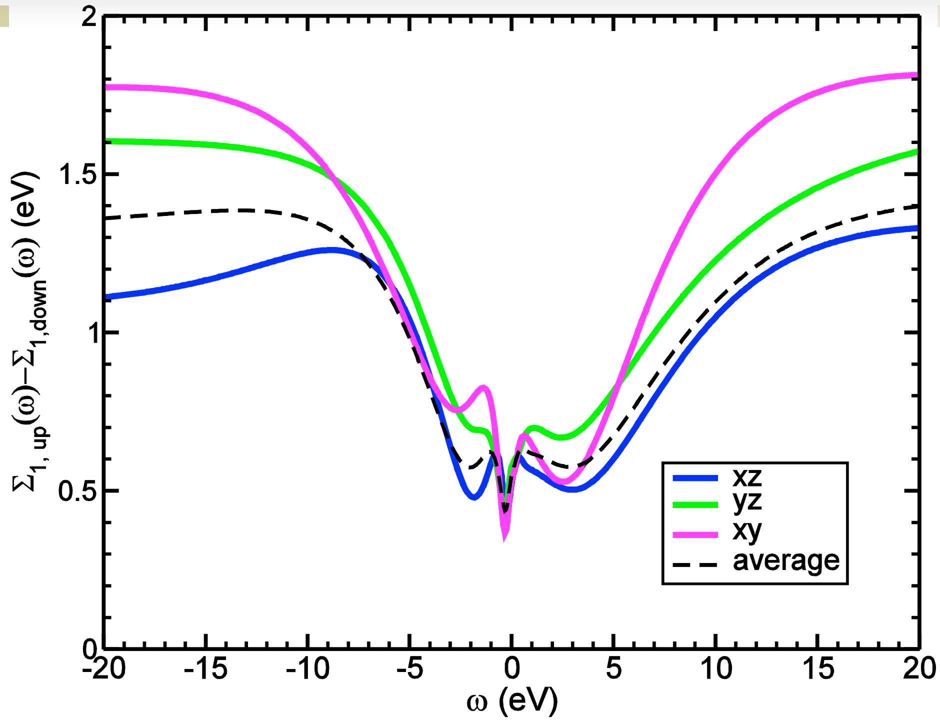
Orbital polarization-low energy phenomena



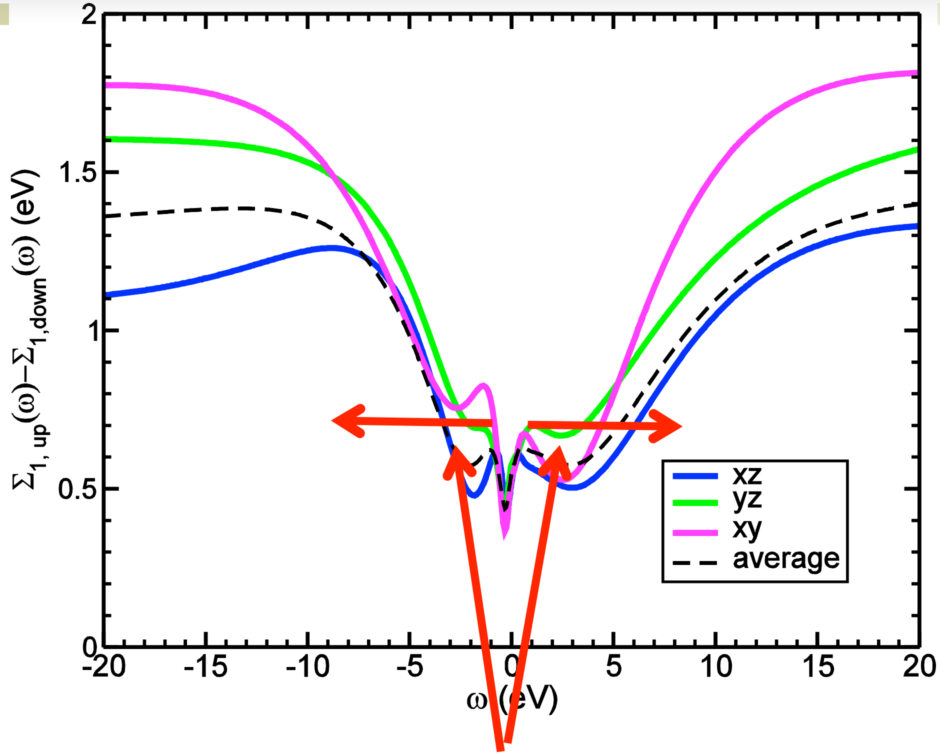
Orbital polarization large at low energy (within 300 meV)

Spin polarization-high energy phenomena

Spin polarization-high energy phenomena

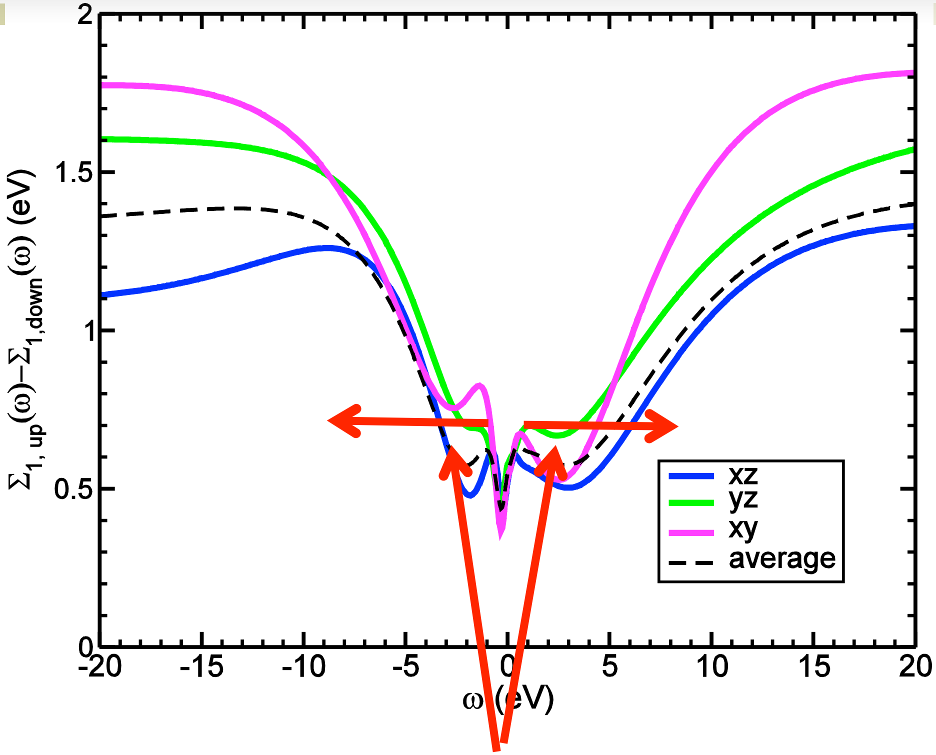


Spin polarization-high energy phenomena



Spin polarization large at high energy

Spin polarization-high energy phenomena



Spin polarization large at high energy

Spin moment lives at high energy with orbital polarization at low energy

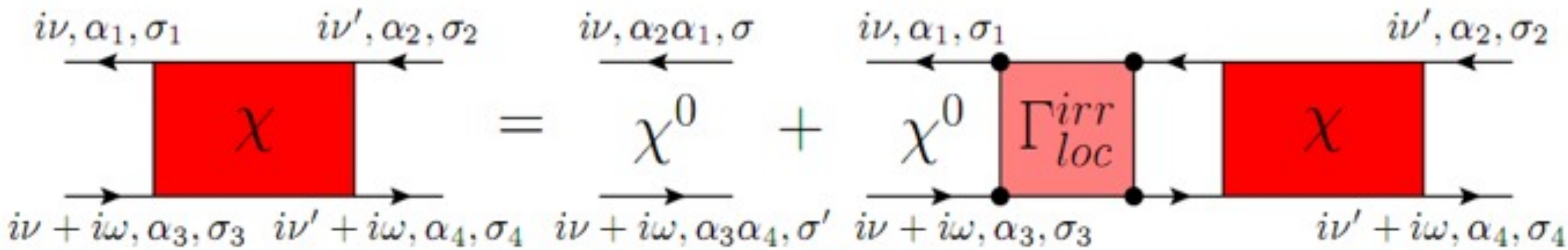
Dynamical structure factor

$$S(\mathbf{q},\omega)=\frac{\chi''(\mathbf{q},\omega)}{1-e^{-\hbar\omega/k_B T}}$$

Dynamical structure factor

$$S(\mathbf{q},\omega)=\frac{\chi''(\mathbf{q},\omega)}{1-e^{-\hbar\omega/k_BT}}$$

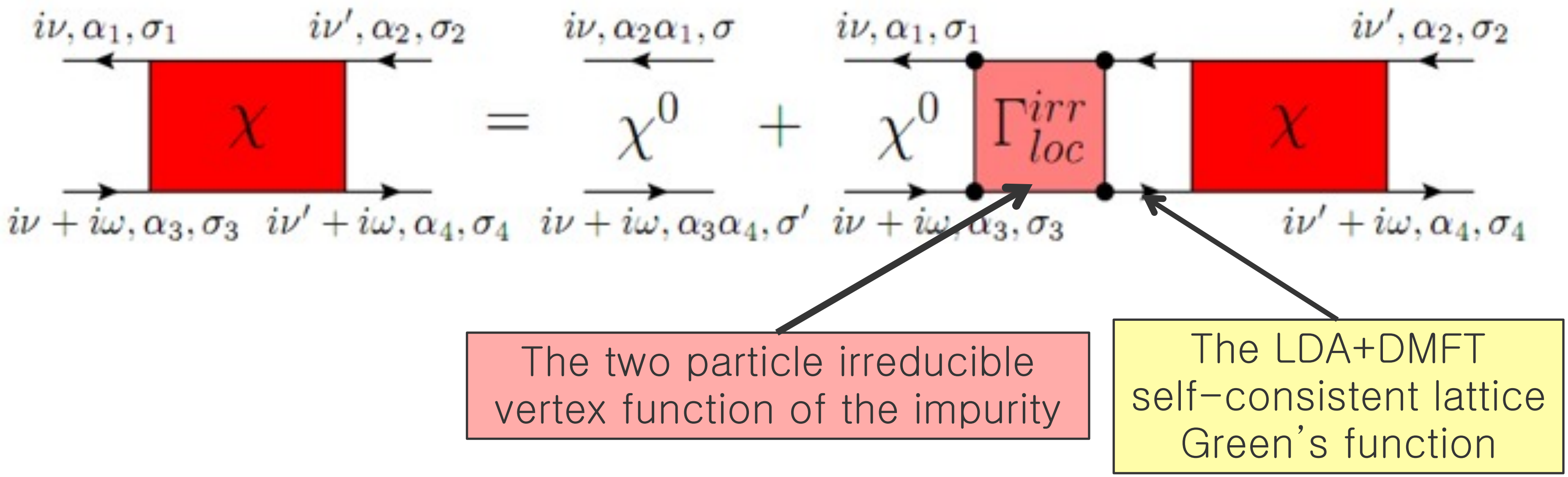
Computed from the two particle response functions using the fact that the irreducible vertex is local.



Dynamical structure factor

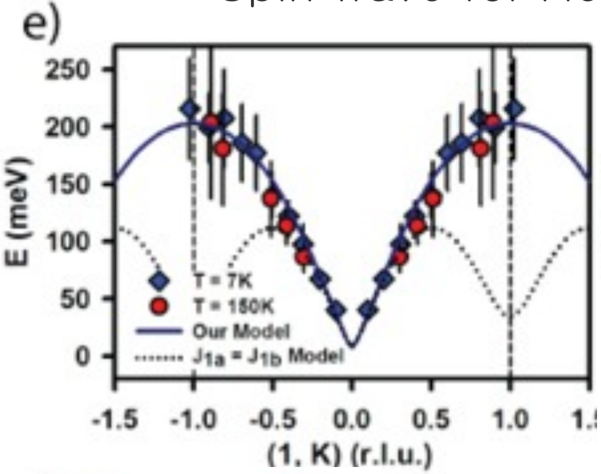
$$S(\mathbf{q},\omega)=\frac{\chi''(\mathbf{q},\omega)}{1-e^{-\hbar\omega/k_BT}}$$

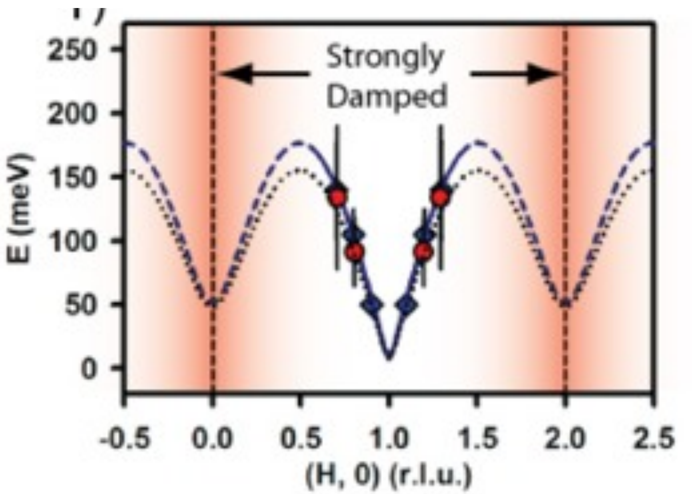
Computed from the two particle response functions using the fact that the irreducible vertex is local.

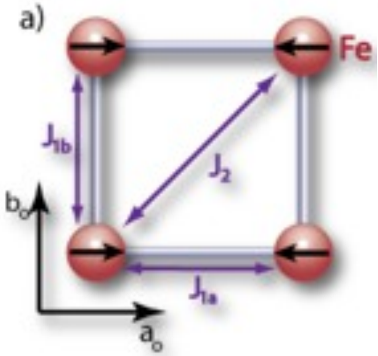


Dynamical structure factor

Spin wave for Heissenberg model



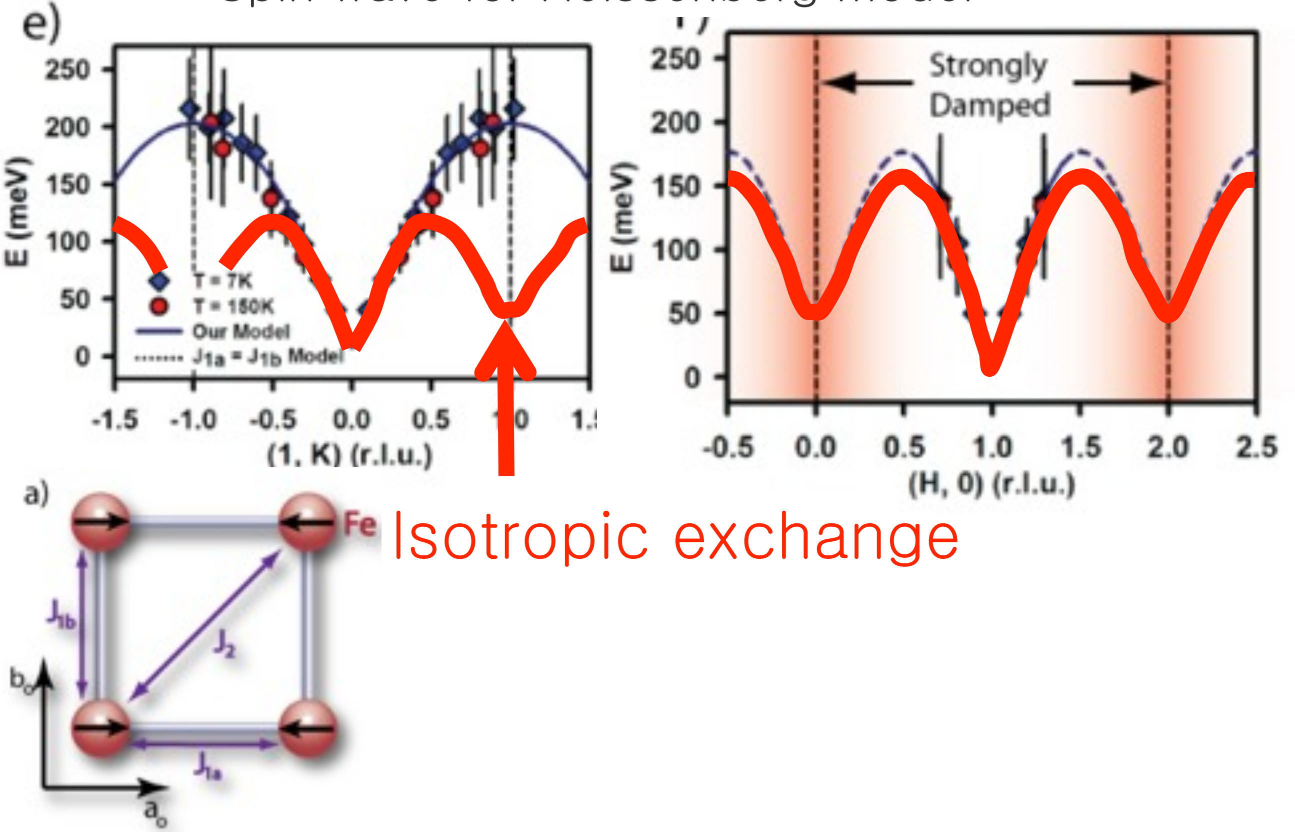




Leland W. Harriger, Pengcheng Dai et al., arXiv:1011.3771

Dynamical structure factor

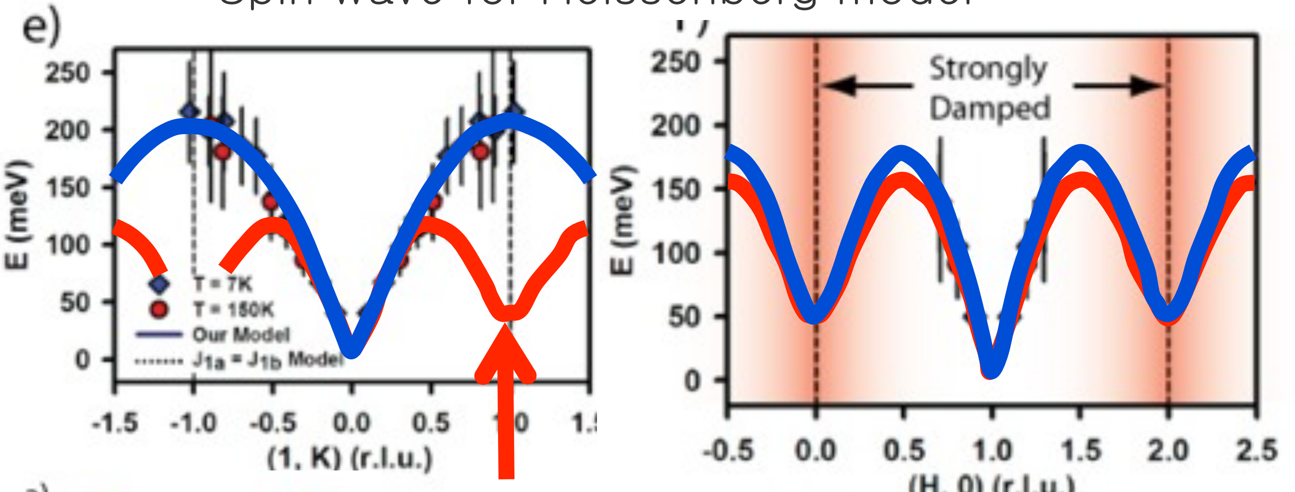
Spin wave for Heissenberg model

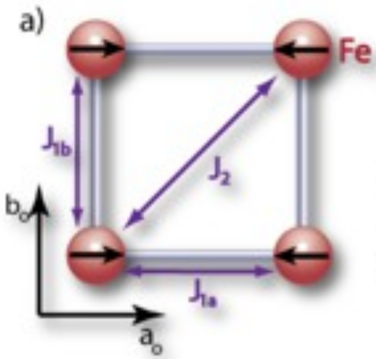


Leland W. Harriger, Pengcheng Dai et al., arXiv:1011.3771

Dynamical structure factor

Spin wave for Heissenberg model





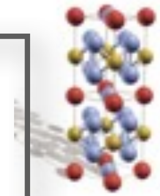
Very anisotropic exchange

$$SJ_{1a} \approx 59.2meV$$

$$SJ_{1b} \approx -9.2meV$$

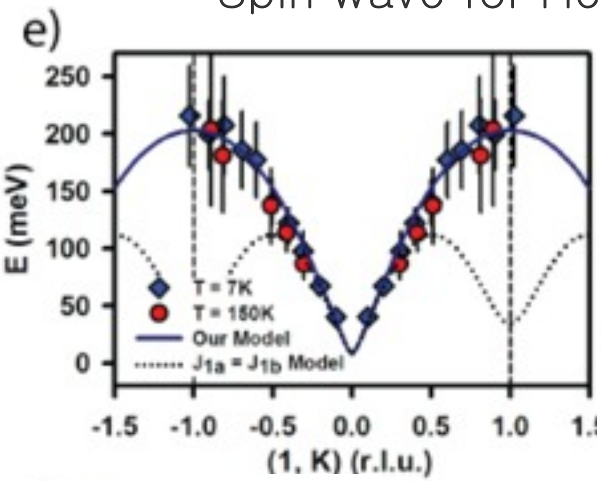
$$SJ_2 \approx 13.6meV$$

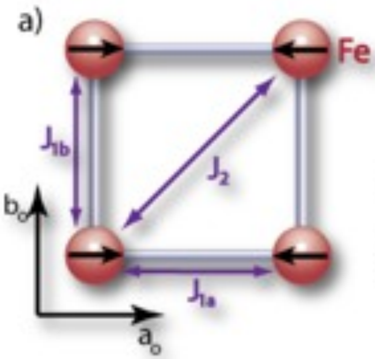
Leland W. Harriger, Pengcheng Dai et al., arXiv:1011.3771



Dynamical structure factor

Spin wave for Heissenberg model



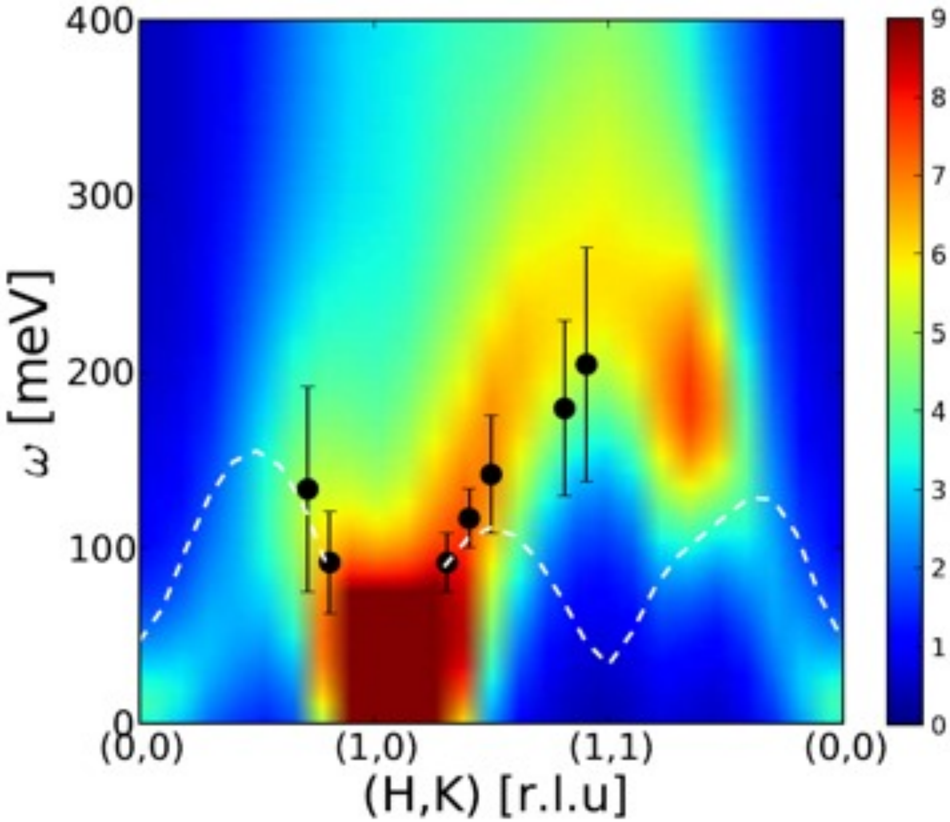


Very ar

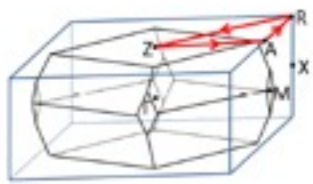
$SJ_{1a} \approx$

$SJ_{1b} \approx$

$SJ_2 \approx$

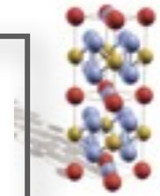


DMFT

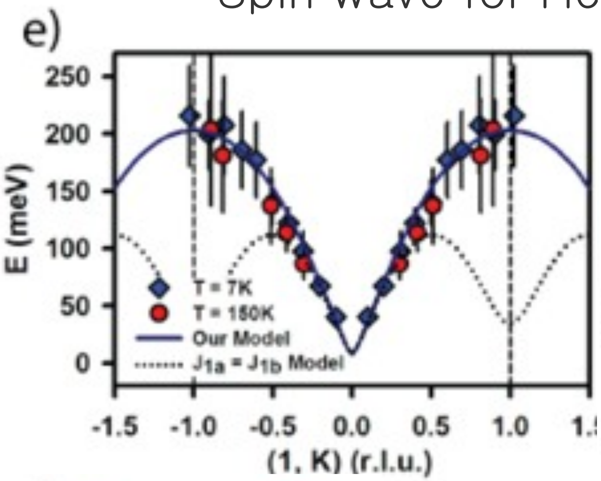


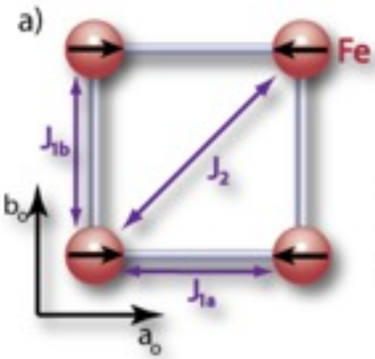
Leland W. Harriger, Pengcheng Dai et al., arXiv:1011.3771

Dynamical structure factor



Spin wave for Heissenberg model



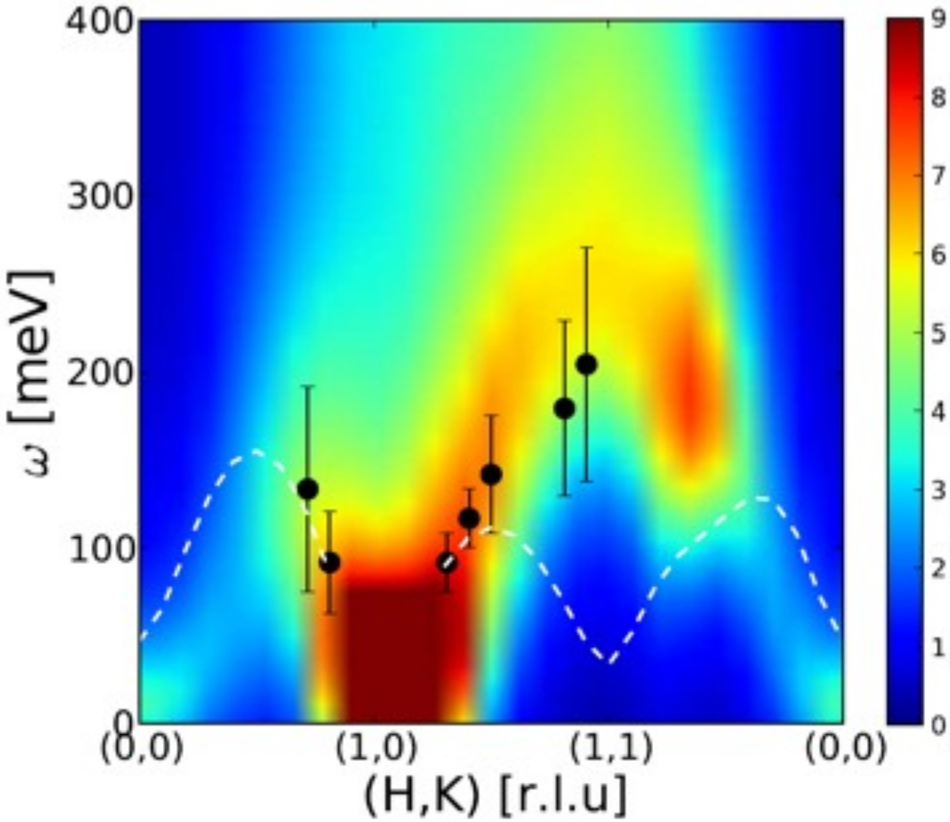


Very ar

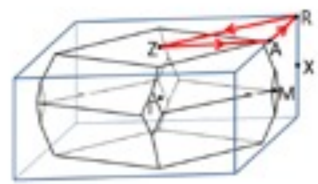
$SJ_{1a} \approx$

$SJ_{1b} \approx$

$SJ_2 \approx$



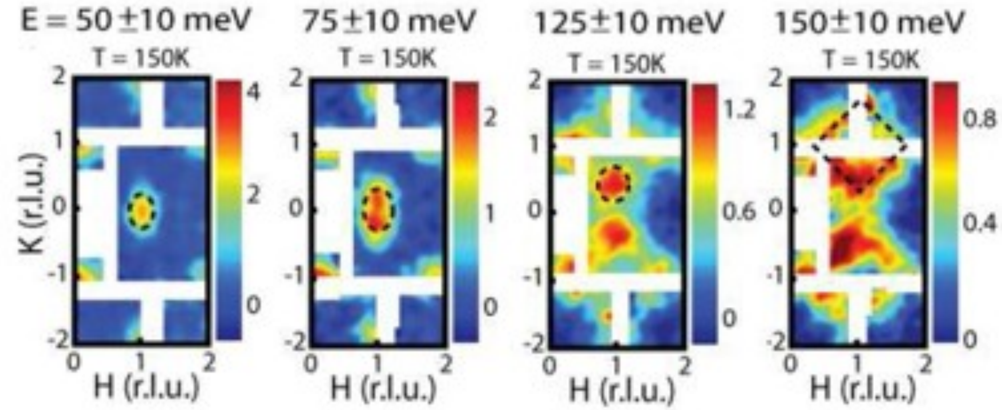
DMFT



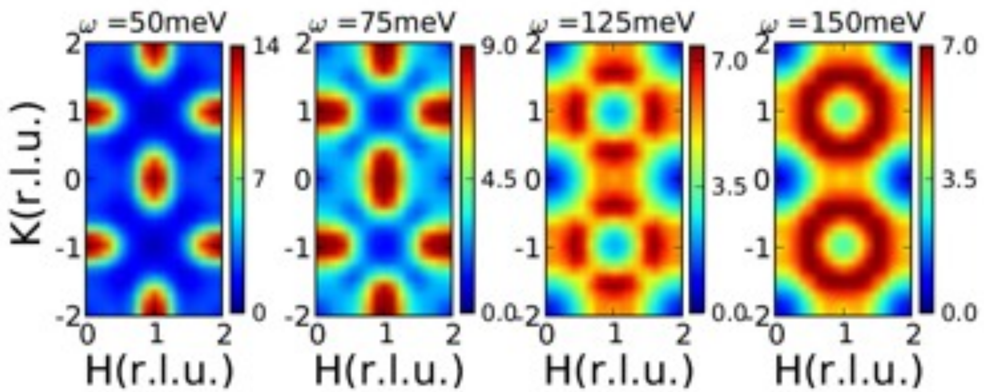
Leland W. Harriger, Pengcheng Dai et al., arXiv:1011.3771

