Spin Dynamics and Pairing in Iron Superconductors from DMFT perspective

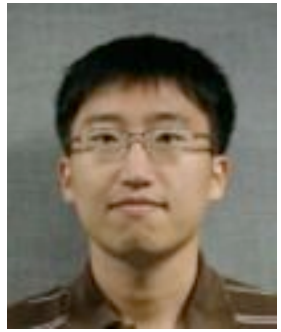
RUTGERS
THE STATE UNIVERSITY OF NEW JERSEY

Kristjan Haule

Support:
NSF
ALFRED P. SLOAN FOUNDATION 1934
ACS Chemistry for Life

Boston, 2013

Work mainly contributed by



Zhiping Yin, (Rutgers)

G. Kotliar (Rutgers)

Hyowon Park: (Columbia)

Building Computational Theoretical Tools

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

Computational tool
developed at Rutgers

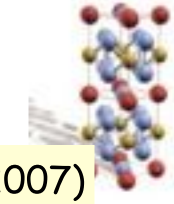
Wien2K+DMFT
multiorbital CTQMC, full potential basis, charge self-consistent.

Thermoelectricity in FeSi as Hunds semiconductors

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

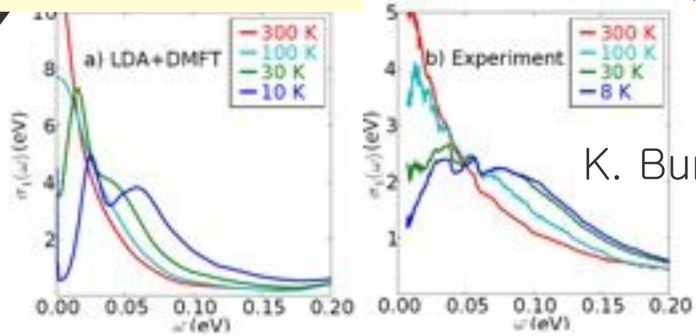
MIT in FeO

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)

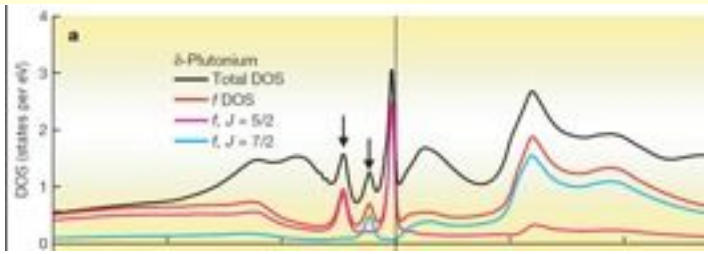


K. Burch et.al.

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

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)

Magnetism and Charge Dynamics in Iron Pnictides.

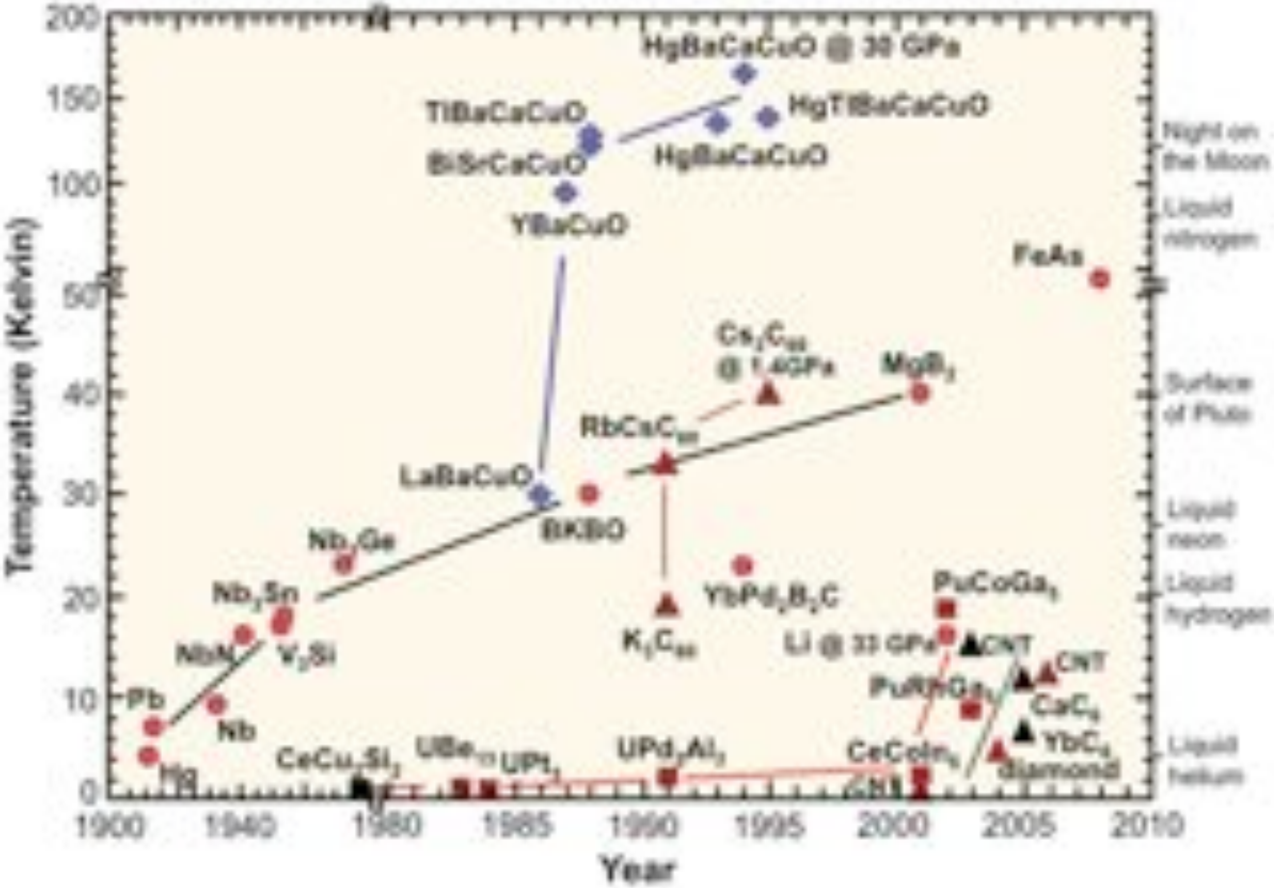
Z. P. Yin, KH, G. Kotliar, Nature Physics (2011)

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

Hidden Order in URu2Si2, Kondo effect and hexadecapole order.

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

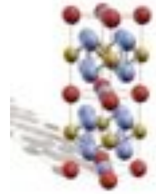
High temperature superconductors

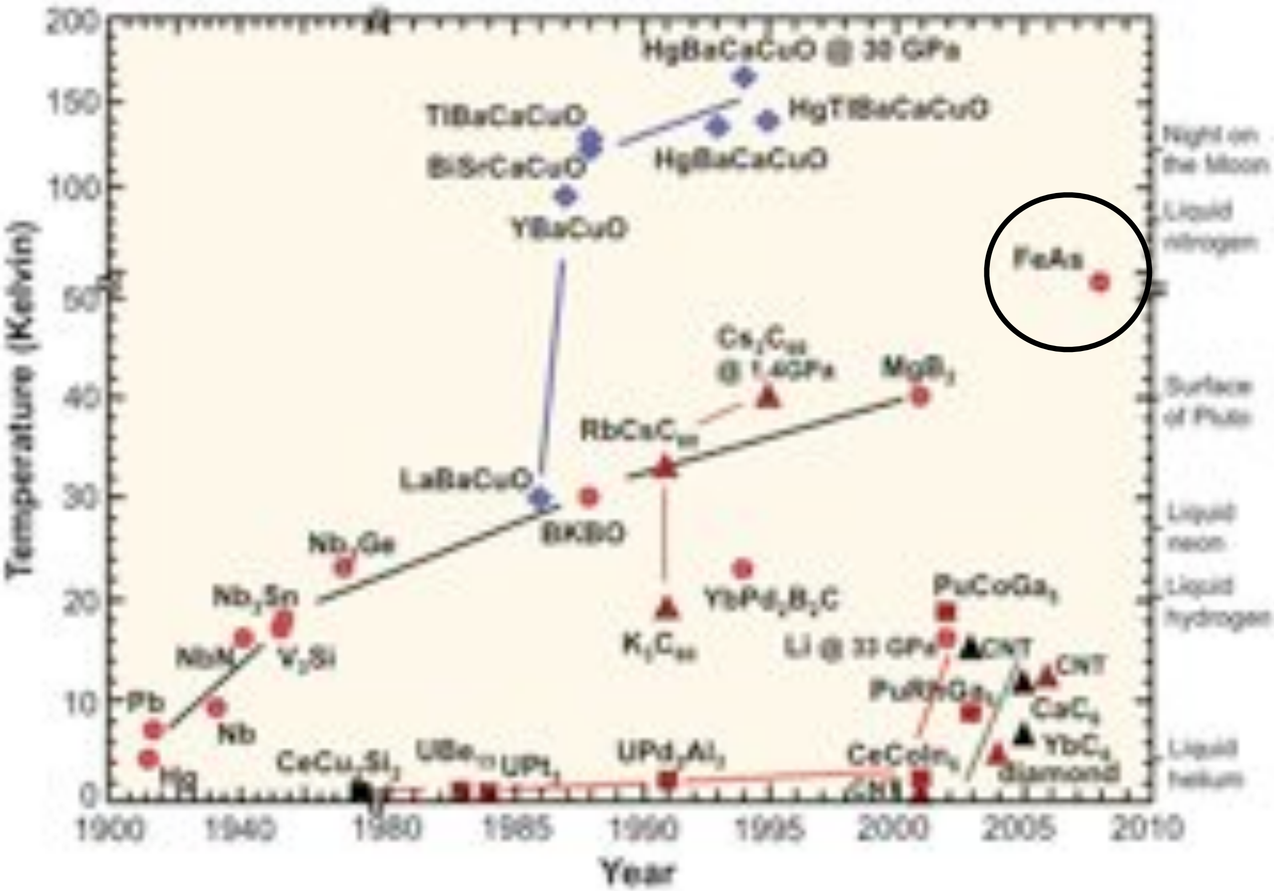


H. Hosono

Reenergize high-Tc field

High temperature superconductors





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Reenergize
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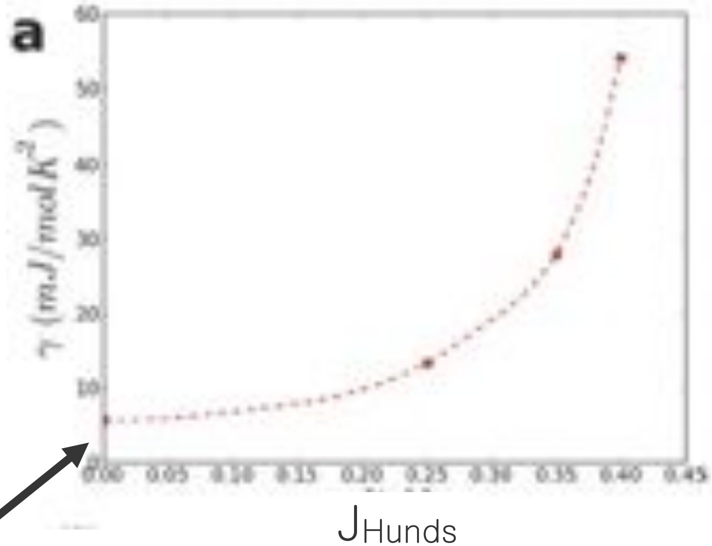
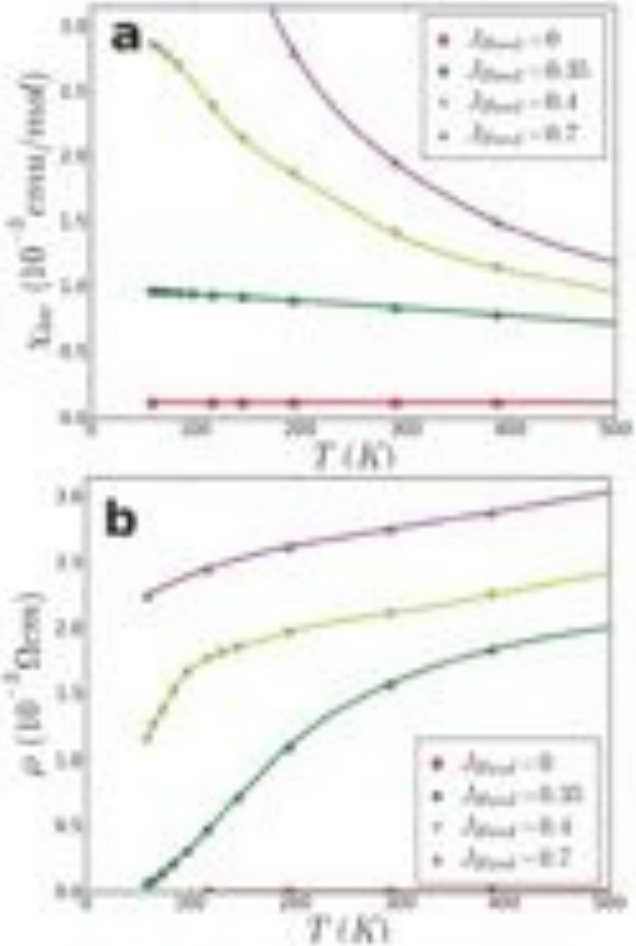
Importance of Hund's rule in pnictides:
Hunds Metals

Significant Correlations in pnictides:
effective mass 3−5 band mass
KH, J.H. Shim, and G. Kotliar, PRL 100, 226402 (2008)





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

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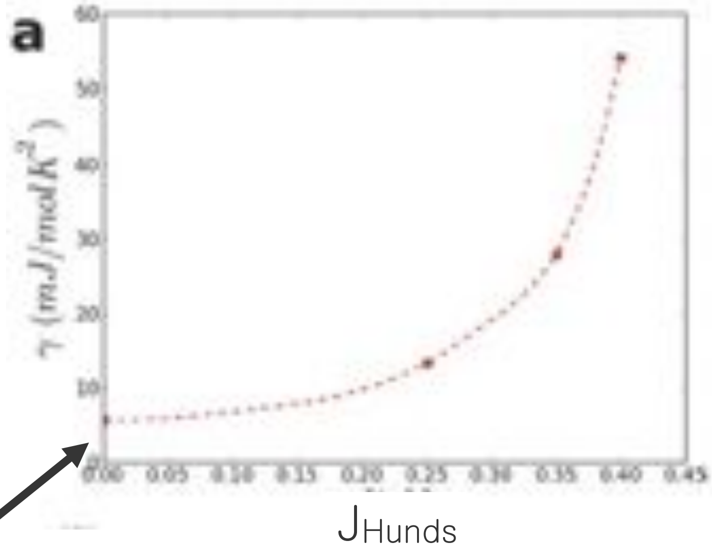
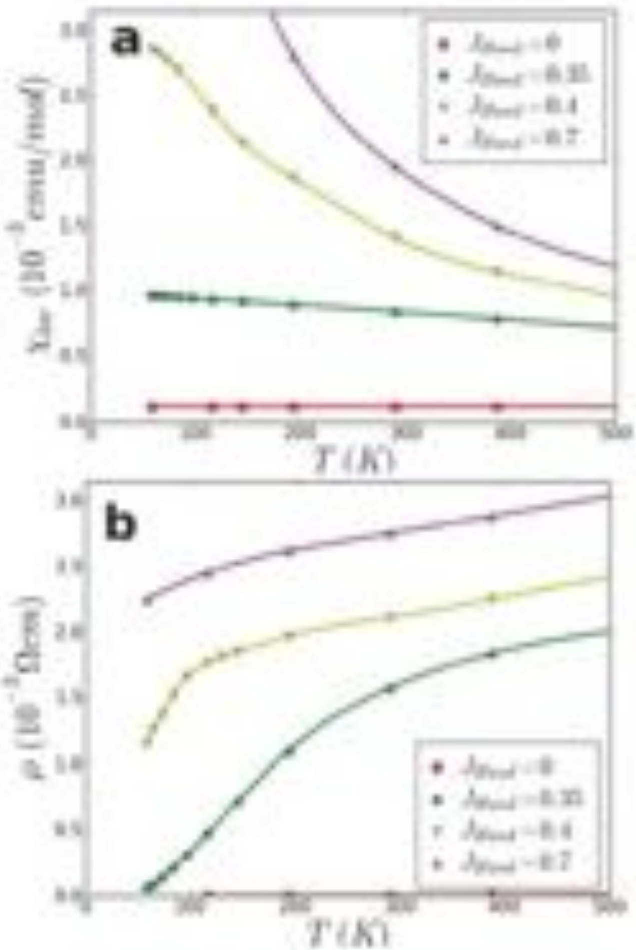


LDA value



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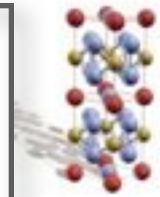

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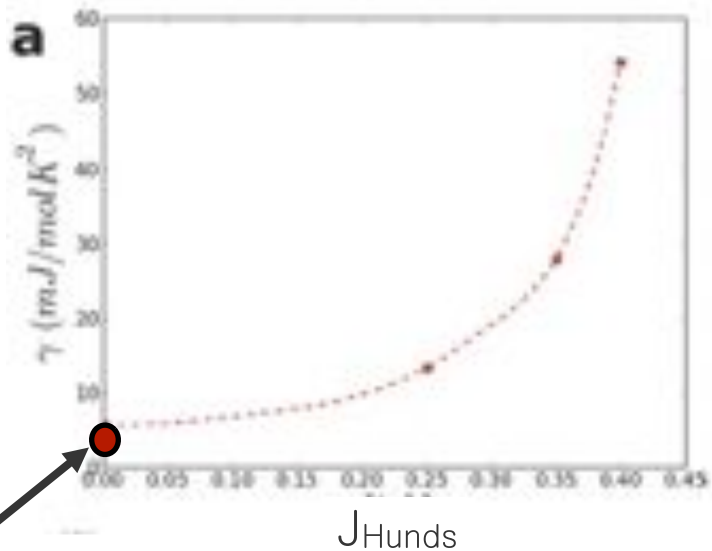
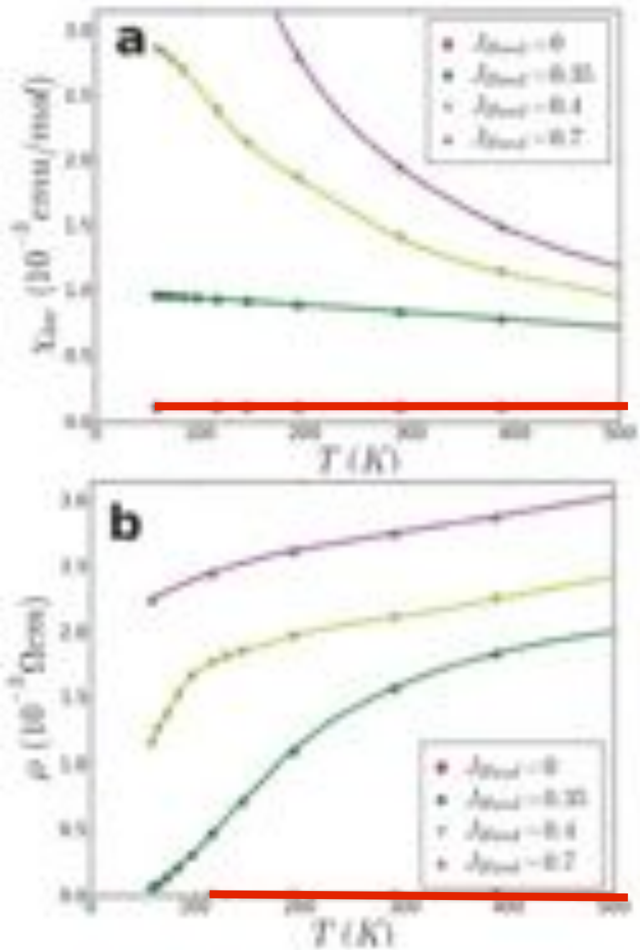


LDA value

J=0



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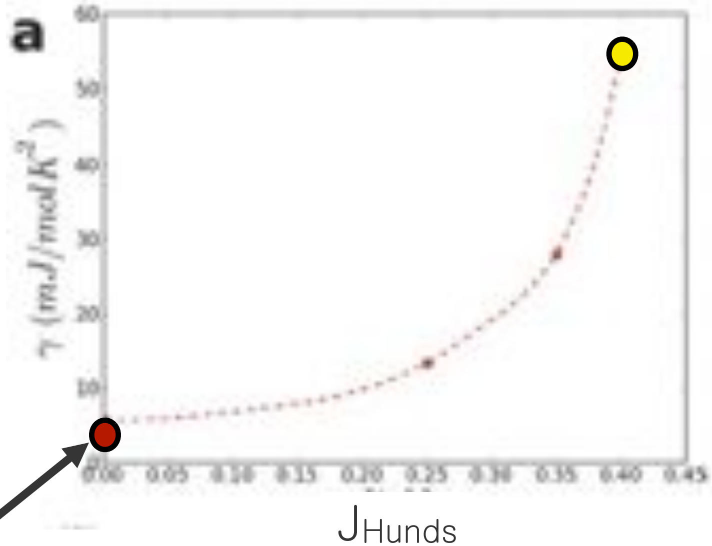
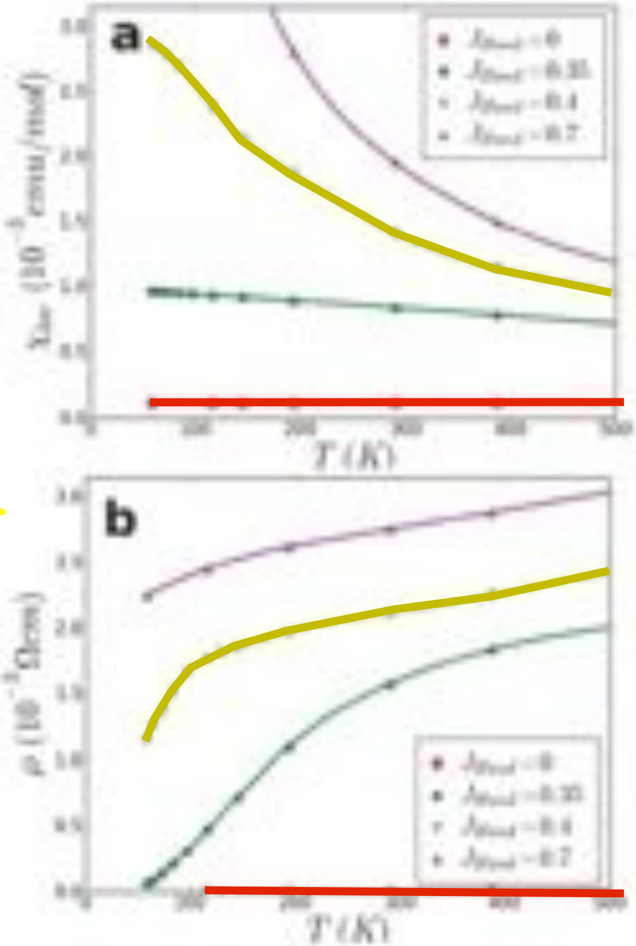