No anysotropy needed (above T_S) to explain neutrons

Dynamical structure factor



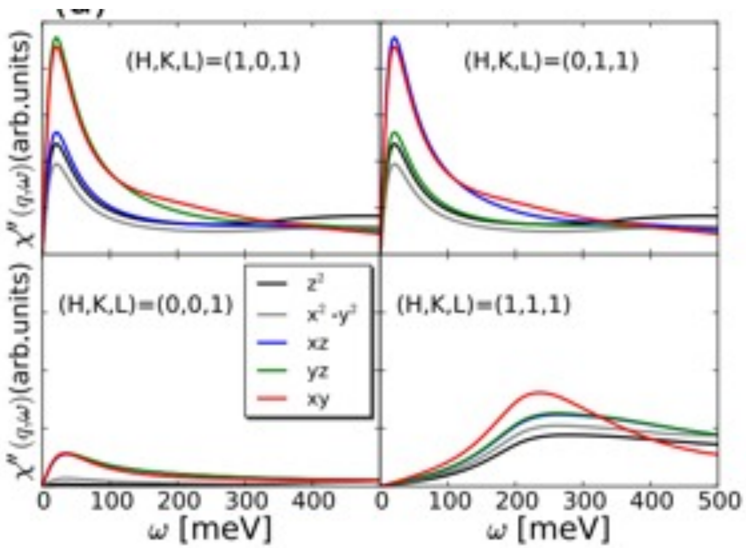
NEUTRONS EXP:
Leland W. Harriger,
Pengcheng Dai et al., arXiv:1011.3771

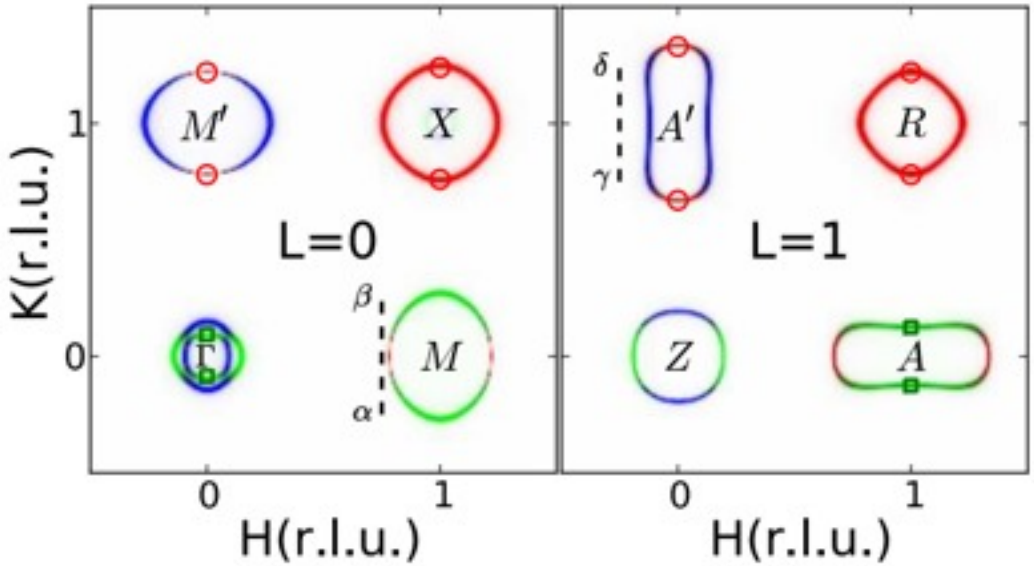


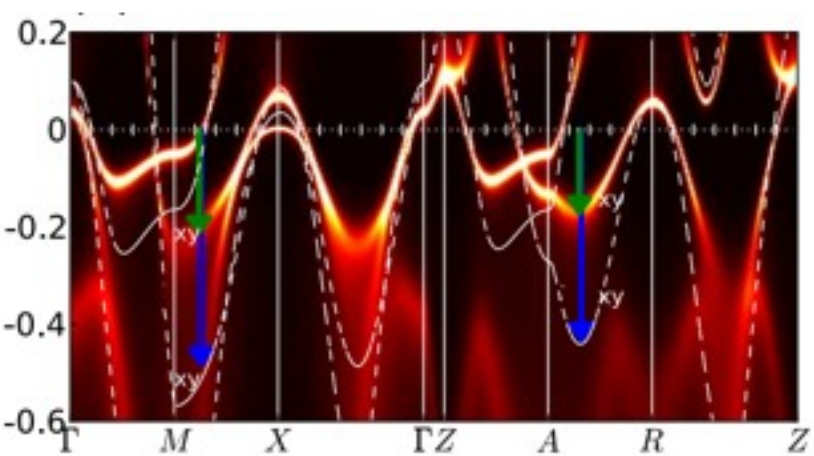
LDA+DMFT

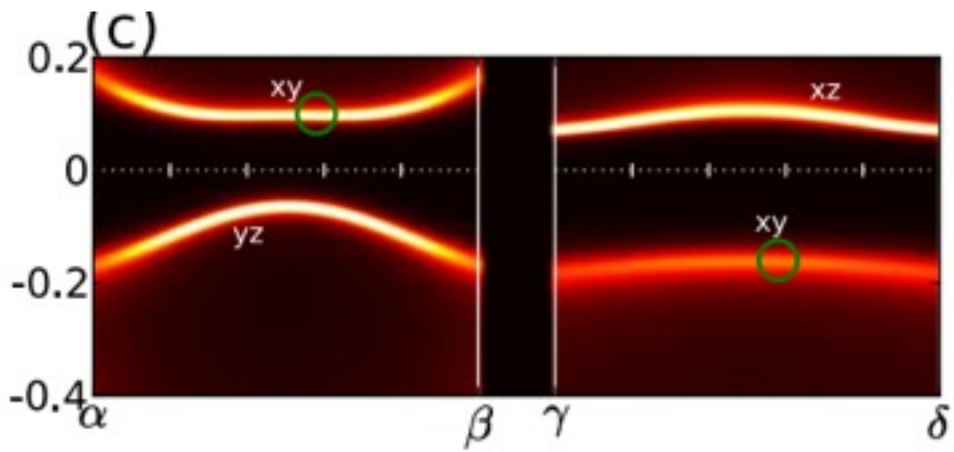
J. T. Park, D. S. Inosov, A. Yaresko, S. Graser, et al.,
Phys. Rev. B 82, 134503 (Oct 2010).

Origin of peaks



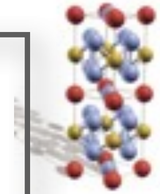






Large fluctuating moment

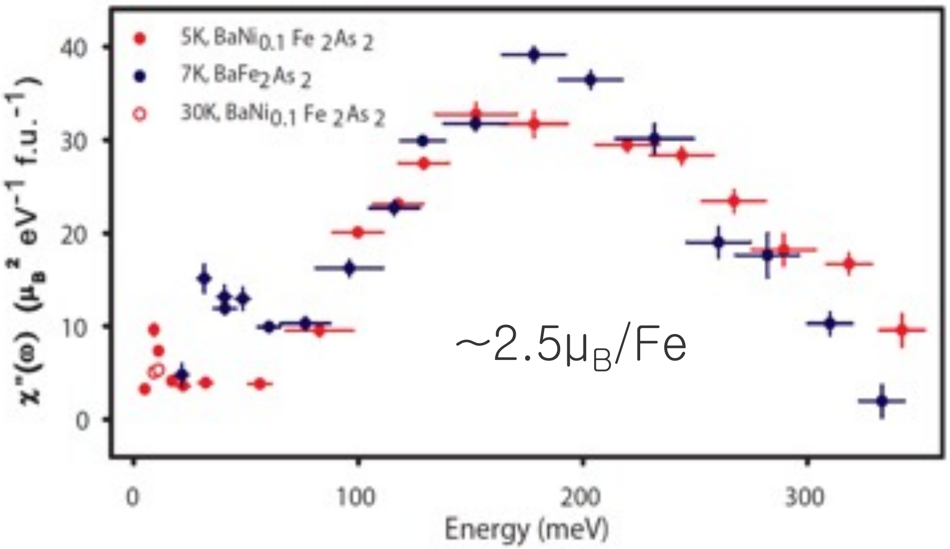
Fluctuating moment by neutrons: $\langle \mu^2 \rangle = \int \frac{d\omega}{\pi} n(\omega) \chi''(\omega)$



Large fluctuating moment

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

Experiment by Pengcheng Dai

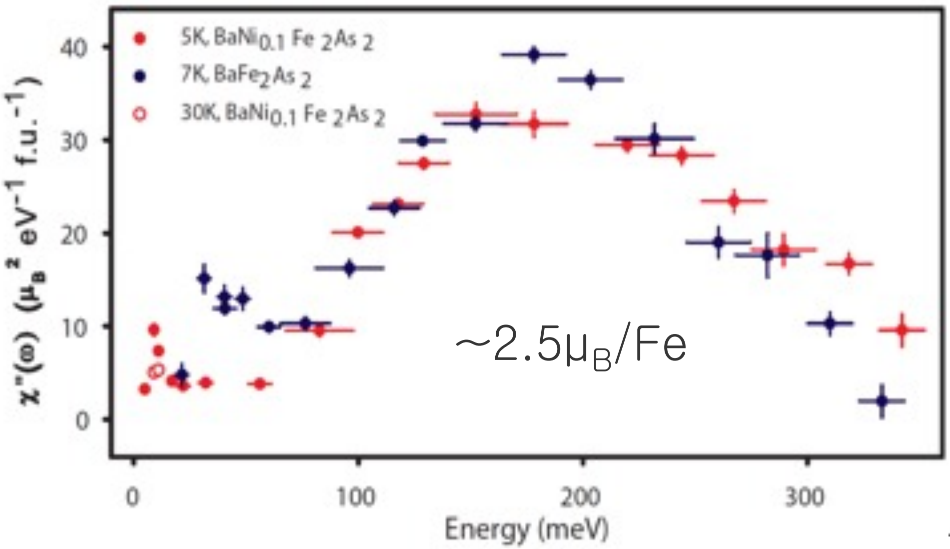


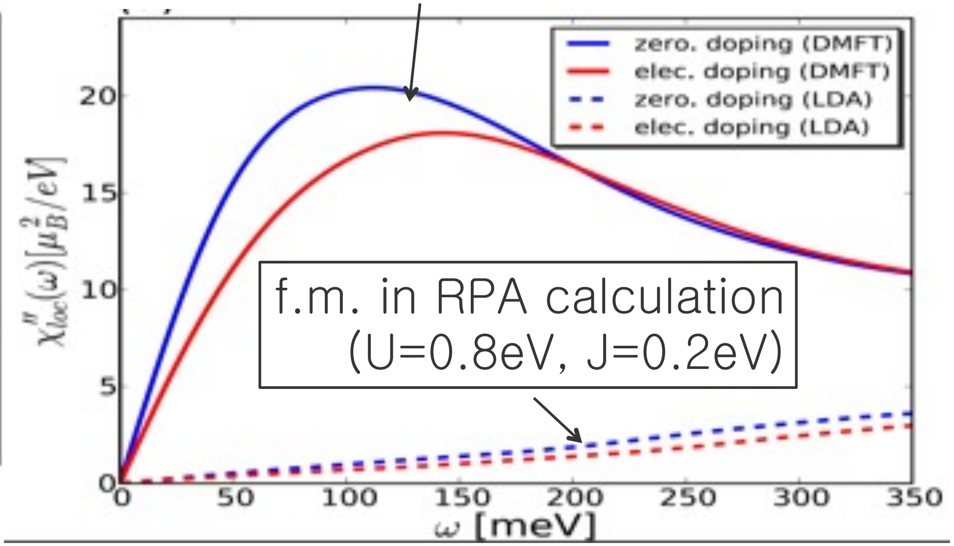
Large fluctuating moment

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

Experiment by Pengcheng Dai

f.m. in DMFT

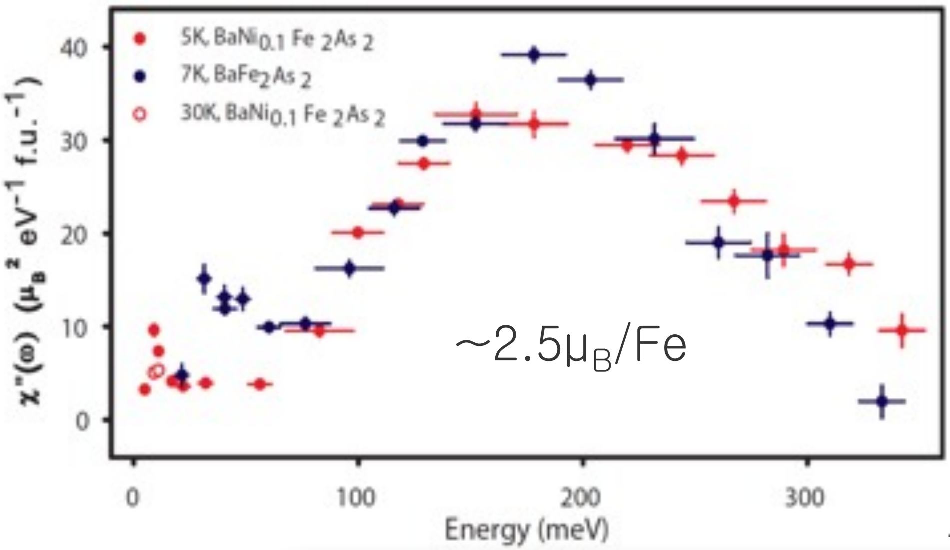


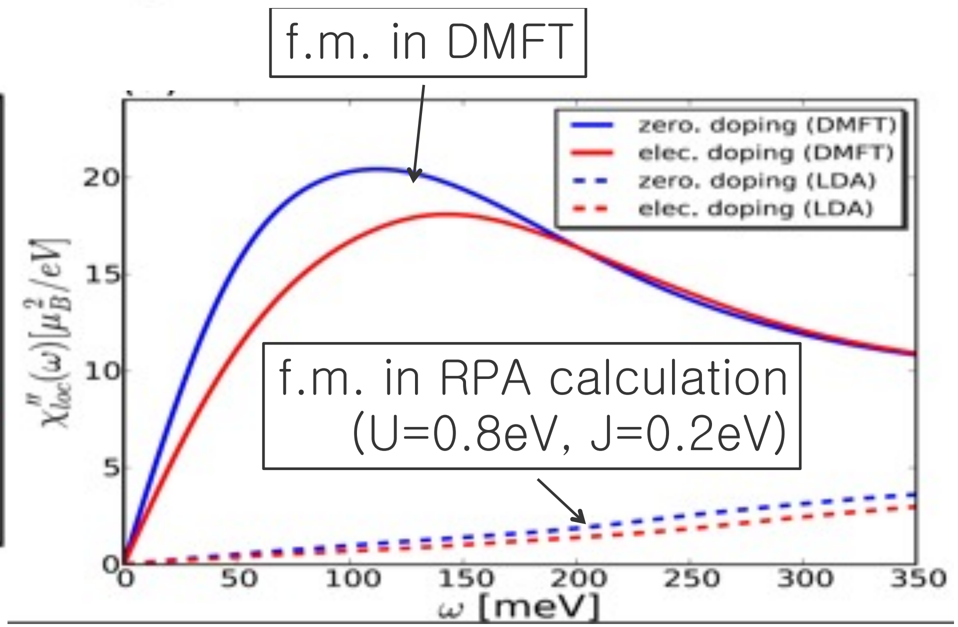


Large fluctuating moment

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

Experiment by Pengcheng Dai

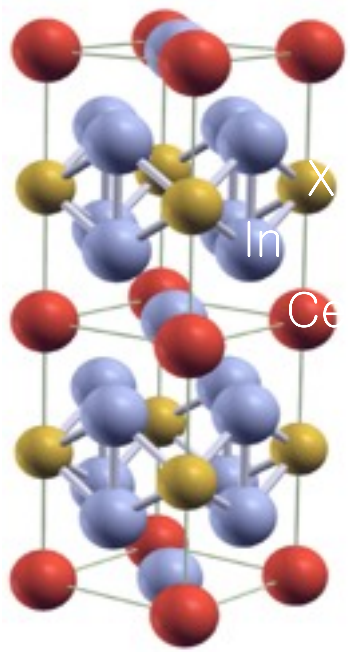


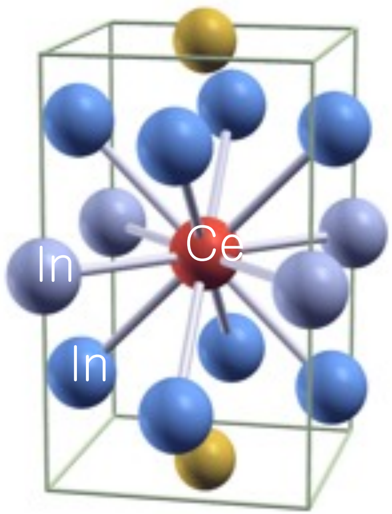


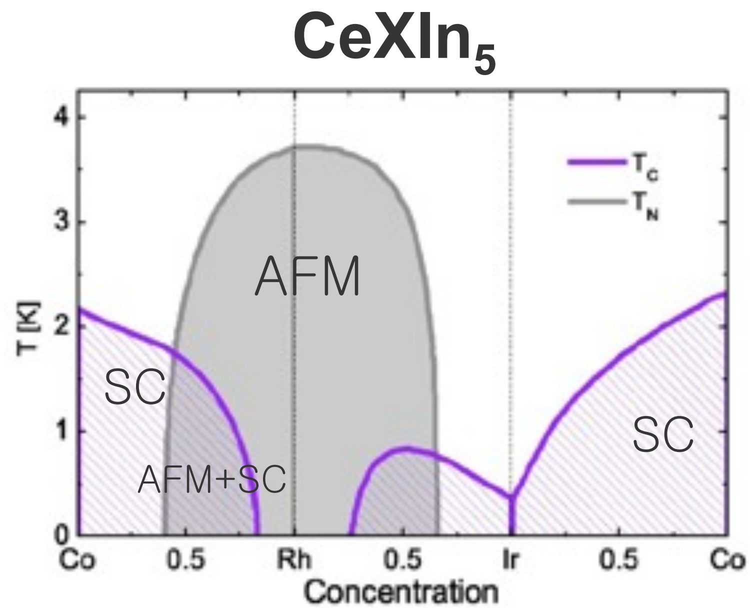
Large fluctuating moment can not be explained by a purely itinerant model.

The DMFT account for a dual nature of iron d electrons: itinerant and localized nature.

Heavy fermion materials (115)







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

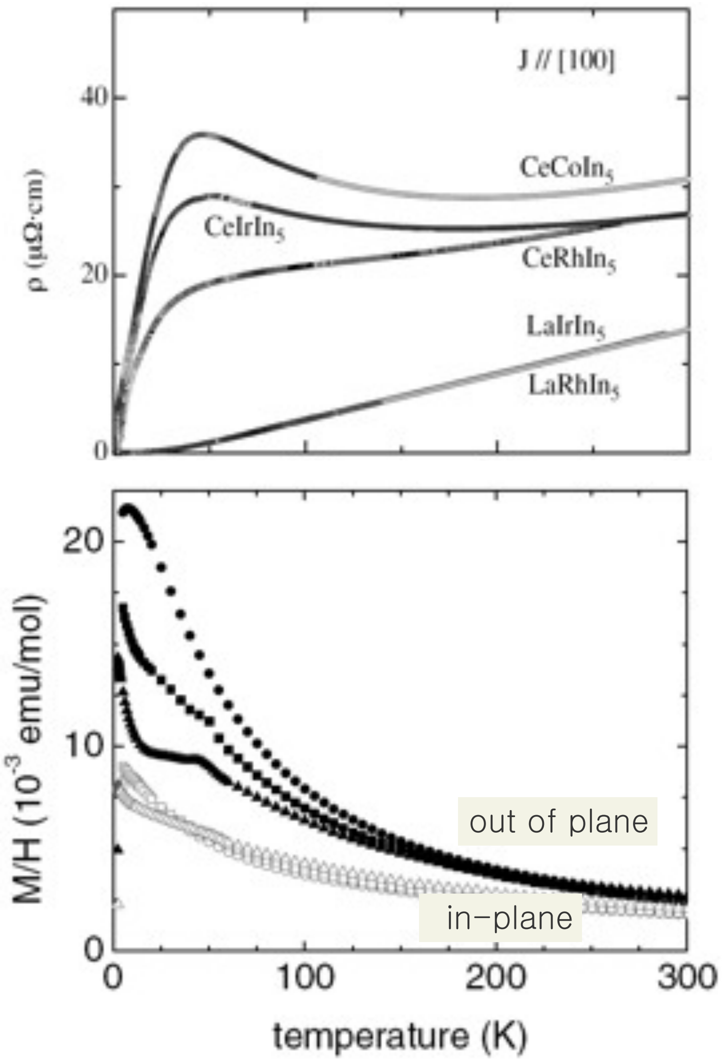
Ce atom in cage of 12 In atoms

Properties can be tuned (substitution, pressure, magnetic field) between

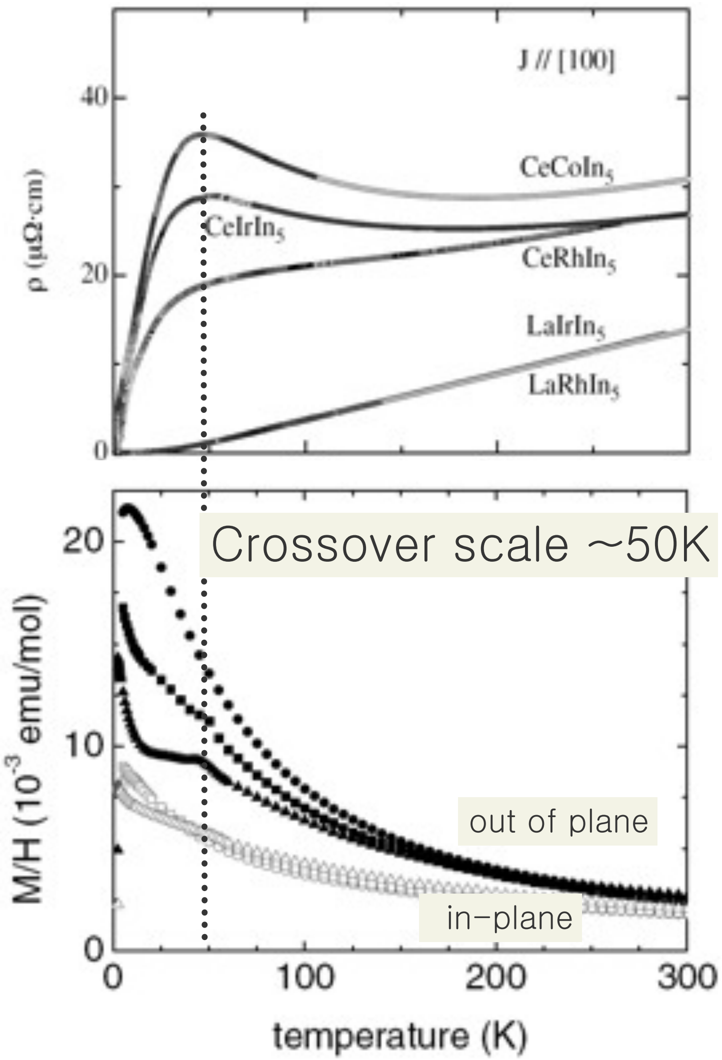
- antiferromagnetism
- superconductivity
- quantum critical point

	$CeCoIn_5$	$CeRhIn_5$	$CeIrIn_5$	$PuCoG_5$
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

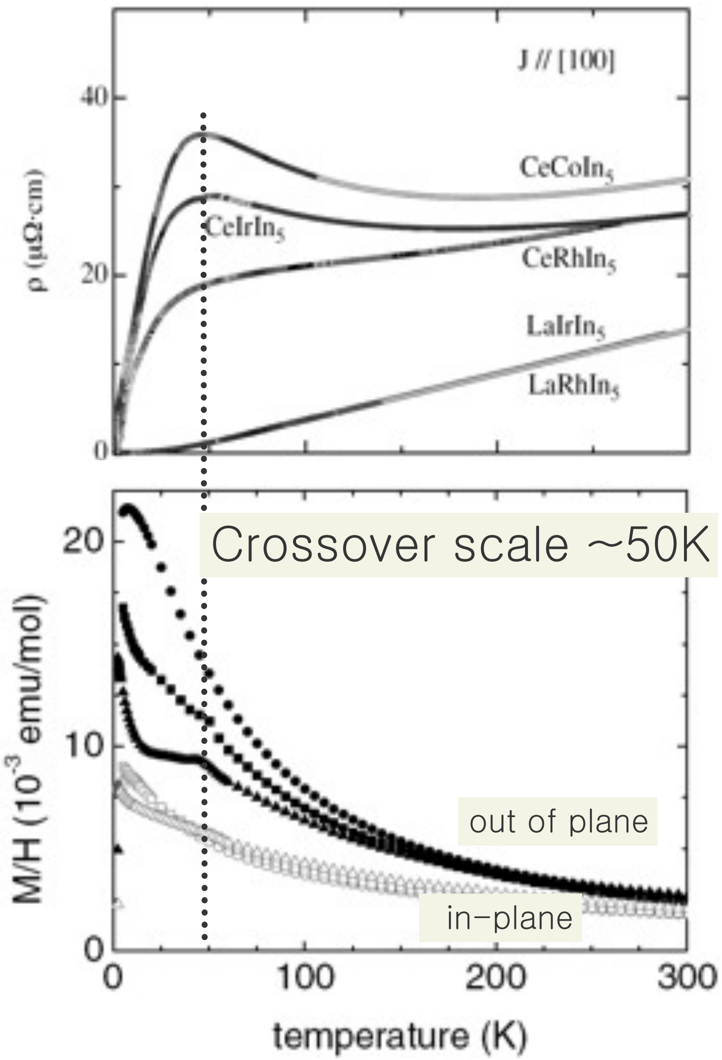
Coherence crossover in exp.

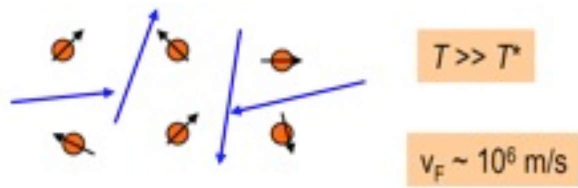


Coherence crossover in exp.



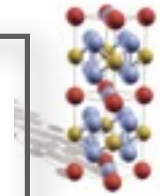
Coherence crossover in exp.

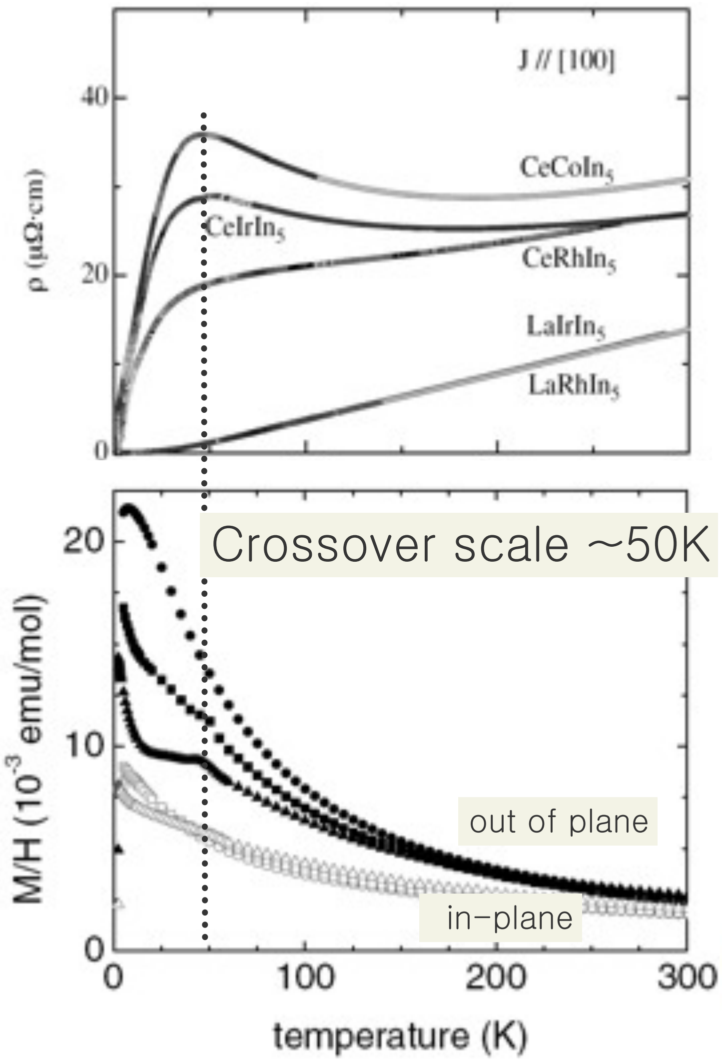


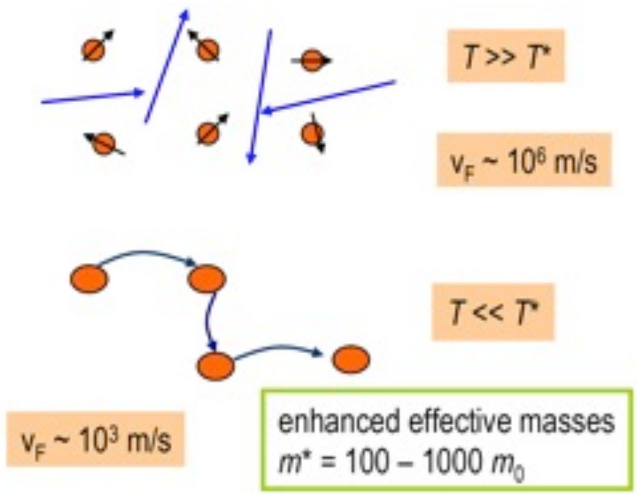


- High temperature Ce-4f local moments

Coherence crossover in exp.



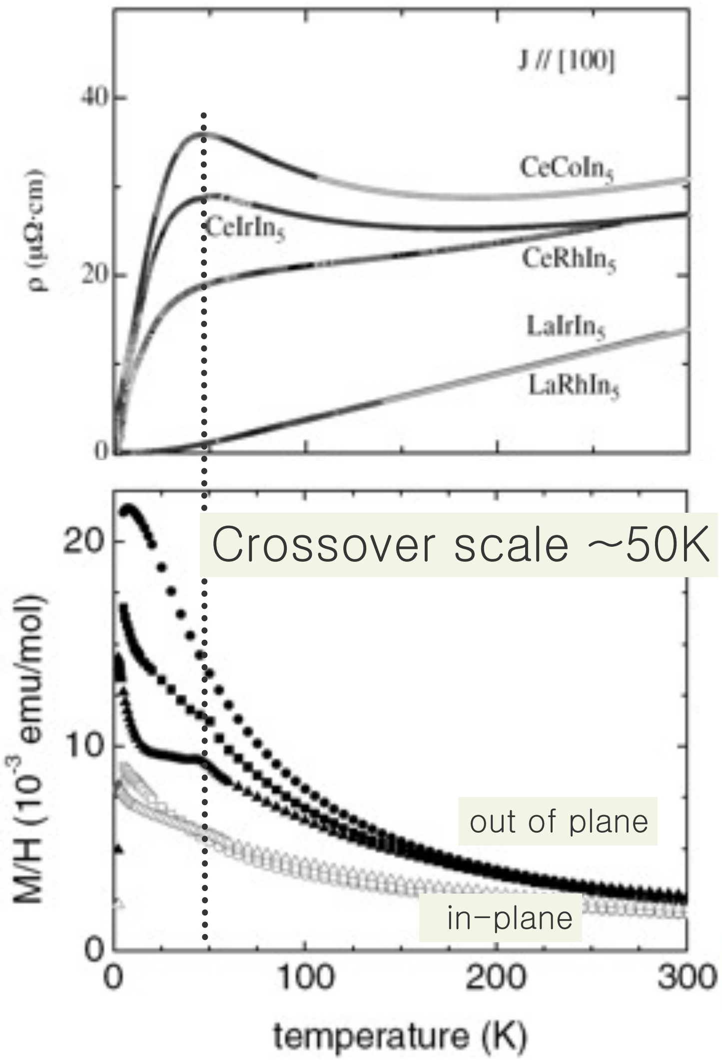


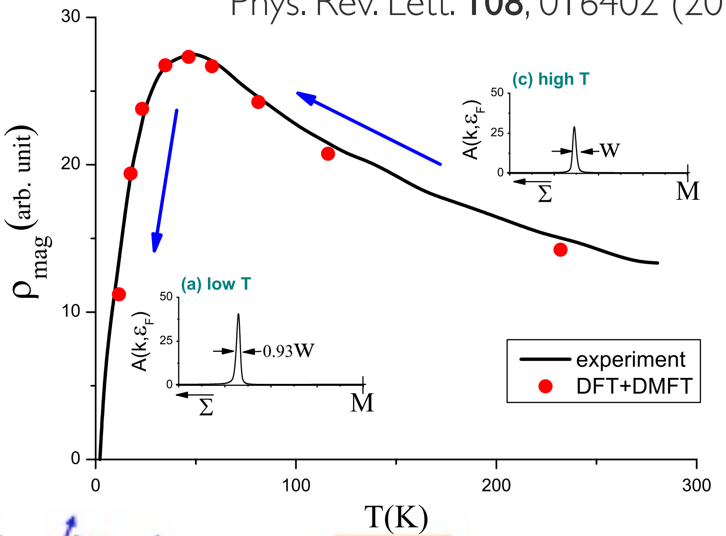


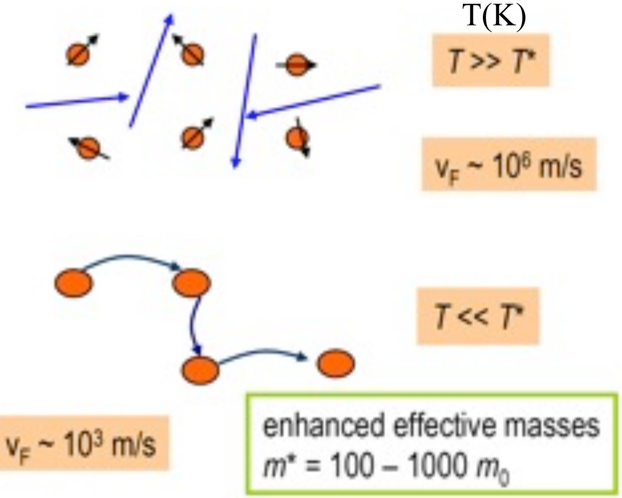
- High temperature Ce-4f local moments
- Low temperature – Itinerant heavy bands

Coherence crossover in exp.

H.C. Choi, B.I. Min, J.H. Shim, K. Haule, G. Kotliar, Phys. Rev. Lett. **108**, 016402 (2012).







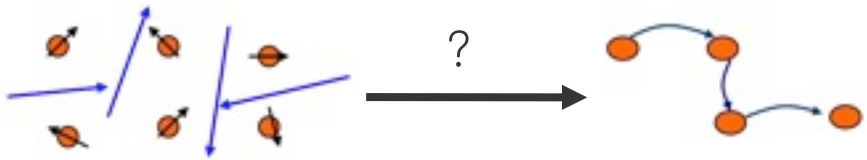
- High temperature Ce−4f local moments

- Low temperature – Itinerant heavy bands

Issues for the specific system

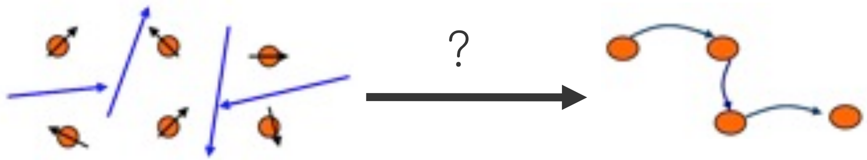
Issues for the specific system

- How does the crossover from localized moments to itinerant q.p. happen?

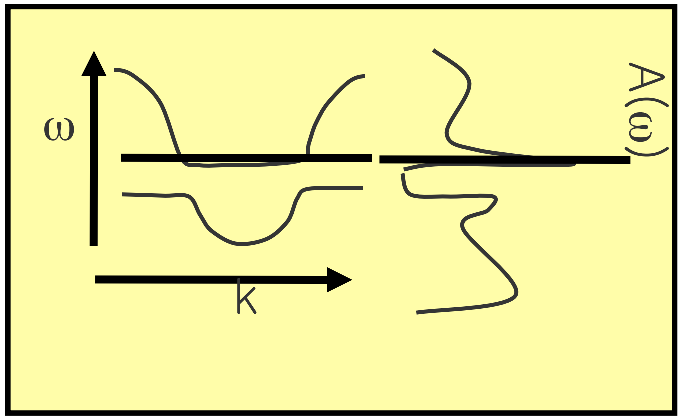


Issues for the specific system

- How does the crossover from localized moments to itinerant q.p. happen?

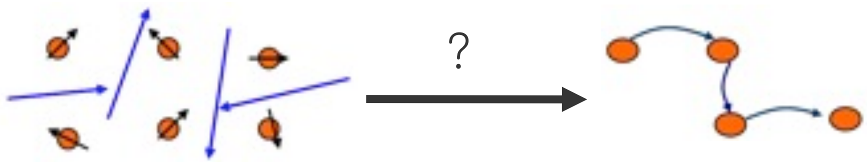


- How does the spectral weight redistribute?



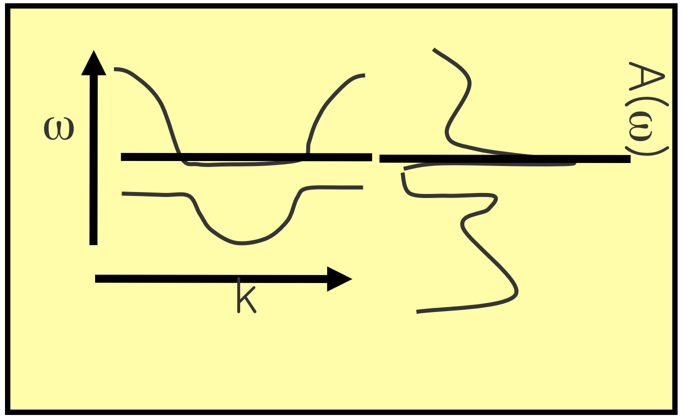
Issues for the specific system

- How does the crossover from localized moments to itinerant q.p. happen?

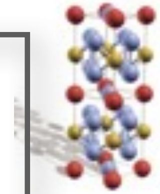


- How does the spectral weight redistribute?

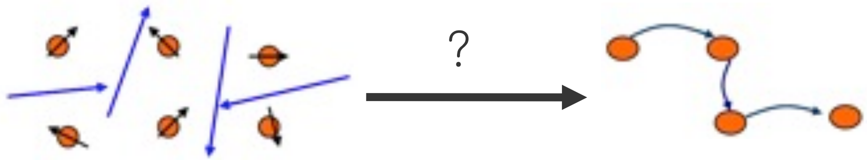
- Where in momentum space q.p. appear?



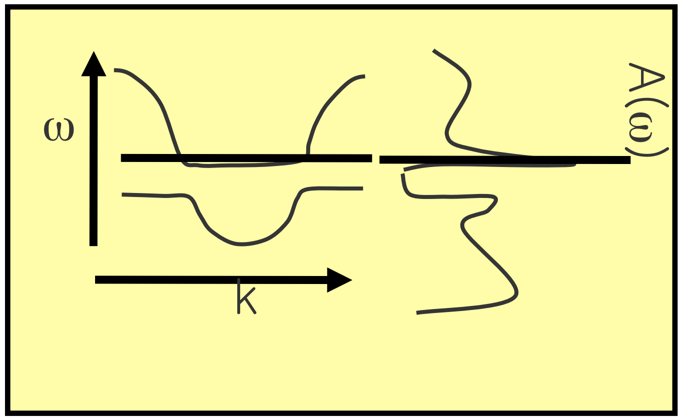
Issues for the specific system



- How does the crossover from localized moments to itinerant q.p. happen?



- How does the spectral weight redistribute?

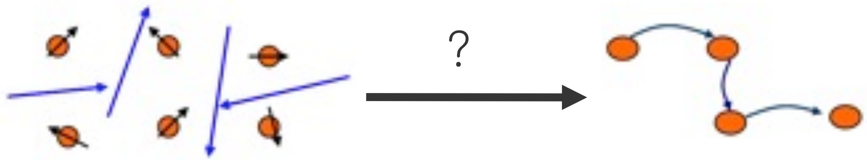


- Where in momentum space q.p. appear?

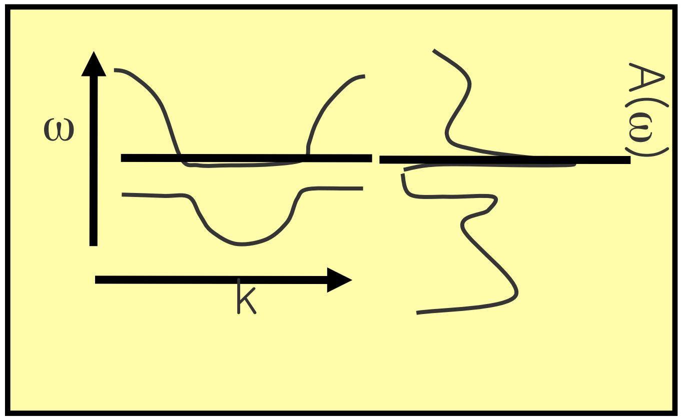
- What is the momentum dispersion of q.p.?

Issues for the specific system

- How does the crossover from localized moments to itinerant q.p. happen?



- How does the spectral weight redistribute?

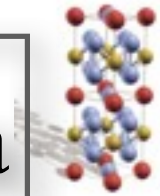


- Where in momentum space q.p. appear?

- What is the momentum dispersion of q.p.?

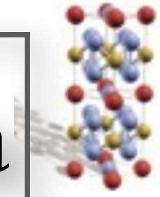
- How does the hybridization gap look like in momentum space?

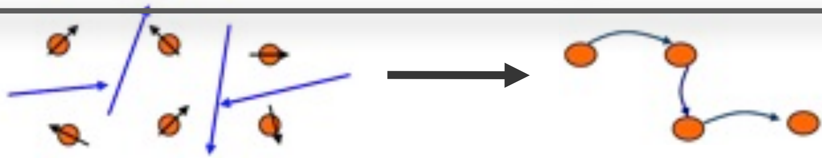
Temperature dep. of the local Ce-4f spectra

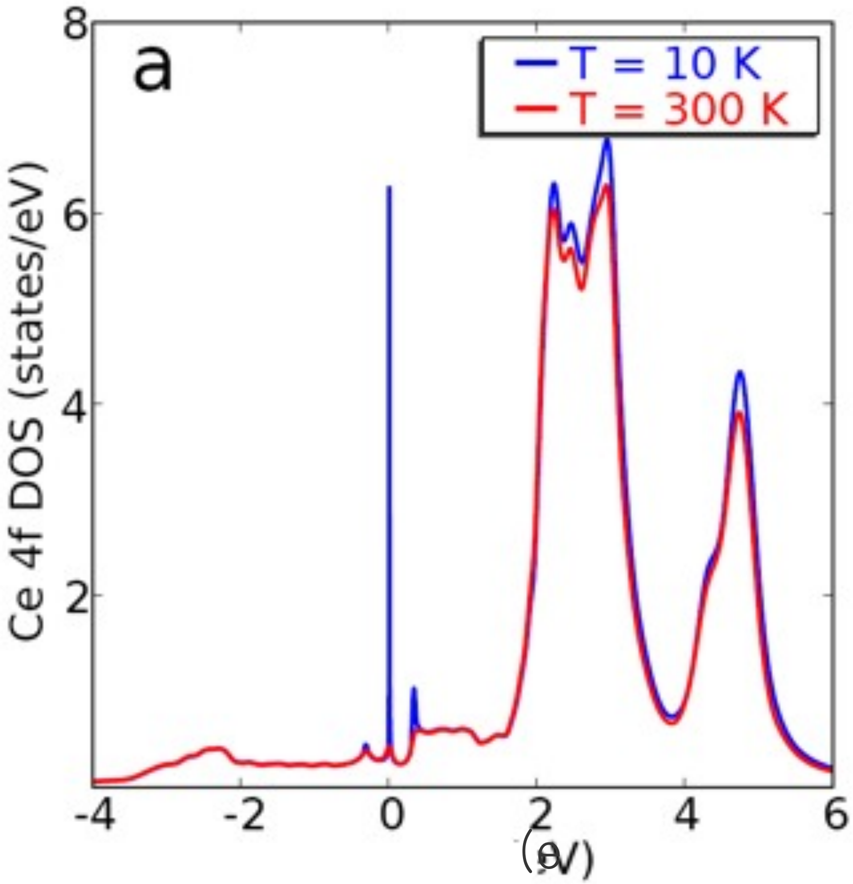


J. H. Shim, KH, and G. Kotliar
Science 318, 1615 (2007)

Temperature dep. of the local Ce-4f spectra

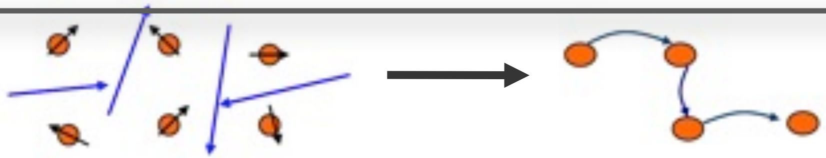


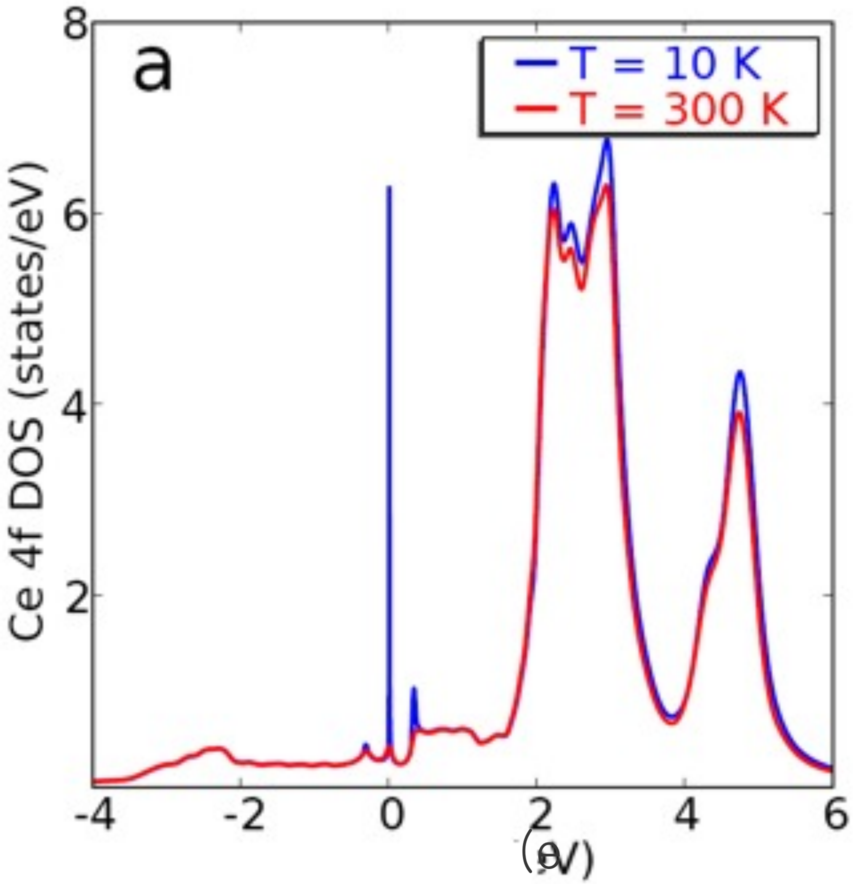




J. H. Shim, KH, and G. Kotliar
Science 318, 1615 (2007)

Temperature dep. of the local Ce-4f spectra

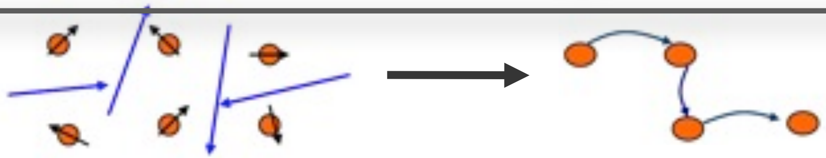


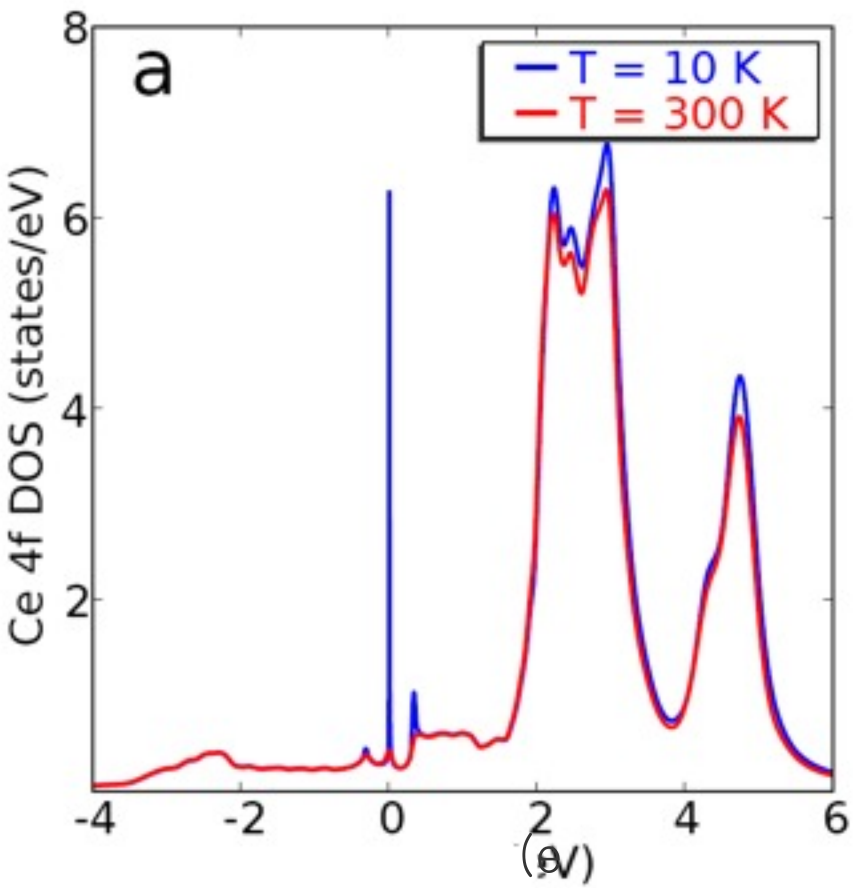


•At 300K, only Hubbard bands

J. H. Shim, KH, and G. Kotliar
Science 318, 1615 (2007)

Temperature dep. of the local Ce-4f spectra



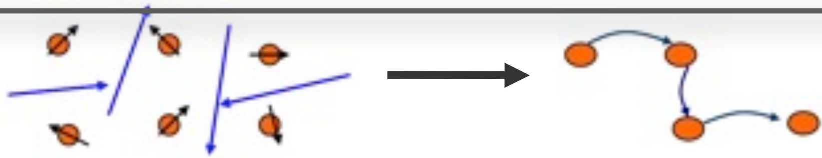


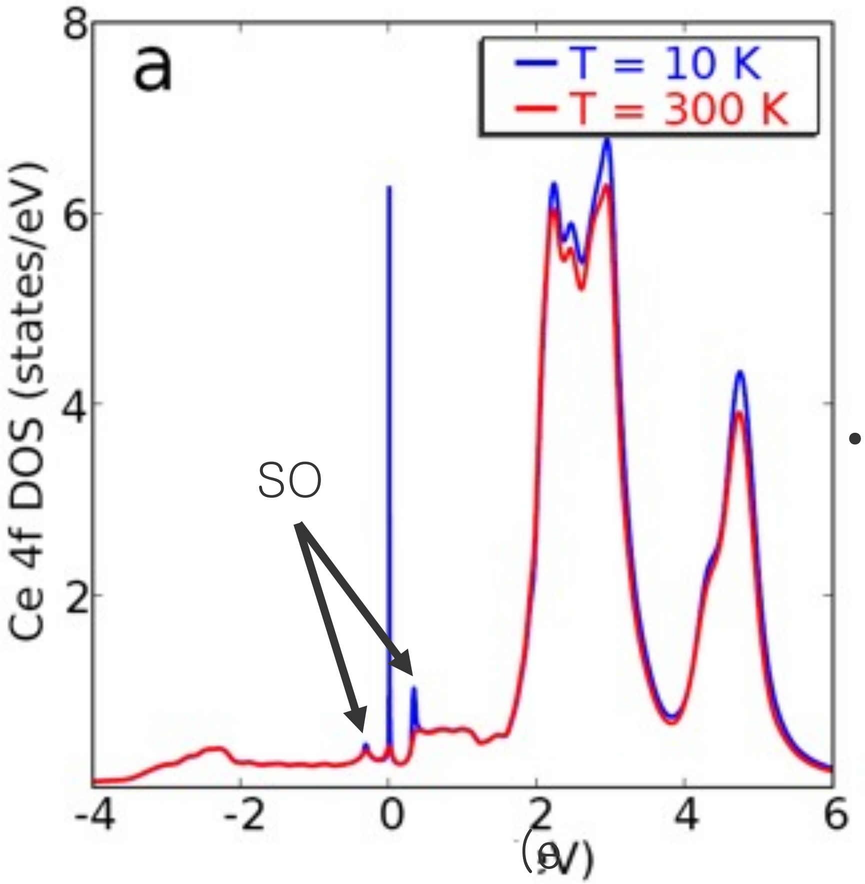
- At 300K, only Hubbard bands

- At low T, very narrow q.p. peak (width ~3meV)

J. H. Shim, KH, and G. Kotliar
Science 318, 1615 (2007)

Temperature dep. of the local Ce-4f spectra

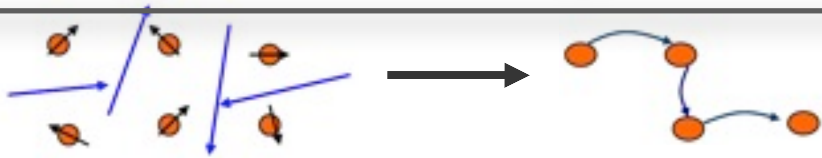


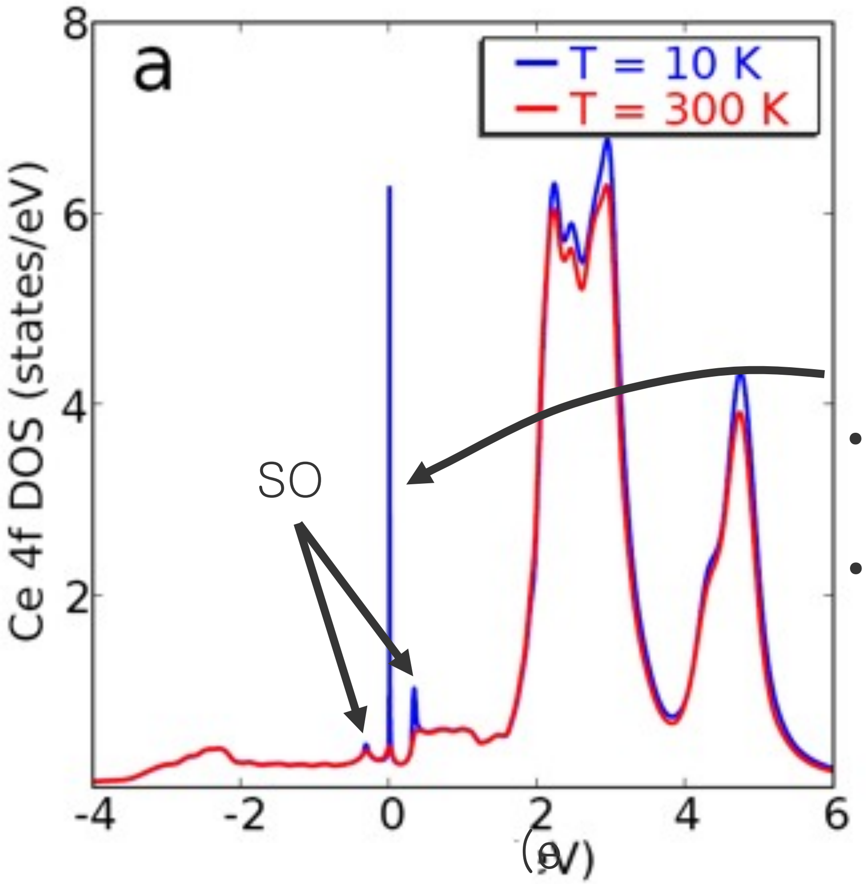


- At 300K, only Hubbard bands
- At low T, very narrow q.p. peak (width ~3meV)
- SO coupling splits q.p.: +-0.28eV

J. H. Shim, KH, and G. Kotliar
Science 318, 1615 (2007)

Temperature dep. of the local Ce-4f spectra





•At 300K, only Hubbard bands

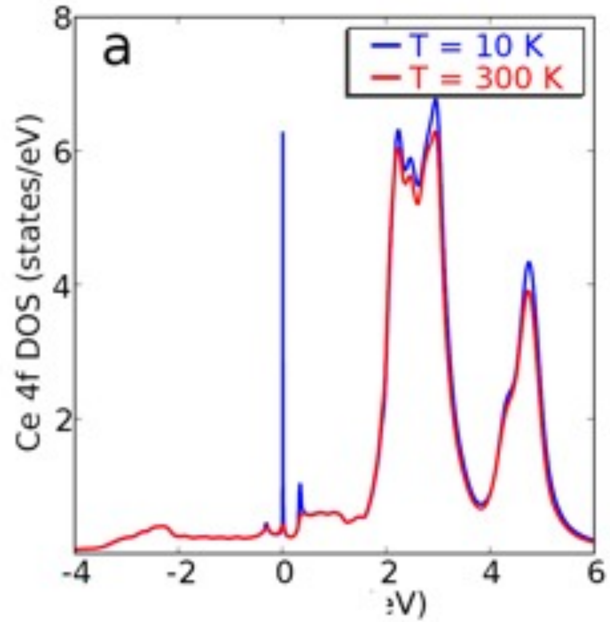
•At low T, very narrow q.p. peak (width ~3meV)

• SO coupling splits q.p.: +−0.28eV

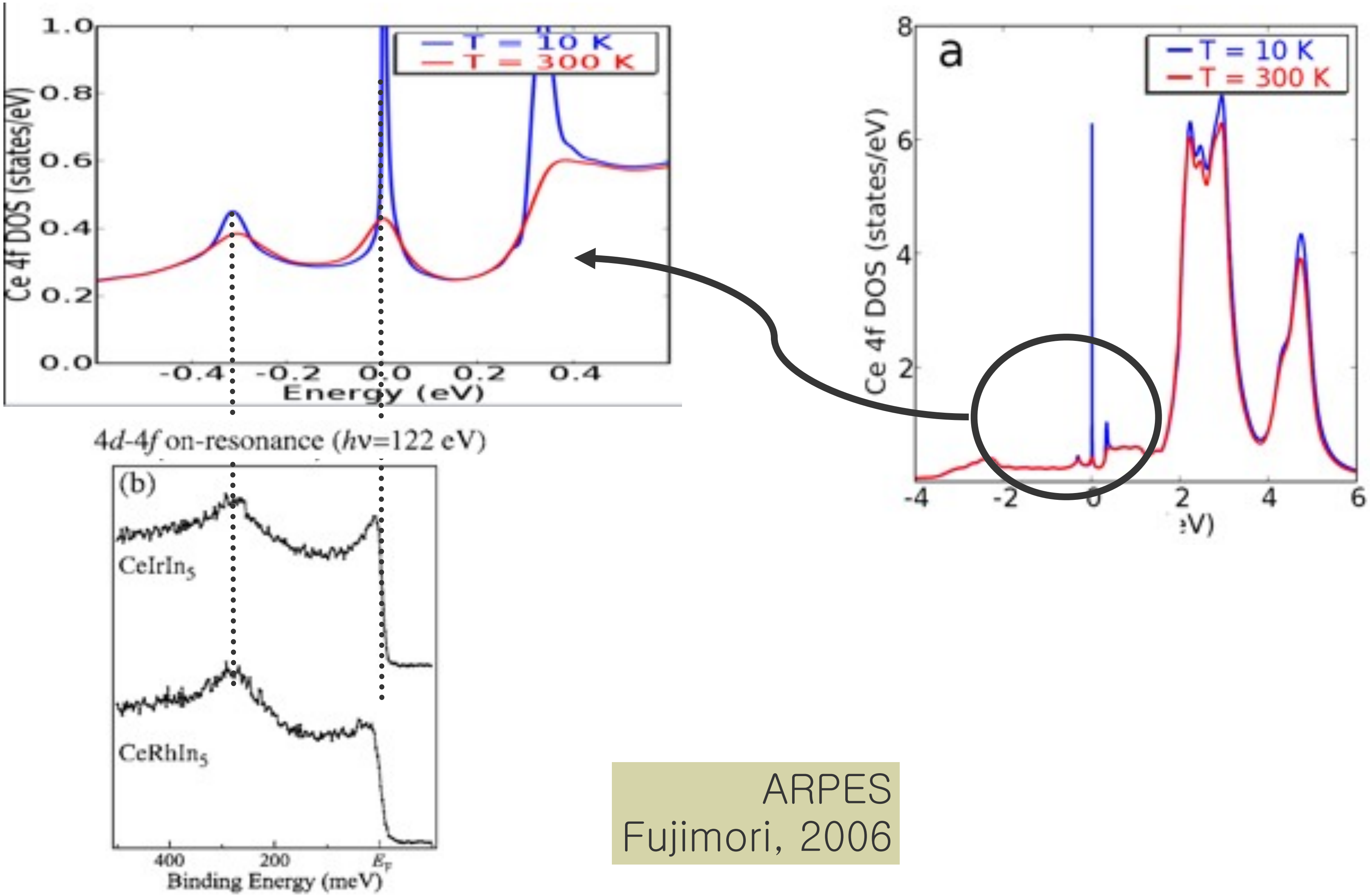
•Redistribution of weight up to very high frequency