LDA value

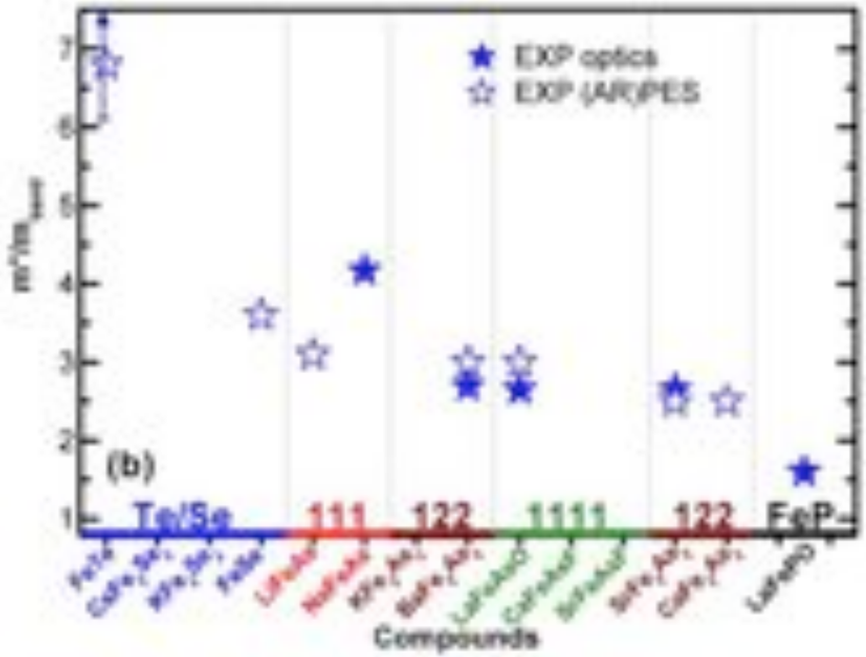
J=0.4



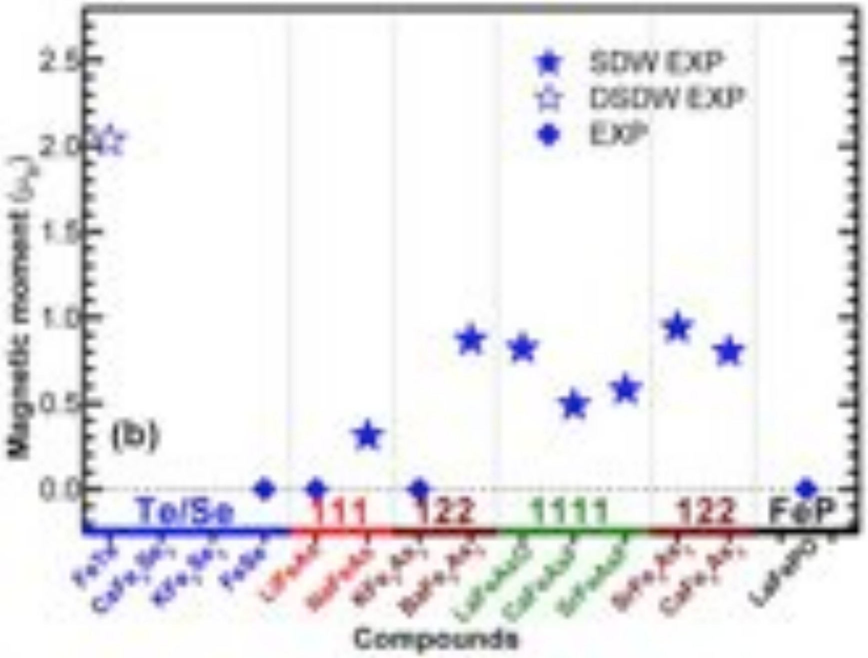
For J=0 there is negligible mass enhancement at U~W!

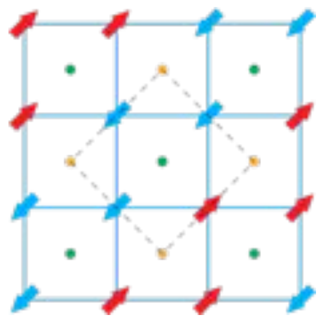
All FeSCs share the same FePn layer, but there are large variations among them.

Mass enhancement in the PM phase.

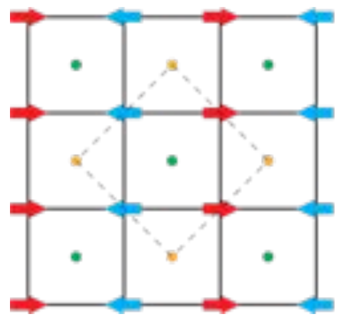


Magnetic moment in the ordered phases.





DSDW



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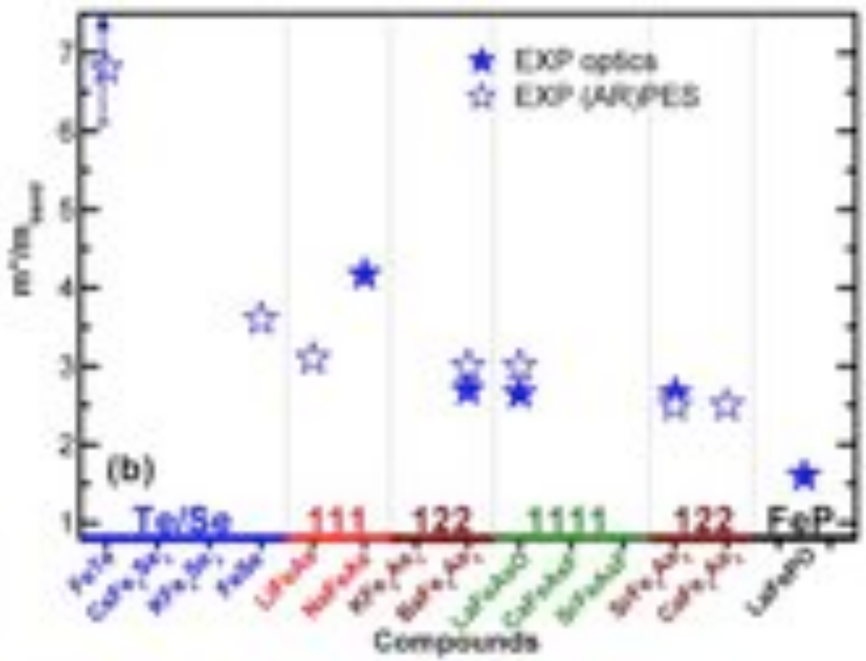

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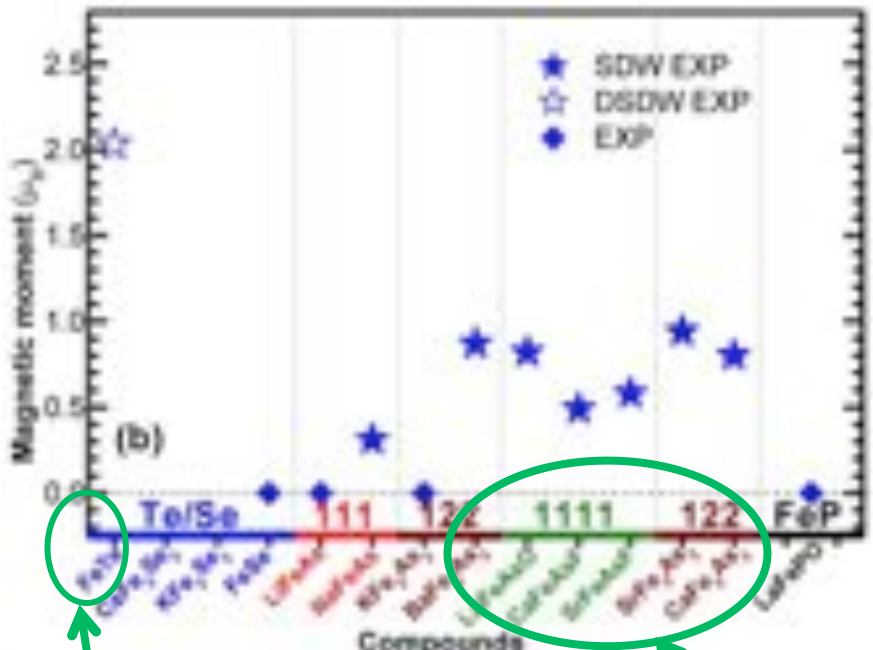
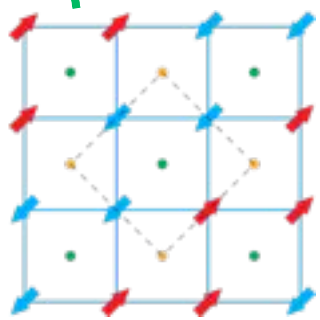
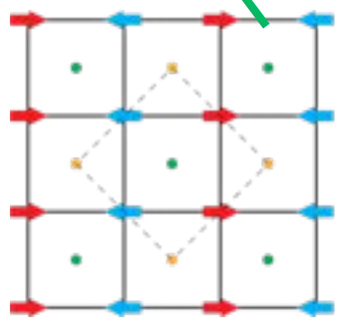




DSDW



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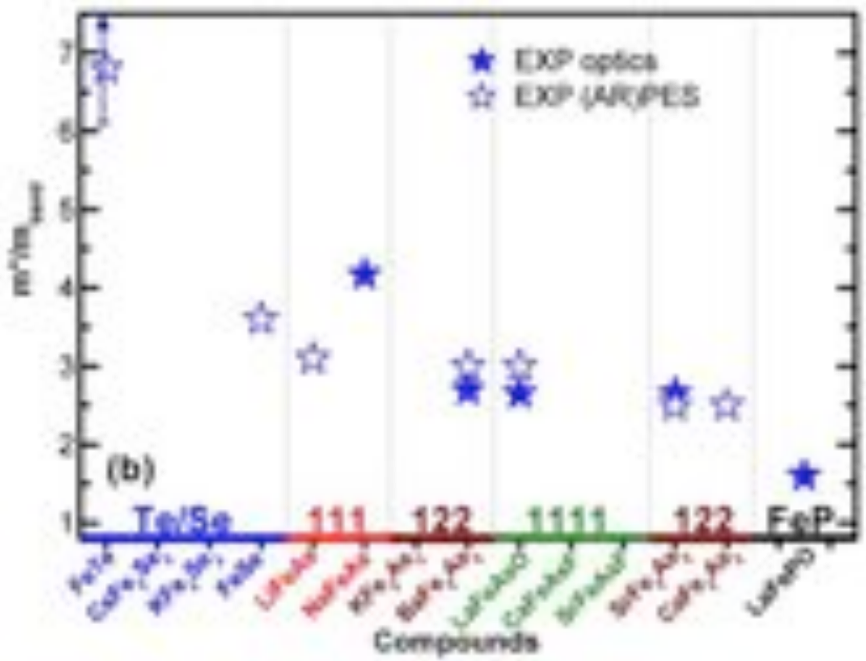

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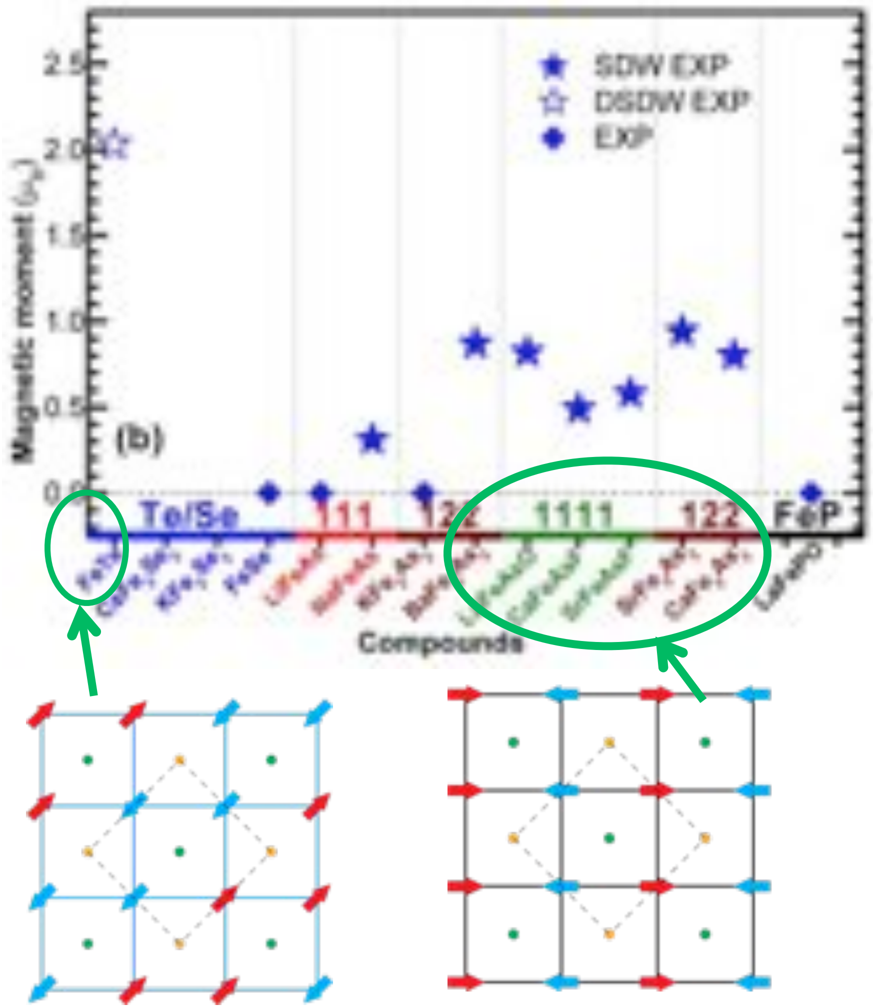


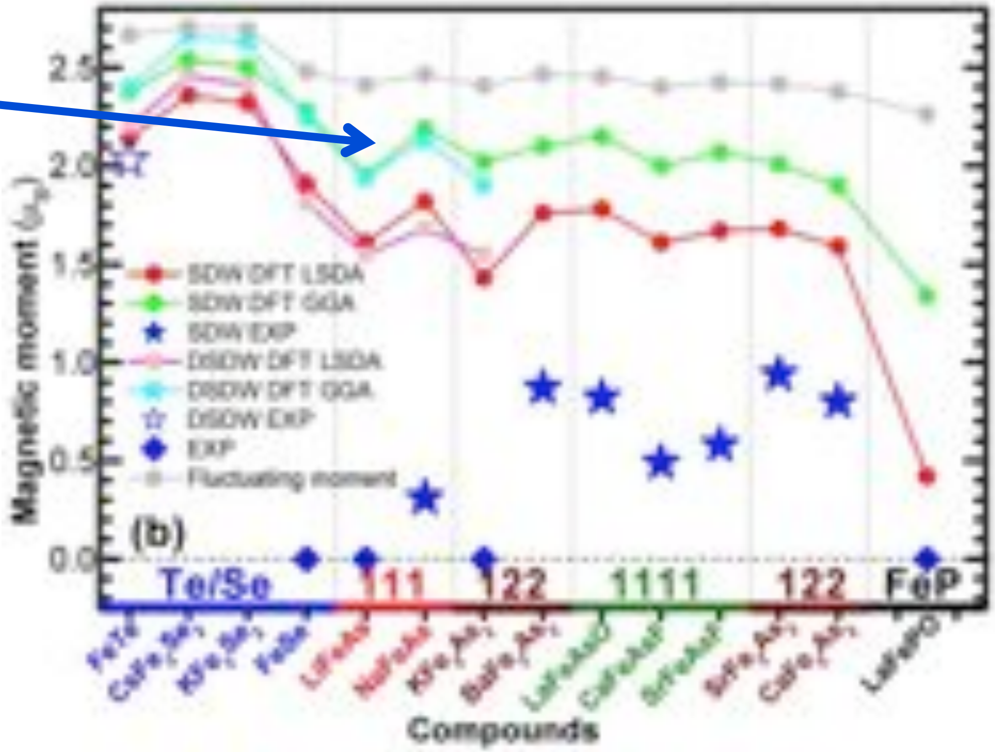
DSDW

SDW

Neither the local picture nor the itinerant picture can fully describe them.

Moments and Magnetism

Moments by DFT are around 2 μ_B, overestimated by a factor of two (ZPY et al, PRL **101**, 047001 (2008).)



Experimental moment (μ_B):

FeTe: 2.03, W. Bao *et al.*, PRL **102**, 247001 (2009).
NaFeAs: 0.31, L. Ma *et al.*, PRB **83**, 132501 (2011).
Ba122: 0.87, Q. Huang *et al.*, PRL **101**, 257003 (2008).
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CaFeAsF: 0.49, Y. Xiao *et al.*, PRB **79**, 060504(R) (2009).
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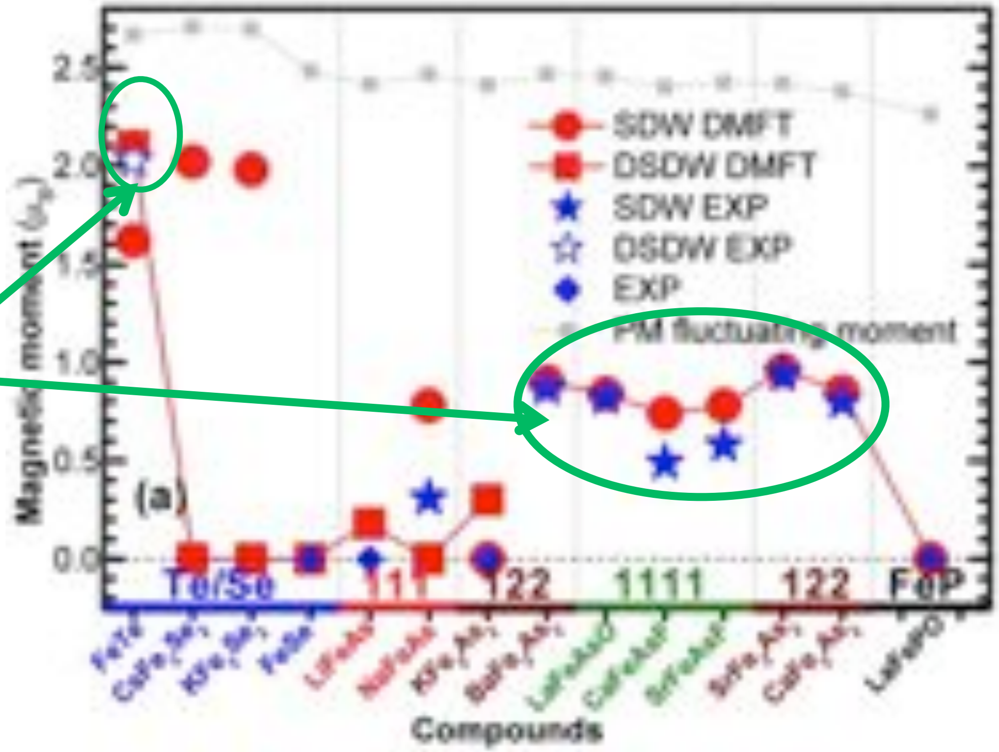
Moments by DFT+DMFT are in good agreement with experiments



Theory
ZPY, K. Haule and G. Kotliar, Nature Materials **10**, 932 (2011).

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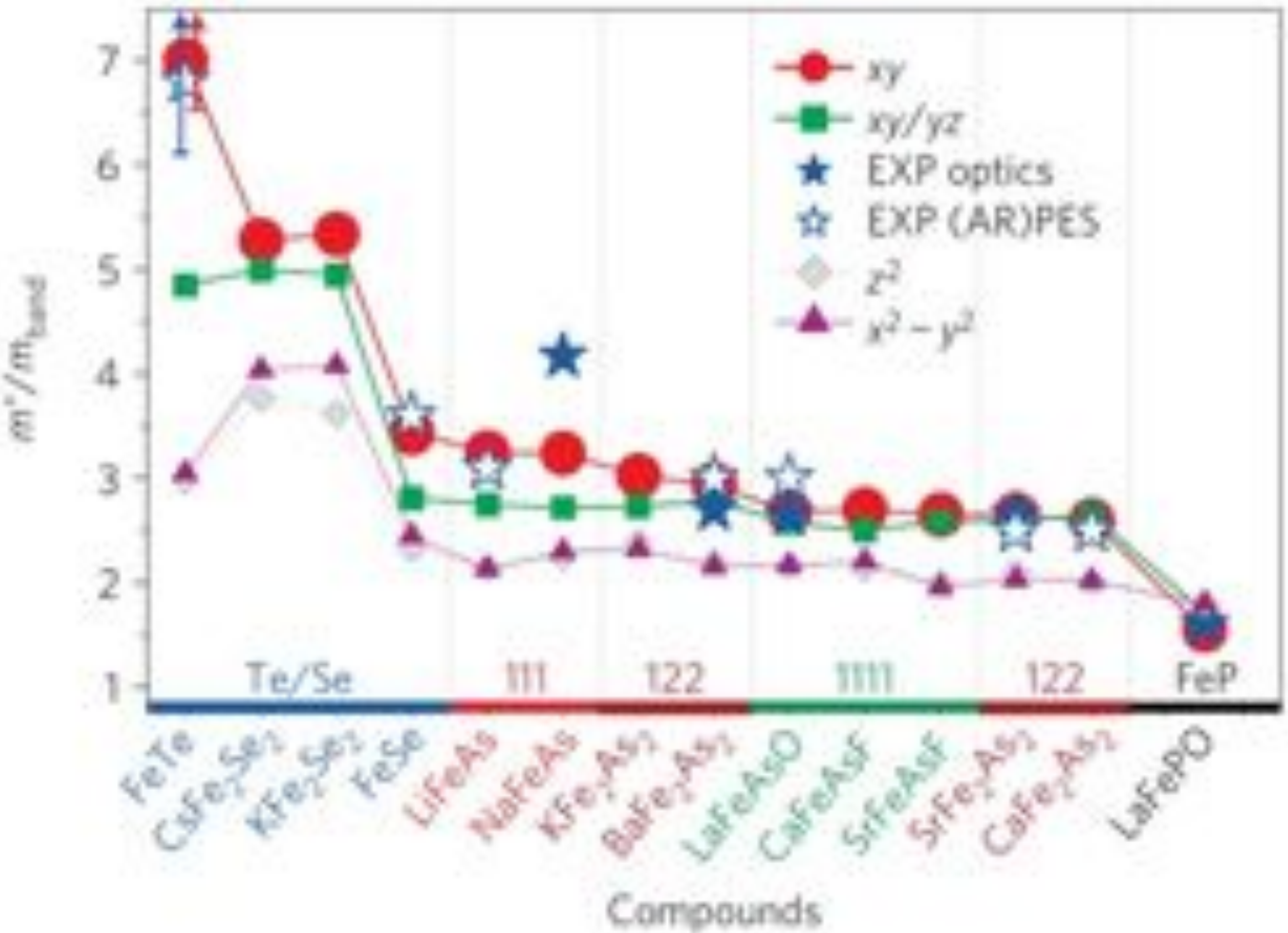
Mass enhancement



ZPY, K. Haule and G. Kotliar,
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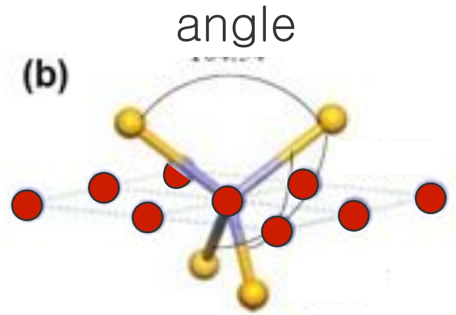
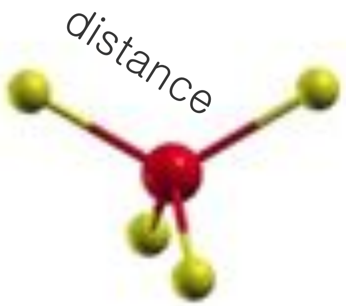
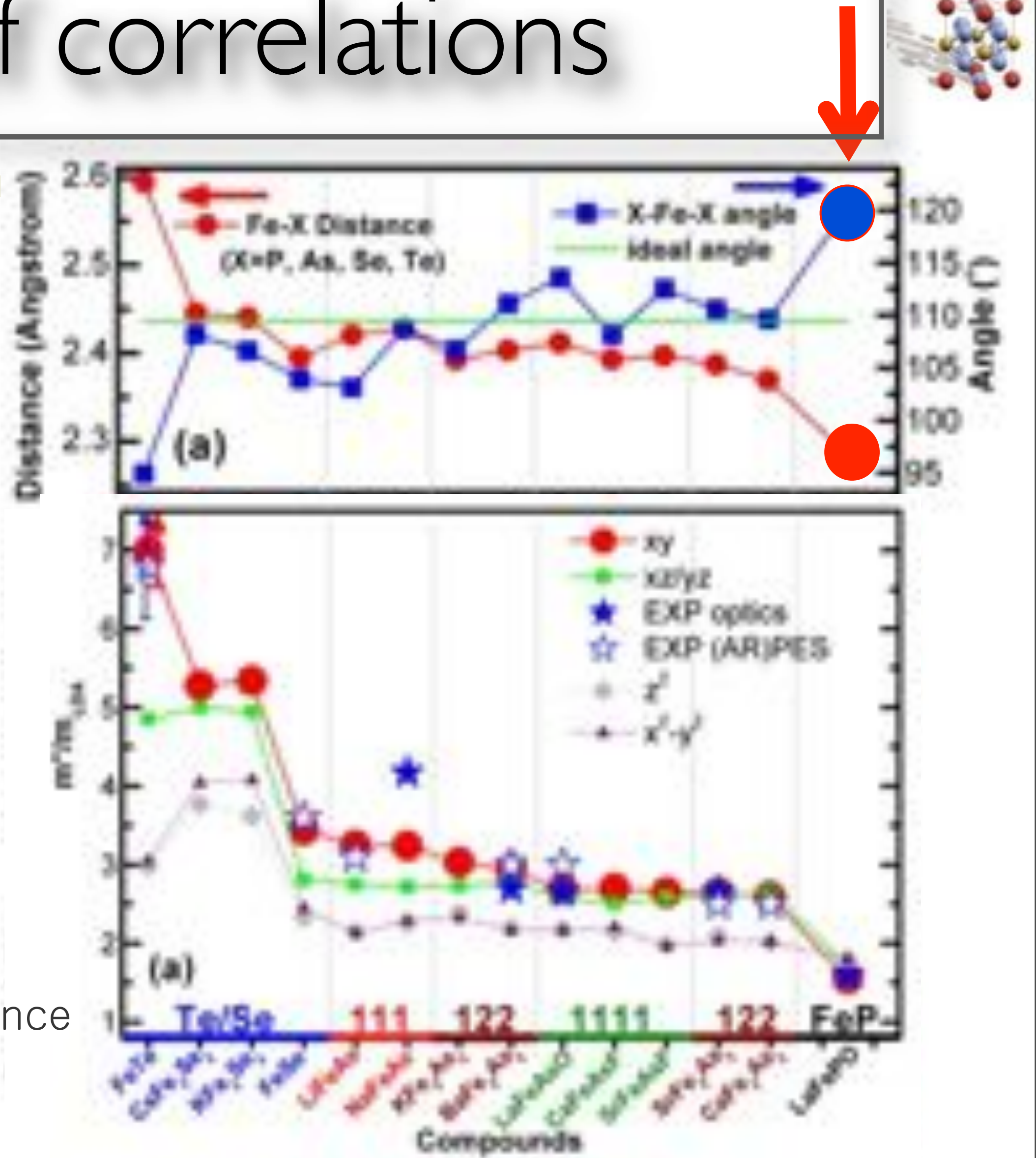
DFT+DMFT accounts for the variations in all families without tuning parameter (U or J)!

Strength of correlations



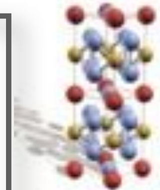


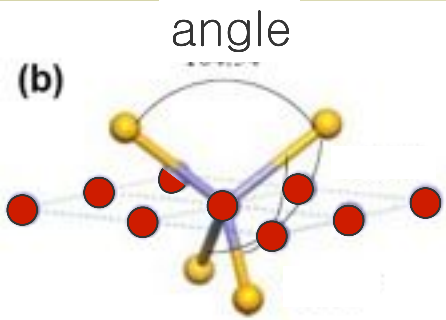


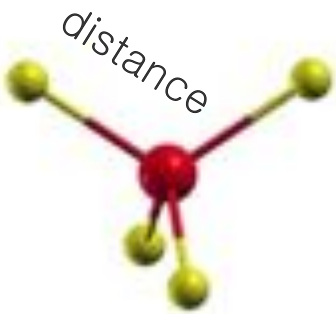
Overal trend consistent with Fe-As distance

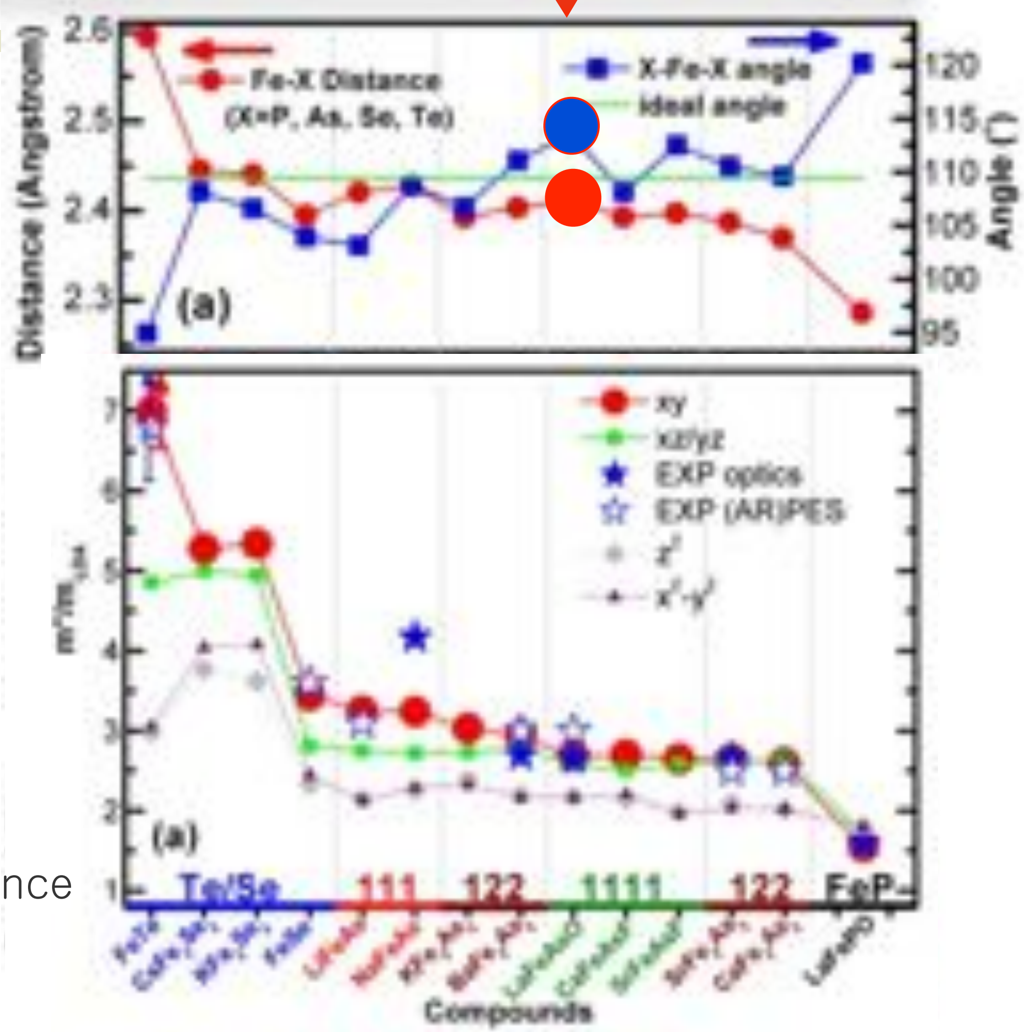
Hybridization with pnictogen

Strength of correlations









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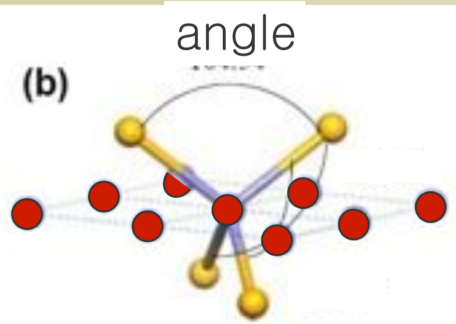

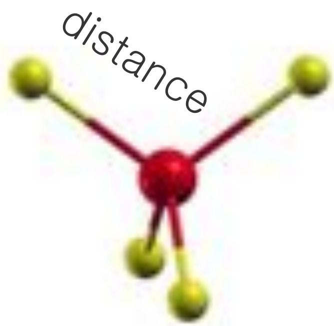

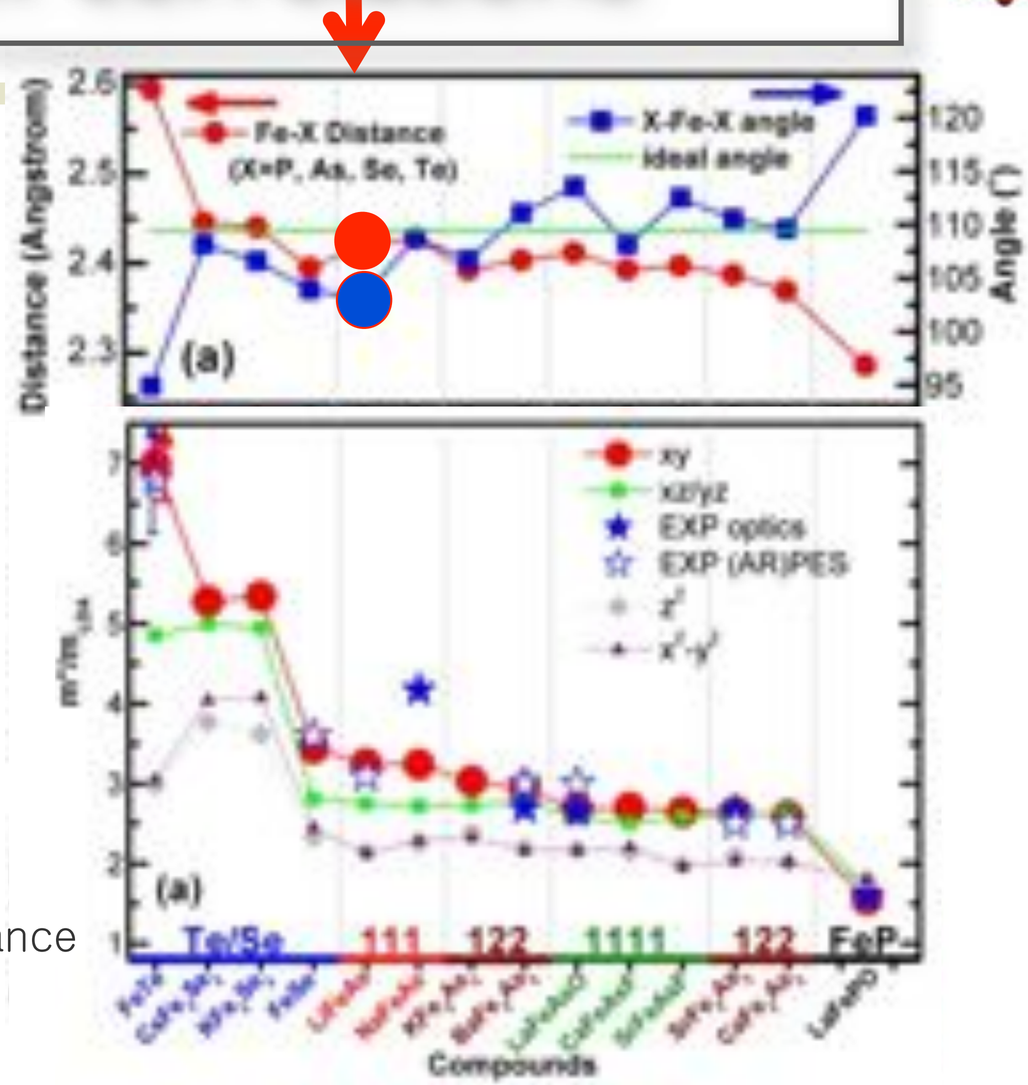

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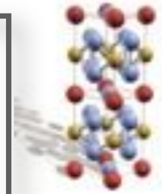
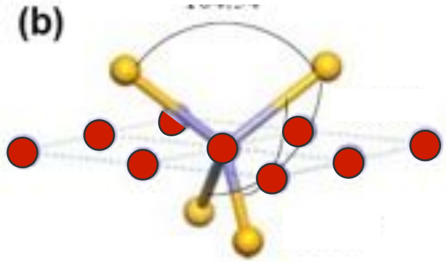
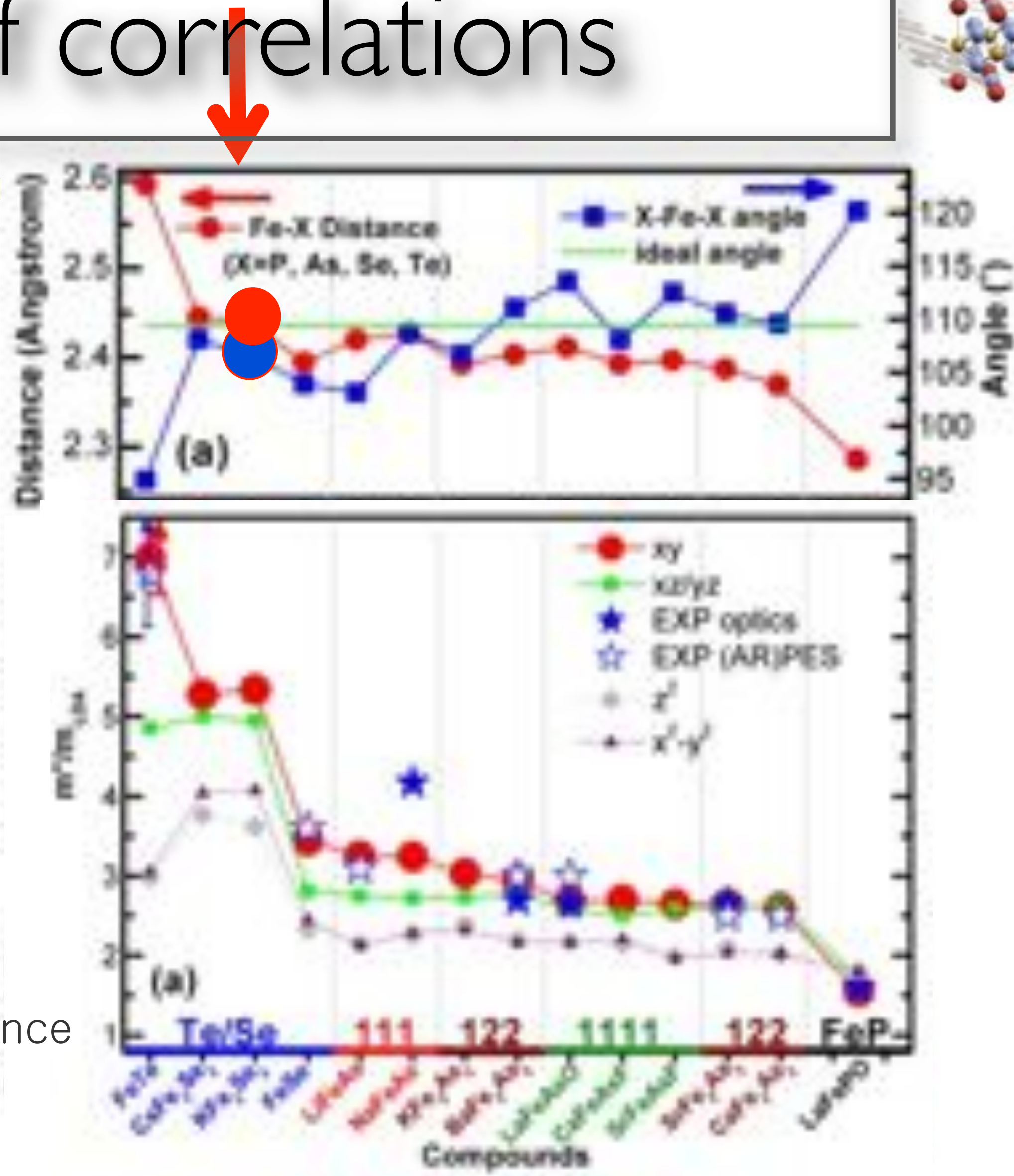


angle

(b)





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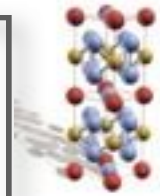