J. H. Shim, KH, and G. Kotliar
Science 318, 1615 (2007)

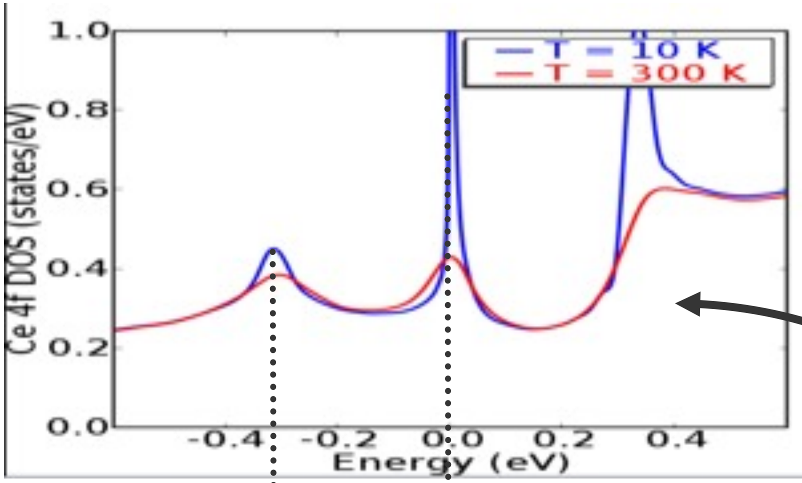
Angle integrated photoemission vs DMFT

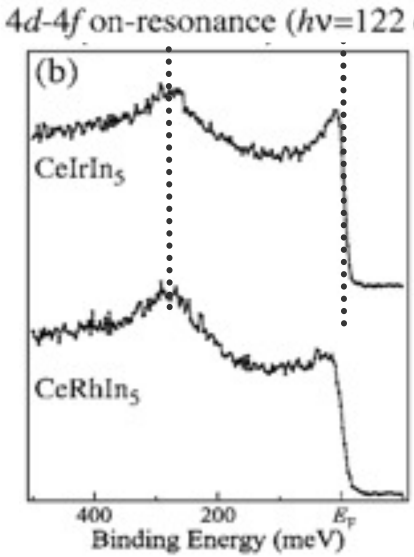


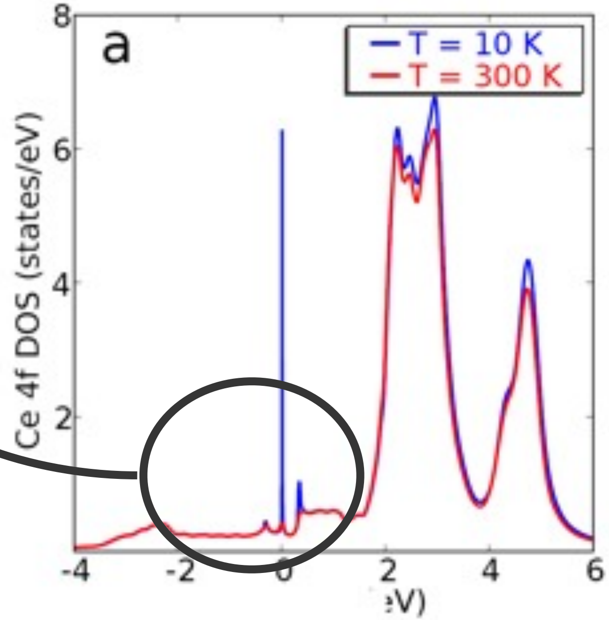
Angle integrated photoemission vs DMFT



Angle integrated photoemission vs DMFT



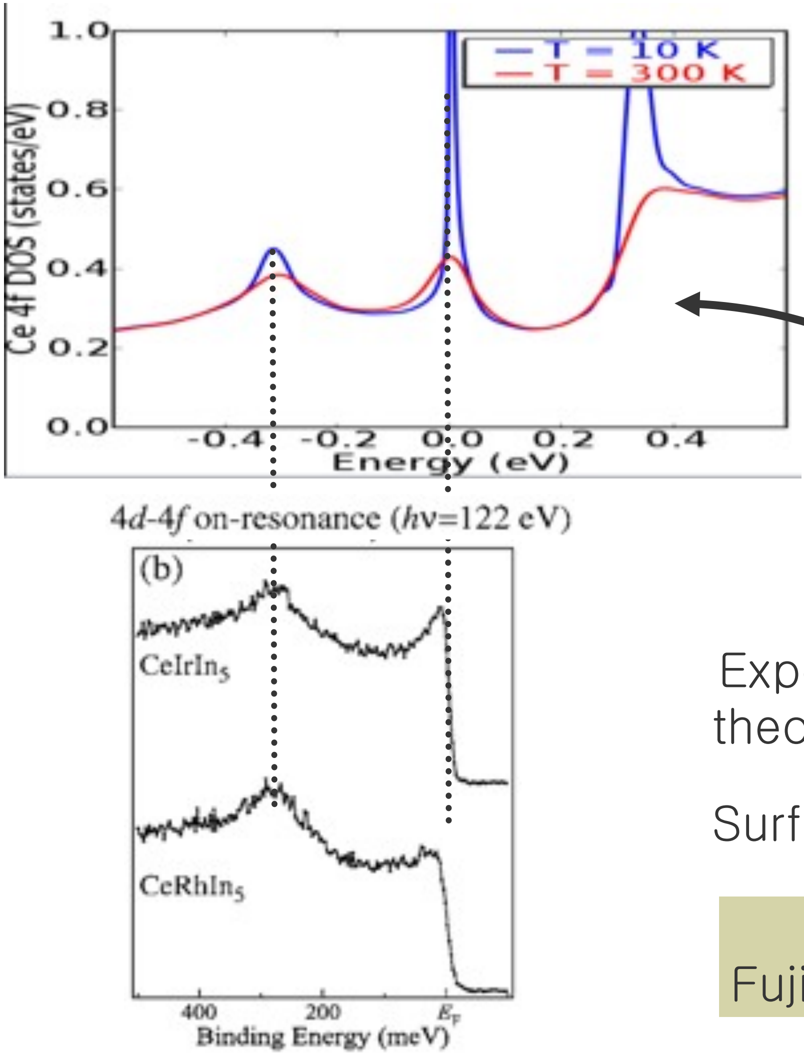


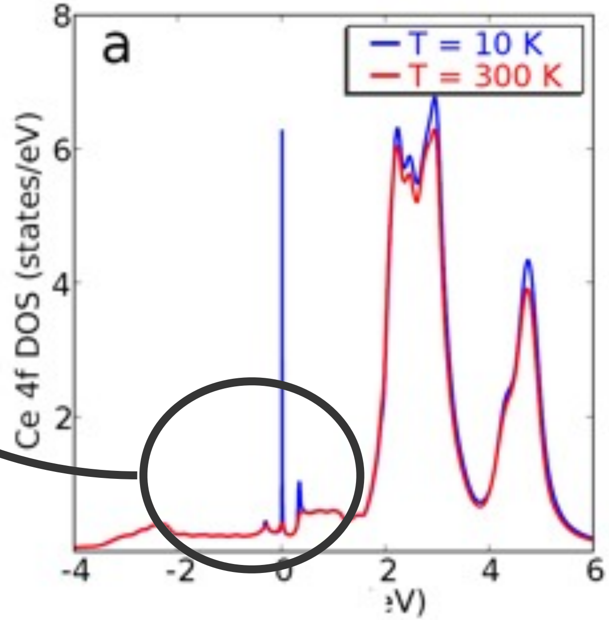


Experimental resolution ~30meV,
theory predicts 3meV broad band

ARPES
Fujimori, 2006

Angle integrated photoemission vs DMFT



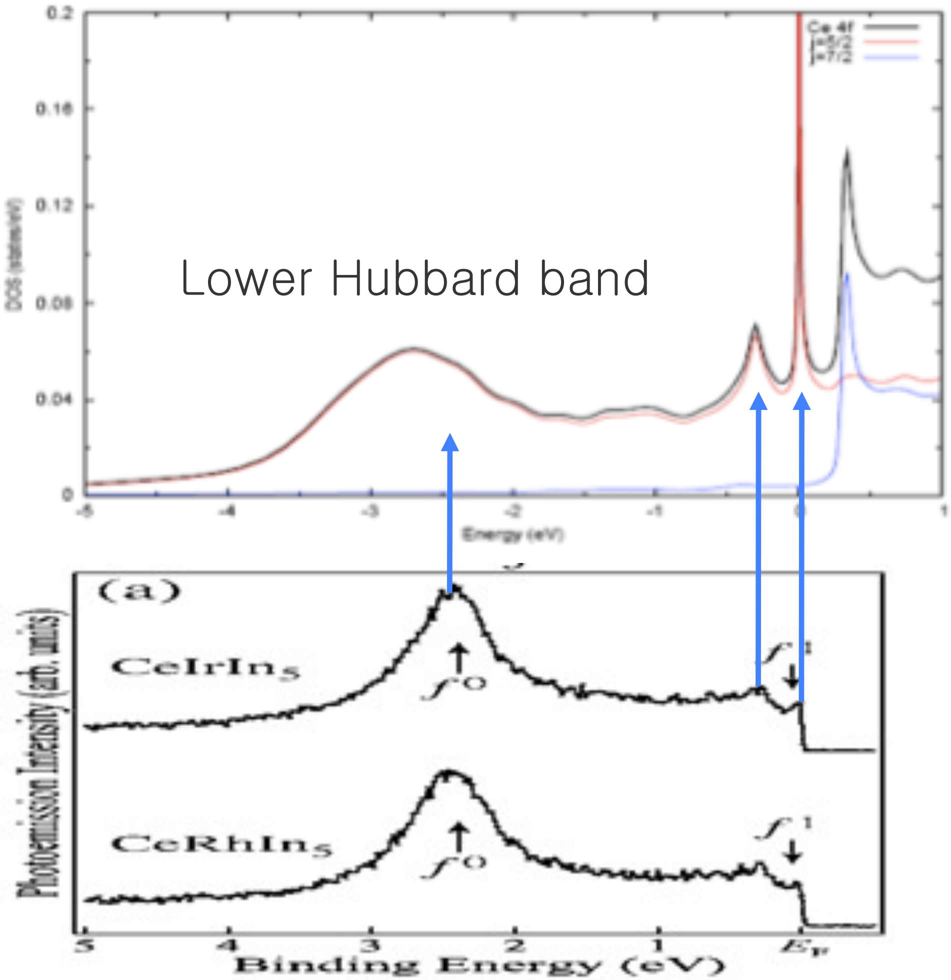


Experimental resolution ~30meV, theory predicts 3meV broad band

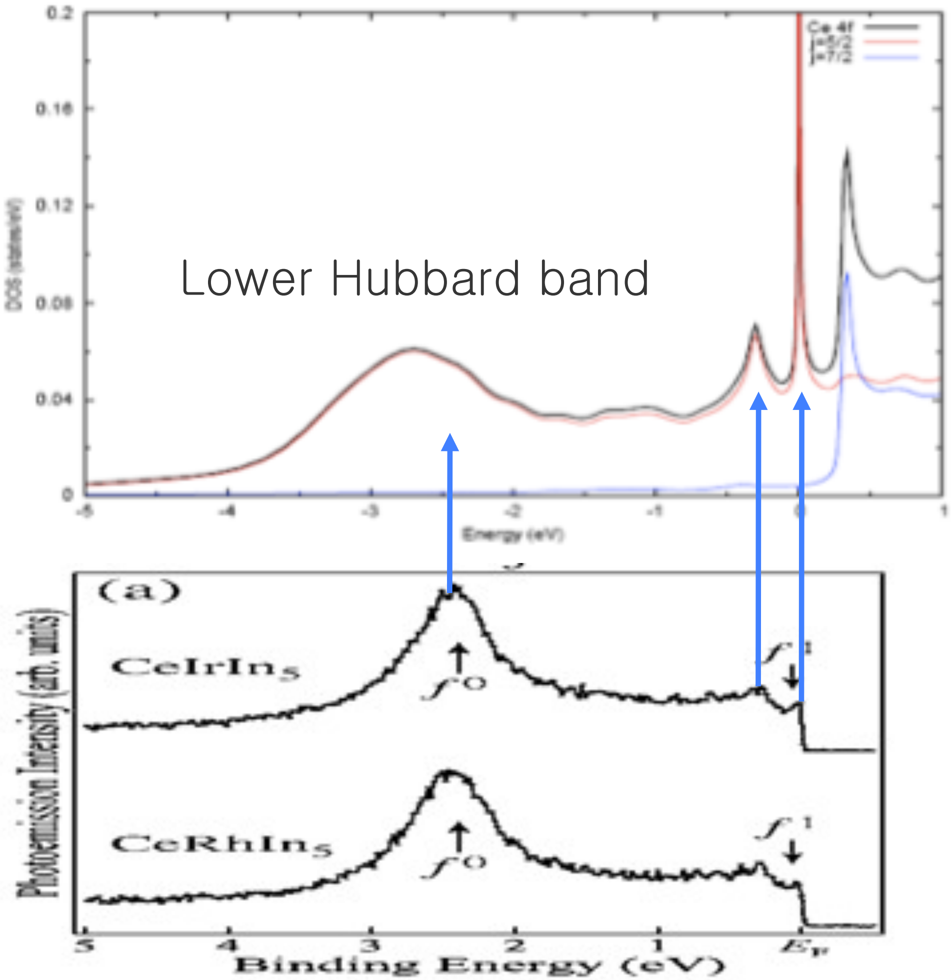
Surface sensitive at 122eV

ARPES
Fujimori, 2006

Angle integrated photoemission vs DMFT

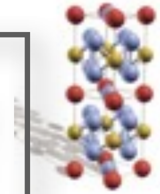


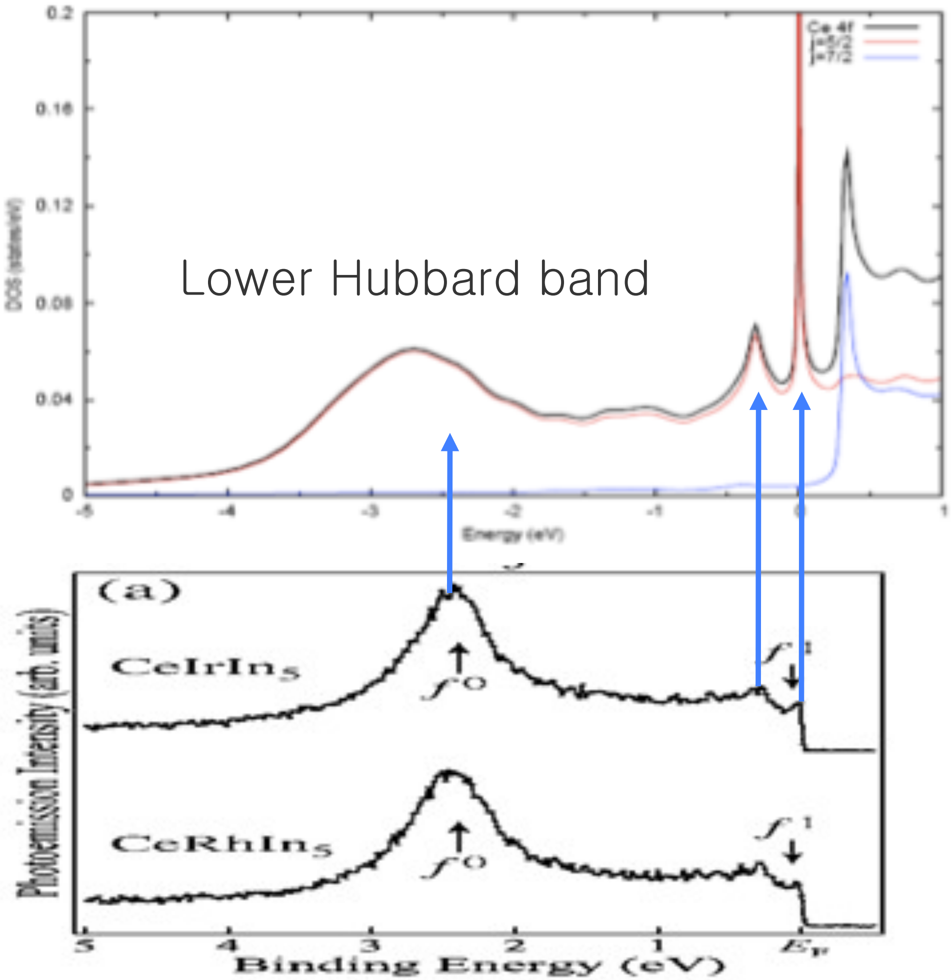
Angle integrated photoemission vs DMFT



ARPES
Fujimori, 2006

Angle integrated photoemission vs DMFT





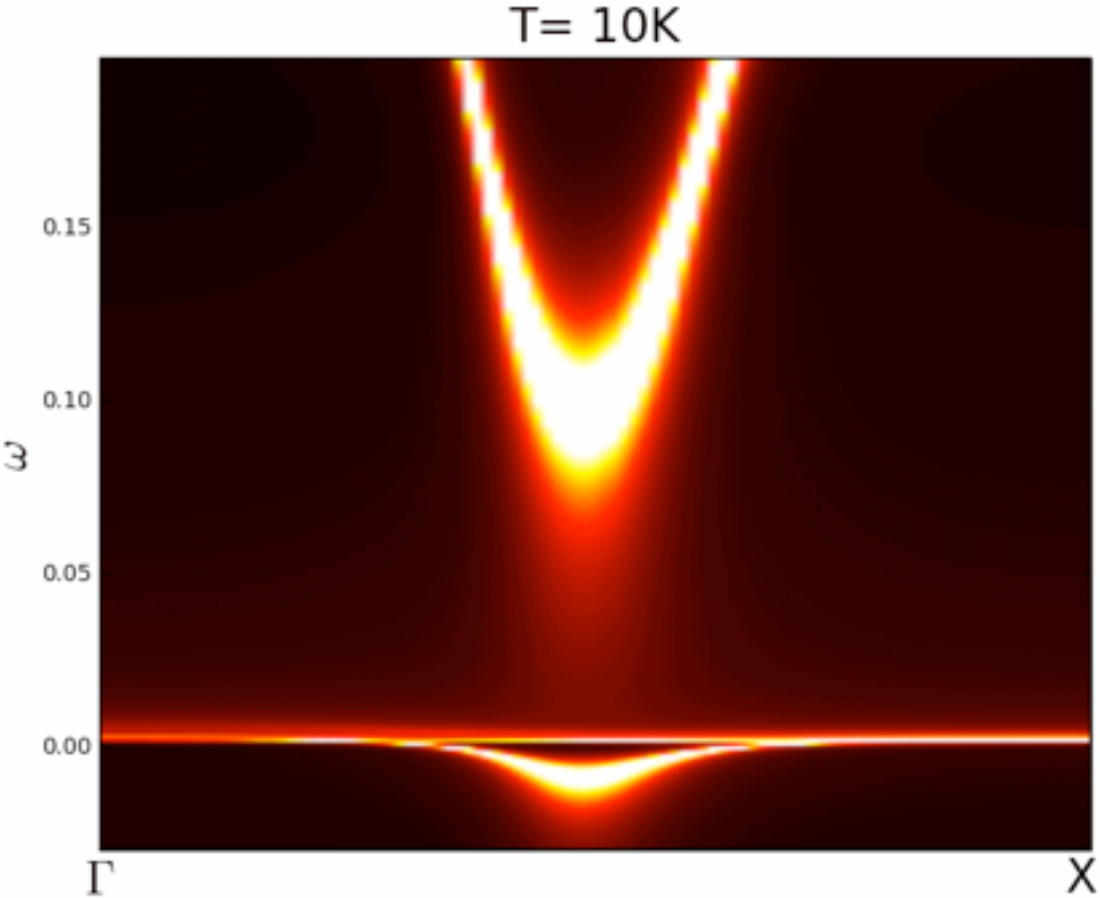
Nice agreement for the
• Hubbard band position
•SO split qp peak

Hard to see narrow resonance in ARPES since very little weight of q.p. is below Ef

ARPES
Fujimori, 2006

T-dep momentum resolved photoemission

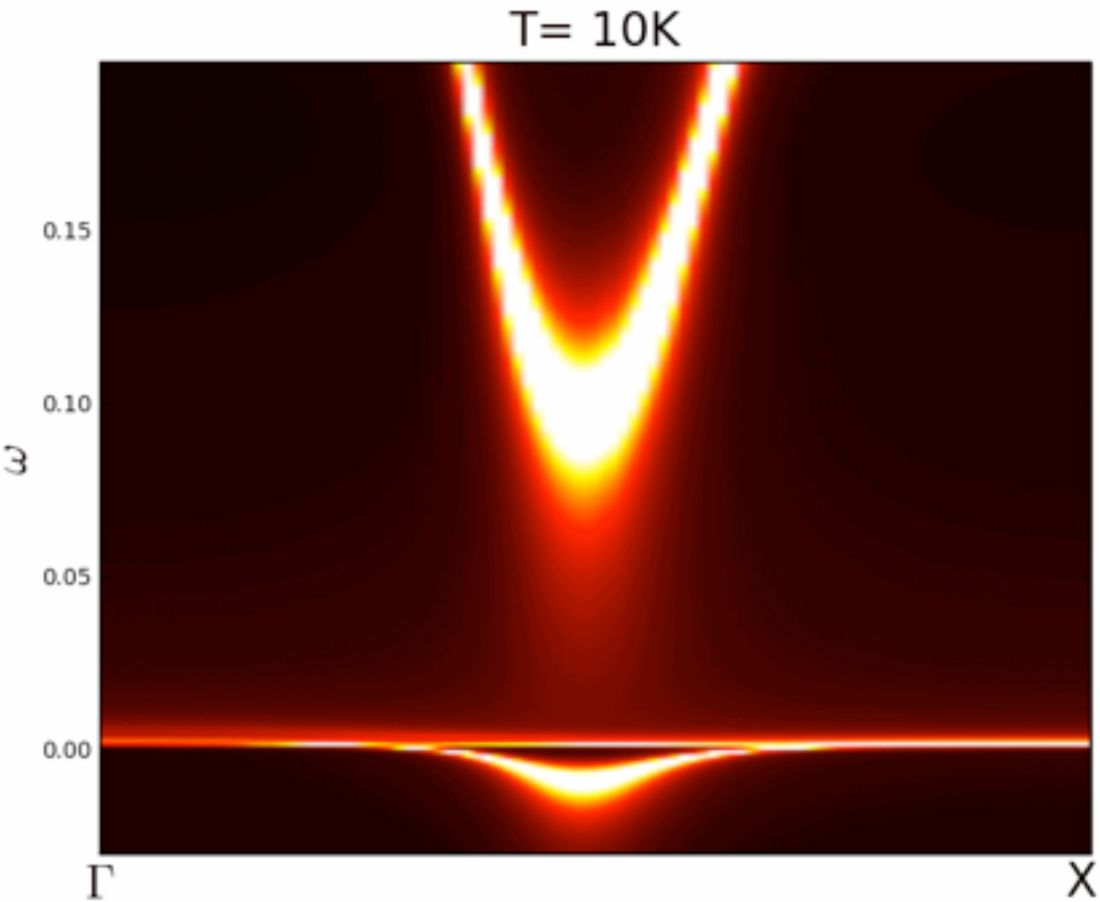
spectral function: $A(k,\omega)$



T-dep momentum resolved photoemission

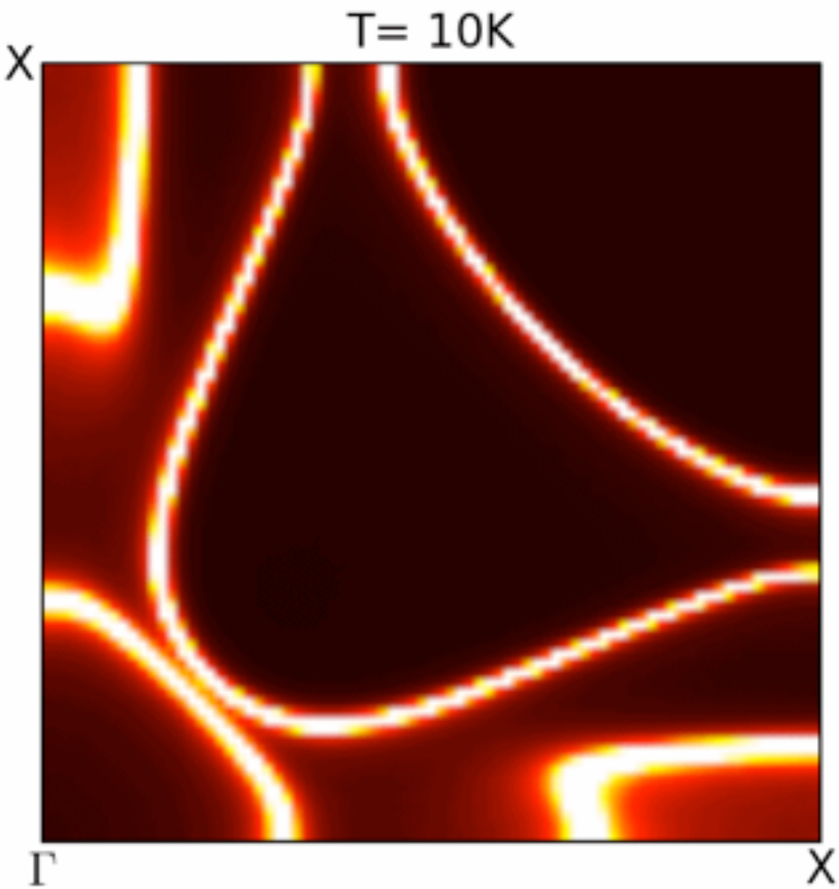
spectral function: $A(k,\omega)$

H.C. Choi, B.I. Min, J.H. Shim, K. Haule, G. Kotliar, Phys. Rev. Lett. **108**, 016402 (2012).

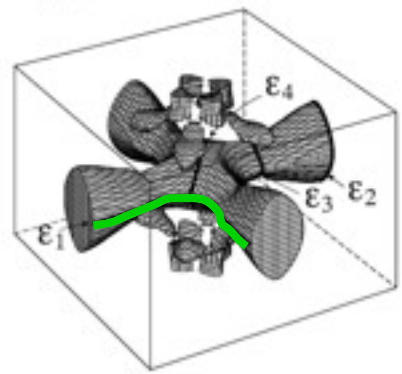


T-dep Fermi surface-topological change

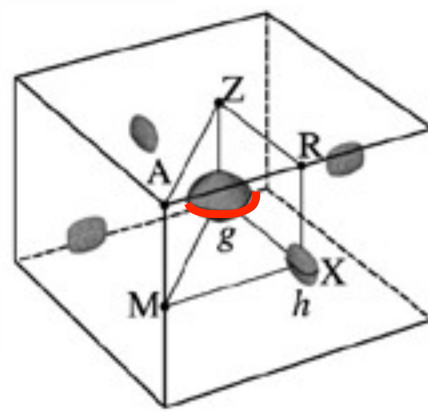
Fermi surface in the Γ plane



high –T

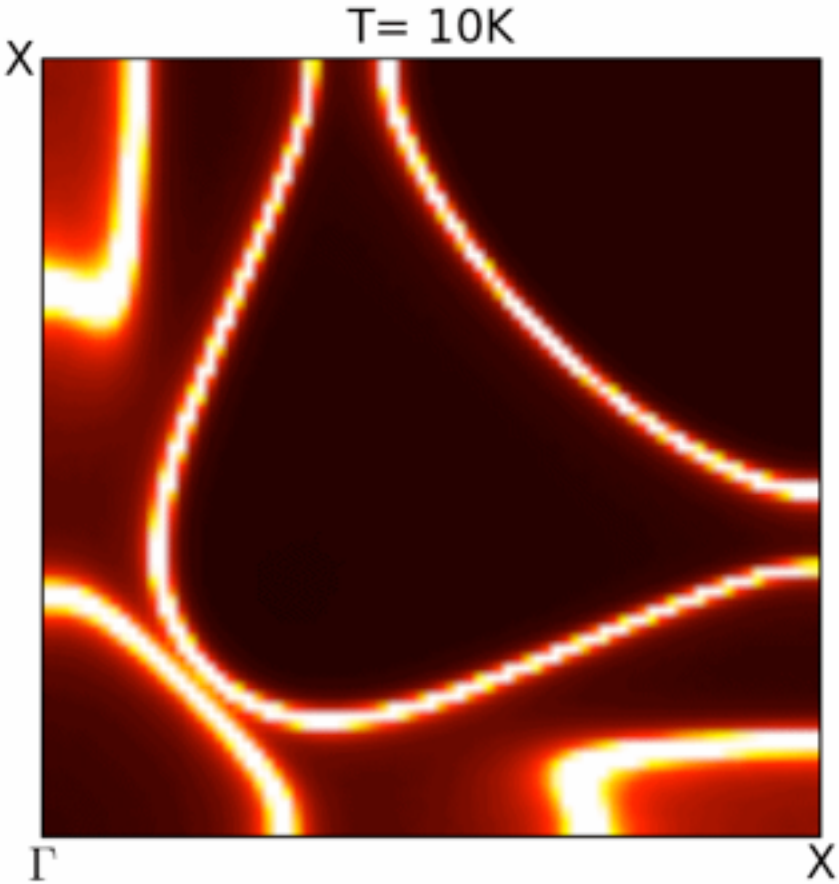


low –T

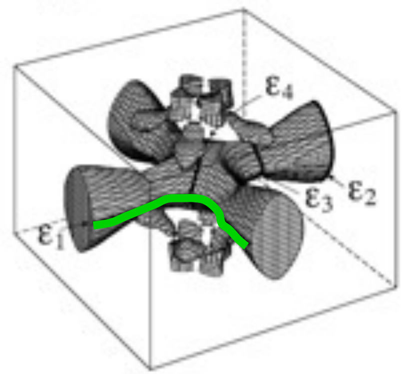


T-dep Fermi surface-topological change

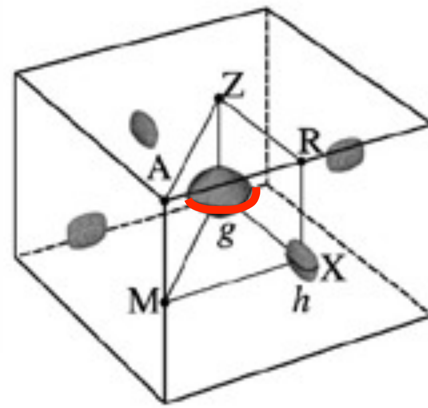
Fermi surface in the
Γ plane



high –T



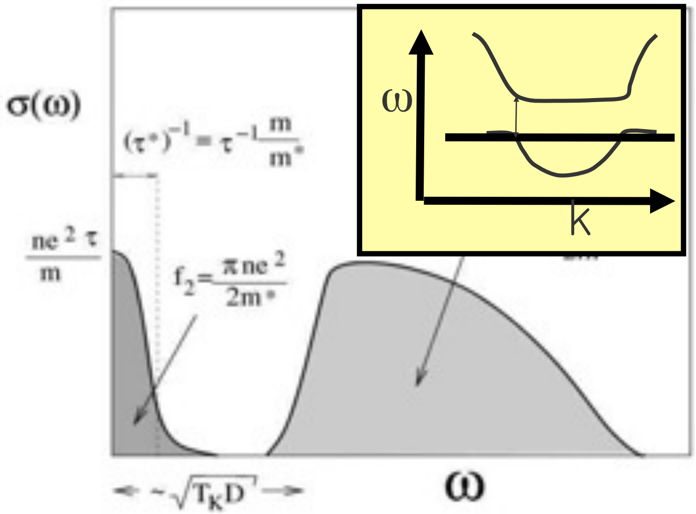
low –T



H.C. Choi, B.I. Min, J.H. Shim, K. Haule, G. Kotliar,
Phys. Rev. Lett. **108**, 016402 (2012).