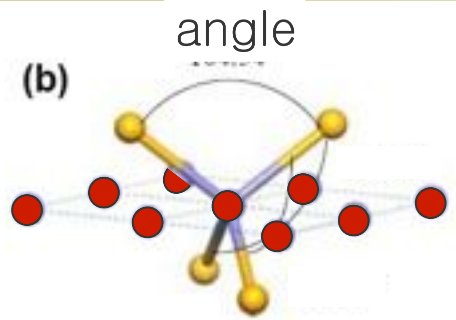

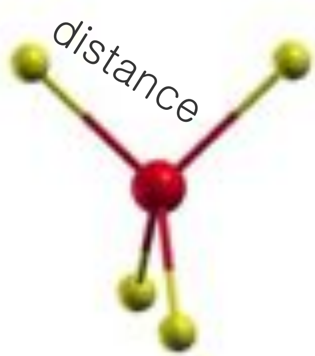

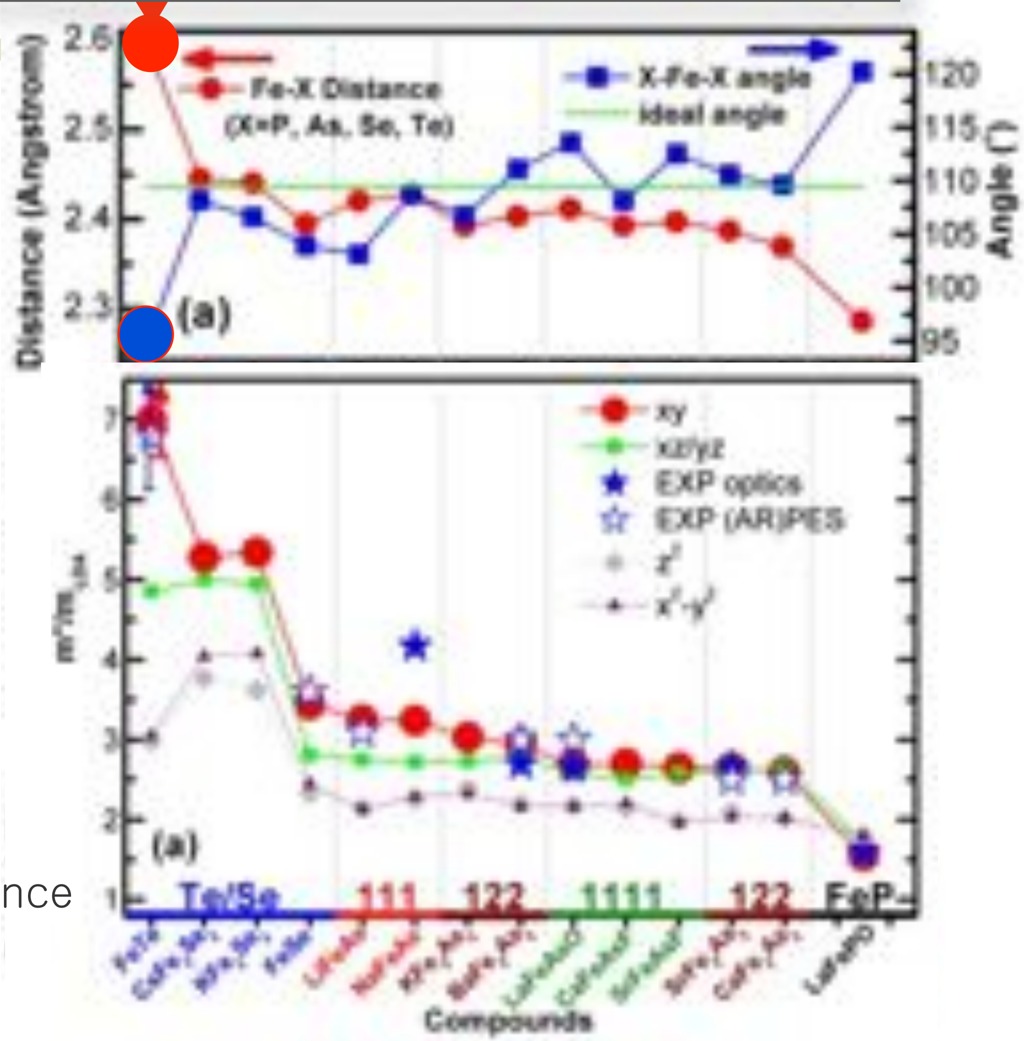

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Hybridization with pnictogen

Two particle response of Hund's metals: Dynamical structure factor

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

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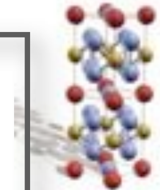
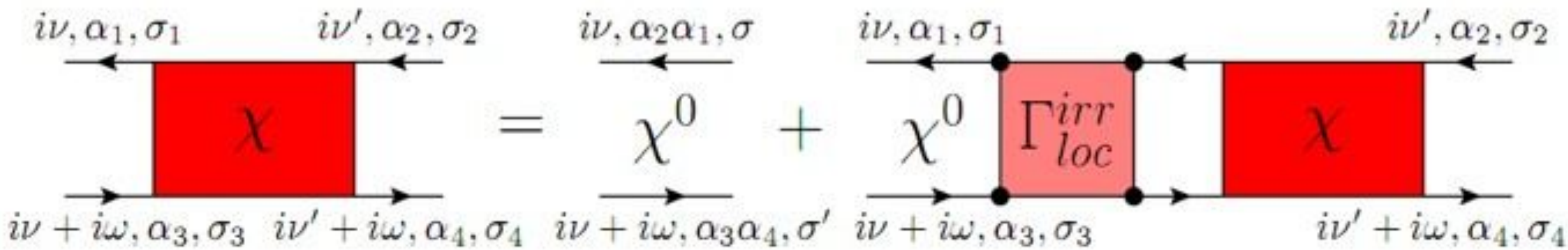


$$S(\mathbf{q},\omega)=\frac{\chi''(\mathbf{q},\omega)}{1-e^{-\hbar\omega/k_B T}}$$

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



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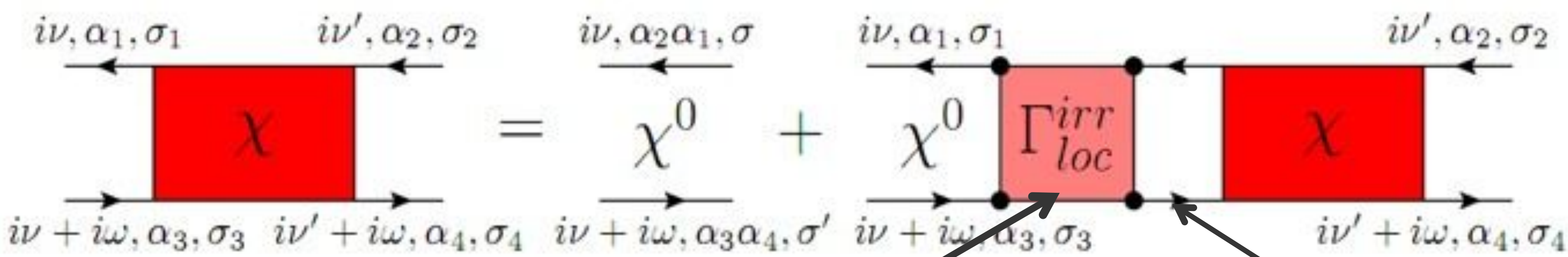
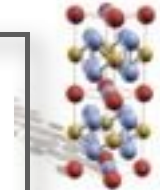


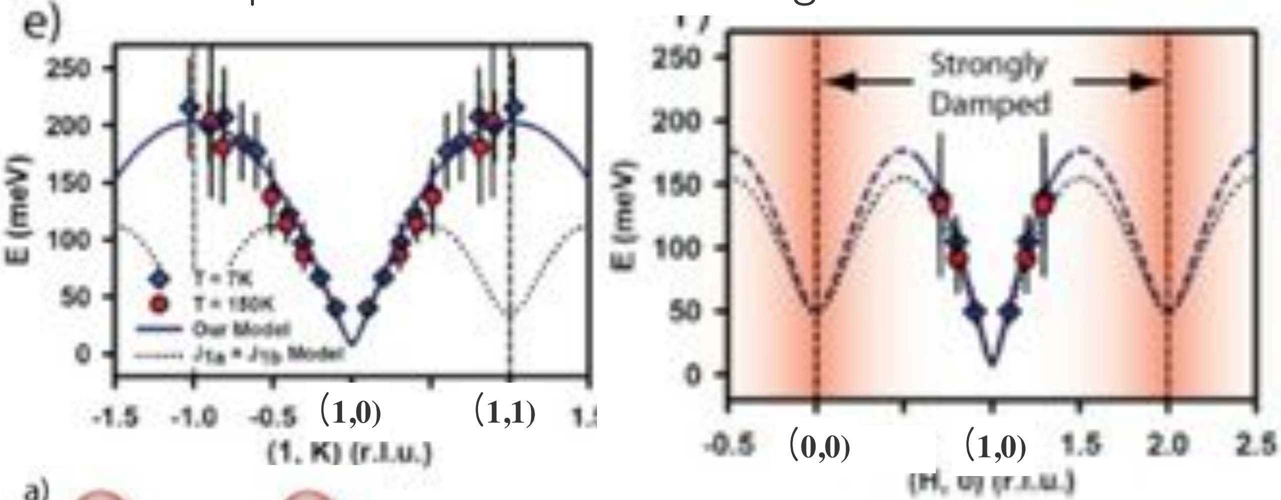
The two particle irreducible vertex function of the impurity

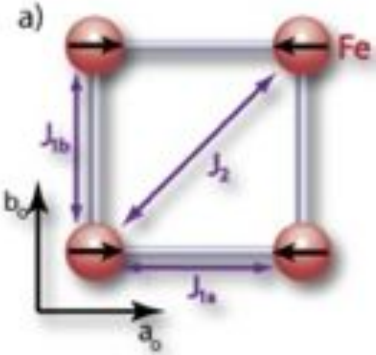
The LDA+DMFT self-consistent lattice Green's function



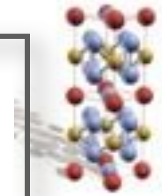
Dynamical structure factor of $BaFe_2As_2$

Spin wave for Heissenberg model





Leland W. Harriger, Pengcheng Dai et al., PRB 84, 054544 (2011).



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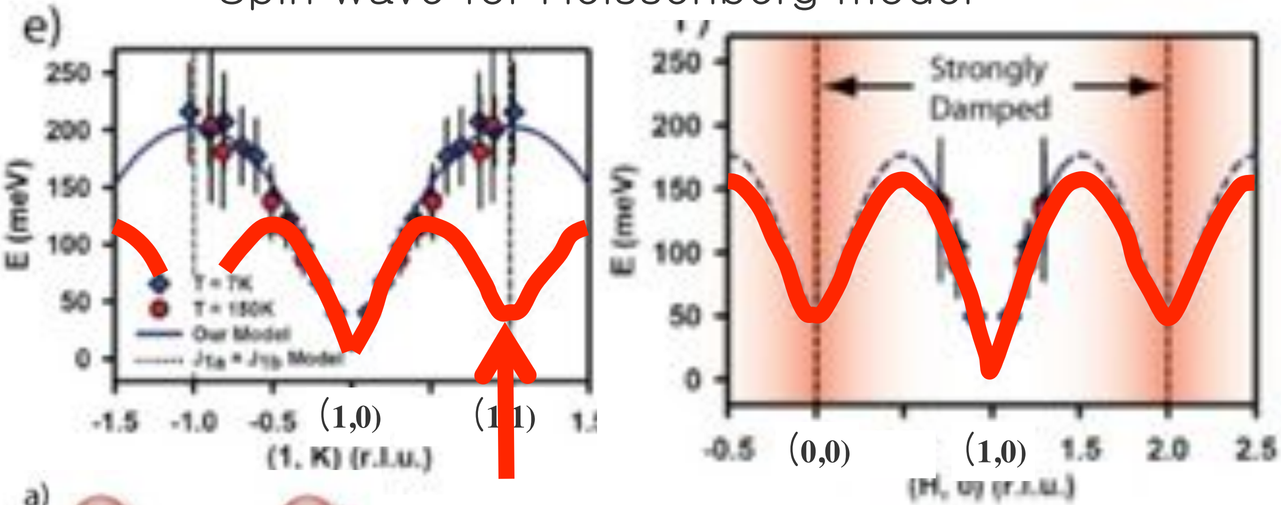
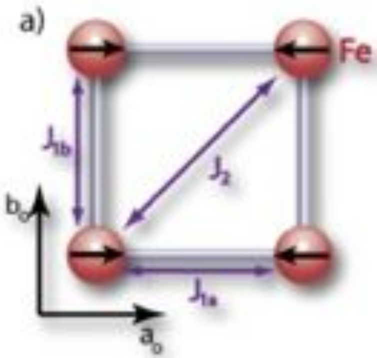


Isotropic exchange



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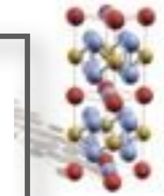
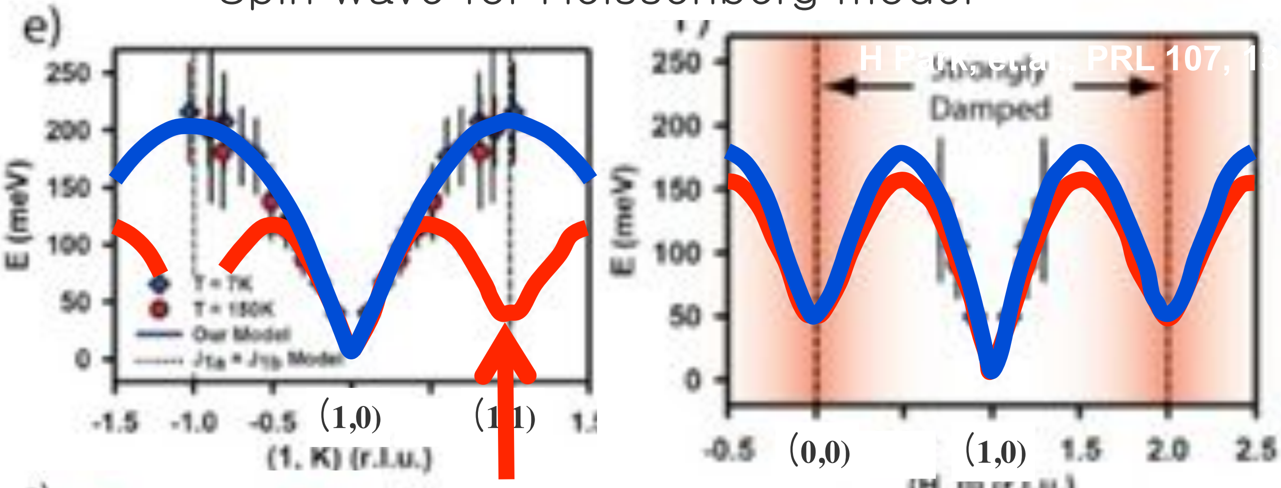
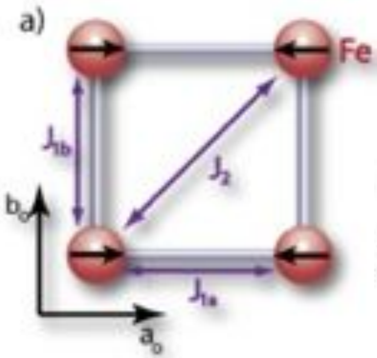
Dynamical structure factor of $BaFe_2As_2$



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., PRB 84, 054544 (2011).

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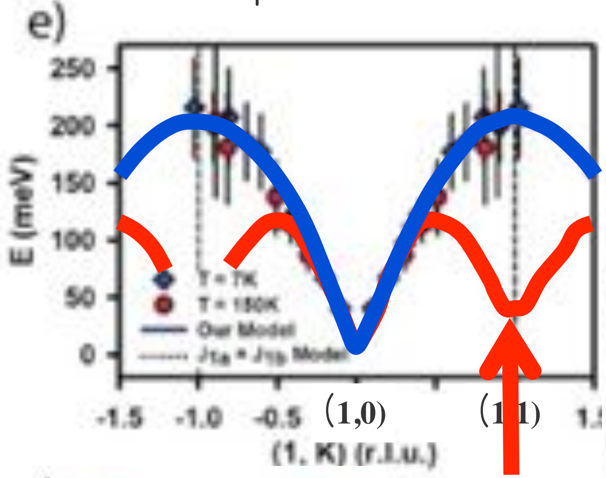
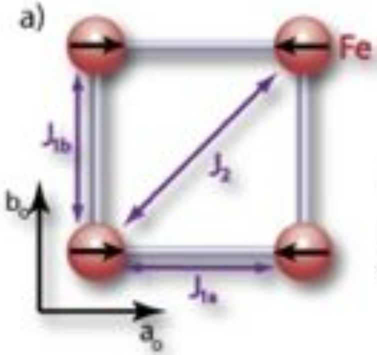


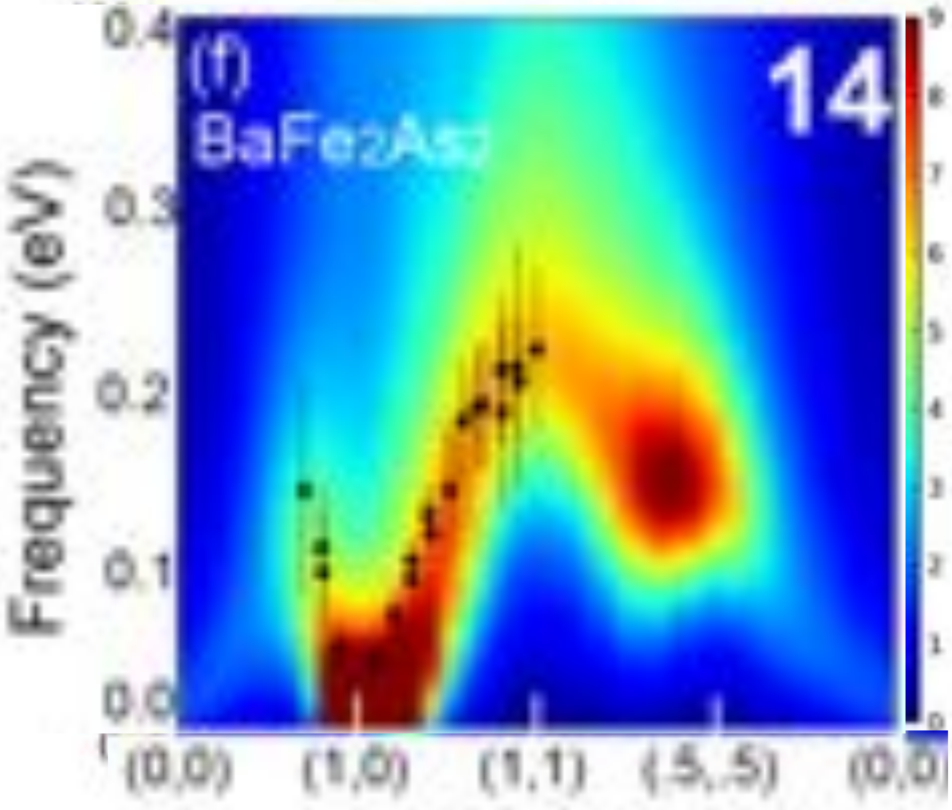


Very ar

$SJ_{1a} \approx$

$SJ_{1b} \approx$

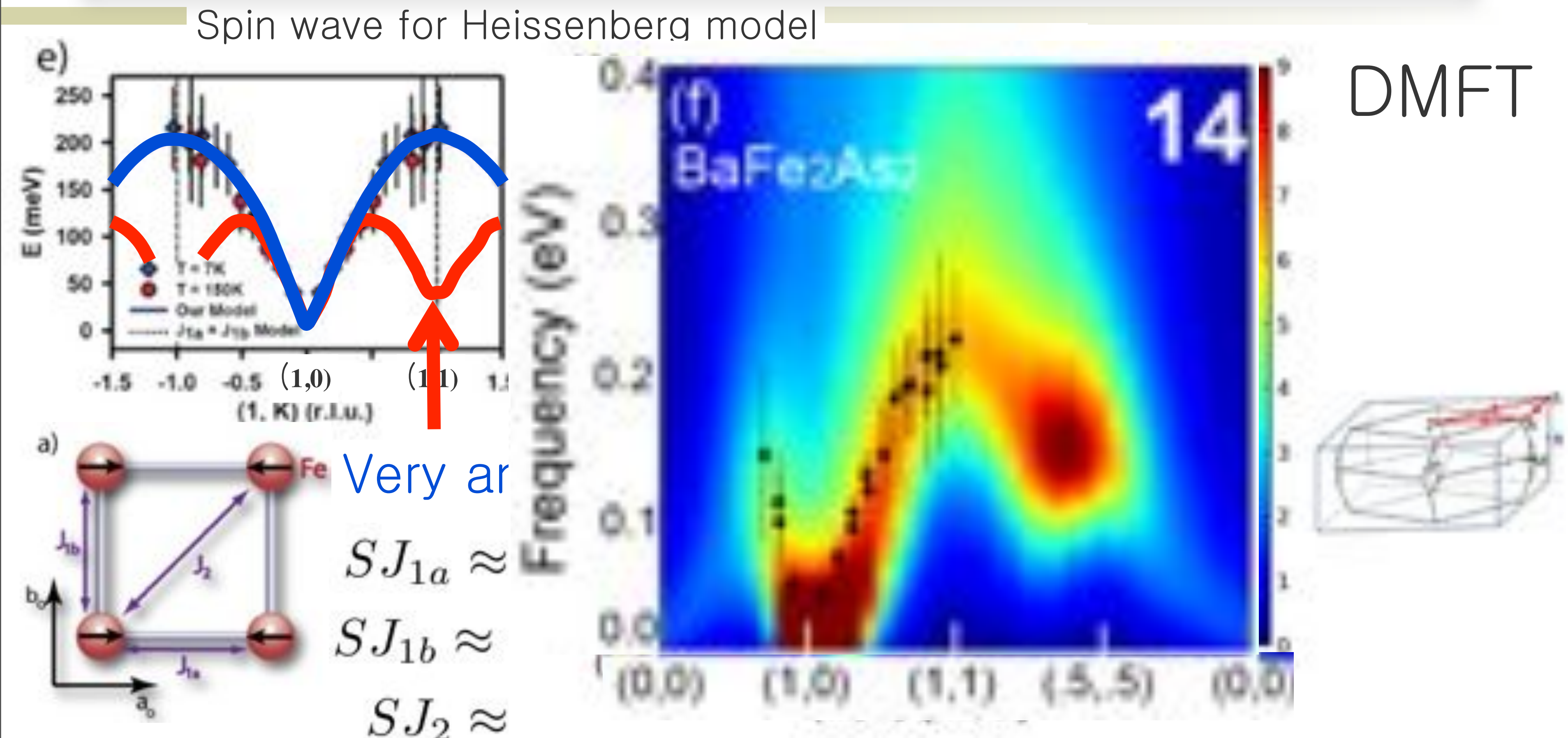
$SJ_2 \approx$



DMFT

Leland W. Harriger, Pengcheng Dai et al., PRB 84, 054544 (2011).