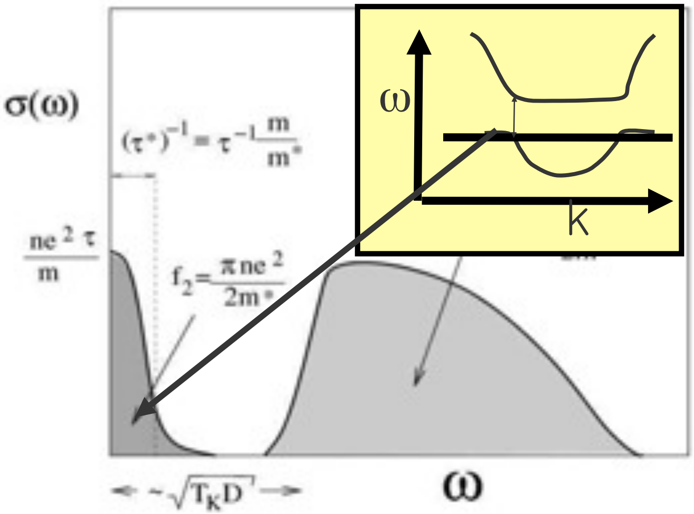
Optical conductivity

Typical heavy fermion at low T:



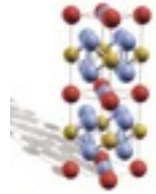
Optical conductivity

Typical heavy fermion at low T:

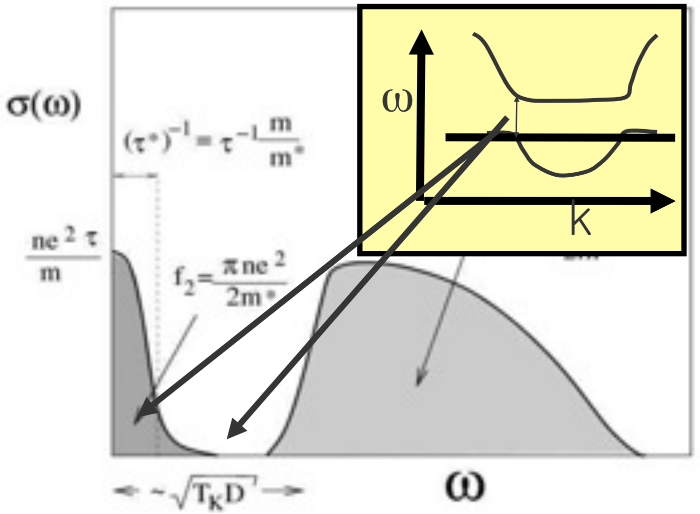


Narrow Drude peak (narrow q.p. band)

Optical conductivity



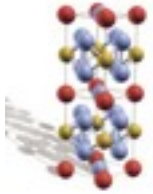
Typical heavy fermion at low T:



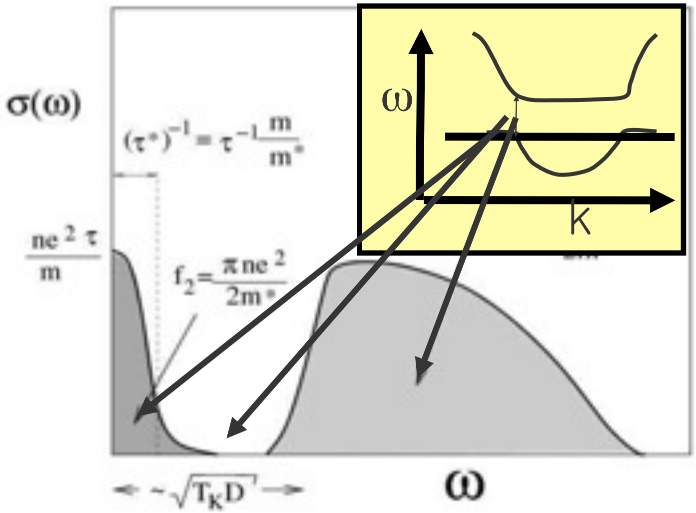
Narrow Drude peak (narrow q.p. band)

Hybridization gap

Optical conductivity



Typical heavy fermion at low T:



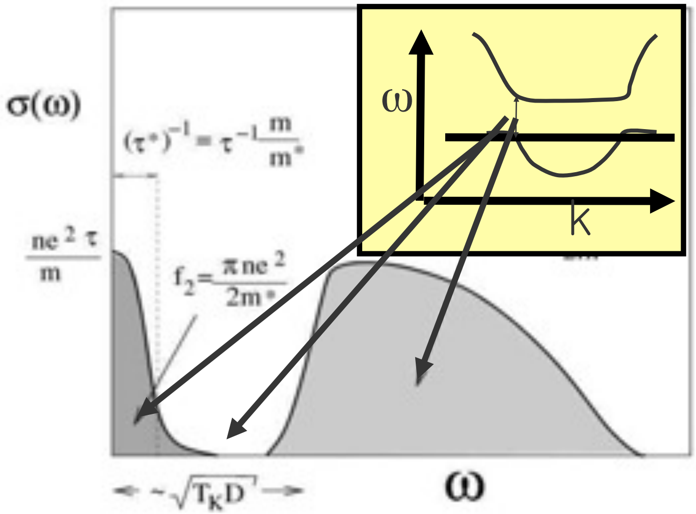
Narrow Drude peak (narrow q.p. band)

Hybridization gap

Interband transitions across hybridization gap -> mid IR peak

Optical conductivity

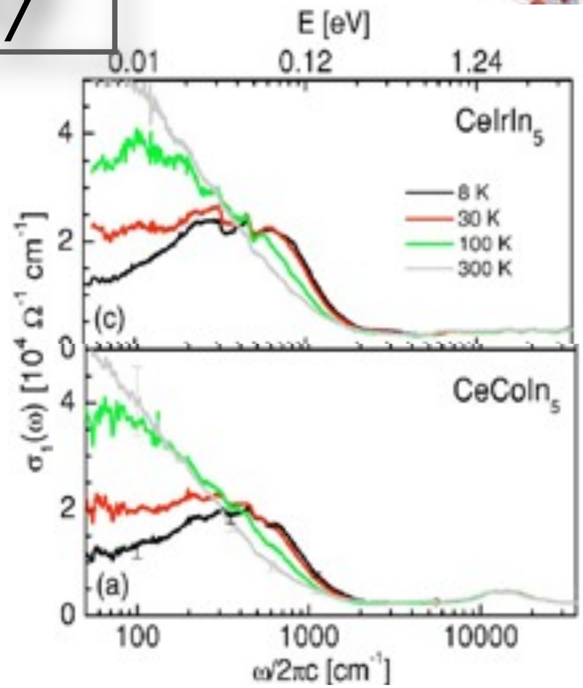
Typical heavy fermion at low T:

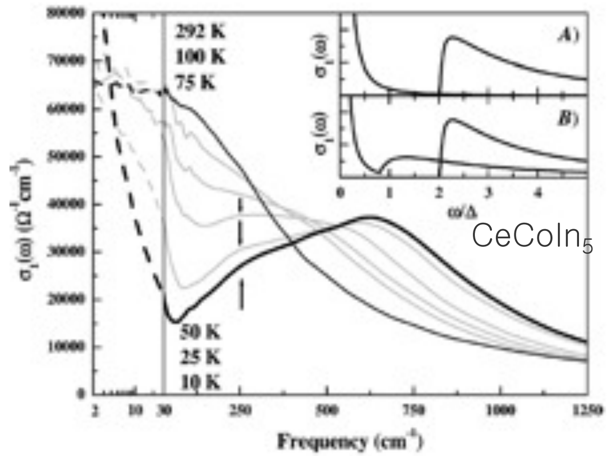


Narrow Drude peak (narrow q.p. band)

Hybridization gap

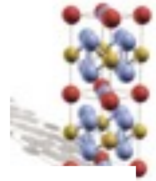
Interband transitions across hybridization gap -> mid IR peak





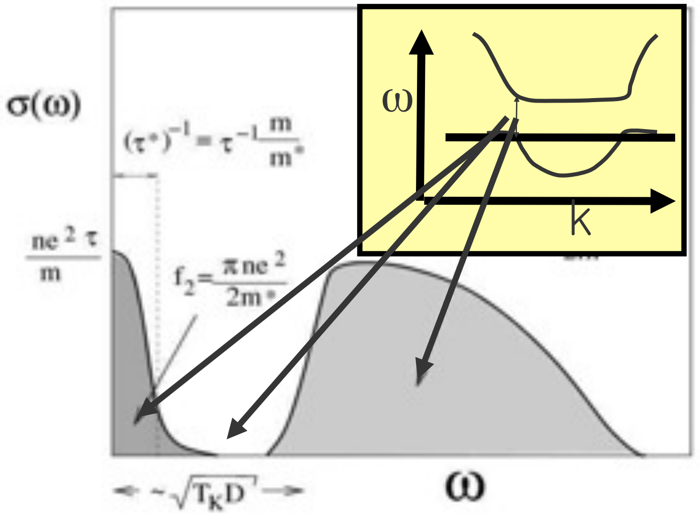
F.P. Mena & D.Van der Marel, 2005

E.J. Singley & D.N Basov, 2002

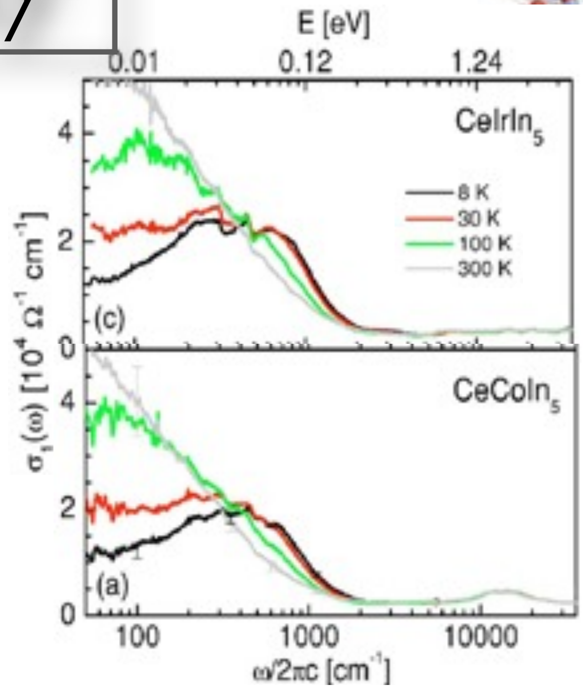


Optical conductivity

Typical heavy fermion at low T:



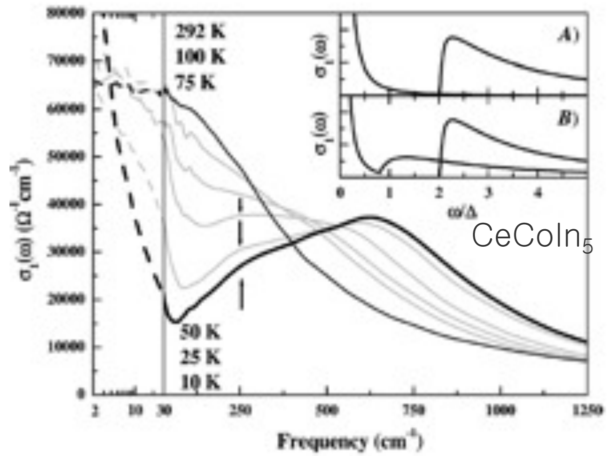
no visible Drude peak



Narrow Drude peak (narrow q.p. band)

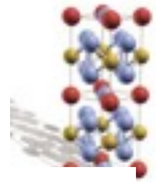
Hybridization gap

Interband transitions across hybridization gap -> mid IR peak

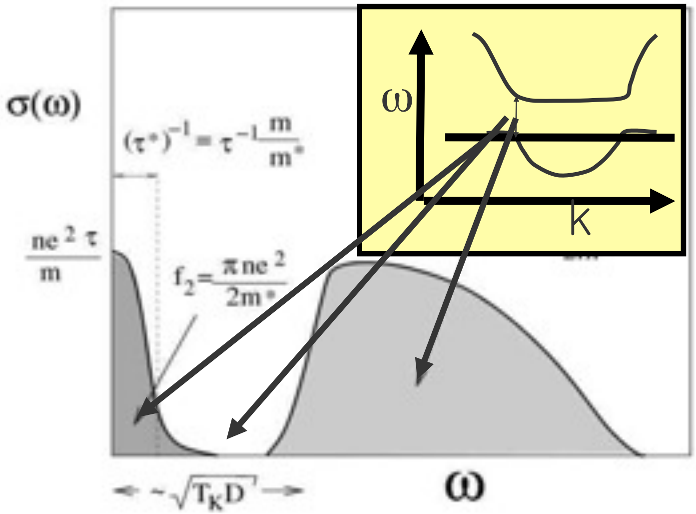


F.P. Mena & D.Van der Marel, 2005 | E.J. Singley & D.N Basov, 2002

Optical conductivity

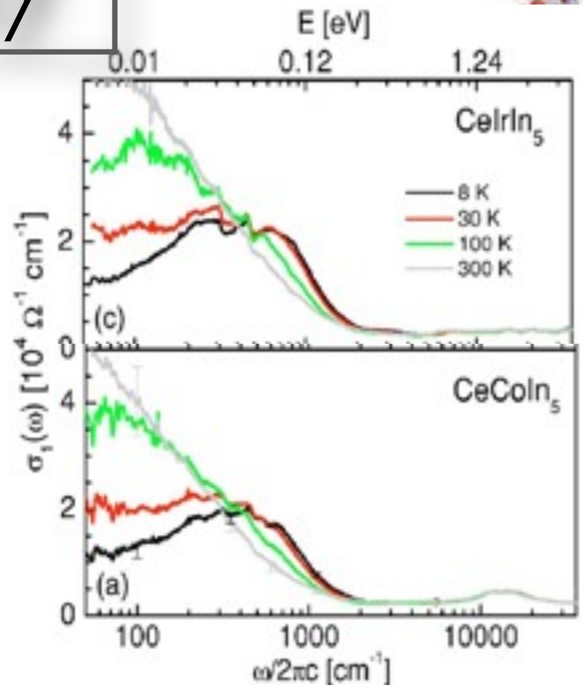


Typical heavy fermion at low T:



no visible Drude peak

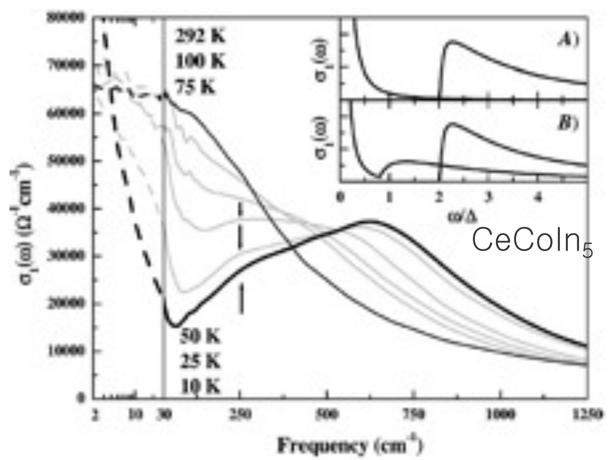
no sharp hybridization gap



Narrow Drude peak (narrow q.p. band)

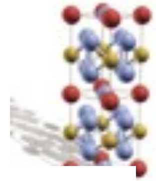
Hybridization gap

Interband transitions across hybridization gap -> mid IR peak

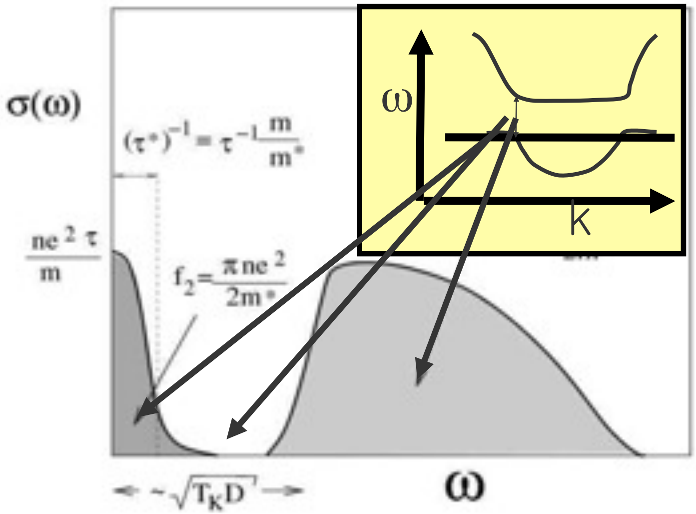


F.P. Mena & D.Van der Marel, 2005 | E.J. Singley & D.N Basov, 2002

Optical conductivity



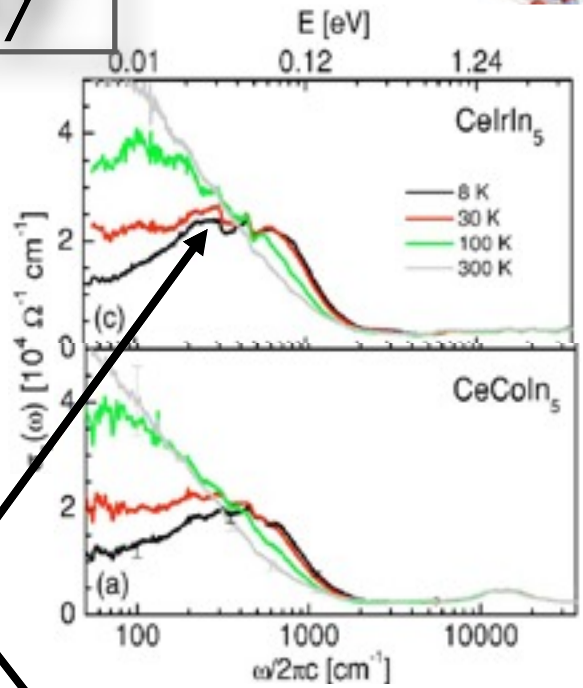
Typical heavy fermion at low T:

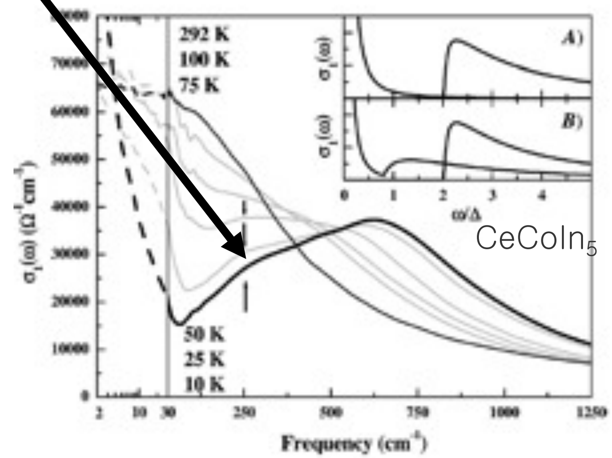


no visible Drude peak

no sharp hybridization gap

first mid-IR peak at 250 cm^{-1}





Narrow Drude peak (narrow q.p. band)

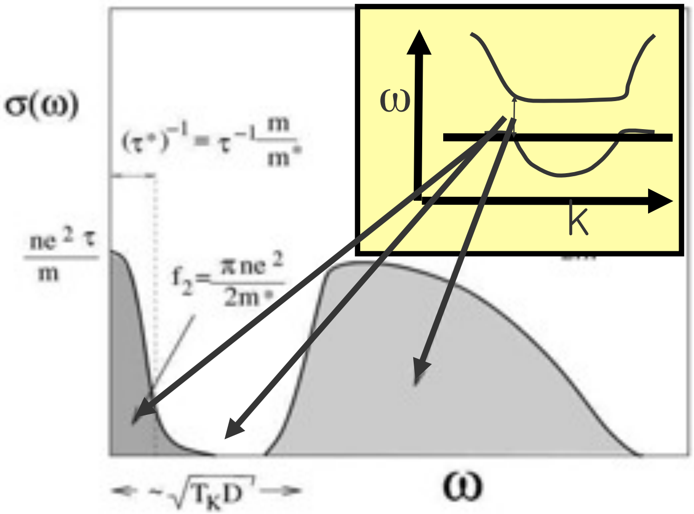
Hybridization gap

Interband transitions across hybridization gap -> mid IR peak

F.P. Mena & D.Van der Marel, 2005 | E.J. Singley & D.N Basov, 2002

Optical conductivity

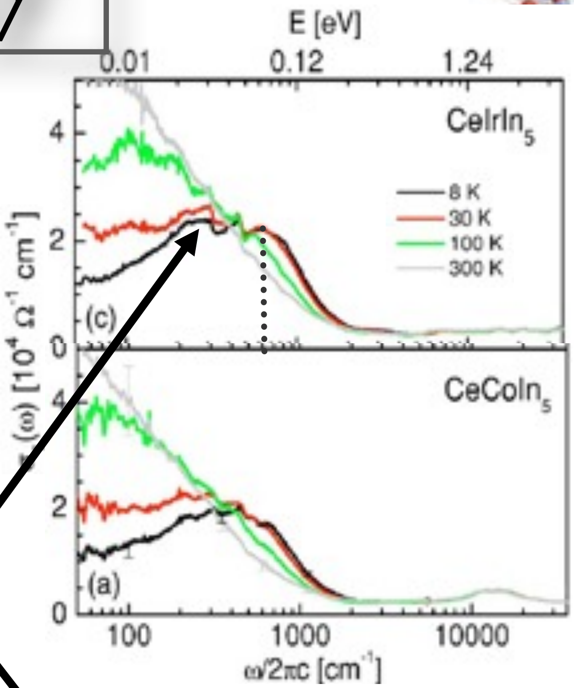
Typical heavy fermion at low T:



no visible Drude peak

no sharp hybridization gap

first mid–IR peak at 250 cm^{-1}

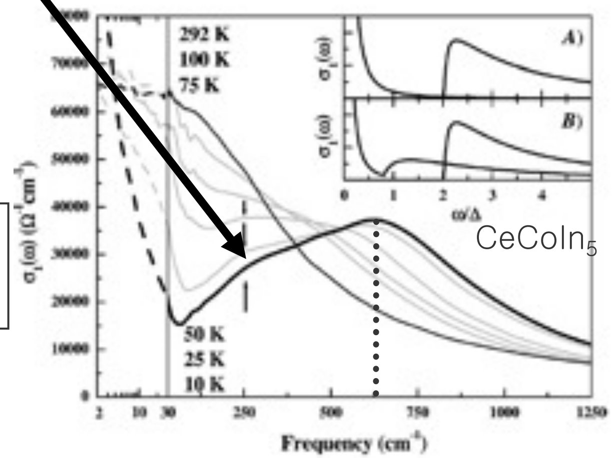


Narrow Drude peak (narrow q.p. band)

Hybridization gap

Interband transitions across hybridization gap –> mid IR peak

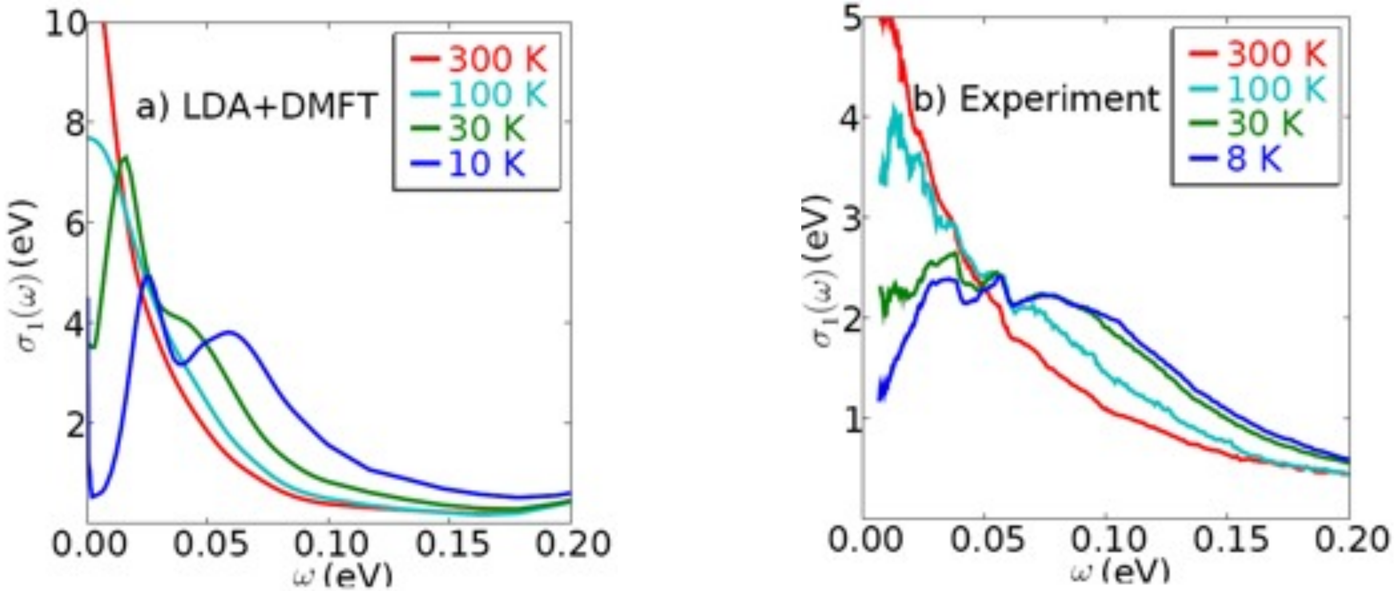
second mid IR peak at 600 cm^{-1}



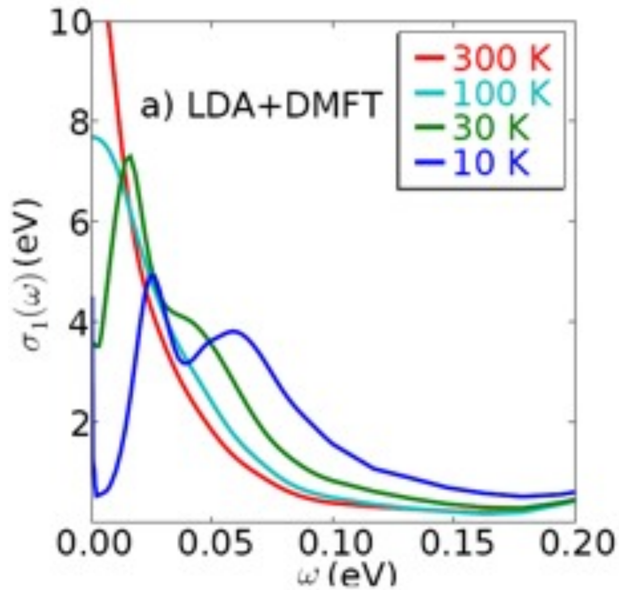
F.P. Mena & D.Van der Marel, 2005 | E.J. Singley & D.N Basov, 2002

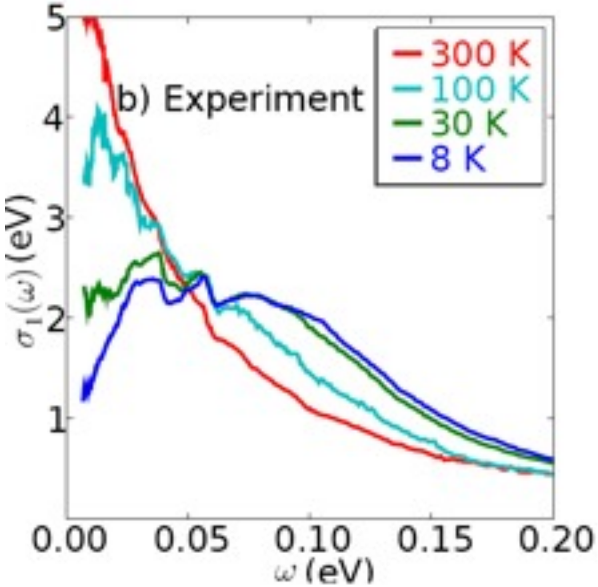
Thursday, January 12, 12

Optical conductivity in LDA+DMFT



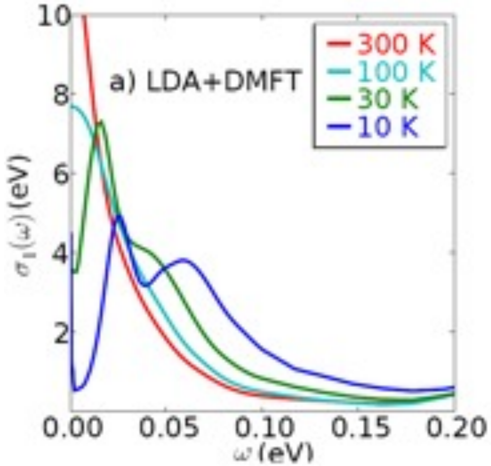
Optical conductivity in LDA+DMFT



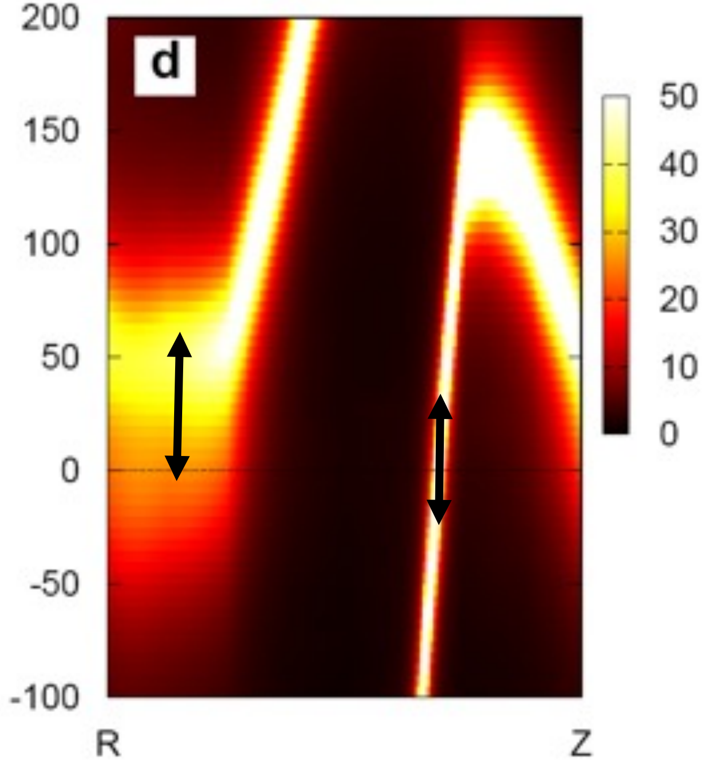


- At 300K very broad Drude peak (e-e scattering, spd lifetime~0.1eV)
- At 10K:
  - very narrow Drude peak
  - First MI peak at 0.03eV~250cm^{-1}
  - Second MI peak at 0.07eV~600cm^{-1}