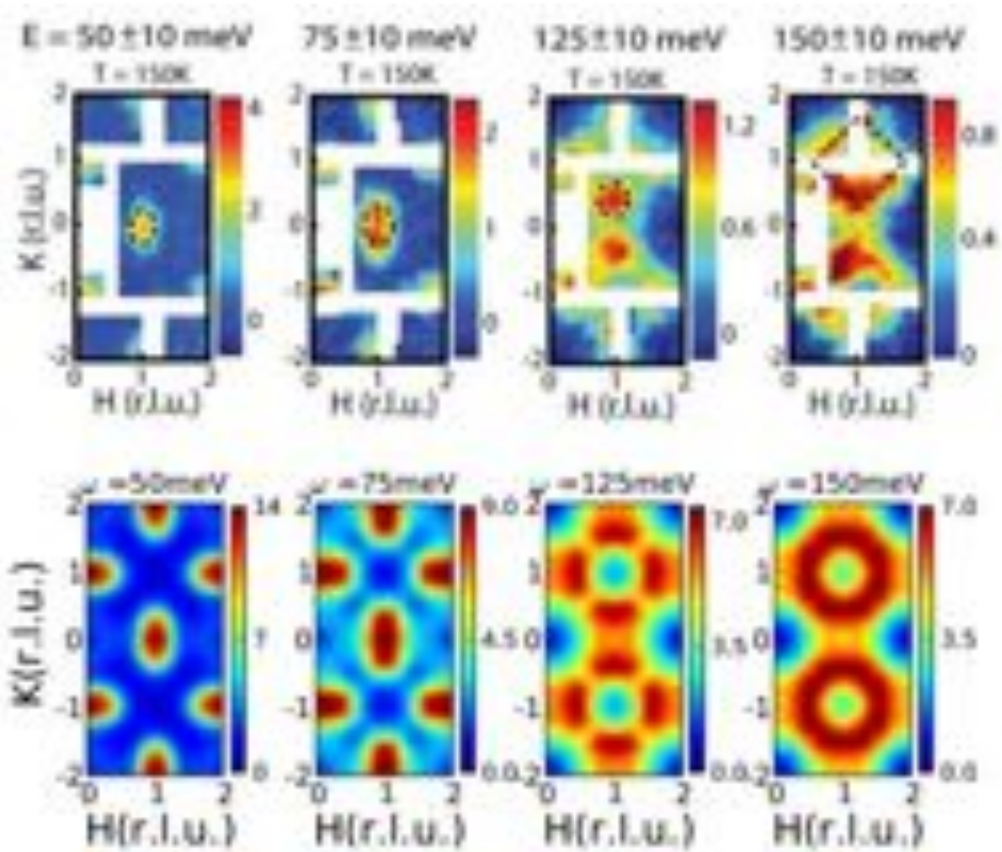
Dynamical structure factor of $BaFe_2As_2$



Leland W. Harriger, Pengcheng Dai et al., PRB 84, 054544 (2011).

S(q,ω) in paramagnetic phase similar to AFM phase!
No anysotropy needed (above T_S) to explain neutrons.

Dynamical structure factor



Experiment: J. T. Park, et al., PRB 82, 134503 (Oct 2010).

LDA+DMFT: H. Park, et.al., PRL 107, 137007 (2011)

Large fluctuating moment

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

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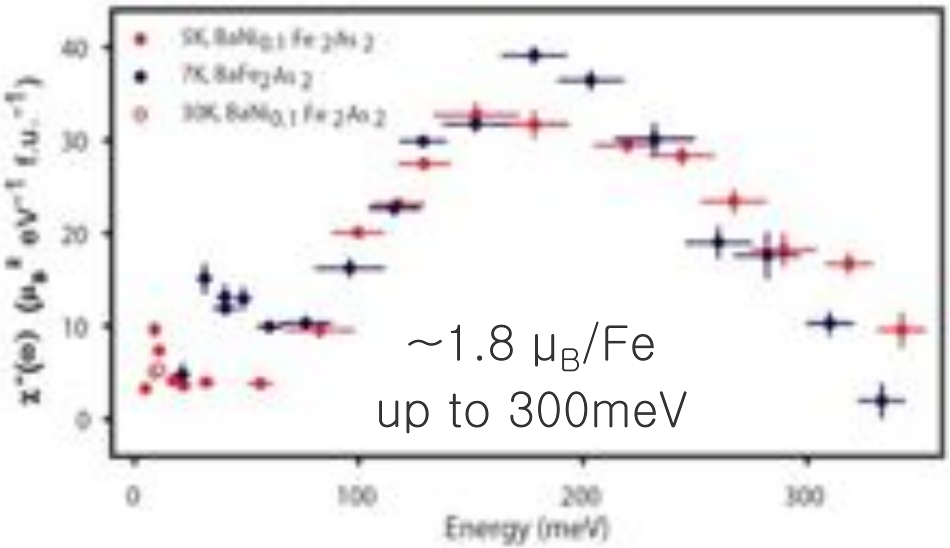
Experiment by Pengcheng Dai



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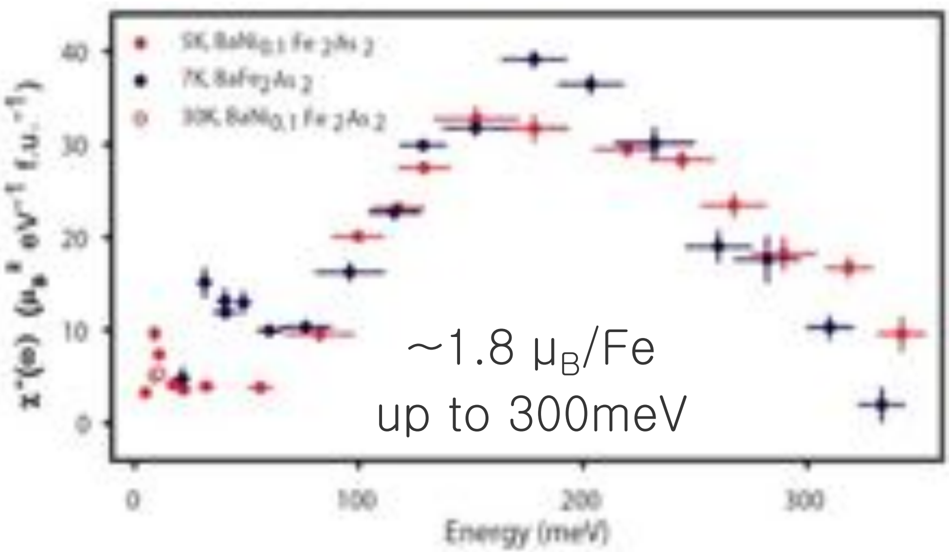

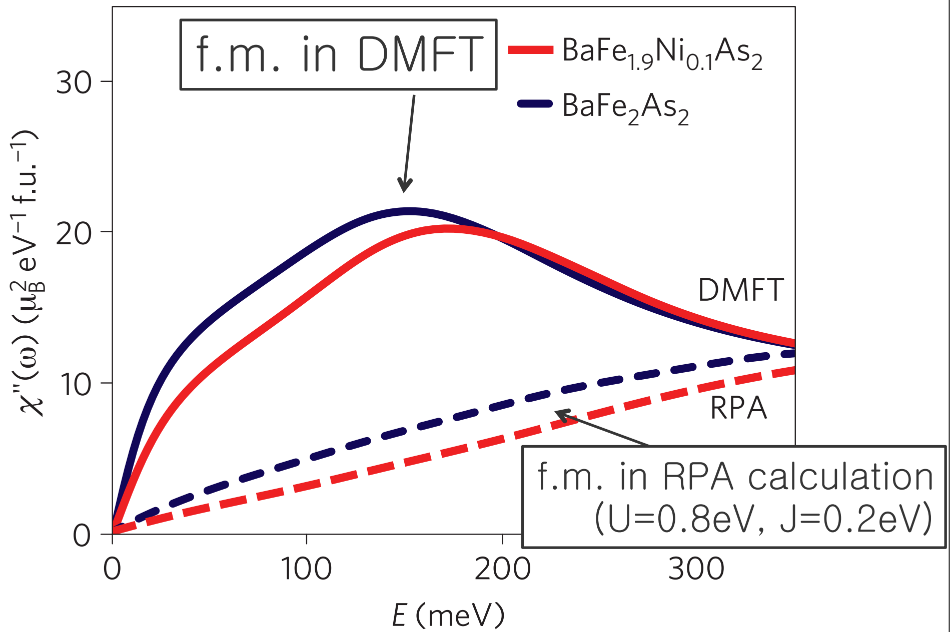

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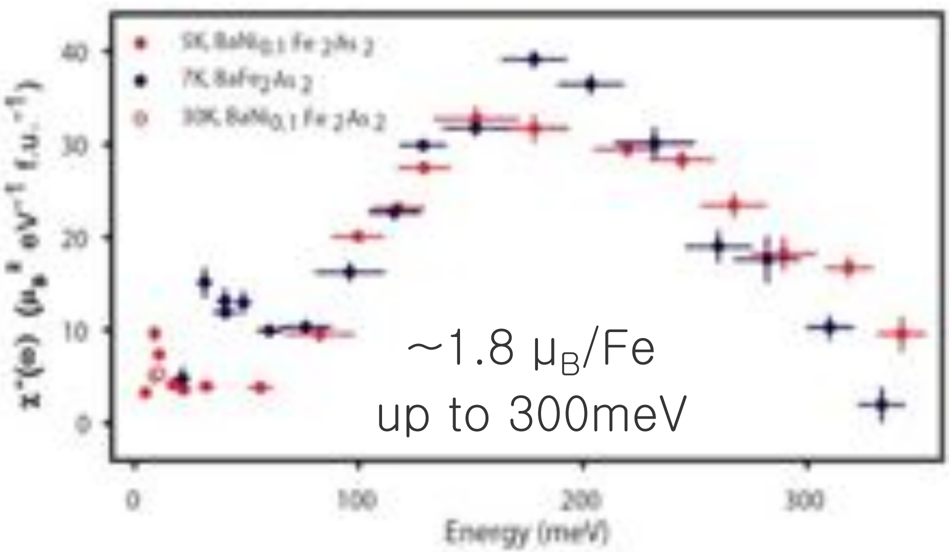
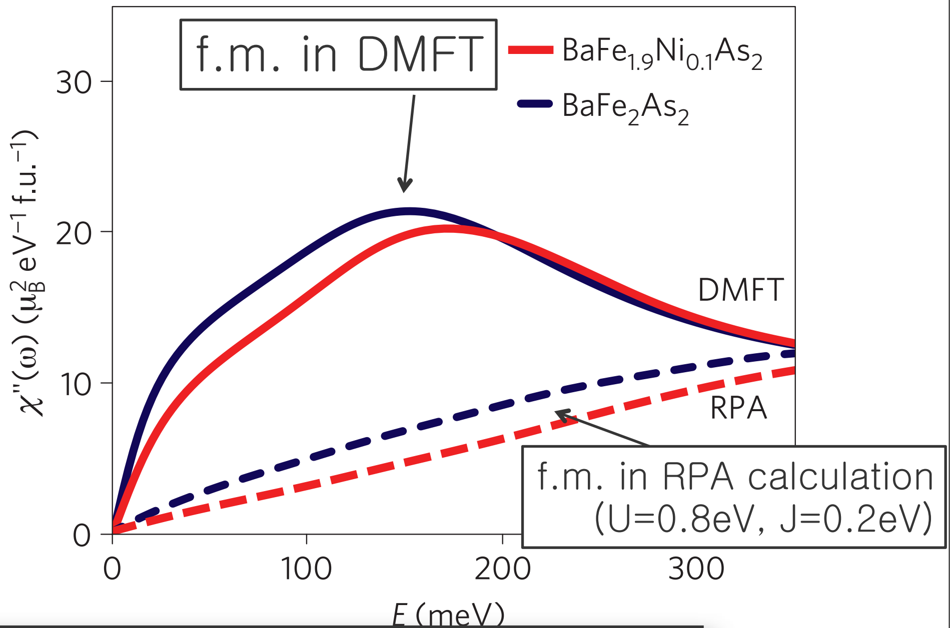


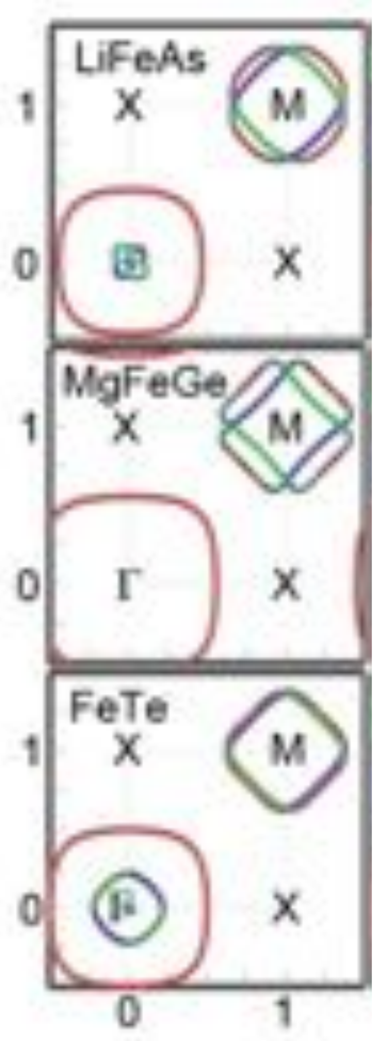


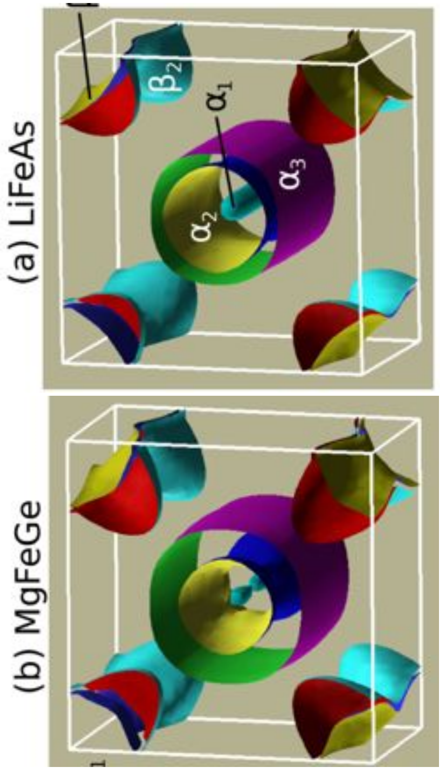
Large fluctuating moment can not be explained by a purely itinerant model - property of Hundsness!

The DMFT account for a dual nature of electrons in Hund's metals: itinerant and localized nature.

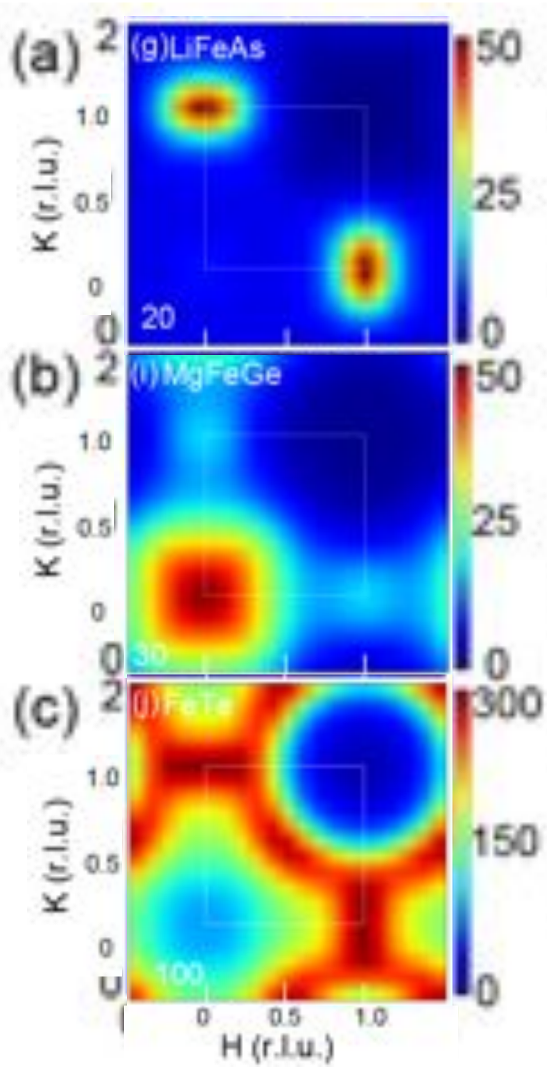
Magnetism not determined only by FS!

Theory: DFT+DMFT





ω=5 meV



ZPY et al, to be published.

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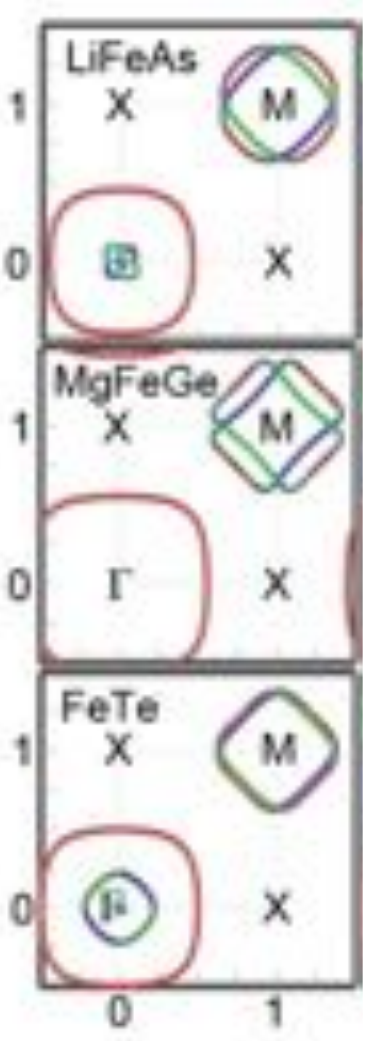
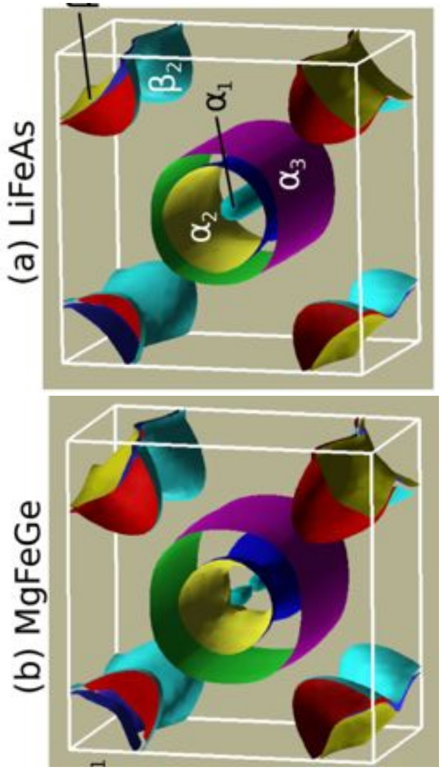
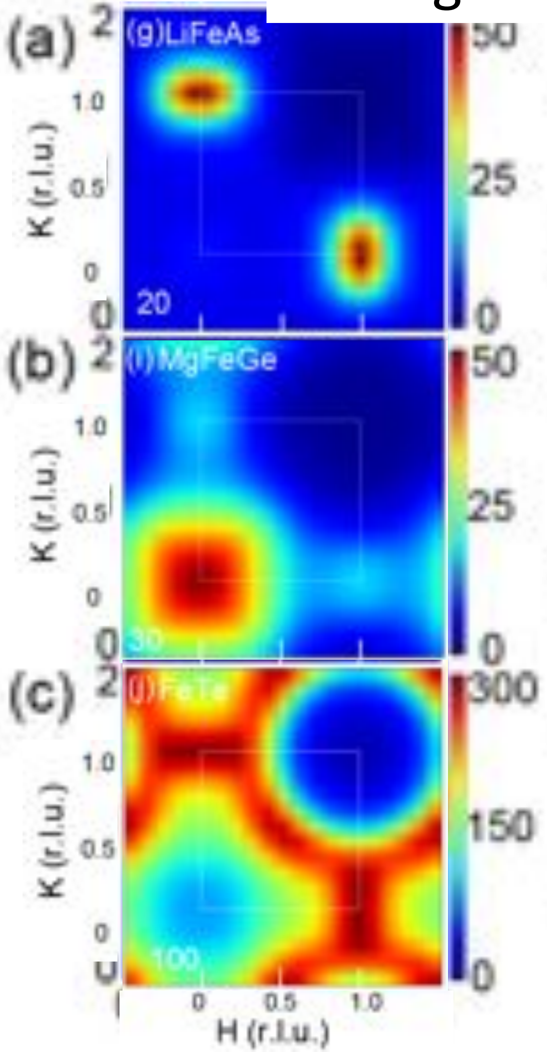




ω=5 meV

Why is LiFeAs SC
but MgFeGe/FeTe not?