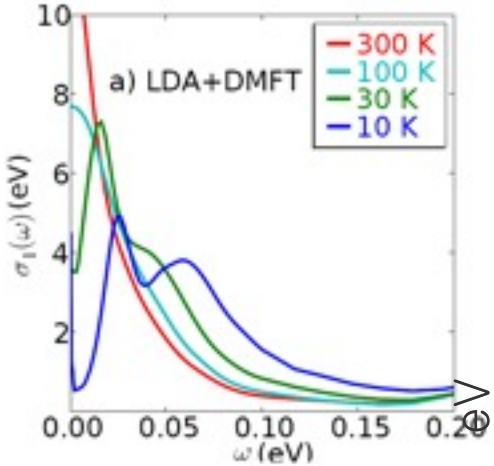
Multiple hybridization gaps

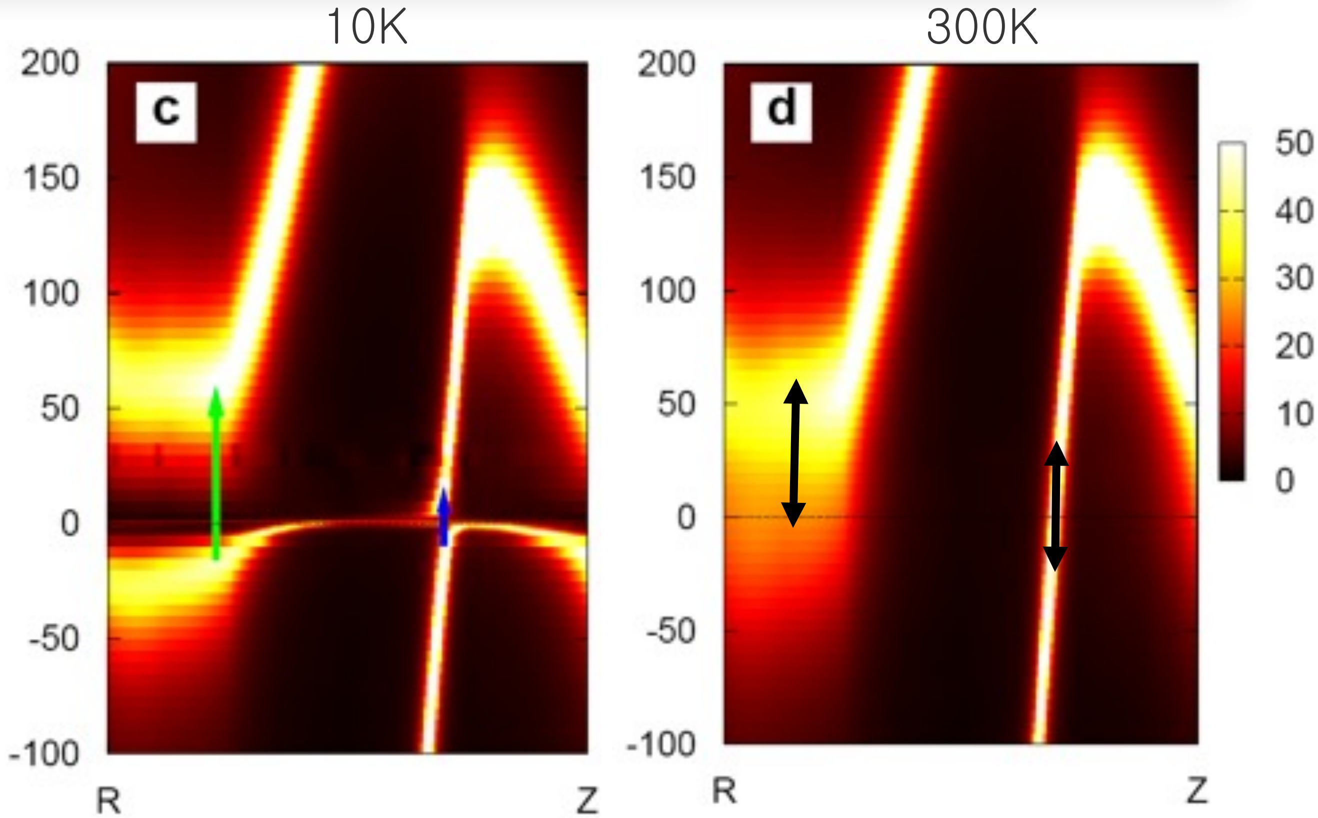


300K

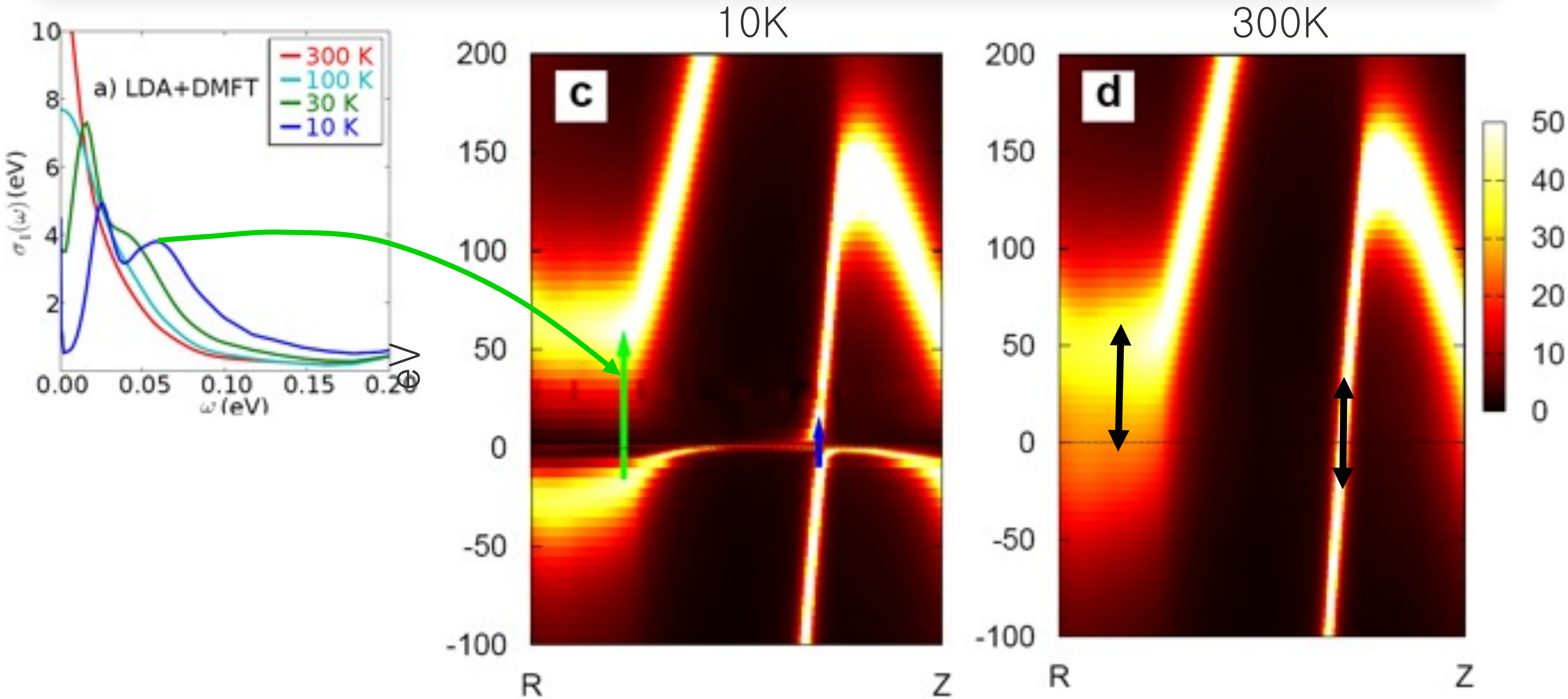


Multiple hybridization gaps

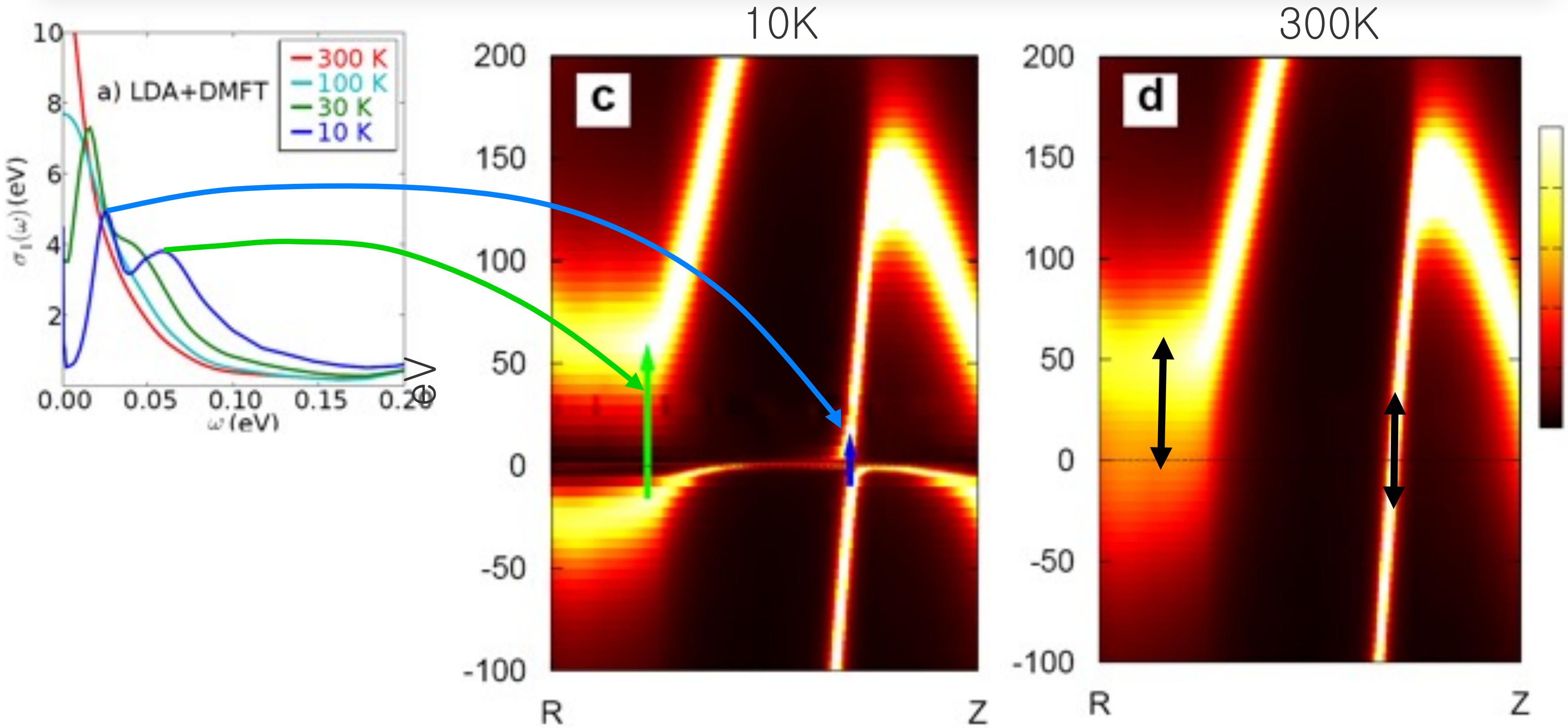




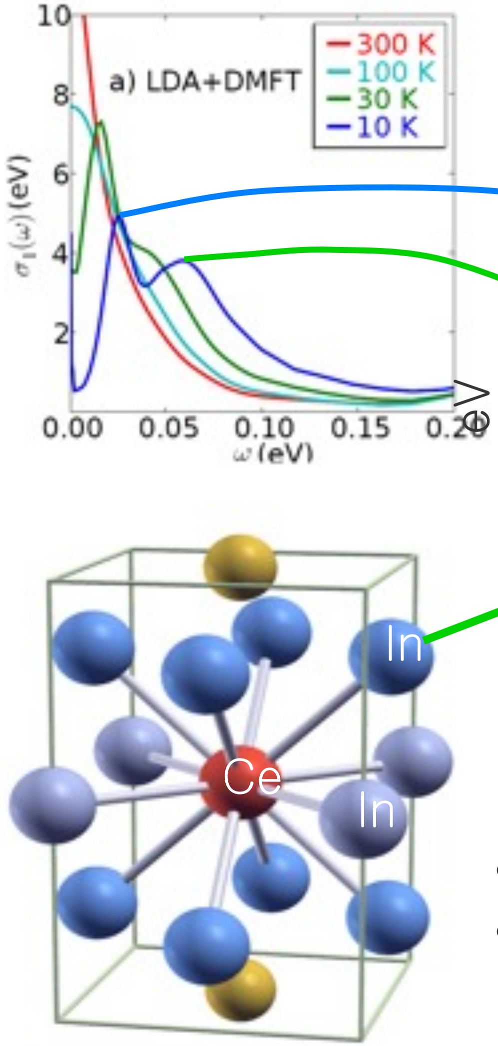
Multiple hybridization gaps

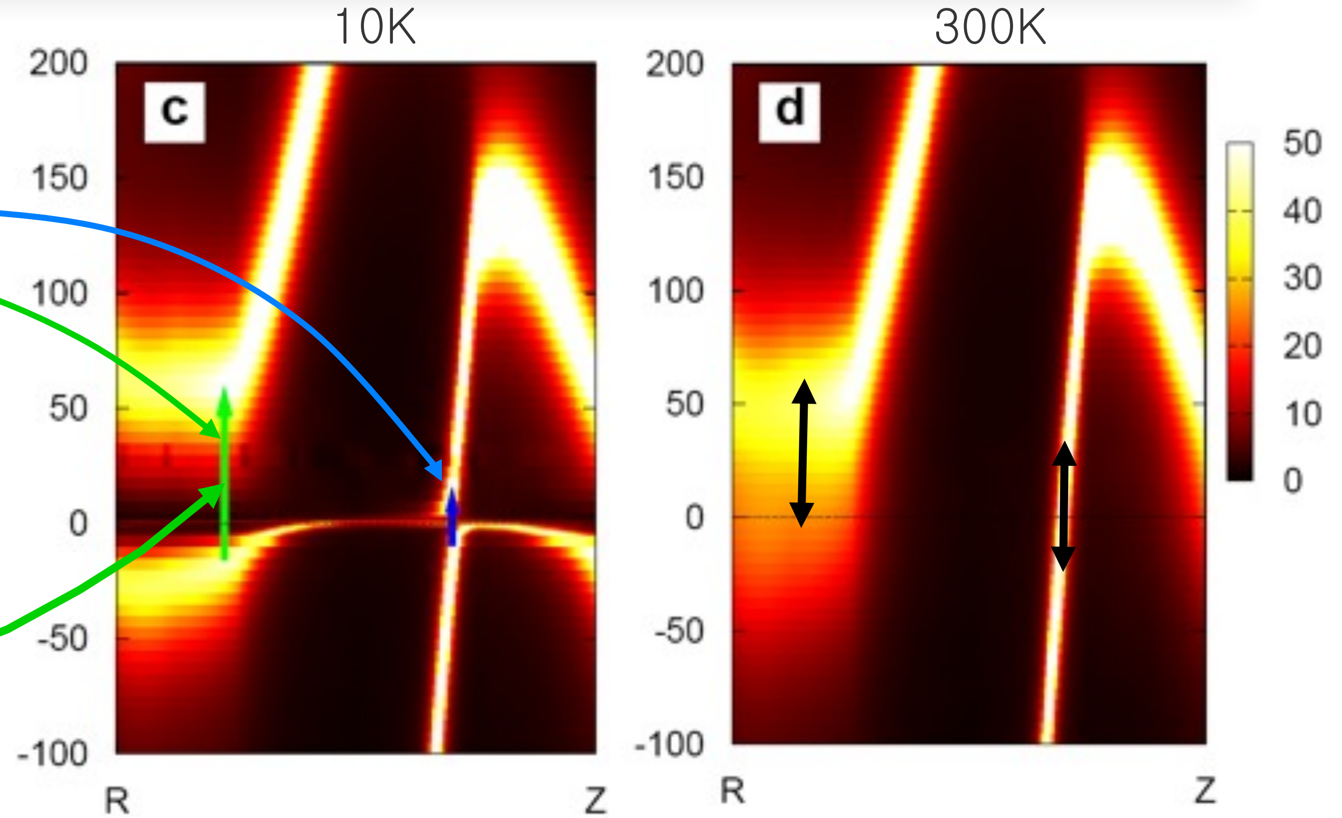


Multiple hybridization gaps



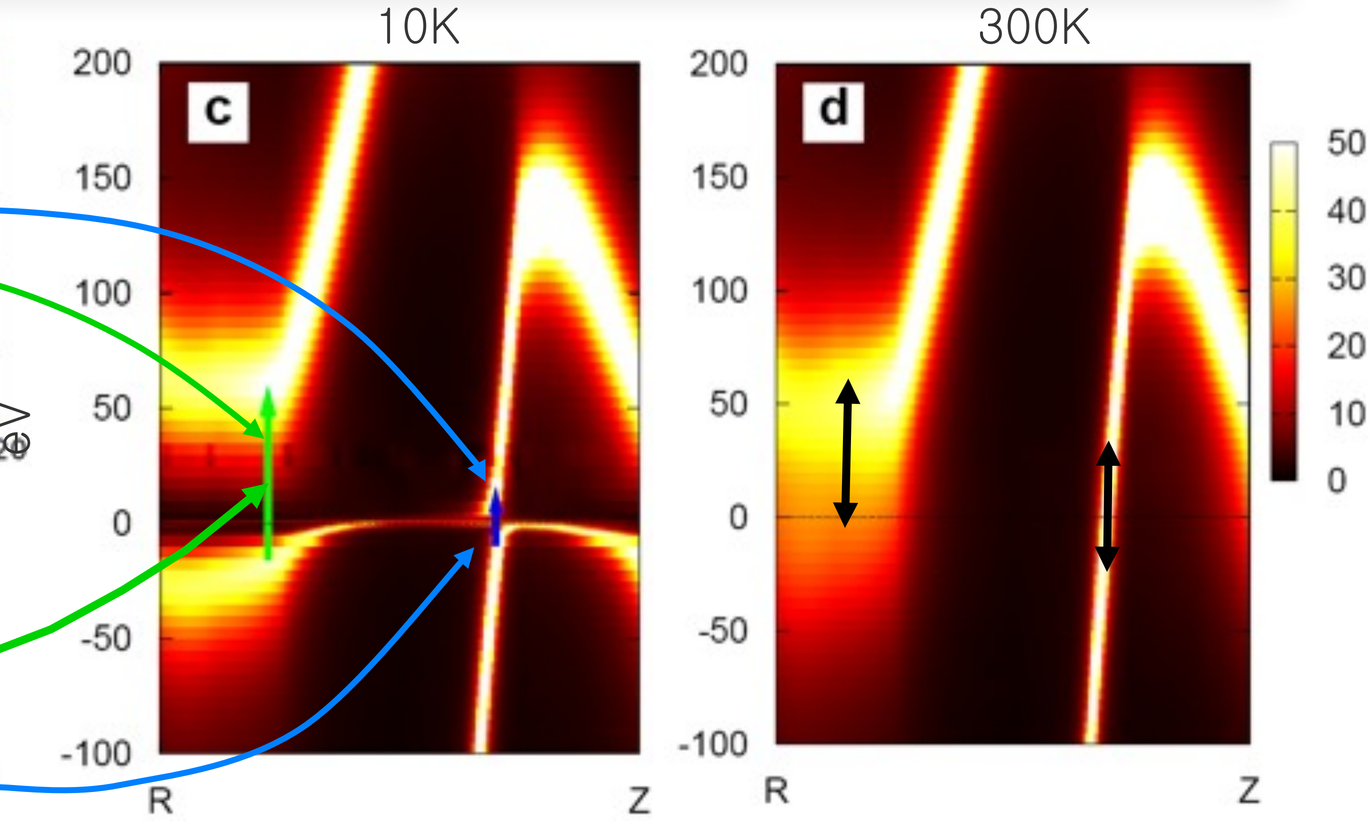
Multiple hybridization gaps

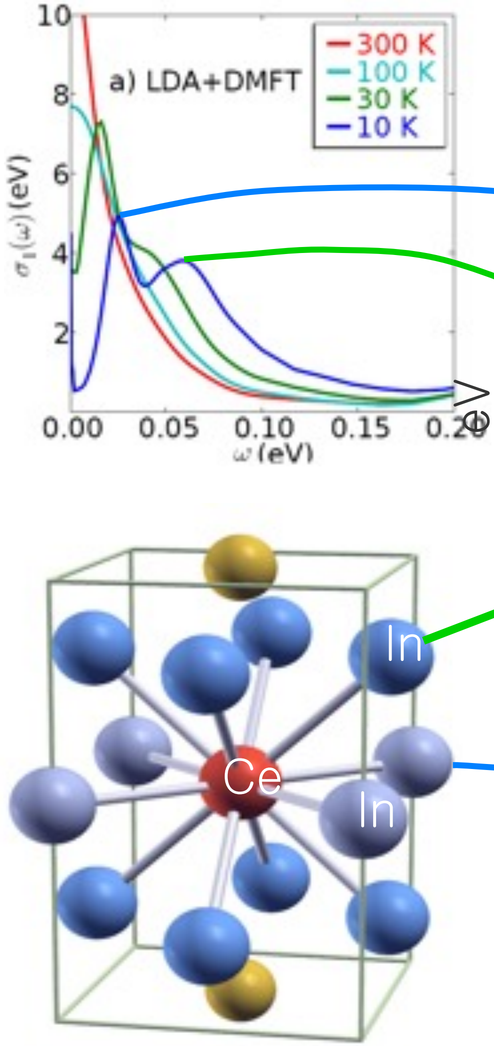




•Larger gap due to hybridization with out of plane In
•Smaller gap due to hybridization with in-plane In

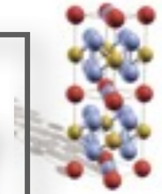
Multiple hybridization gaps

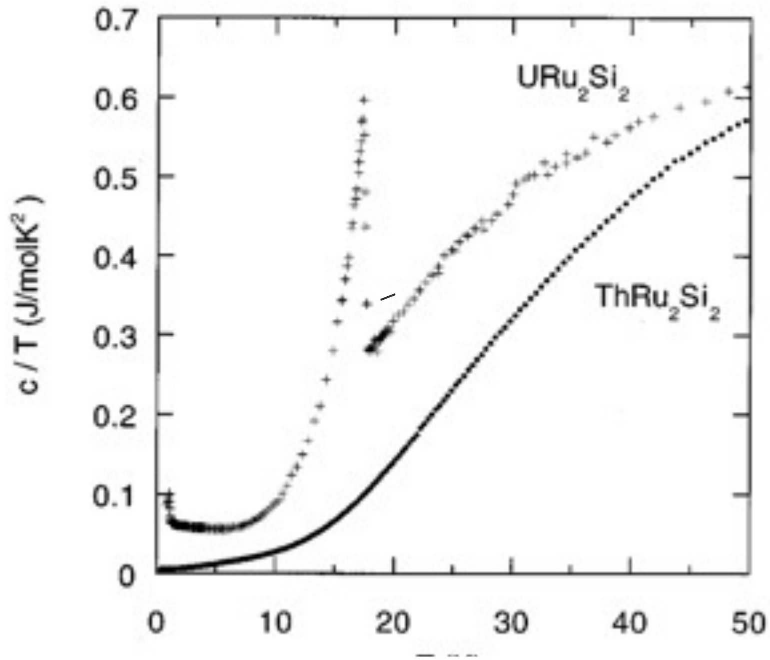


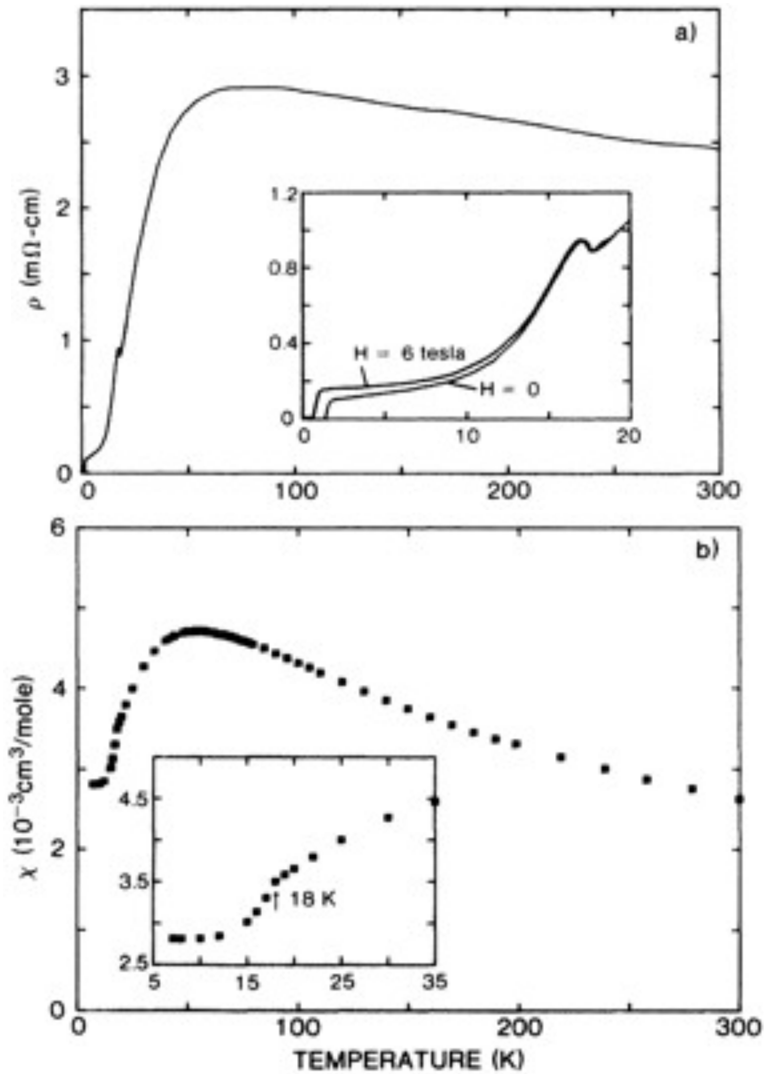


- Larger gap due to hybridization with out of plane In
- Smaller gap due to hybridization with in-plane In

URu_2Si_2 heavy fermion with hidden order

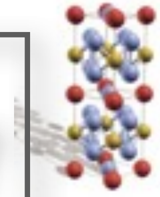




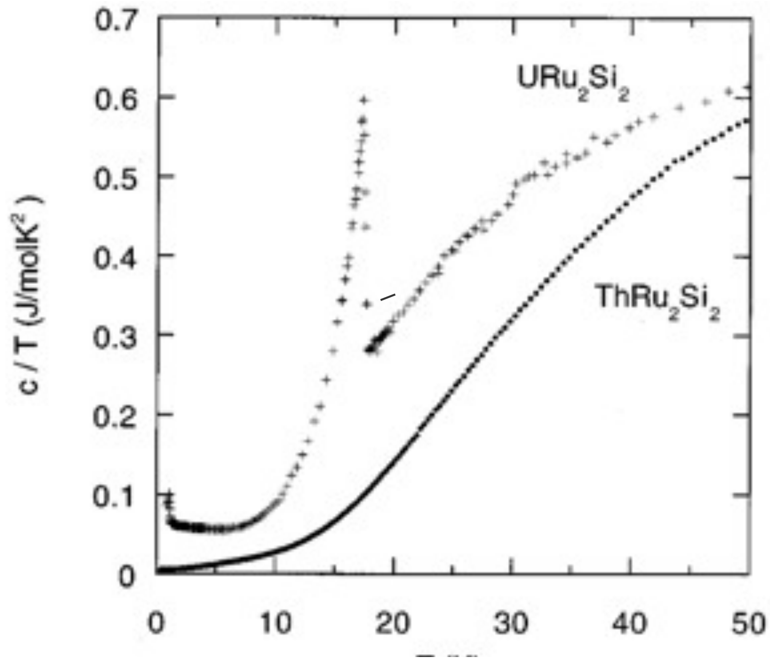


N. H. van Dijk, PRB 56, 14493 (1997).

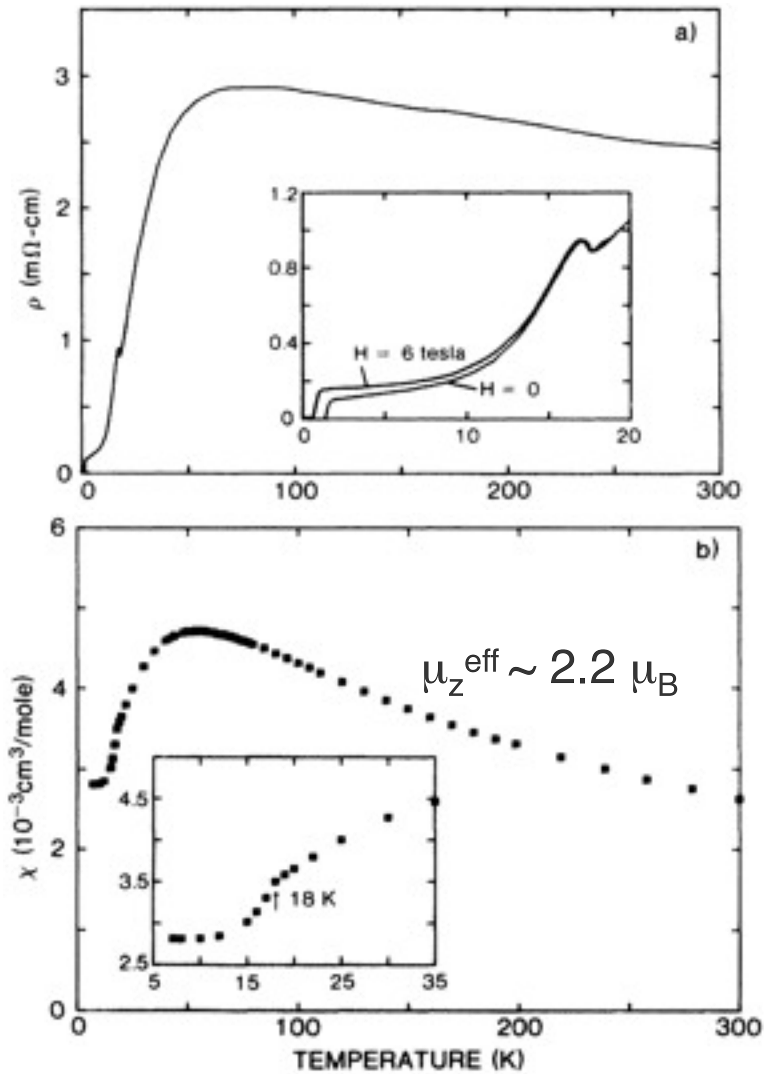
URu_2Si_2 heavy fermion with hidden order



Curie−Weiss: $\mu_z^{eff} \sim 2.2\ \mu_B$



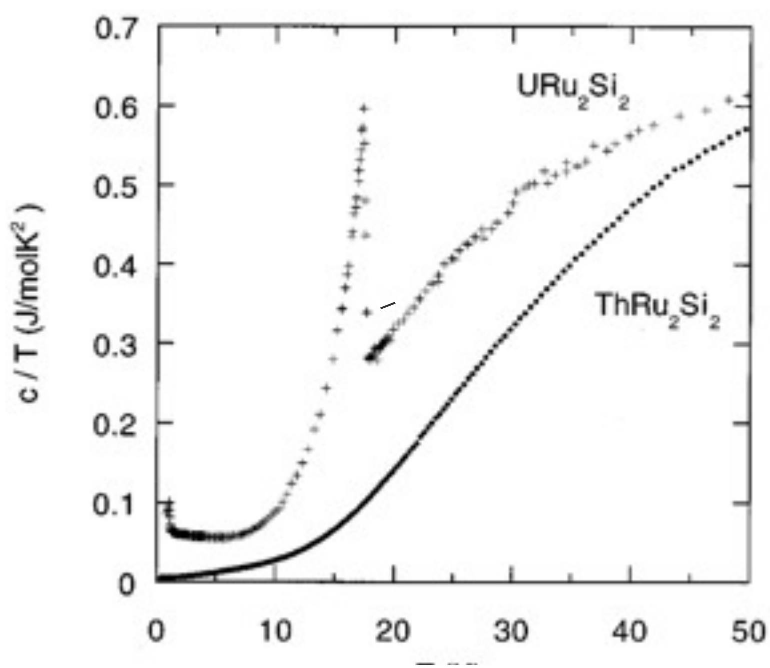
N. H. van Dijk, PRB 56, 14493 (1997).



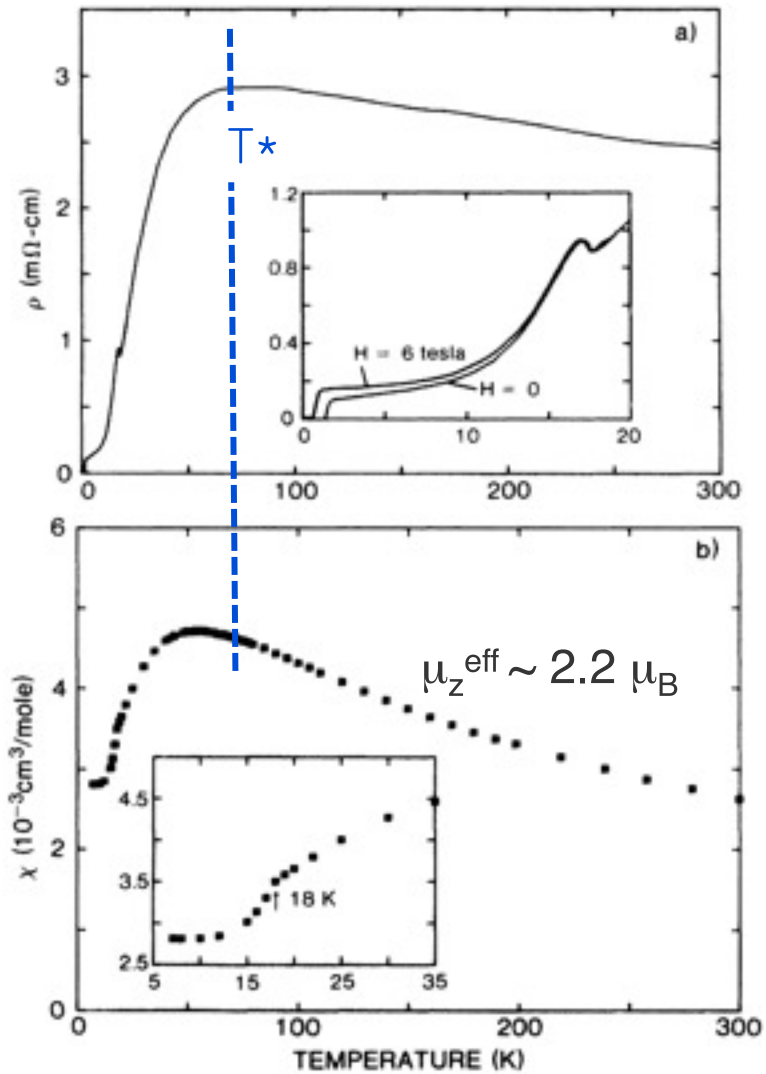
URu_2Si_2 heavy fermion with hidden order

Curie–Weiss: $\mu_z^{eff} \sim 2.2\ \mu_B$

Coherence: T*~70K



N. H. van Dijk, PRB 56, 14493 (1997).

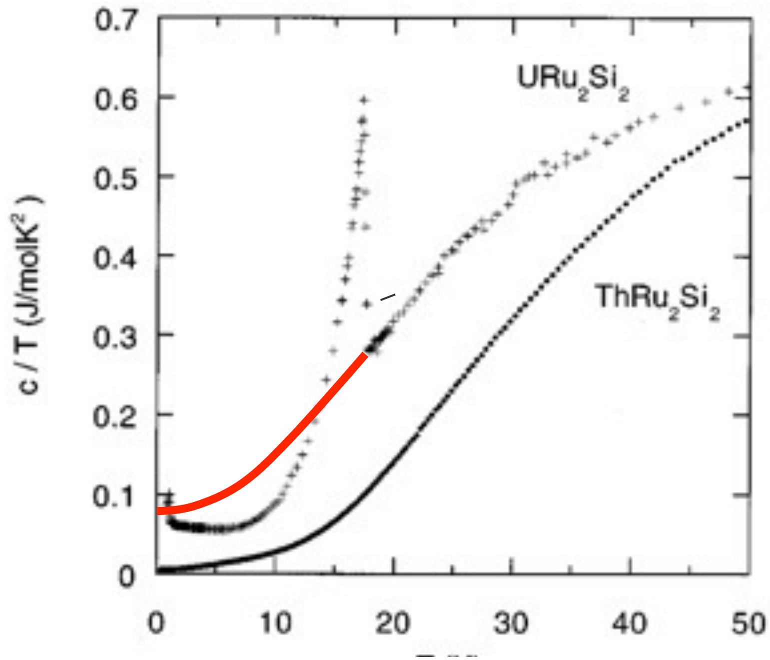


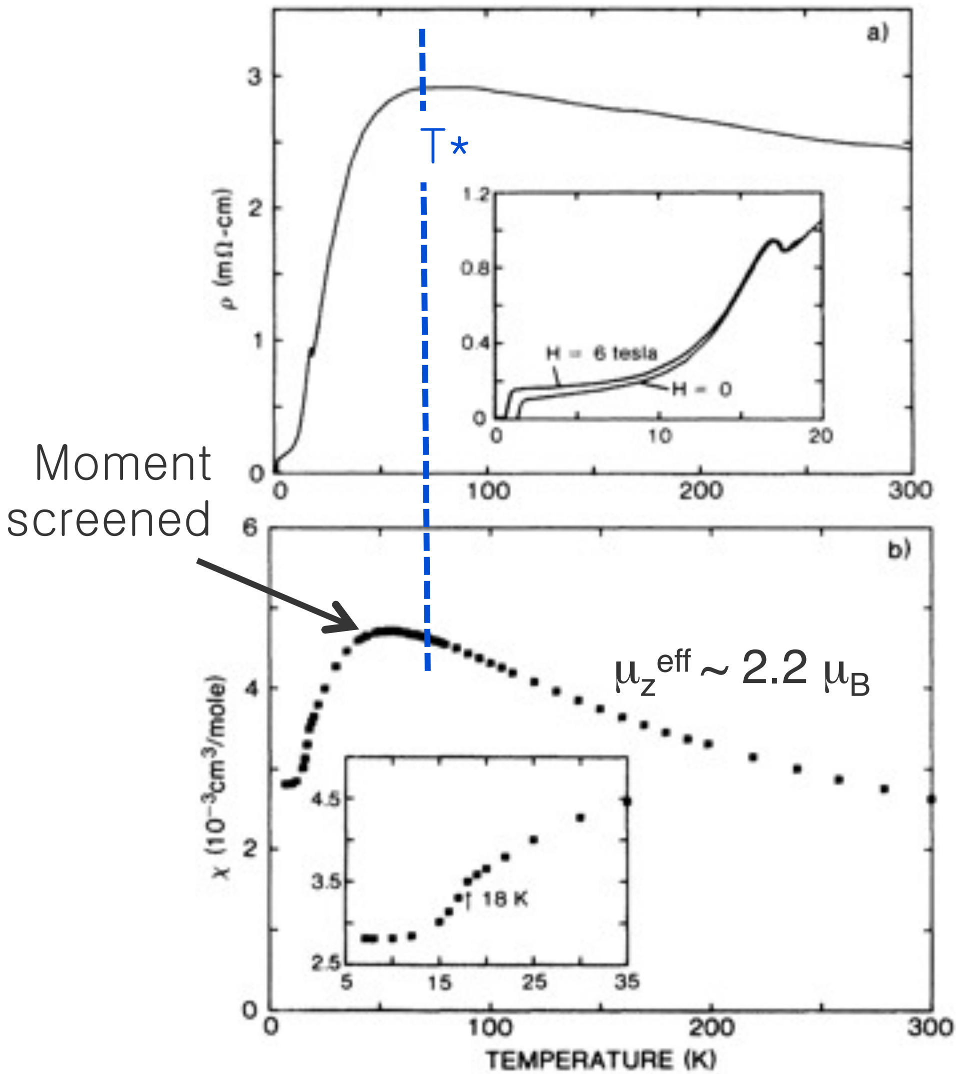
URu_2Si_2 heavy fermion with hidden order

Curie−Weiss: $\mu_z^{eff} \sim 2.2\ \mu_B$

Elec. cv: $\gamma \sim 70$ mJ/mol K²

Coherence: T*~70K





N. H. van Dijk, PRB 56, 14493 (1997).

URu_2Si_2 heavy fermion with hidden order

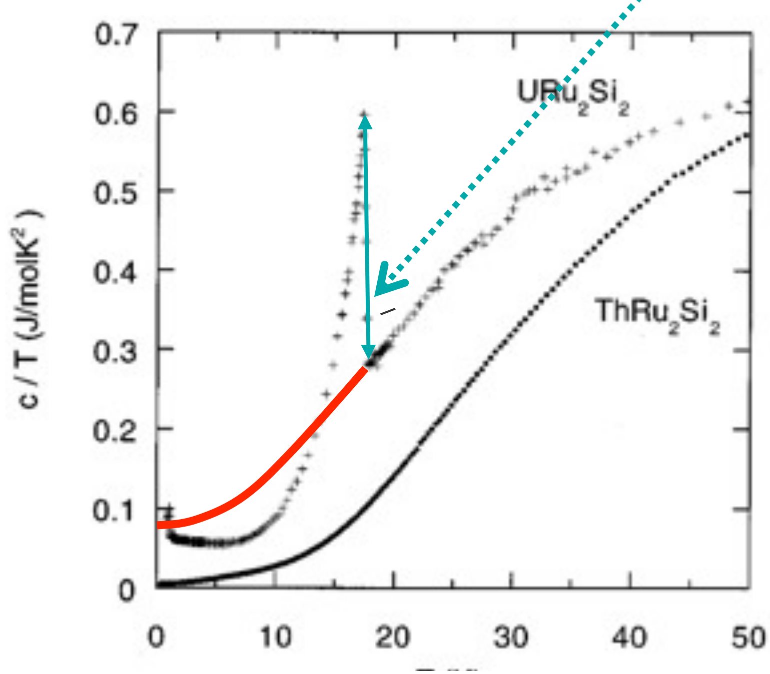
Curie−Weiss: $\mu_z^{eff} \sim 2.2\ \mu_B$

Second order phase transition

Elec. cv: $\gamma \sim 70$ mJ/mol K^2

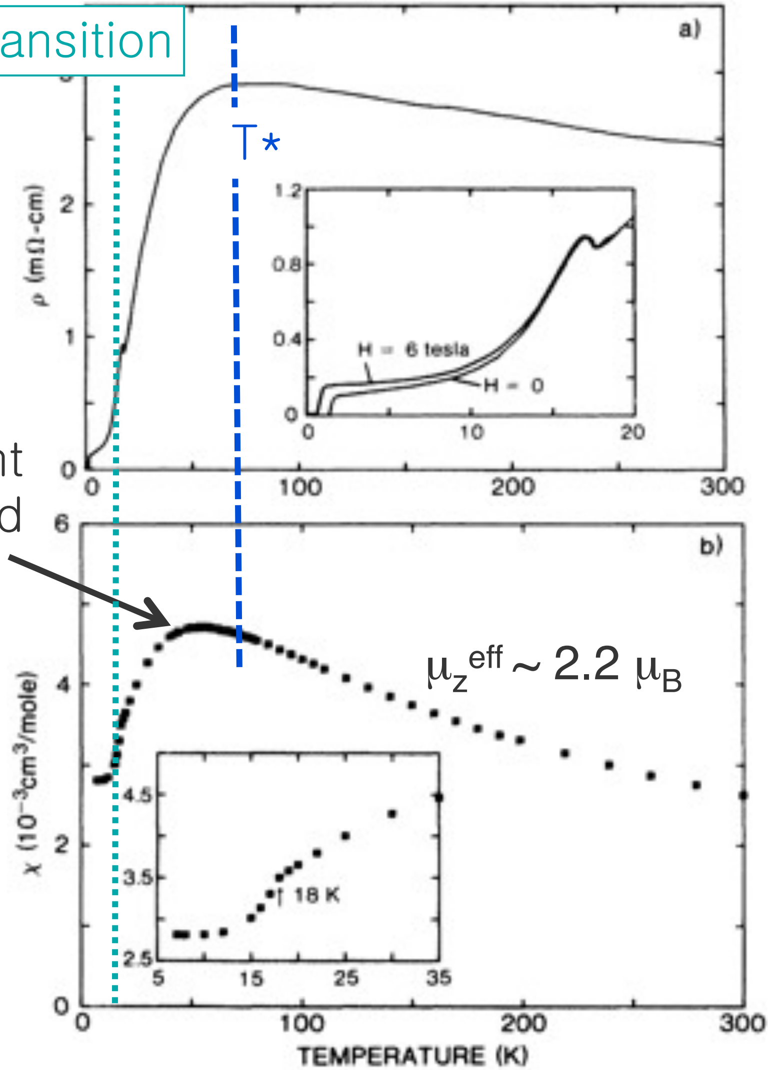
Coherence: T*~70K

SOPT: T_0~17.8K



N. H. van Dijk, PRB 56, 14493 (1997).

Moment screened



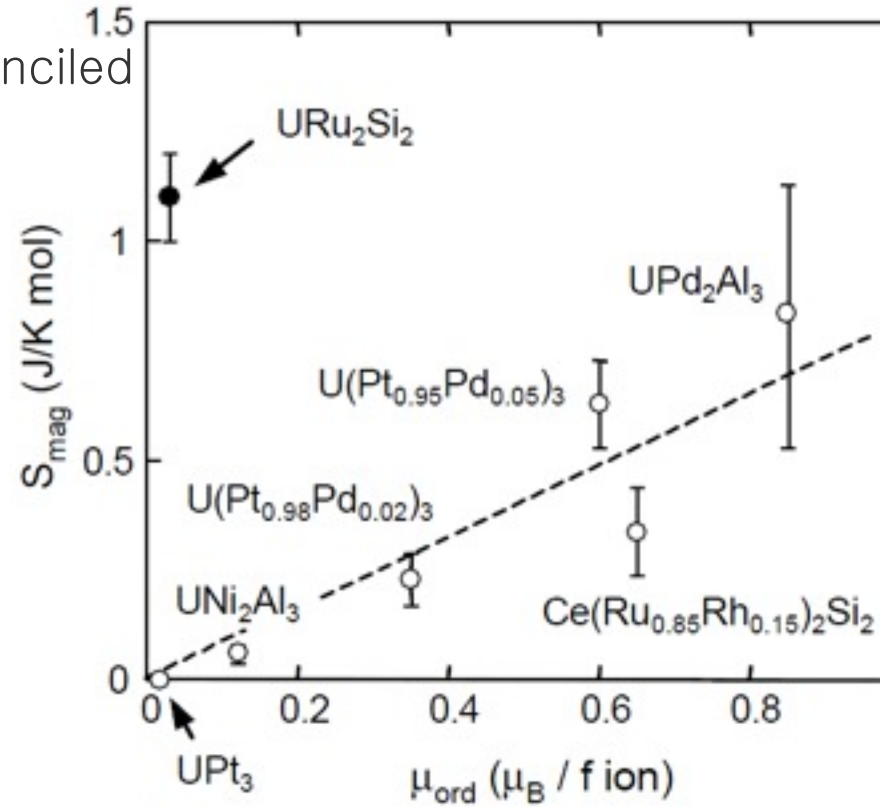
Hidden Order: The CMT dark matter problem

- Moment is tiny
  (likely small admixture of AFM phase)

- Large loss of entropy can not be reconciled by small moment

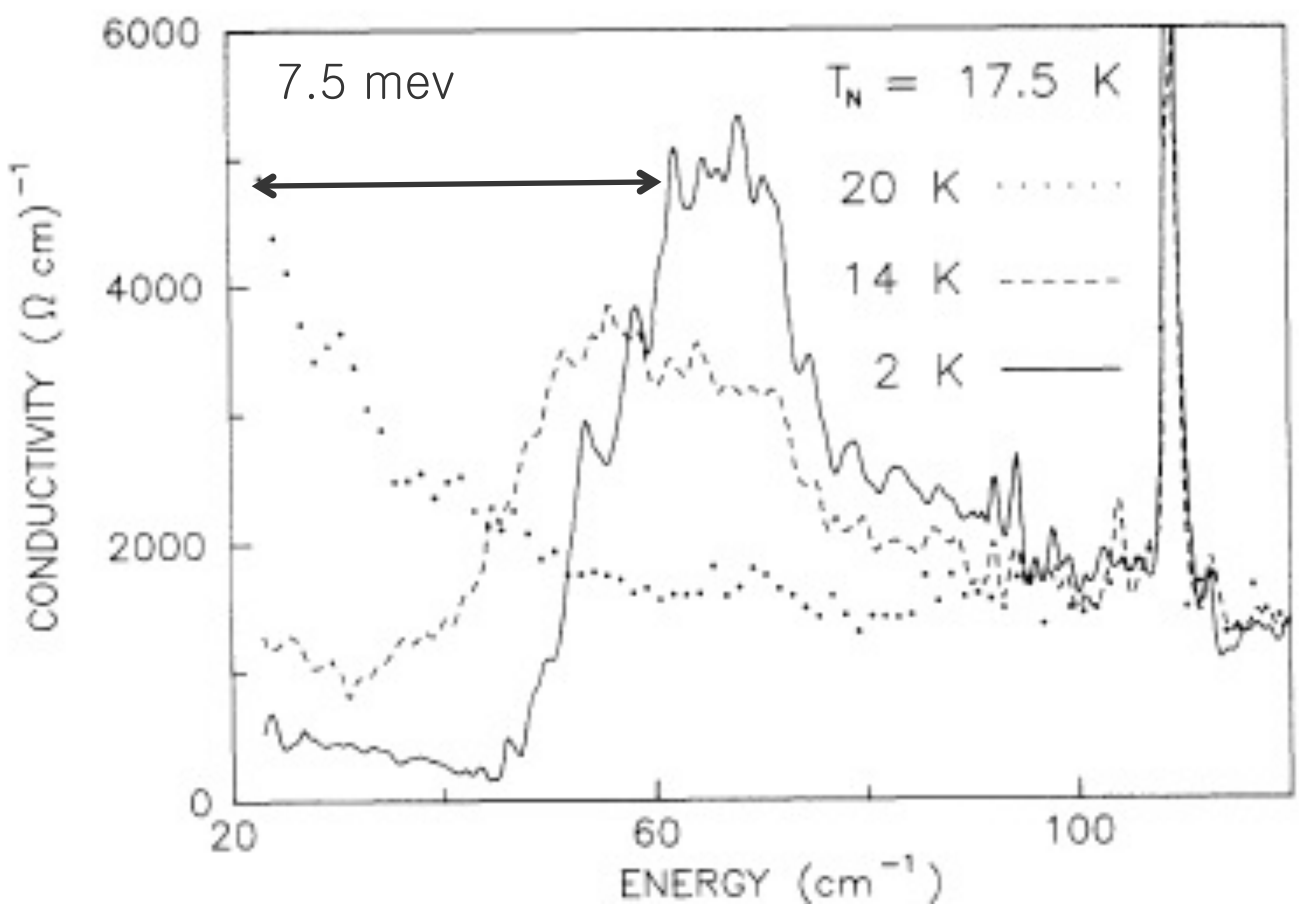
- Some other symmetry breaks.
  Hidden order parameter

WHICH?



Optical conductivity

Pseudo-gap opens at Tc: D. A. Bonn et al. PRL (1988).



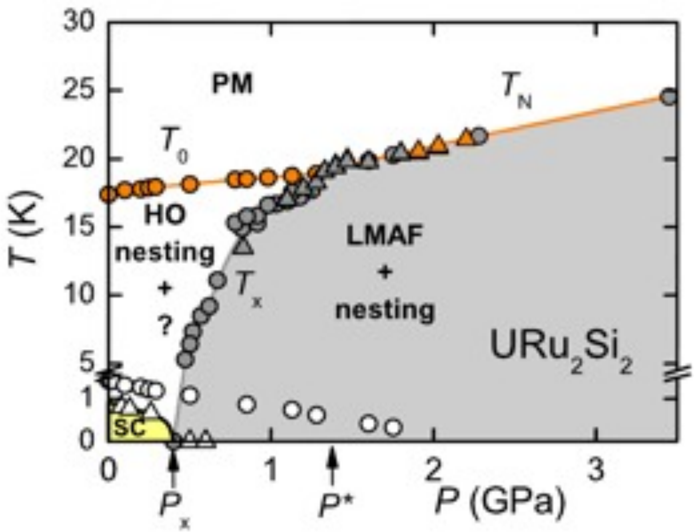
Adiabatic continuity between HO&AFM state

PRL 98, 166404 (2007) PHYSICAL REVIEW LETTERS week ending 20 APRIL 2007

Field-Induced Fermi Surface Reconstruction and Adiabatic Continuity between Antiferromagnetism and the Hidden-Order State in URu_2Si_2

Y. J. Jo,[1] L. Balicas,[1] C. Capan,[2] K. Behnia,[3] P. Lejay,[4] J. Flouquet,[5] J. A. Mydosh,[6] and P. Schlottmann[1]

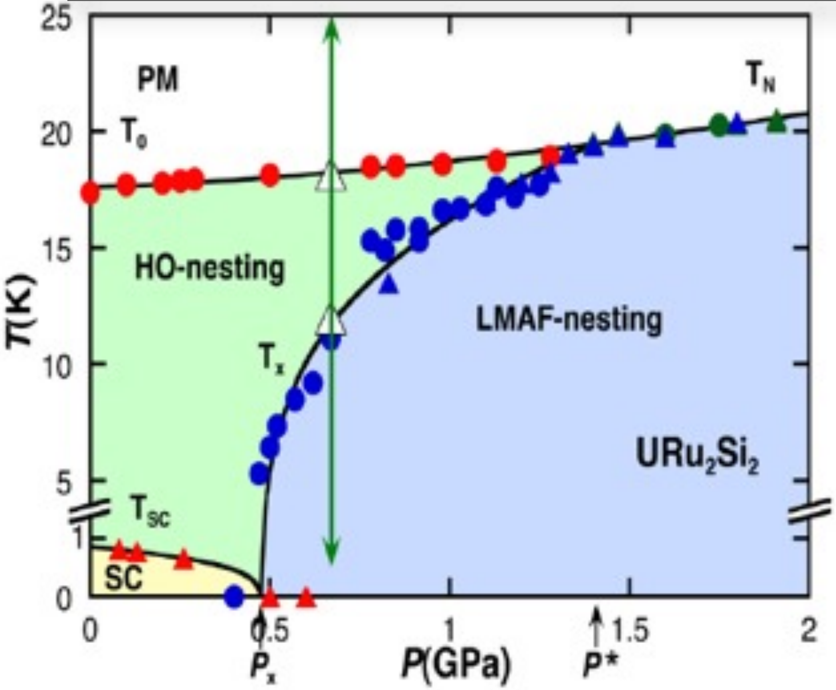
$H - T$ phase diagram. Instead of phase separation between HO and antiferromagnetism our observations indicate adiabatic continuity between both orderings with field and pressure changing their relative weight.

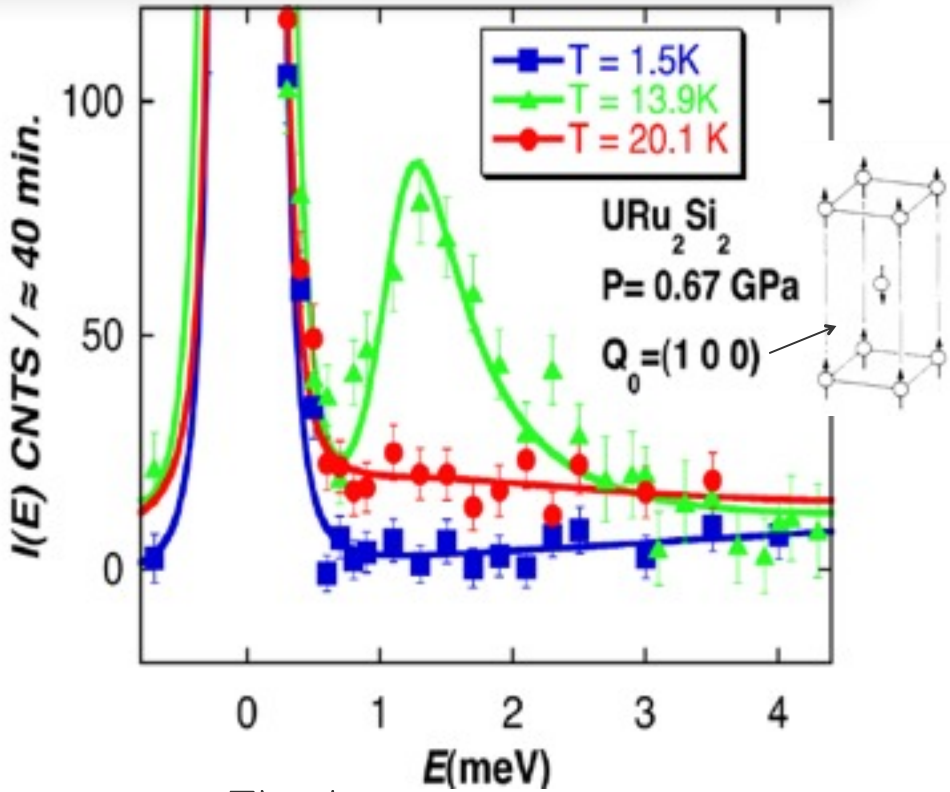


- HO under pressure converted to AFM phase through 1st order transition
- Similar T_0 and T_N
- Almost identical thermodynamic
  - quantities (jump in Cv), quantum osc

E. Hassinger et.al. PRL 77, 115117 (2008)

Key experiment: Neutron scattering





The low energy resonance

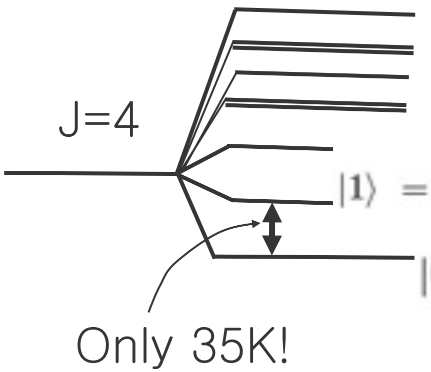
A.Villaume, F. Bourdarot, E. Hassinger, S. Raymond, V. Taufour, D. Aoki, and J. Flouquet, PRB 78, 012504 (2008)

Origin of gapping?

Partial DOS

Small effects on spd electrons
Large effect on U−f's

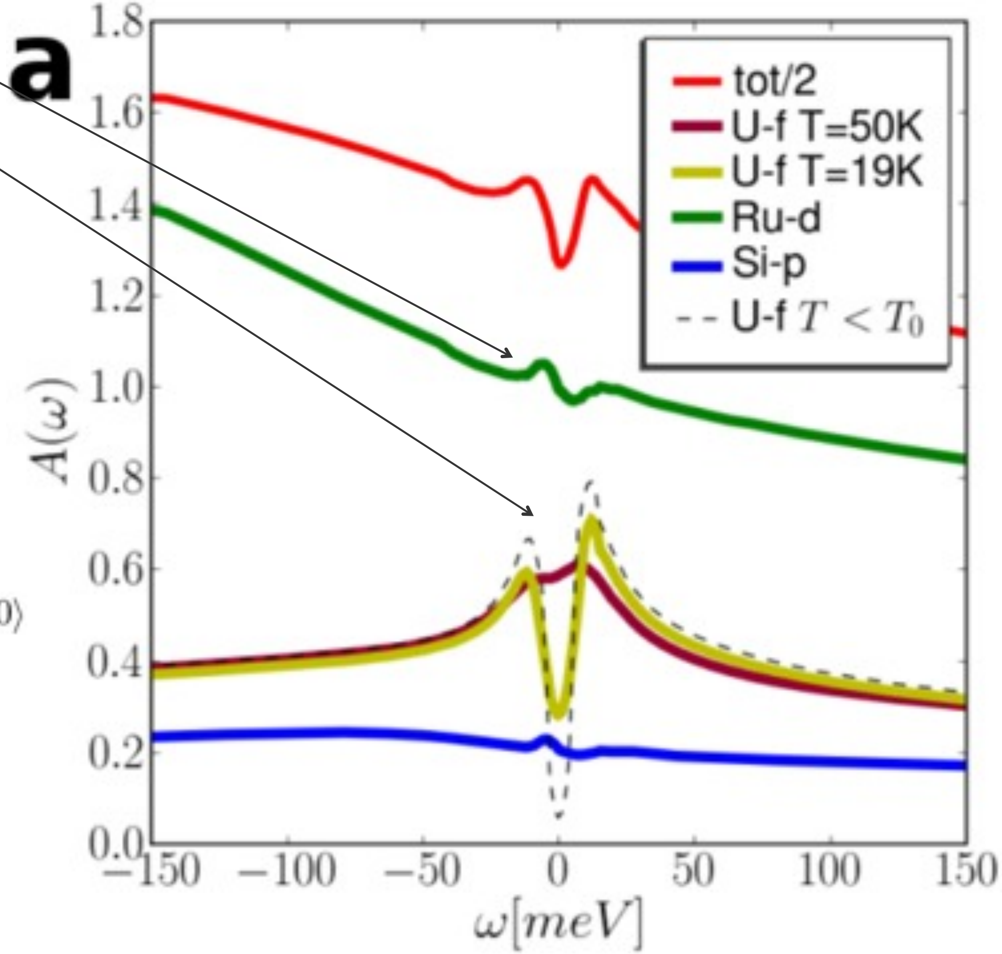
Ground state atomic multiplet of f^2 configuration in tetragonal field



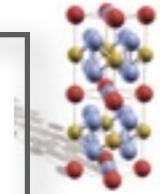
$$|1\rangle = \frac{\cos(\phi)}{\sqrt{2}}(|4\rangle + |-4\rangle) - \sin(\phi)|0\rangle$$

$$|0\rangle = \frac{i}{\sqrt{2}}(|4\rangle - |-4\rangle)$$

|state>==|J=4,Jz>

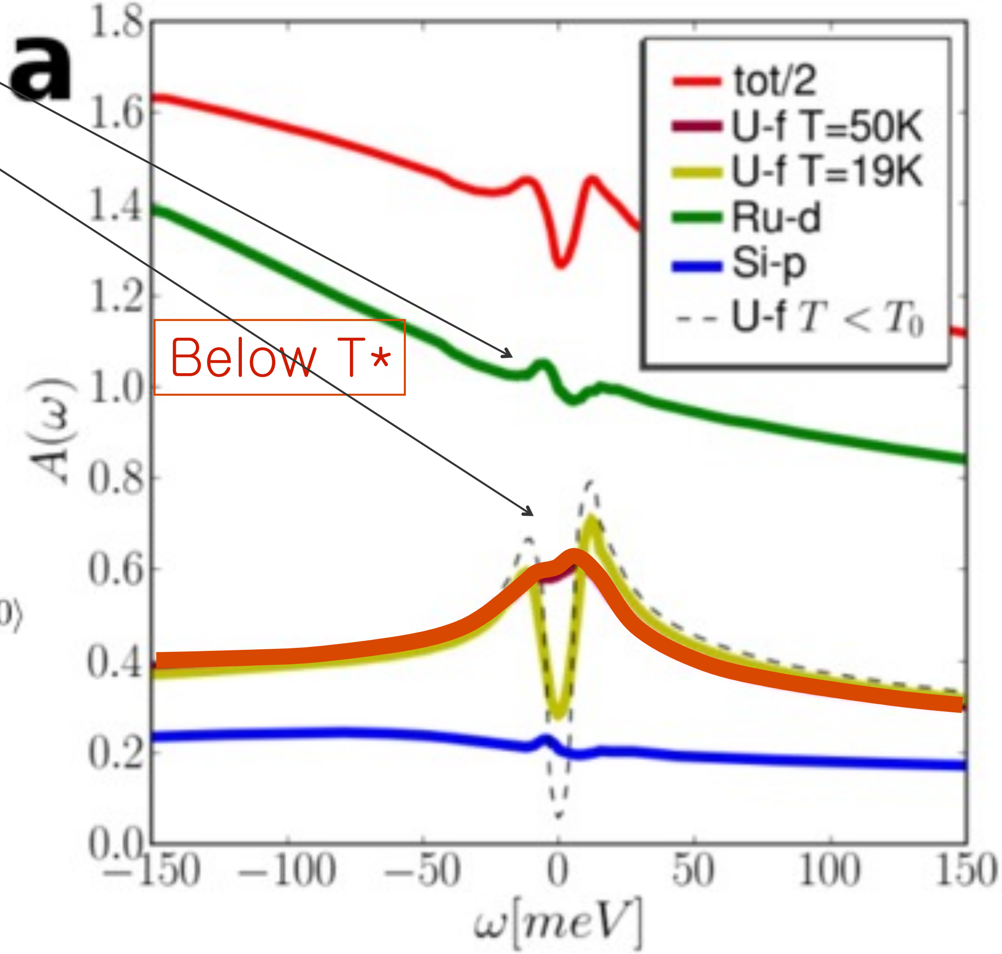


Origin of gapping?

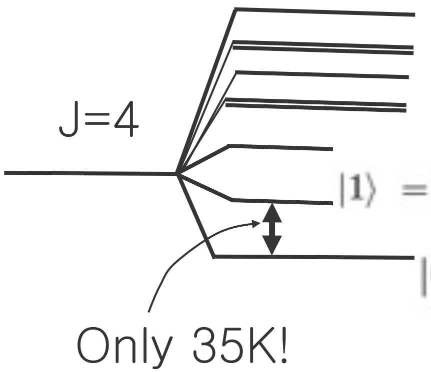


Partial DOS

Small effects on spd electrons
Large effect on U−f's



Ground state atomic multiplet of f^2 configuration in tetragonal field

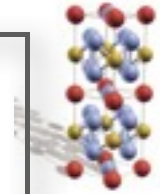


$$|1\rangle = \frac{\cos(\phi)}{\sqrt{2}}(|4\rangle + |-4\rangle) - \sin(\phi)|0\rangle$$

$$|0\rangle = \frac{i}{\sqrt{2}}(|4\rangle - |-4\rangle)$$

|state>==|J=4,Jz>

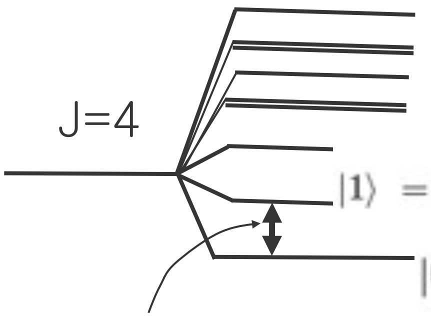
Origin of gapping?