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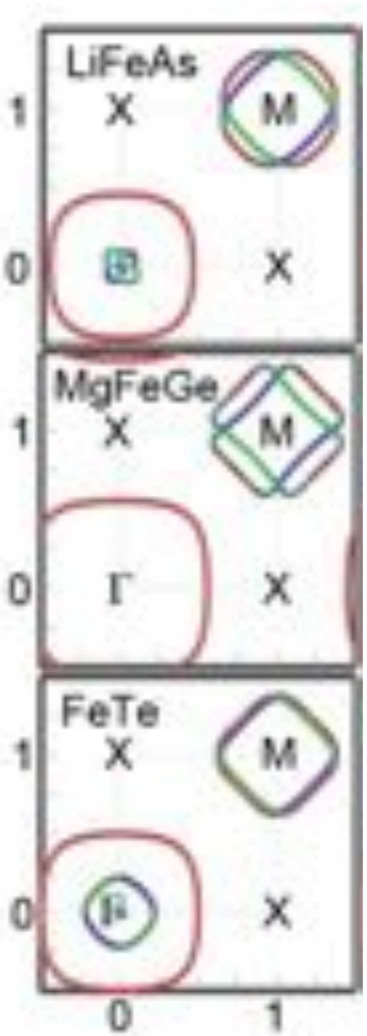

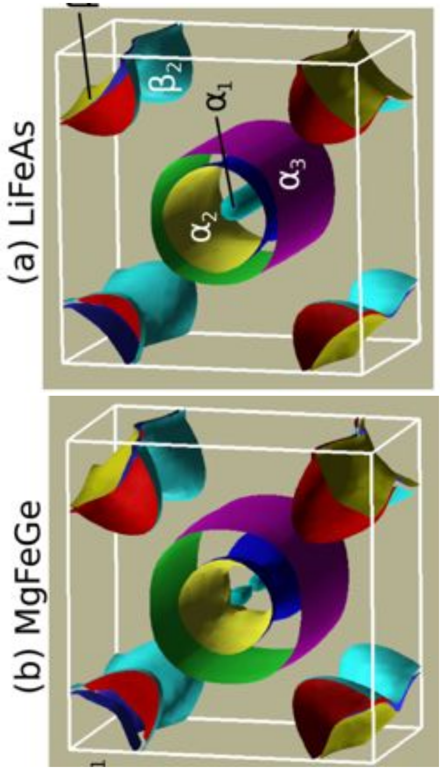

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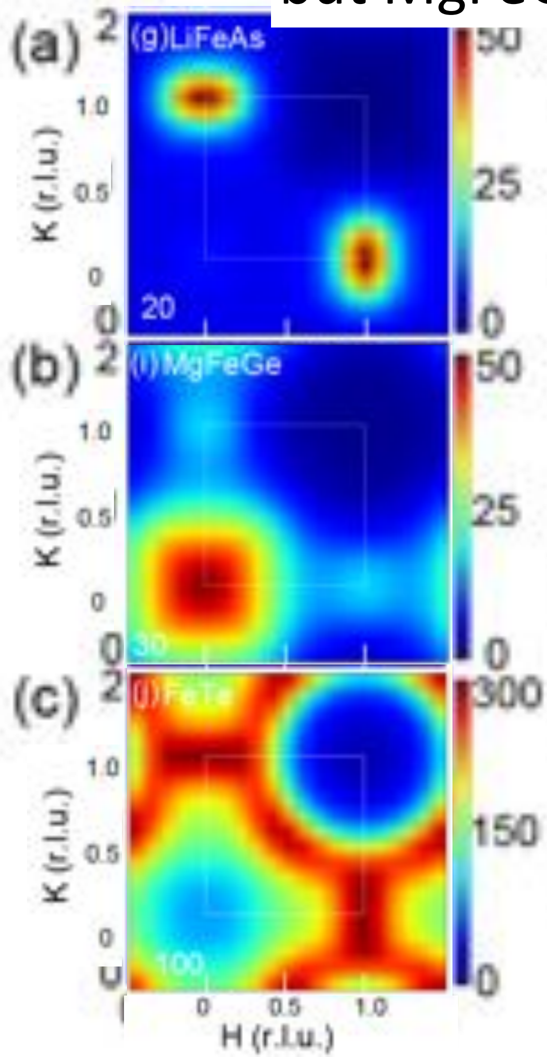
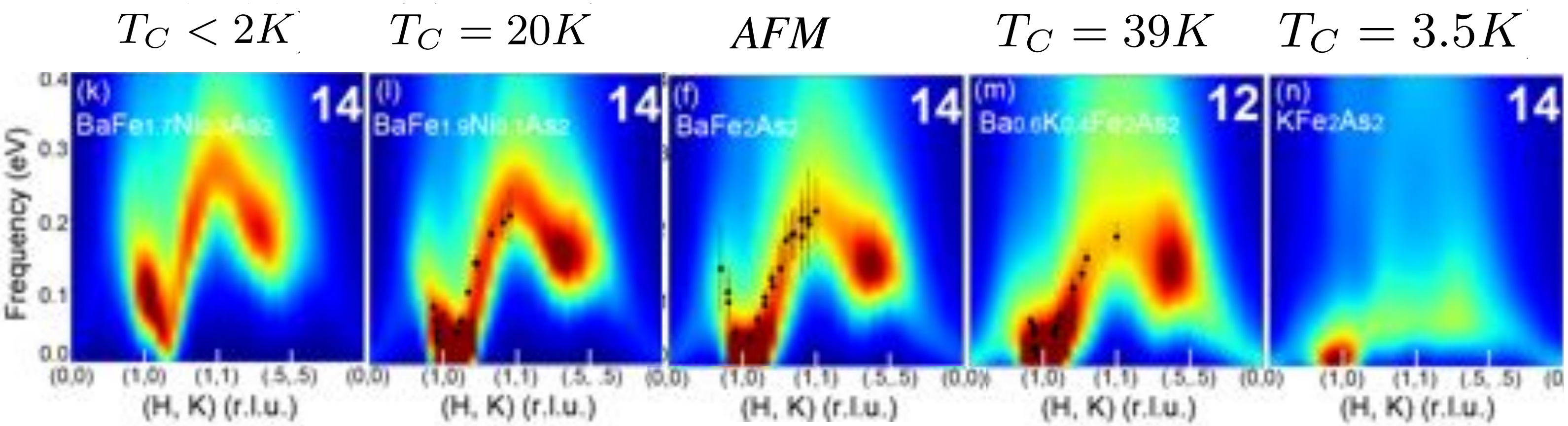


Very different magnetic excitations

ZPY et al, to be published.

Theoretical Magnetic excitations

Doping variation

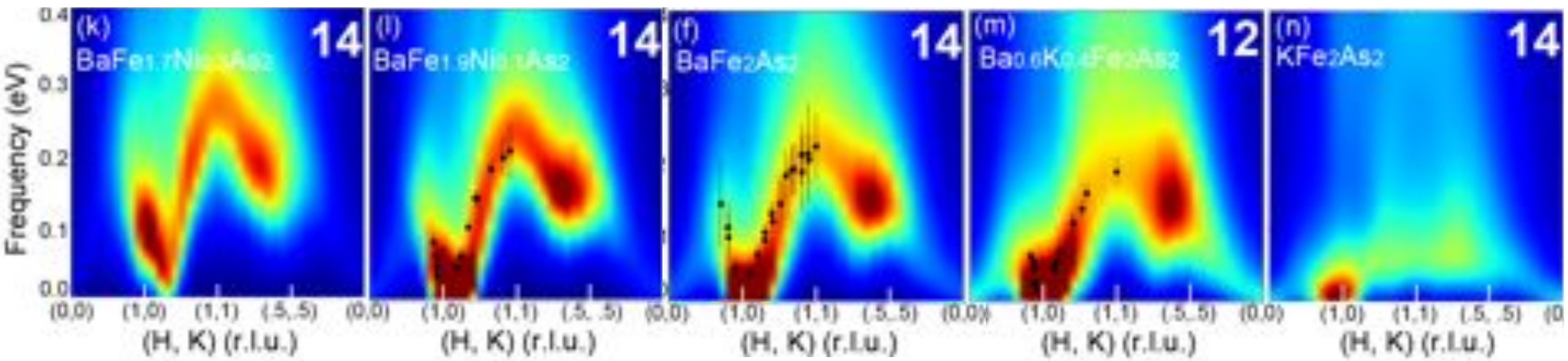


Theoretical Magnetic excitations

Doping variation

electron doping ←

$T_C < 2K$ $T_C = 20K$ AFM $T_C = 39K$ $T_C = 3.5K$



Theoretical Magnetic excitations

Doping variation

electron doping ← → hole doping

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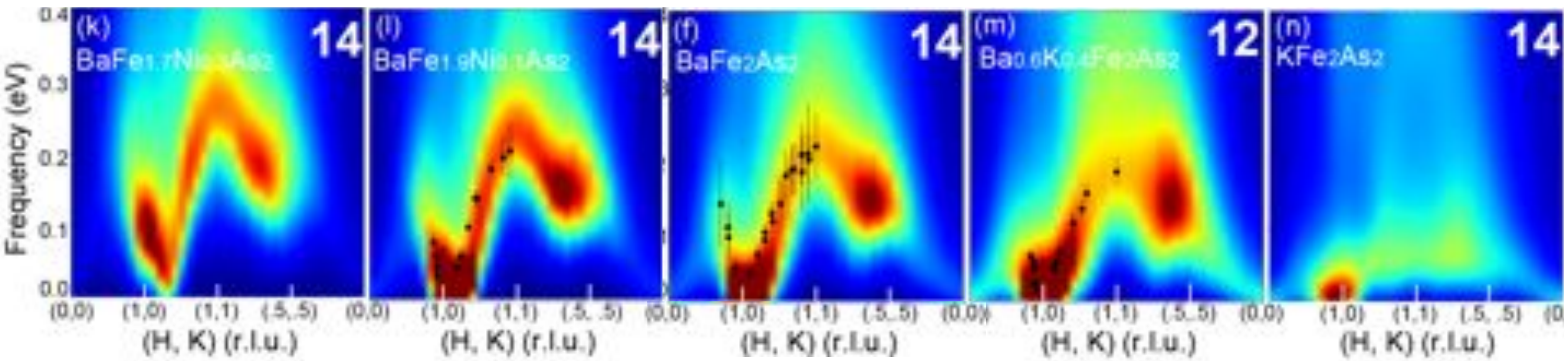

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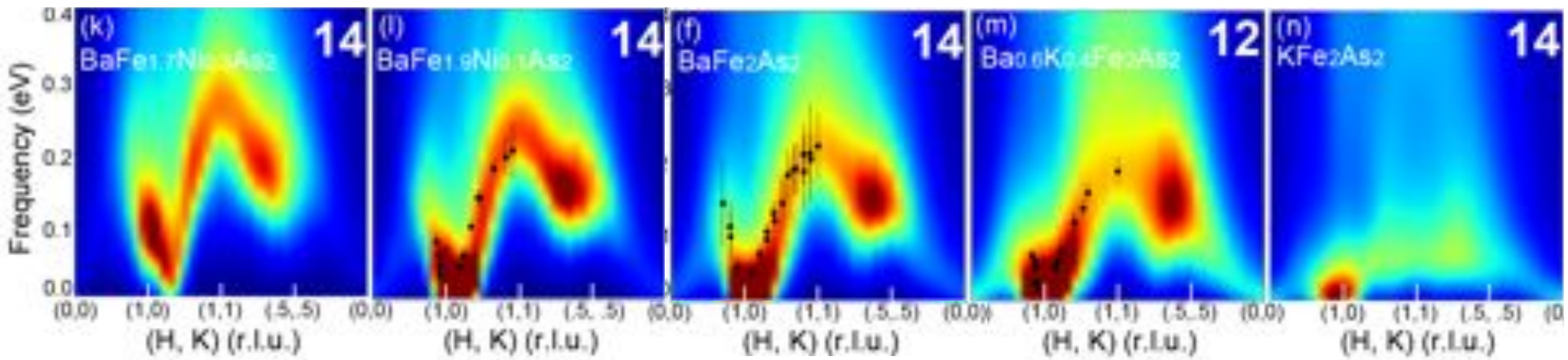
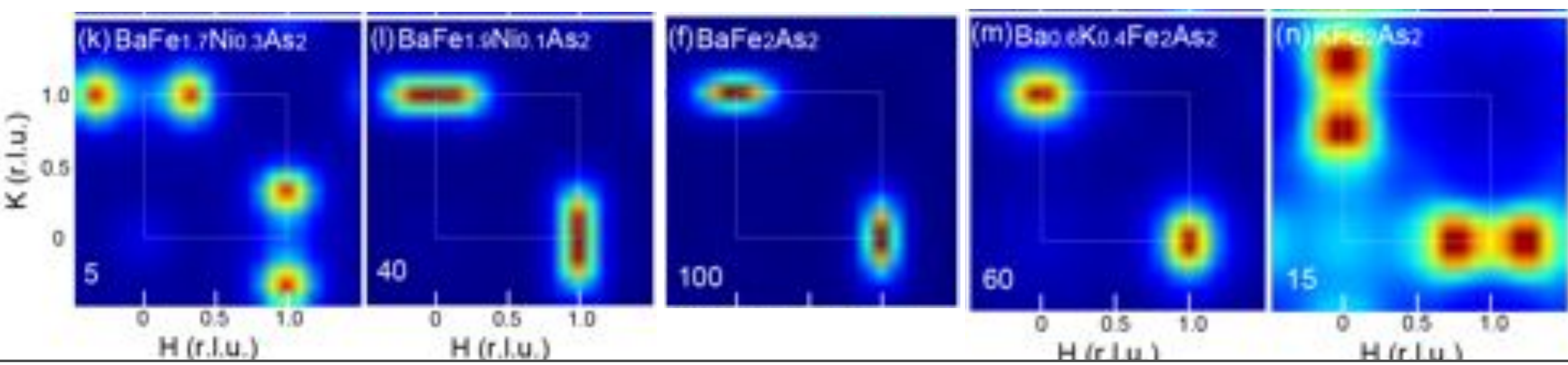
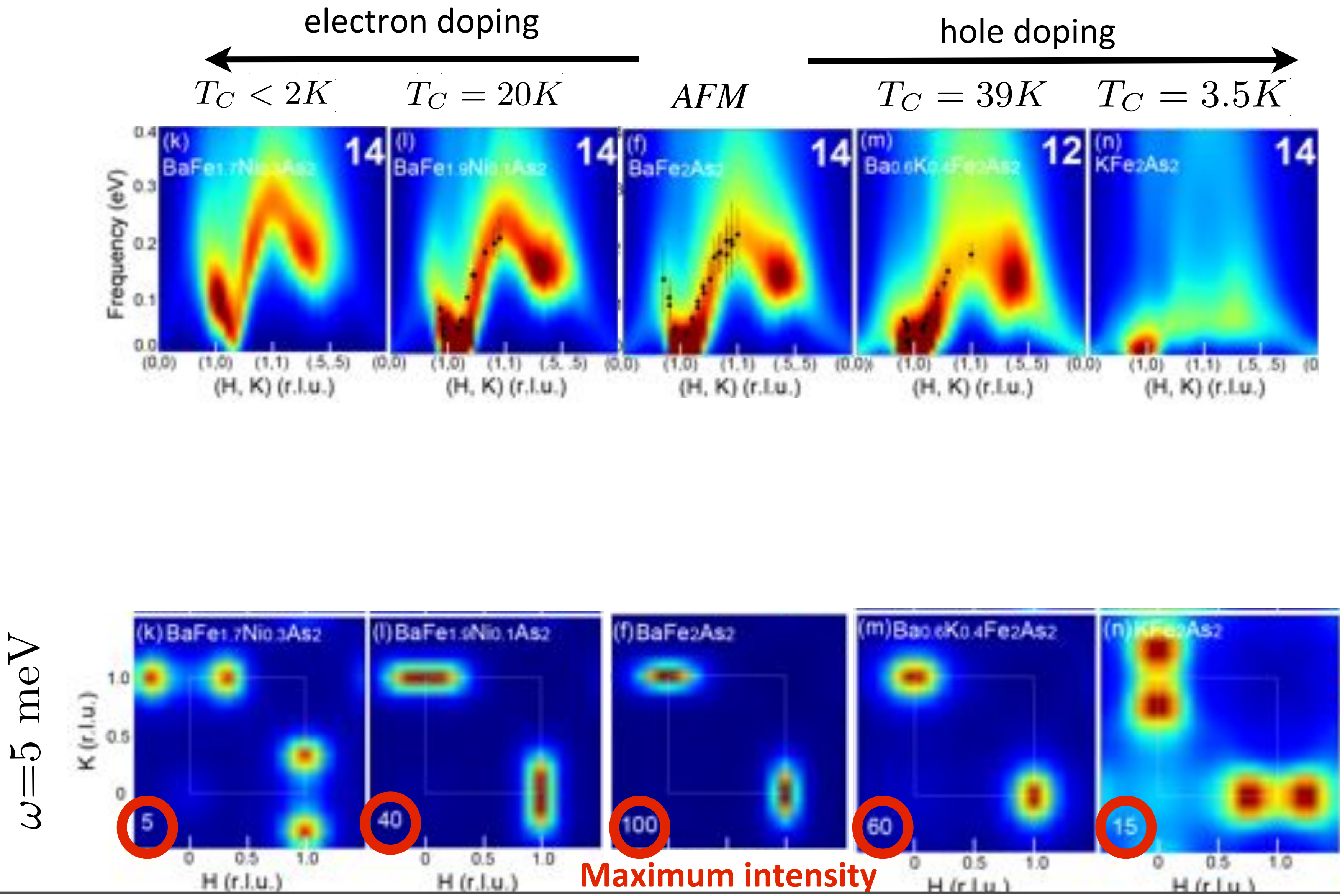




Theoretical Magnetic excitations

Doping variation



Theoretical Magnetic excitations

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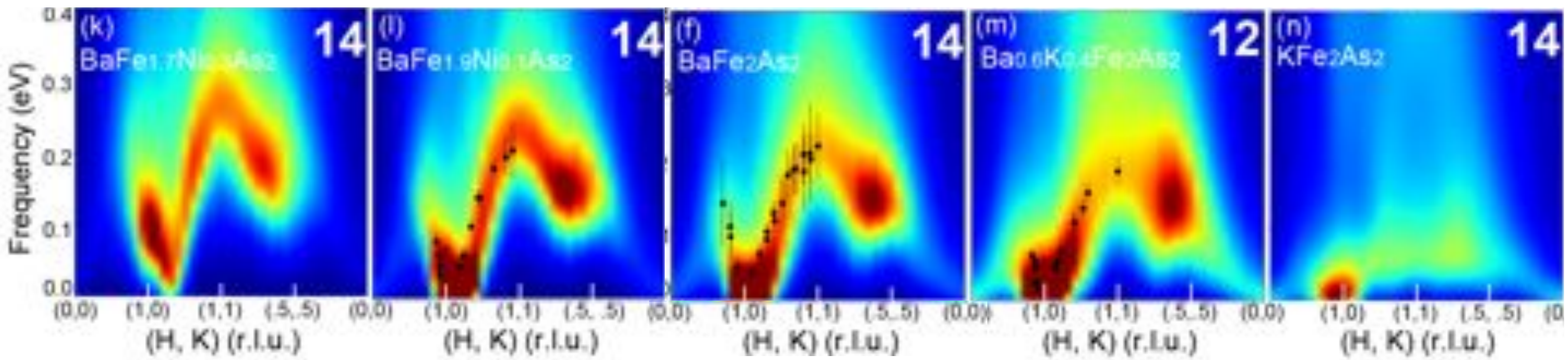
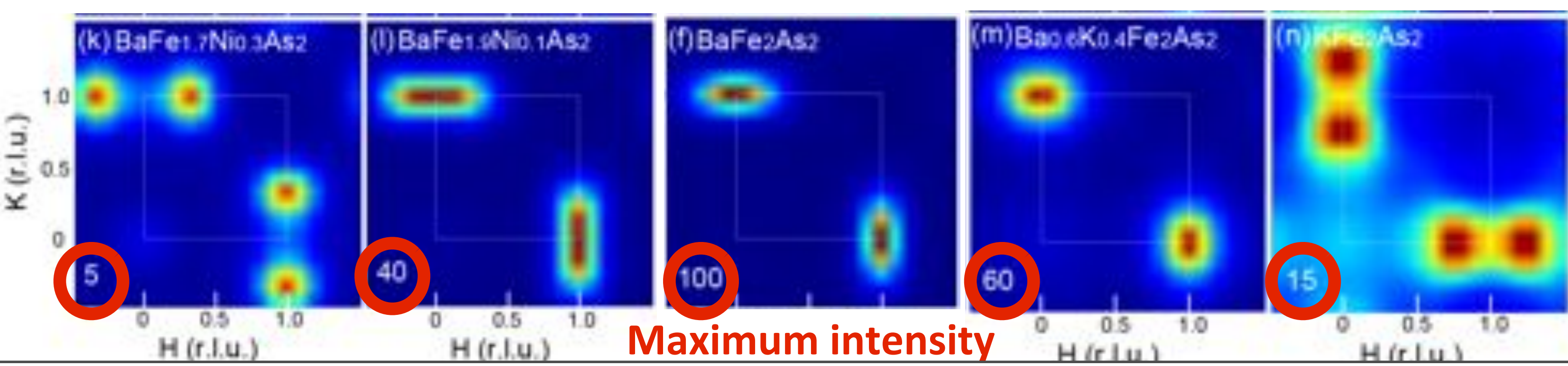


electron overdoped:
low energy spin excitations
very weak
and become **incommensurate**

$\omega = 5$ meV



Maximum intensity

Theoretical Magnetic excitations

Doping variation

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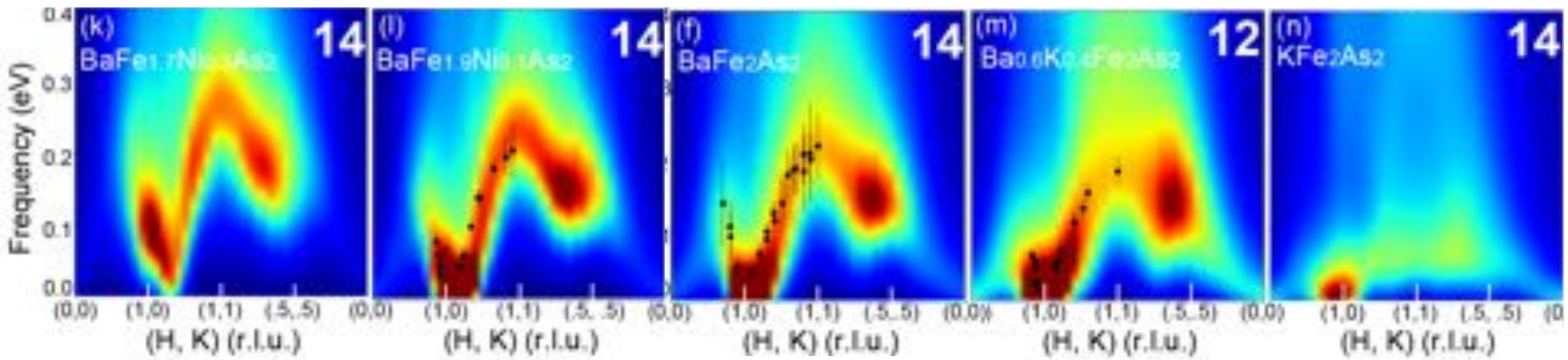
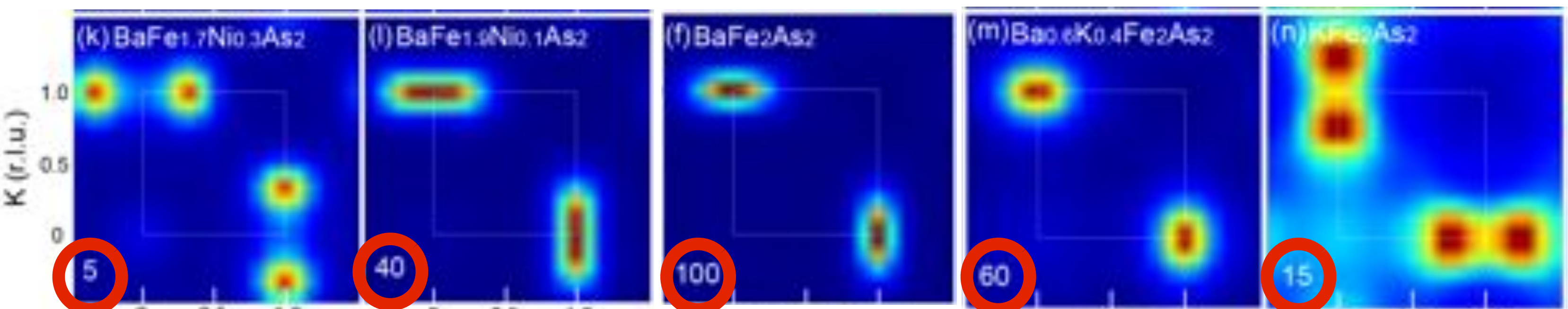


electron overdoped:
low energy spin excitations
very weak
and become **incommensurate**

hole overdoped:
low energy spin excitations
weaker
and **incommensurate**

$\omega = 5$ meV



Maximum intensity

Sunday, September 29, 13

Theoretical Magnetic excitations

Doping variation

electron doping ← → hole doping

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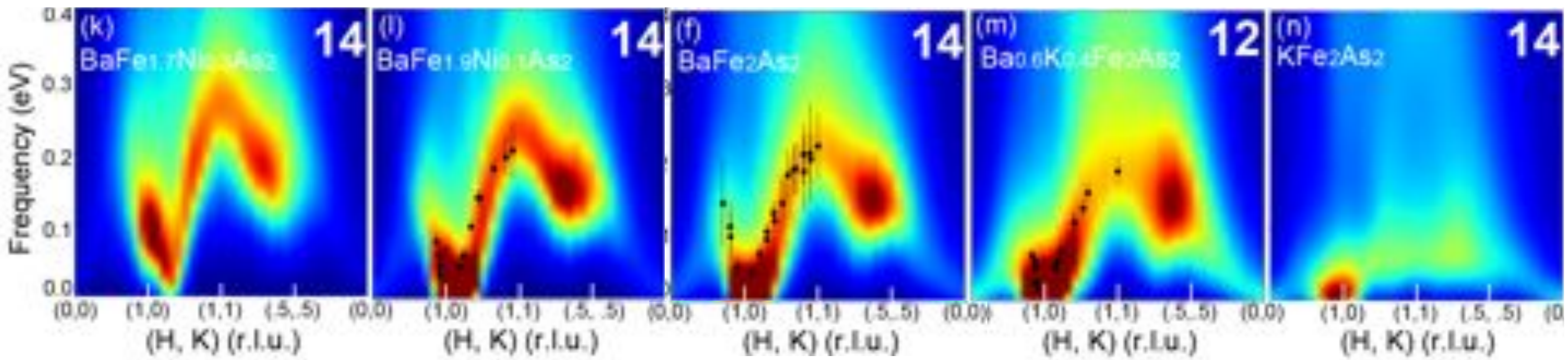
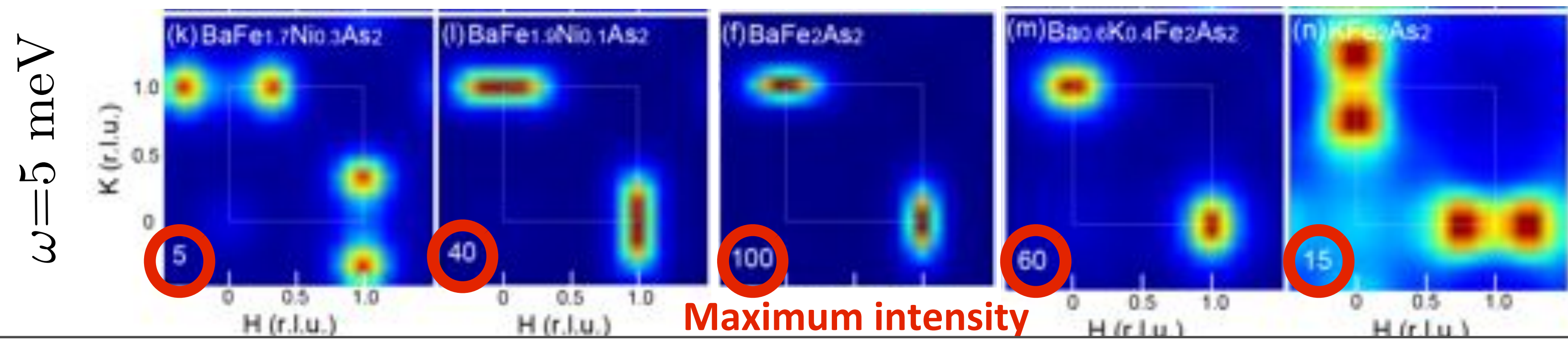


electron overdoped:
low energy spin excitations
very weak
and become **incommensurate**

Optimally doped:
Commensurate low energy
strong low energy
strong high energy

hole overdoped:
low energy spin excitations
weaker
and **incommensurate**

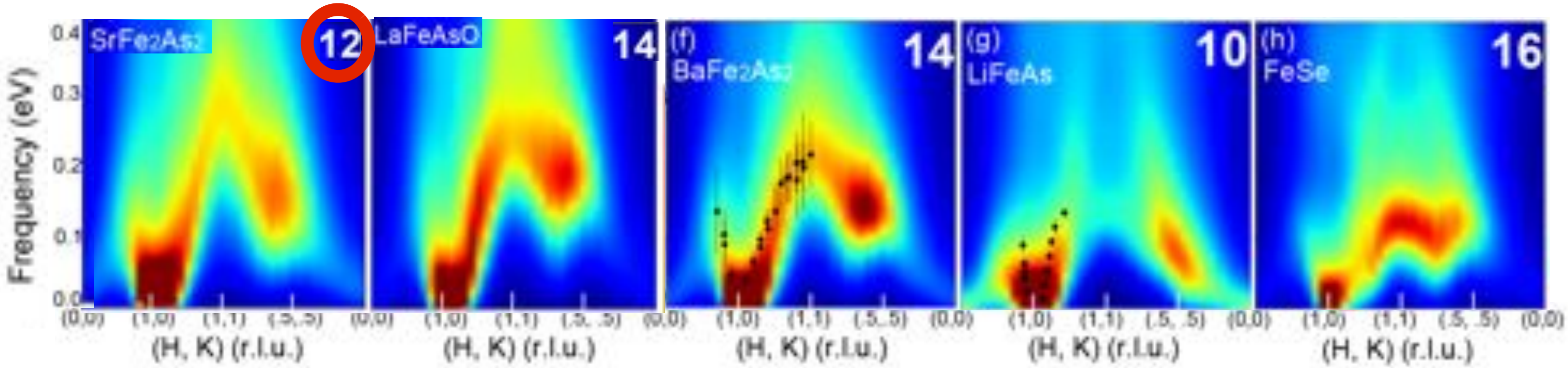


Sunday, September 29, 13

Variation across families

High-Tc compounds

$T_C^{max} = 37K$ $T_C^{max} = 43K$ $T_C^{max} = 39K$ $T_C = 18K$ $T_C^{max} = 37K$



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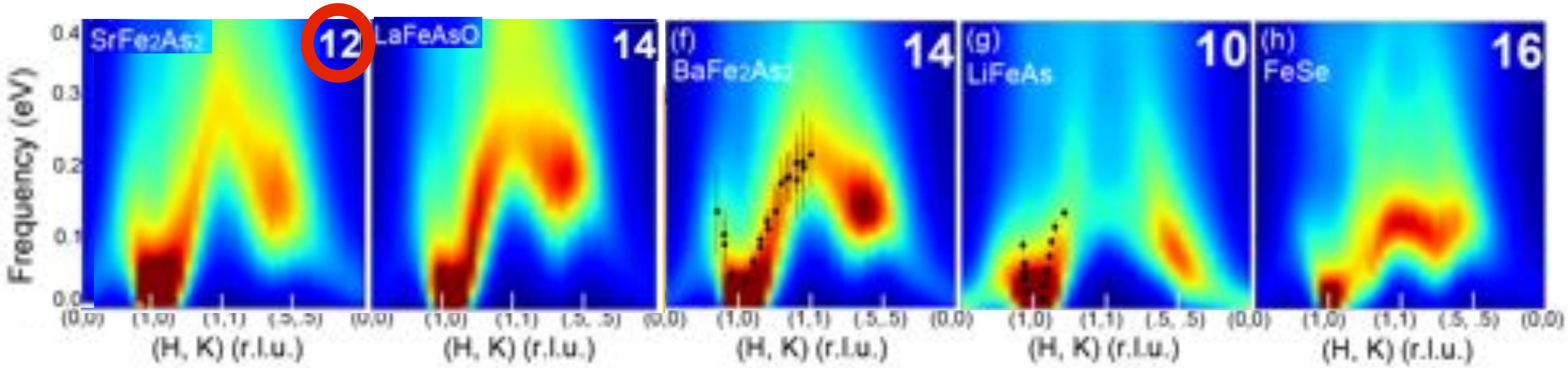

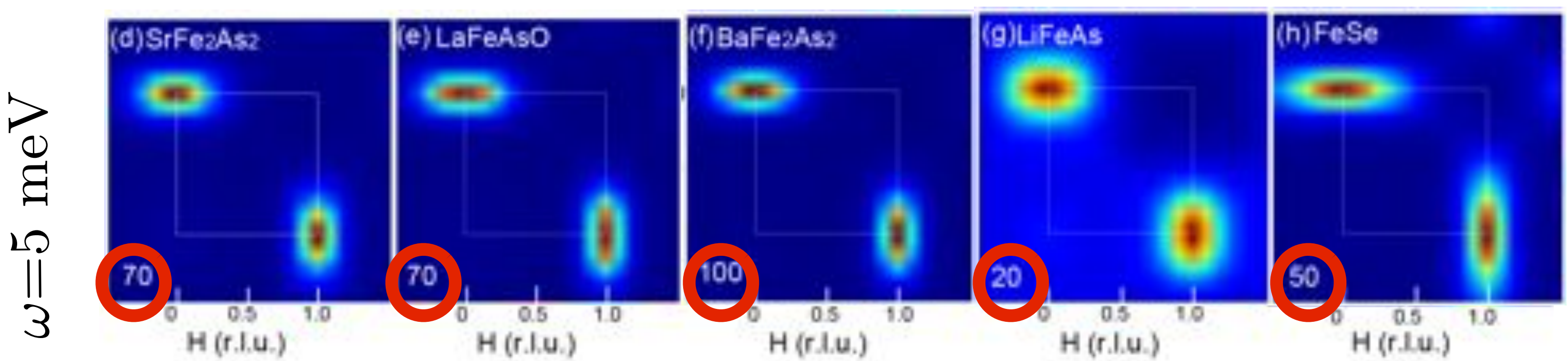

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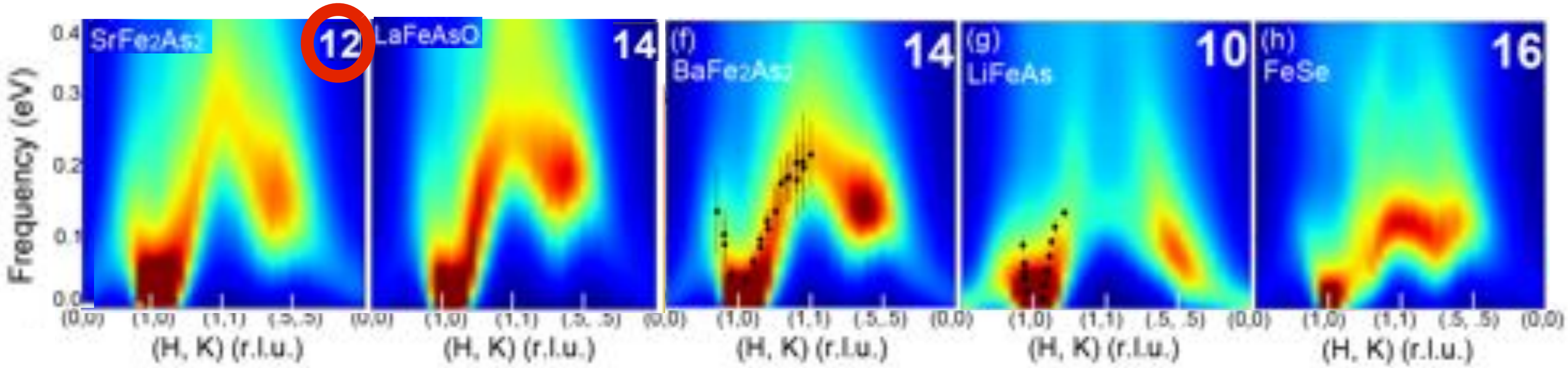
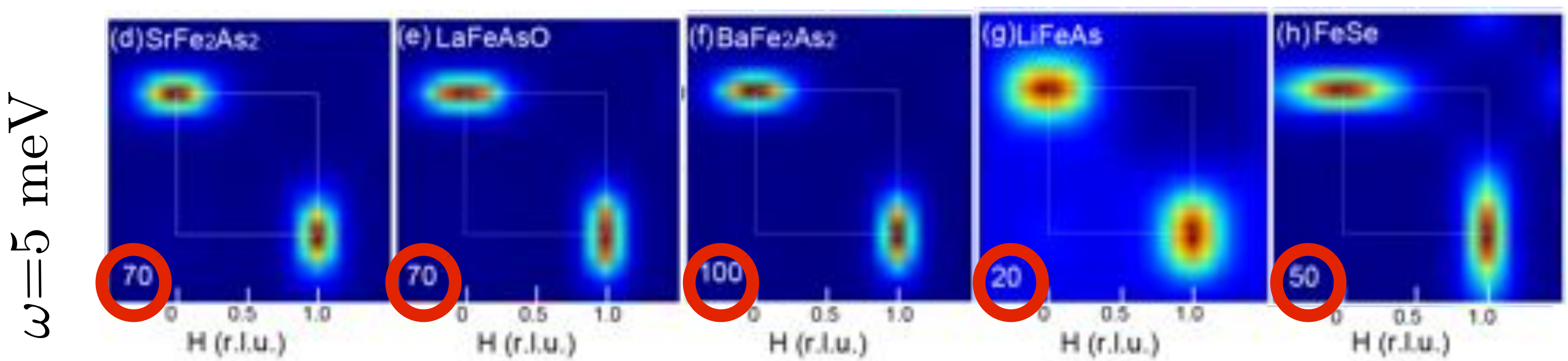


high Tc: **Strong commensurate low energy excitations**, strong high energy dispersive exc.

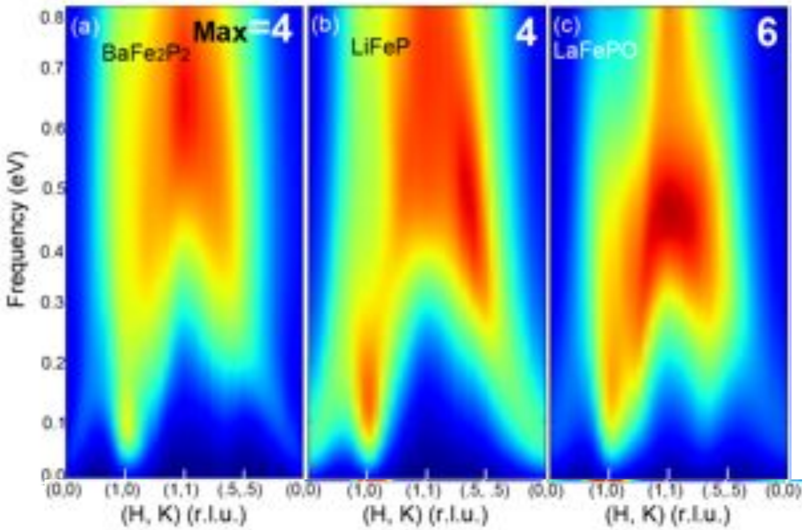


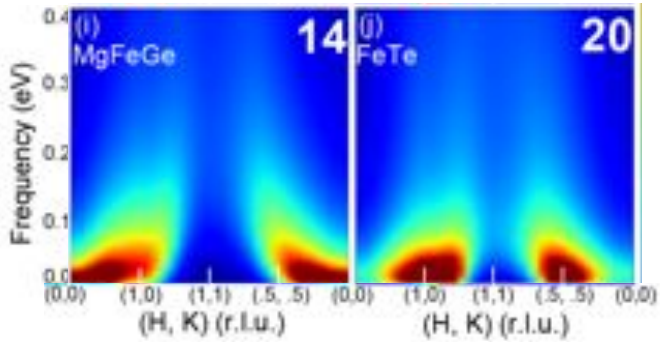
Maximum intensity

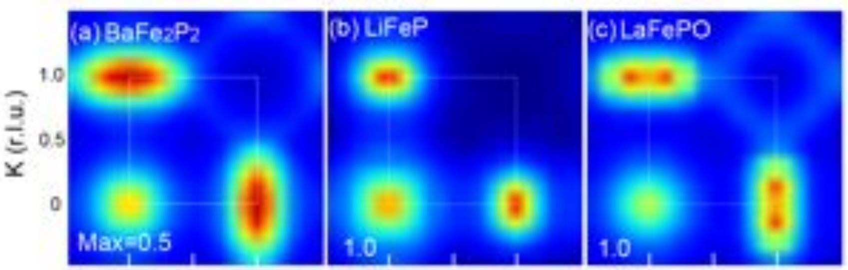
Variation across families

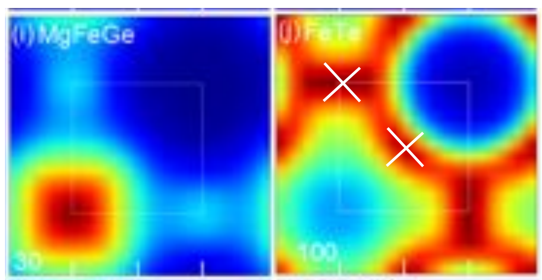
Low-Tc compounds

$T_C^{max} < 2K$ $T_C = 6K$ $T_C = 7K$ $T_C^{max} = 0$ $T_C^{max} = 0$









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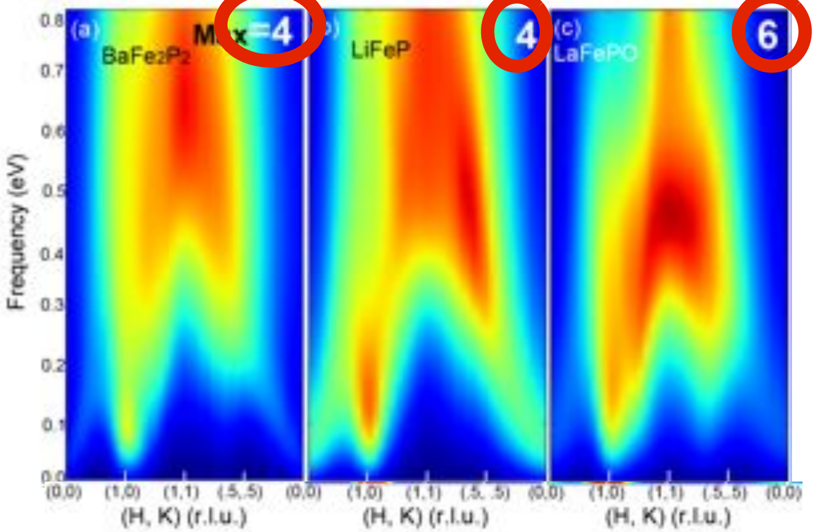