Partial DOS

Small effects on spd electrons
Large effect on U−f's

Ground state atomic multiplet of f^2 configuration in tetragonal field

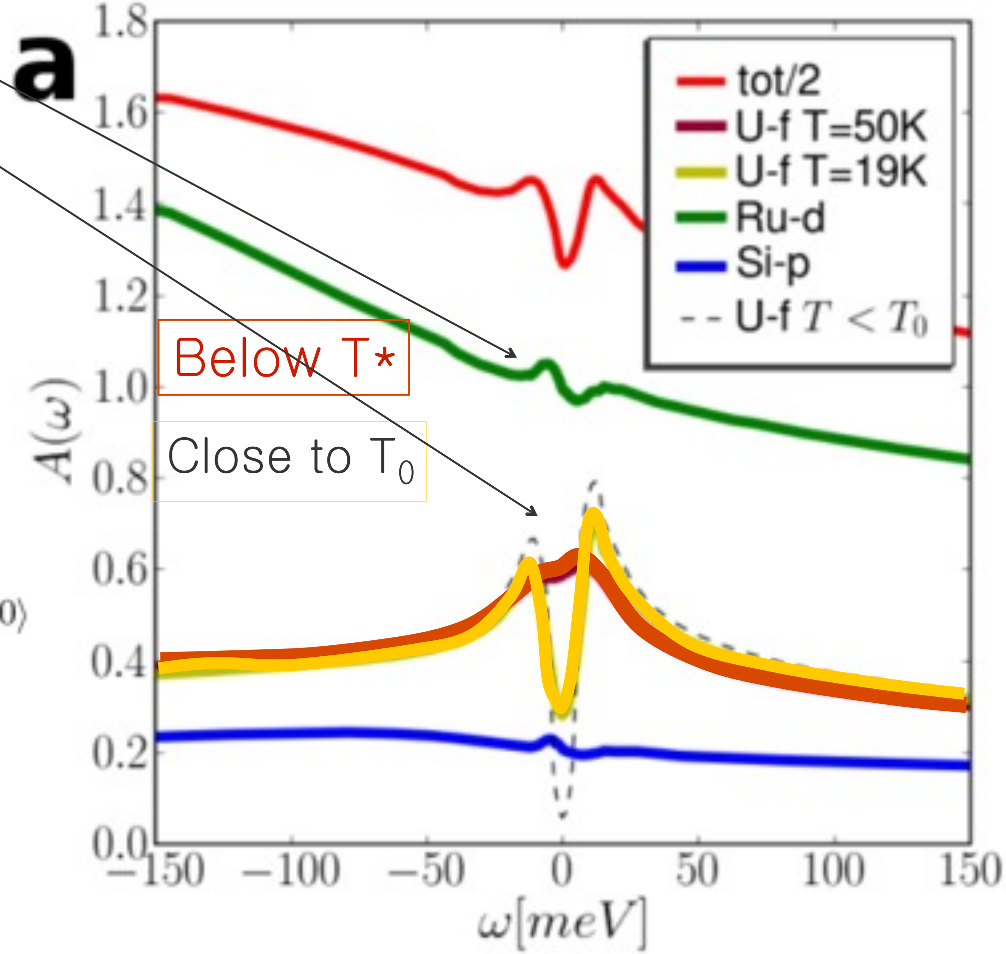


$$|1\rangle = \frac{\cos(\phi)}{\sqrt{2}}(|4\rangle + |-4\rangle) - \sin(\phi)|0\rangle$$

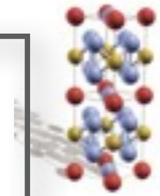
$$|0\rangle = \frac{i}{\sqrt{2}}(|4\rangle - |-4\rangle)$$

Only 35K!

|state>==|J=4,Jz>



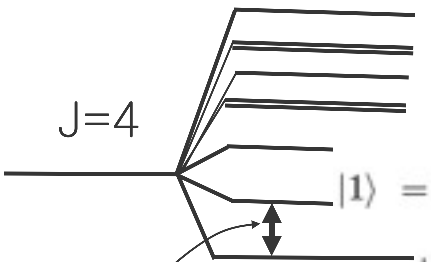
Origin of gapping?



Small effects on spd electrons
Large effect on U−f’s

Ground state atomic multiplet of f^2 configuration in tetragonal field

J=4



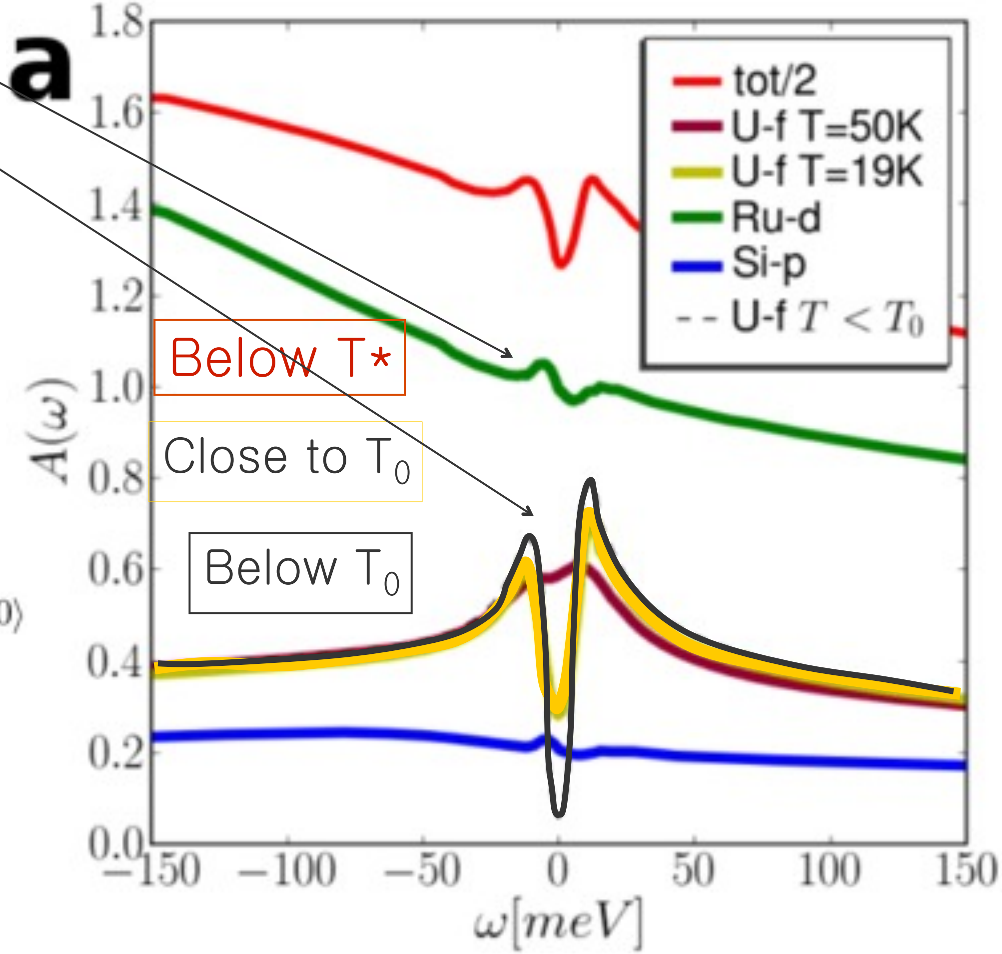
$$|1\rangle = \frac{\cos(\phi)}{\sqrt{2}}(|4\rangle + |-4\rangle) - \sin(\phi)|0\rangle$$

$$|0\rangle = \frac{i}{\sqrt{2}}(|4\rangle - |-4\rangle)$$

Only 35K!

|state>==|J=4,Jz>

Partial DOS

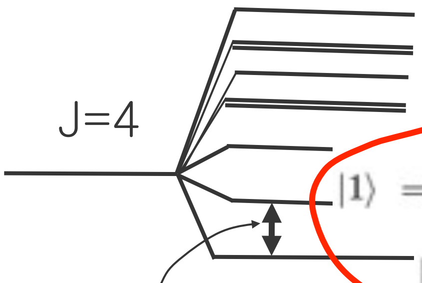


Origin of gapping?

Partial DOS

Small effects on spd electrons
Large effect on U−f's

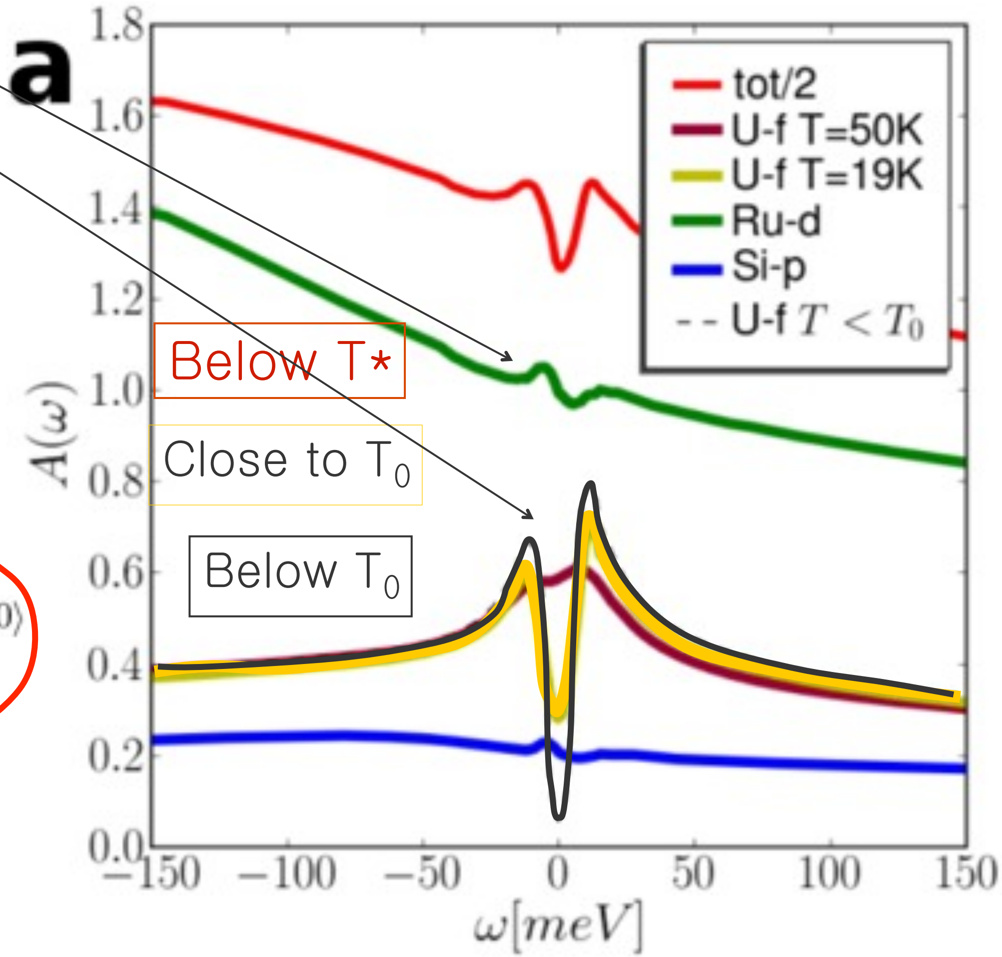
Ground state atomic multiplet of f[2] configuration in tetragonal field

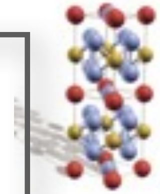


$$|1\rangle = \frac{\cos(\phi)}{\sqrt{2}}(|4\rangle + |-4\rangle) - \sin(\phi)|0\rangle$$

$$|0\rangle = \frac{i}{\sqrt{2}}(|4\rangle - |-4\rangle)$$

|state>==|J=4,Jz>

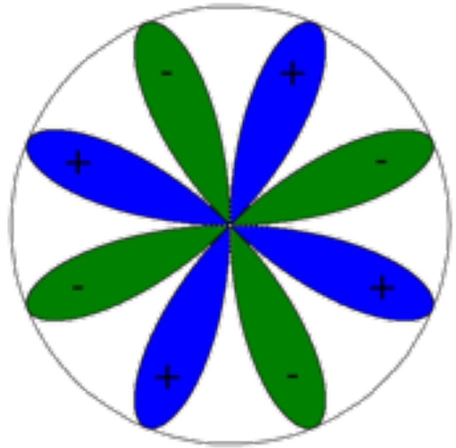




DMFT order parameter

$$|0\rangle = \frac{i}{\sqrt{2}}(|4\rangle - |-4\rangle)$$

$$|1\rangle = \frac{\cos(\phi)}{\sqrt{2}}(|4\rangle + |-4\rangle) - \sin(\phi)|0\rangle$$



Order parameter:

$$\psi_i = \langle X_{01}(\mathbf{R}_i)\rangle$$

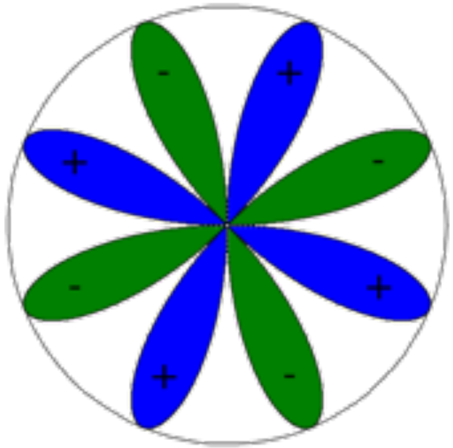
$$\mathrm{Im}\psi \propto \langle J_z\rangle$$

$$\mathrm{Re}\psi \propto \langle(J_xJ_y+J_yJ_x)(J_x^2-J_y^2\rangle$$

DMFT order parameter

$$|0\rangle = \frac{i}{\sqrt{2}}(|4\rangle - |-4\rangle)$$

$$|1\rangle = \frac{\cos(\phi)}{\sqrt{2}}(|4\rangle + |-4\rangle) - \sin(\phi)|0\rangle$$



Order parameter:

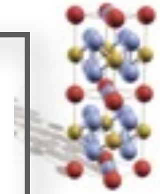
$$\psi_i = \langle X_{01}(\mathbf{R}_i)\rangle$$

$$\text{Im}\psi \propto \langle J_z \rangle$$

$$\text{Re}\psi \propto \langle (J_xJ_y + J_yJ_x)(J_x^2 - J_y^2)\rangle$$

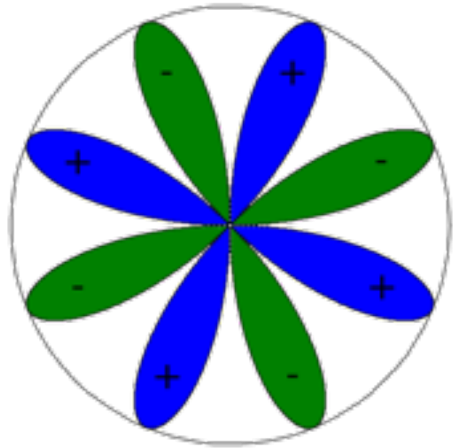
Different orientation gives different phases: adiabatic continuity explained!

DMFT order parameter



$$|0\rangle = \frac{i}{\sqrt{2}}(|4\rangle - |-4\rangle)$$

$$|1\rangle = \frac{\cos(\phi)}{\sqrt{2}}(|4\rangle + |-4\rangle) - \sin(\phi)|0\rangle$$



Order parameter:

$$\psi_i = \langle X_{01}(\mathbf{R}_i)\rangle$$

$$\mathrm{Im}\psi \propto \langle J_z\rangle$$

$$\mathrm{Re}\psi \propto \langle (J_xJ_y + J_yJ_x)(J_x^2 - J_y^2)\rangle$$

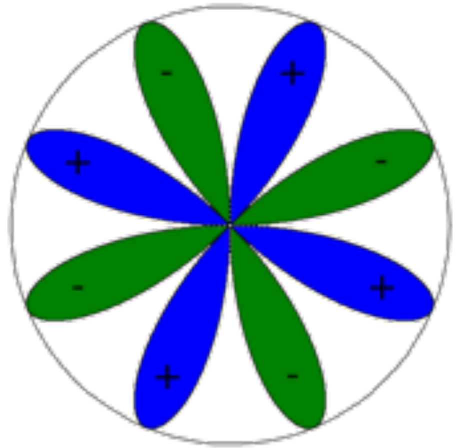
Different orientation gives different phases: adiabatic continuity explained!

Does not break the time reversal, nor C4 symmetry. It breaks inversion symmetry.

DMFT order parameter

$$|0\rangle = \frac{i}{\sqrt{2}}(|4\rangle - |-4\rangle)$$

$$|1\rangle = \frac{\cos(\phi)}{\sqrt{2}}(|4\rangle + |-4\rangle) - \sin(\phi)|0\rangle$$



Order parameter:

$$\psi_i = \langle X_{01}(\mathbf{R}_i)\rangle$$

$$\mathrm{Im}\psi \propto \langle J_z\rangle$$

$$\mathrm{Re}\psi \propto \langle (J_xJ_y + J_yJ_x)(J_x^2 - J_y^2)\rangle$$

Different orientation gives different phases: adiabatic continuity explained!

Does not break the time reversal, nor C4 symmetry. It breaks inversion symmetry.

In the atomic limit:

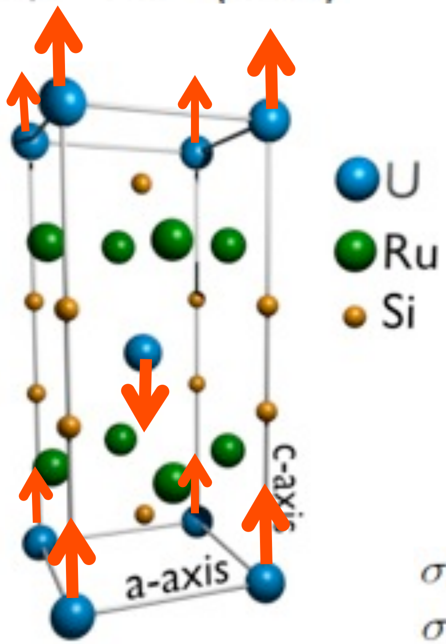
$$|gs\rangle = \cos(\theta)|0\rangle + \sin(\theta)e^{i\varphi}|1\rangle$$

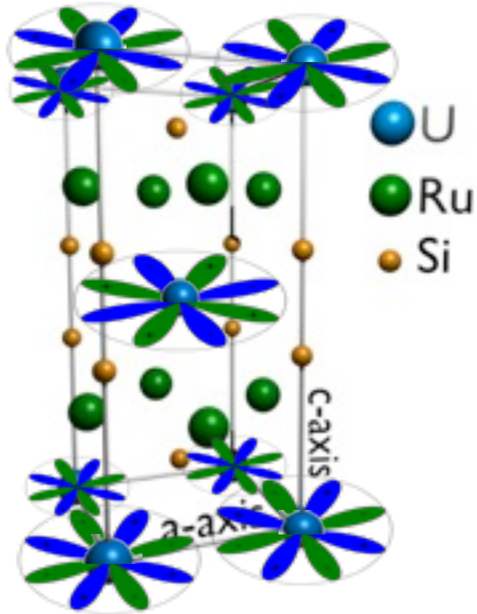
$$\langle gs|\mathbf{J}|gs\rangle = 4\cos(\phi)\sin(2\theta)\sin(\varphi) * (0,0,1)$$

Moment only in z-direction!

The two broken symmetry states

$\mathrm{Im}\psi \propto \langle J_z \rangle$ $\mathrm{Re}\psi \propto \langle (J_x J_y + J_y J_x)(J_x^2 - J_y^2) \rangle$





A toy model

$$\sigma_3 = |\emptyset\rangle\langle\emptyset| - |1\rangle\langle 1|$$
$$\sigma_1 = |\emptyset\rangle\langle 1| + |1\rangle\langle\emptyset|$$
$$\sigma_2 = i(|1\rangle\langle\emptyset| - |\emptyset\rangle\langle 1|)$$

Magnetic moment: y–direction

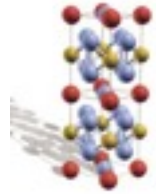
Hexadecapole: x–direction

crystal field: z direction

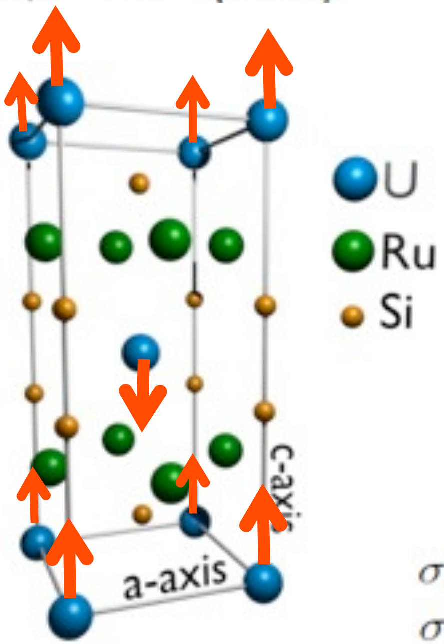
XY–Ising

$$H = \sum_i -\frac{\Delta}{2}\sigma_3^i - \frac{1}{2} g\mu_B B |\langle 1|J_z|\emptyset\rangle| \sigma_2^i + \sum_{i,j} \frac{1}{2}(J_{ij}^1 \sigma_1^i \sigma_1^j + J_{ij}^2 \sigma_2^i \sigma_2^j)$$

The two broken symmetry states

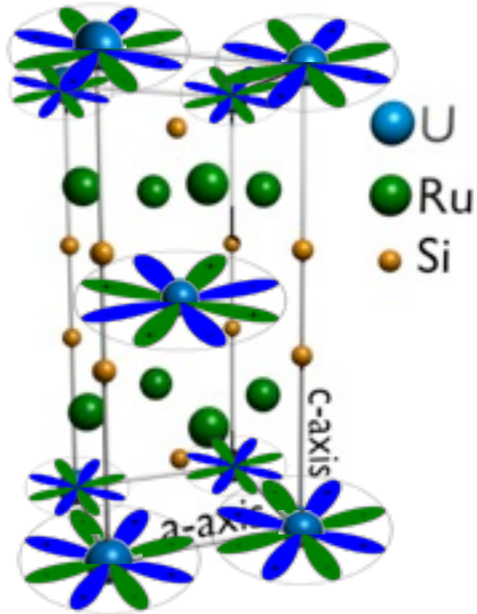


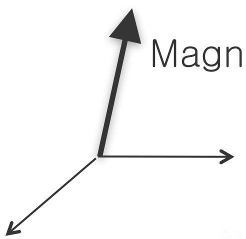
$\mathrm{Im}\psi \propto \langle J_z \rangle$ $\mathrm{Re}\psi \propto \langle (J_x J_y + J_y J_x)(J_x^2 - J_y^2) \rangle$

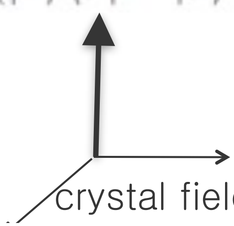


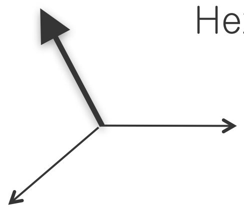
A toy model

$$\sigma_3 = |\emptyset\rangle\langle\emptyset| - |1\rangle\langle 1|$$
$$\sigma_1 = |\emptyset\rangle\langle 1| + |1\rangle\langle\emptyset|$$
$$\sigma_2 = i(|1\rangle\langle\emptyset| - |\emptyset\rangle\langle 1|)$$









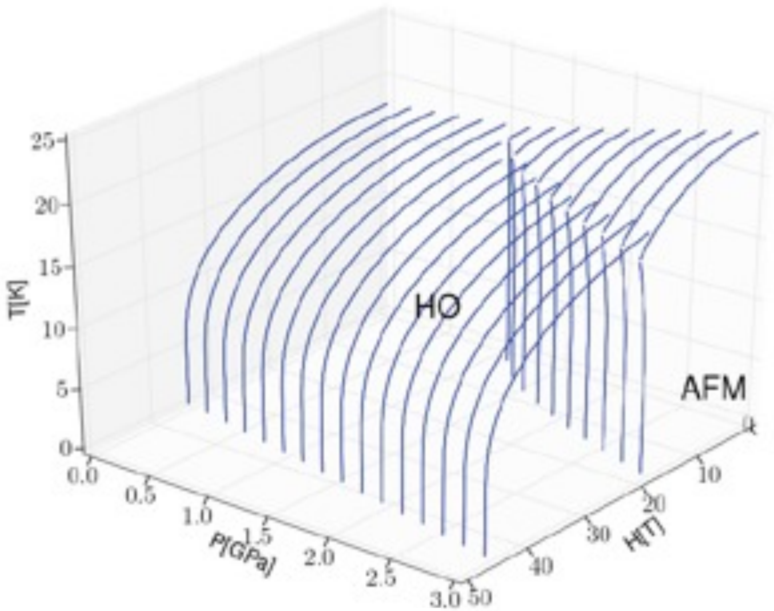
XY−Ising

$$H = \sum_i -\frac{\Delta}{2}\sigma_3^i - \frac{1}{2} g\mu_B B |\langle 1|J_z|\emptyset\rangle| \sigma_2^i + \sum_{i,j} \frac{1}{2}(J_{ij}^1 \sigma_1^i \sigma_1^j + J_{ij}^2 \sigma_2^i \sigma_2^j)$$

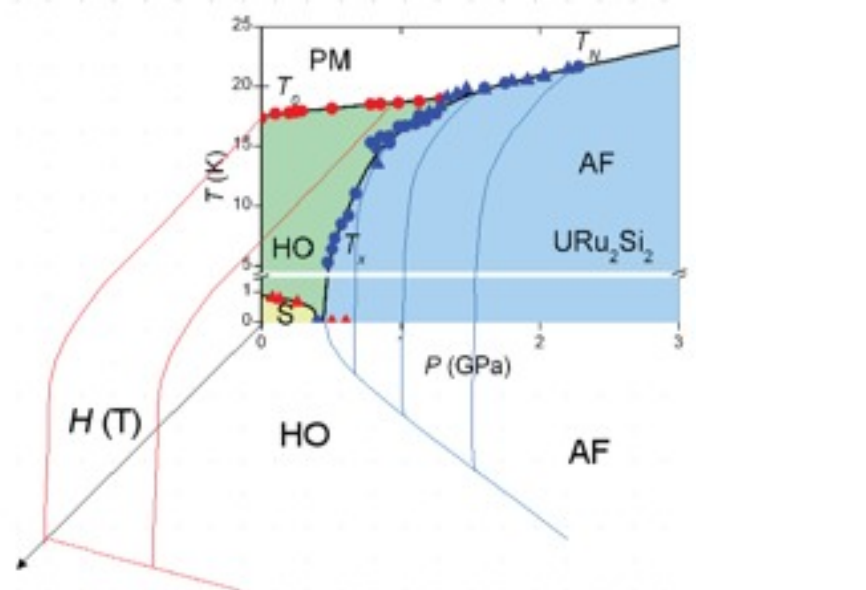
HO&AFM in magnetic field

KH & G.Kotliar, arxiv: arXiv:0907.3892

$$F[h,\psi] = \frac{1}{2}\sum_{ij,\alpha=(1,2)} J^{\alpha}_{ij}\,\psi^{\alpha}_i\psi^{\alpha}_j - \sum_{i,\alpha=(1,2)} (h^{\alpha}_i + b^{\alpha})\psi^{\alpha}_i - T\sum_i \log\left(\cosh\left(\beta\sqrt{(\Delta/2)^2 + (h^1_i)^2/2 + (h^2_i)^2/2}\right)\right)$$



Mean field



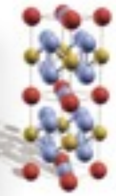
Exp. by E. Hassinger et.al. PRL 77, 115117 (2008)

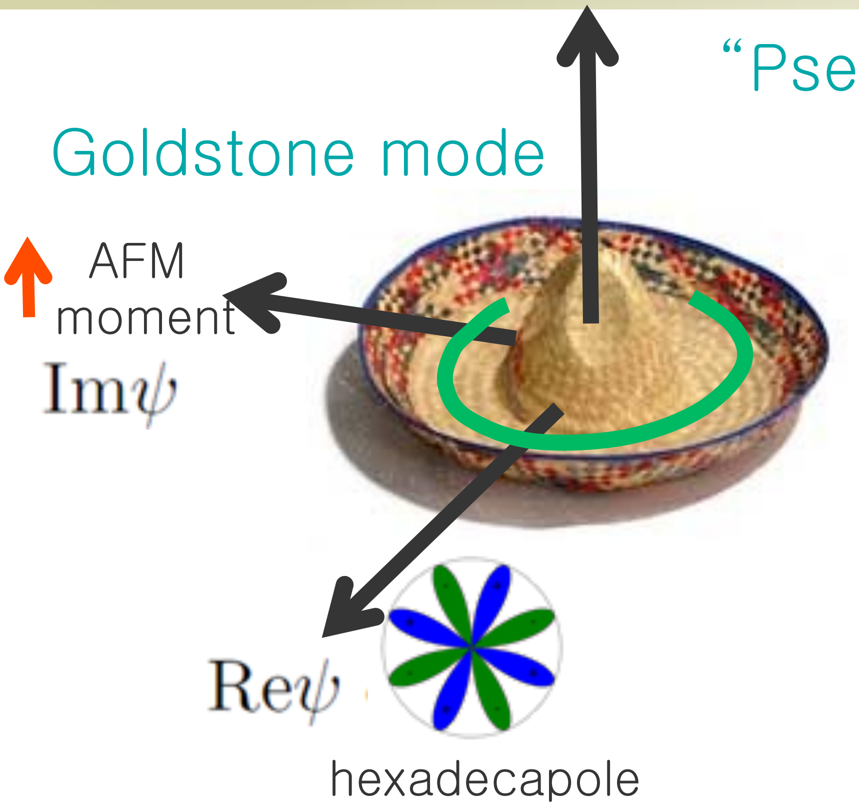
Only two fitting parameters: J_{eff}^1 , J_{eff}^2 $J^1_{eff} = \dfrac{\Delta}{\tanh(\Delta/(2T_0))}$

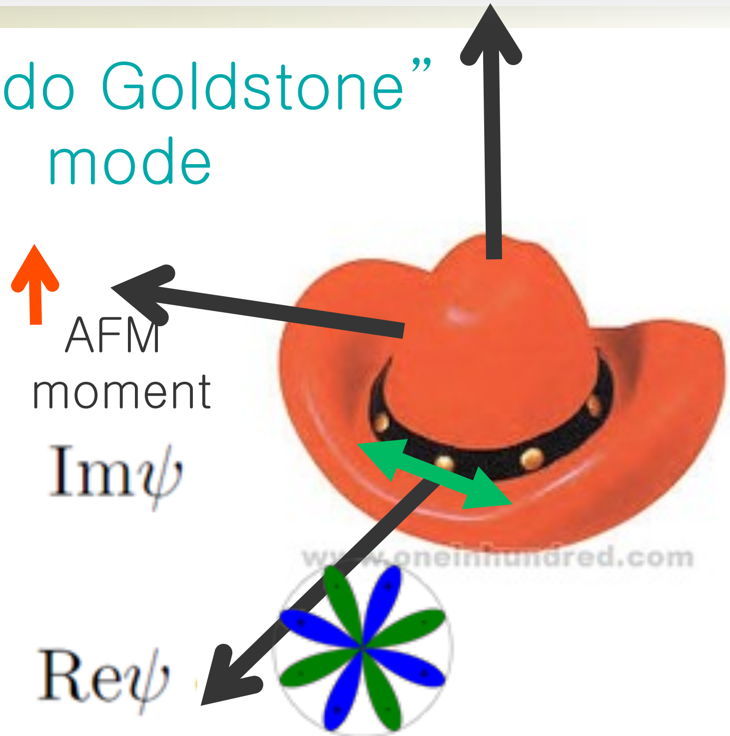
$J_{eff} = 4|J_1| + 8J_2$

determined by exp. transition temperature: $J^2_{eff} = \dfrac{\Delta}{\tanh(\Delta/(2T_N))}$

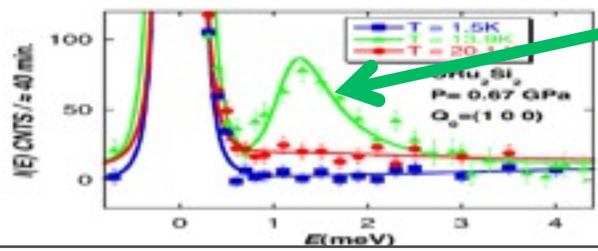
Neutron scattering experiments



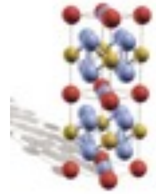




Symmetry is approximate
"Pseudo–Goldstone" mode
Fluctuation of m – finite mass



The exchange constants J
are slightly different in the two phases (~6%)



If you are :

- looking for a postdoc
- interested in materials theory

Please apply to Rutgers NOW :

haule@physics.rutgers.edu

THANKS!