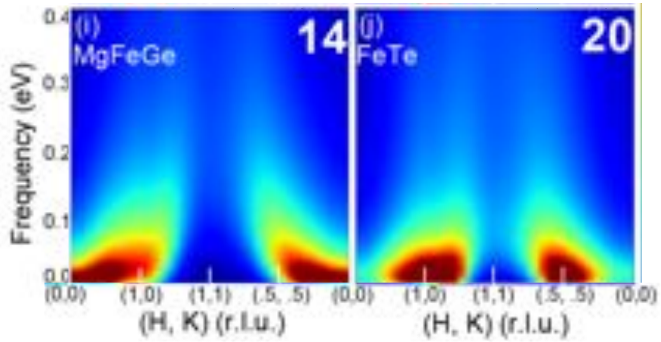

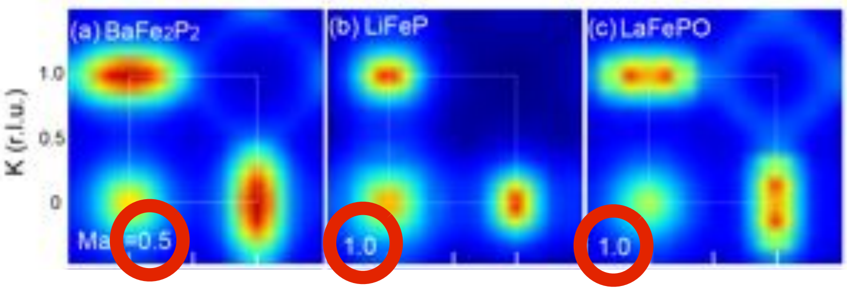

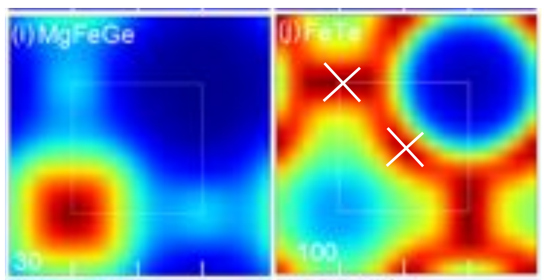

Maximum intensity two orders of magnitude smaller

Variation across families

Low-Tc compounds

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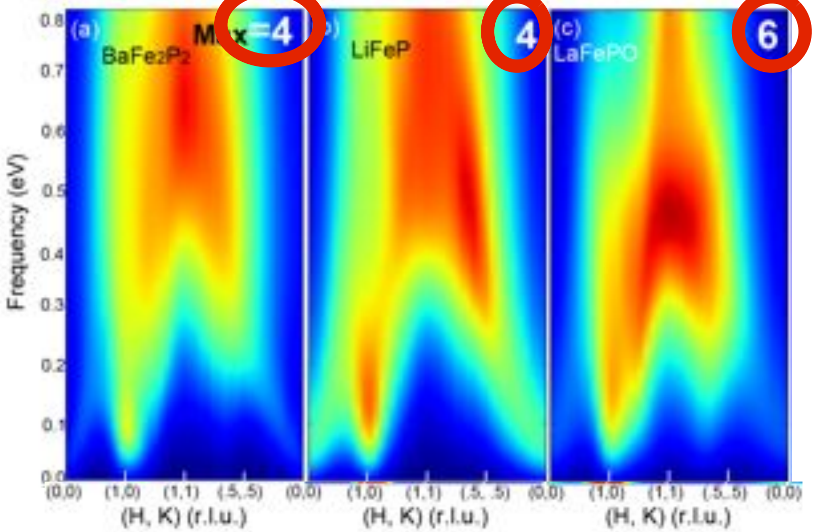
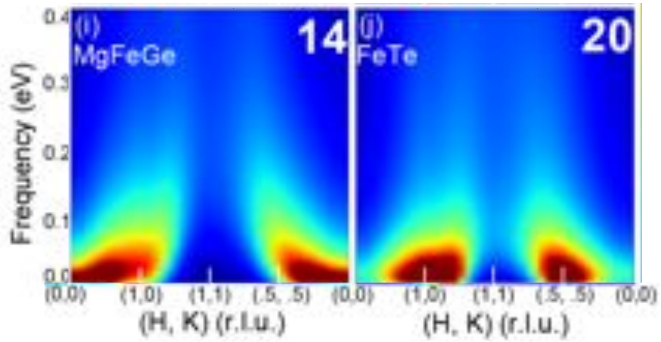
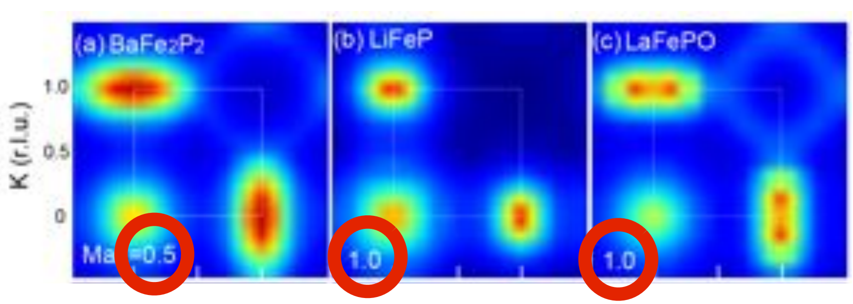
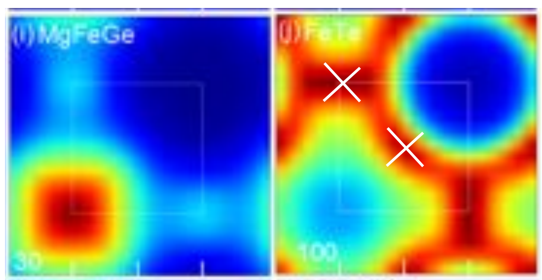


$T_C^{max} = 0$ $T_C^{max} = 0$



very small low energy intensity
competing order at (0,0)!





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Variation across families

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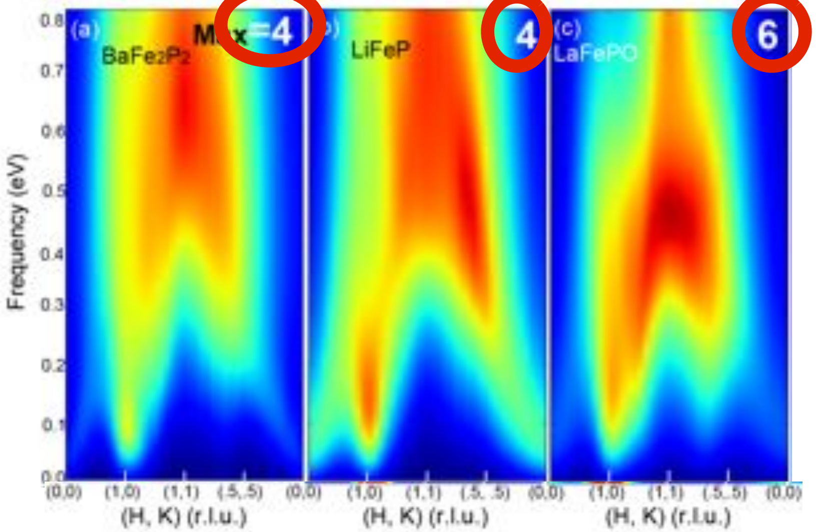

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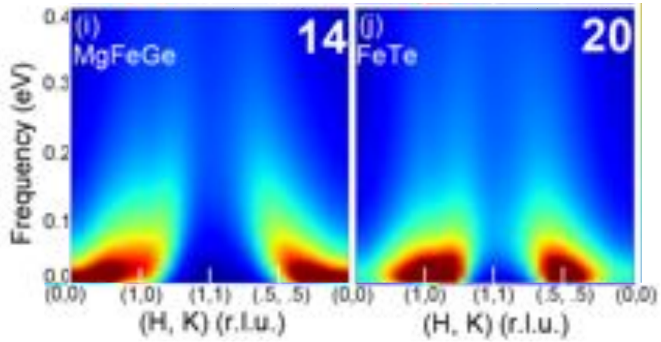
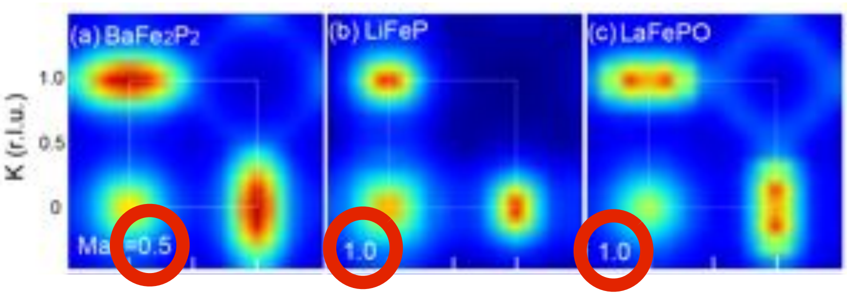
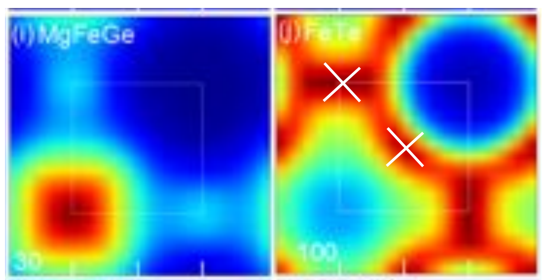


very small low energy intensity
competing order at (0,0)!

broad with
mostly
(0,0) peak





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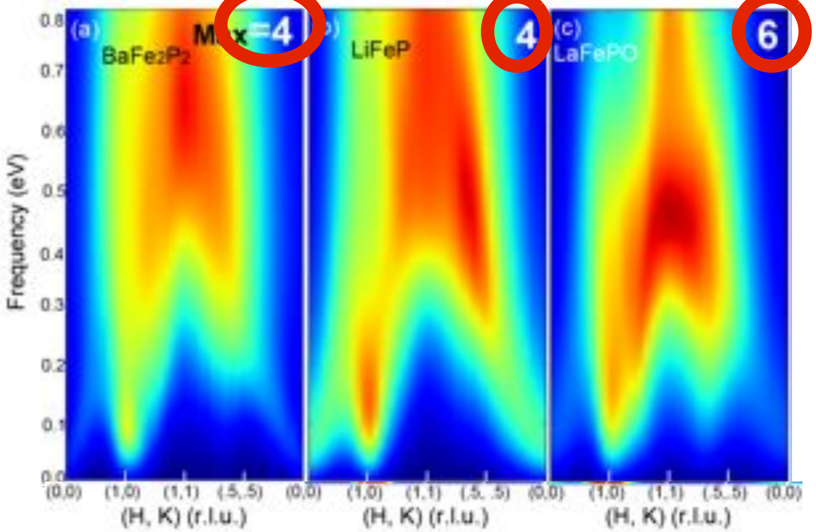

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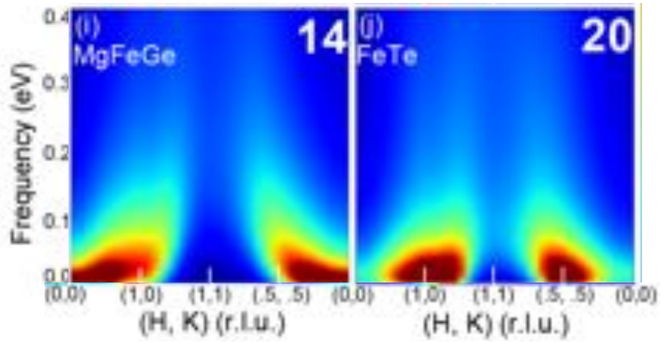
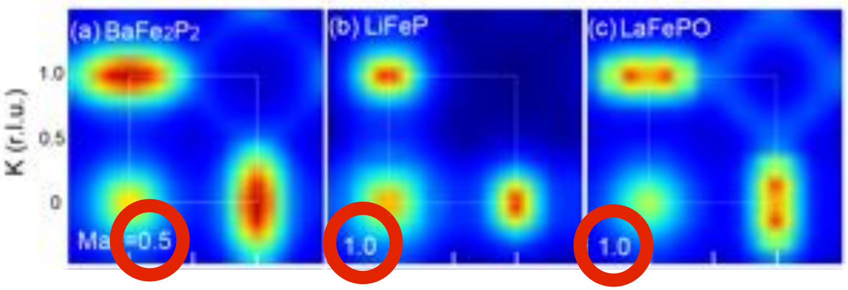
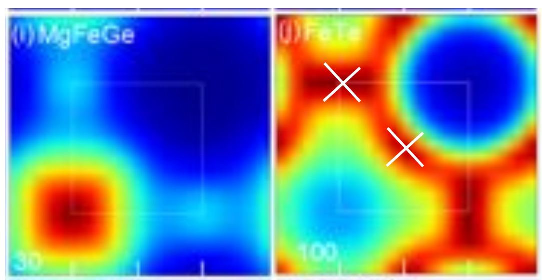


broad with mostly (0,0) peak

two competing orders (1,0)&(1/2,1/2)

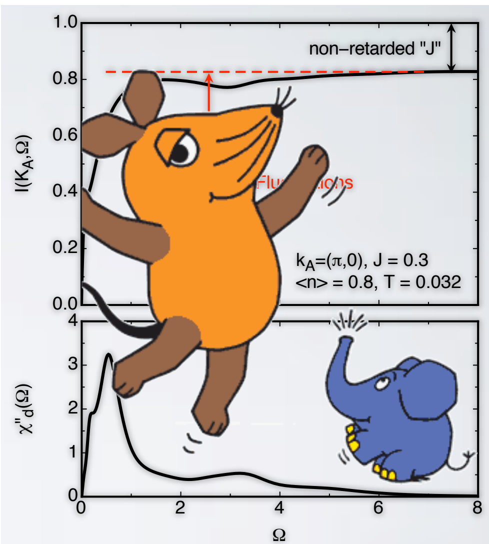




Maximum intensity two orders of magnitude smaller

What do we need for SC?

"We have a mammoth and an elephant in our refrigerator— do we care much if there is also a mouse?"



P.W. Anderson, Science 316, 1705 (2007):

"We have a mammoth (U) and an elephant (J) in our refrigerator -do we care if there is also a mouse (spin fluctuations)?"

D. Scalapino & T. Maier:

Spin fluctuation theory and weak coupling approaches: Only low energy spin fluctuations are important :

"mouse is larger than the elephant"

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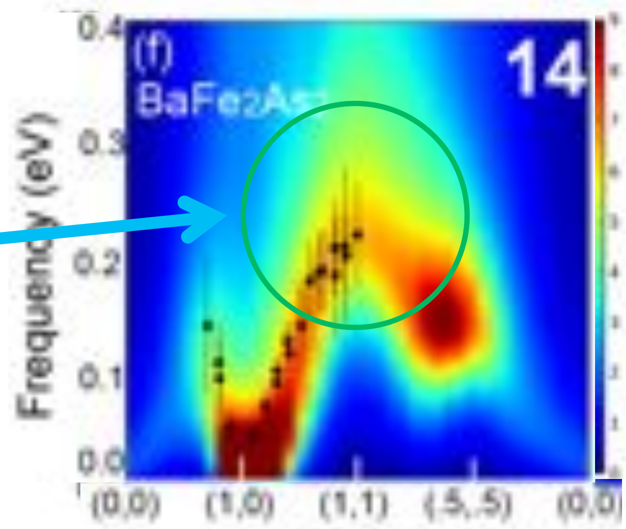
Both appear in iron superconductors:

high-energy magnetic excitations with well-defined dispersion (which give large fluctuating moment)



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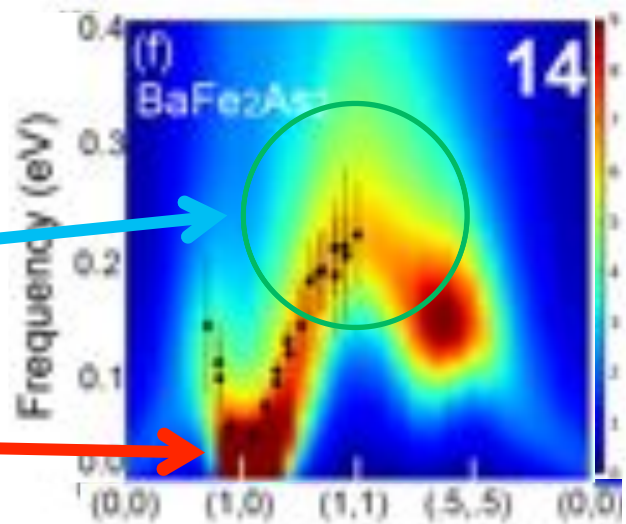
Both appear in iron superconductors:

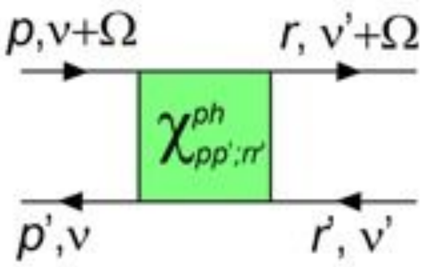
high-energy magnetic excitations with well-defined dispersion (which give large fluctuating moment)

commensurate (1,0) low-energy magnetic excitations (spin fluctuations)



Particle-particle irreducible vertex

have particle hole



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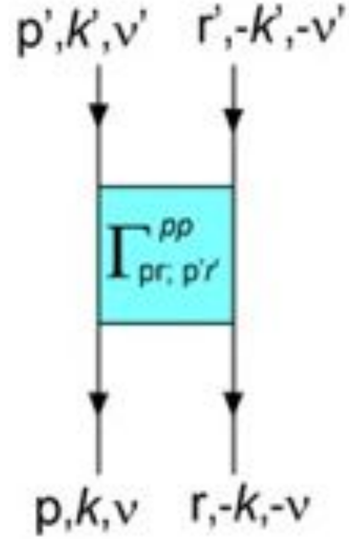

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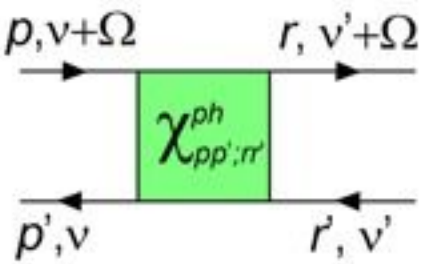

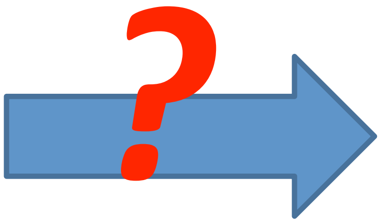

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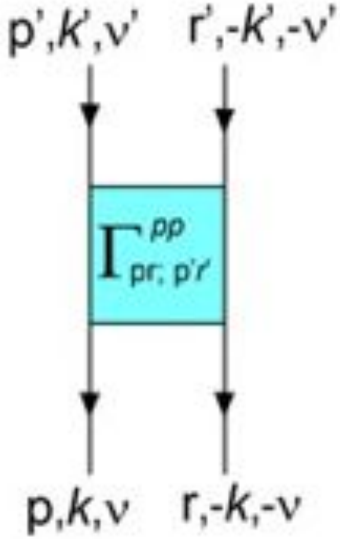

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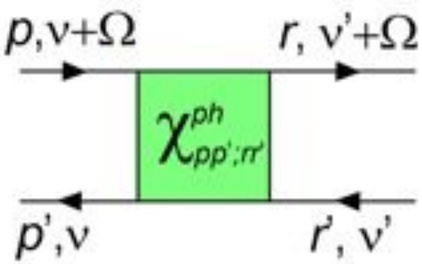

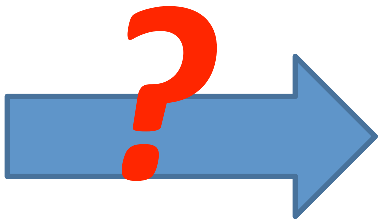

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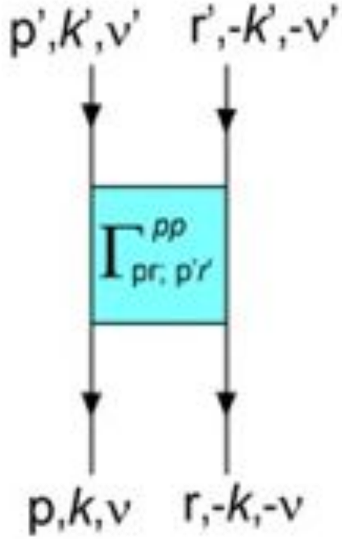

We can compute particle-particle vertex using particle-hole vertex and susceptibility:

Particle-particle irreducible vertex

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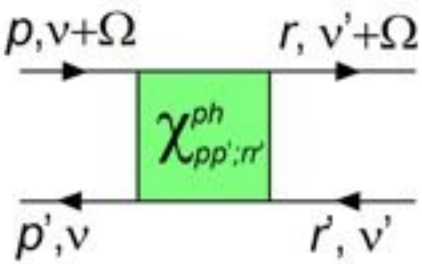

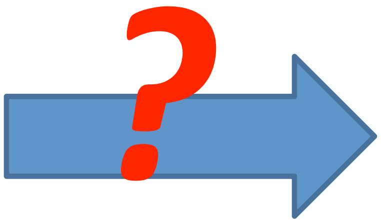

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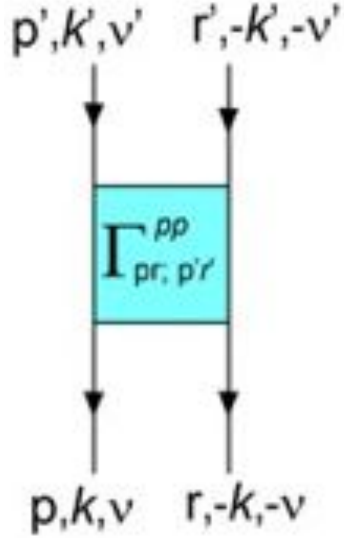

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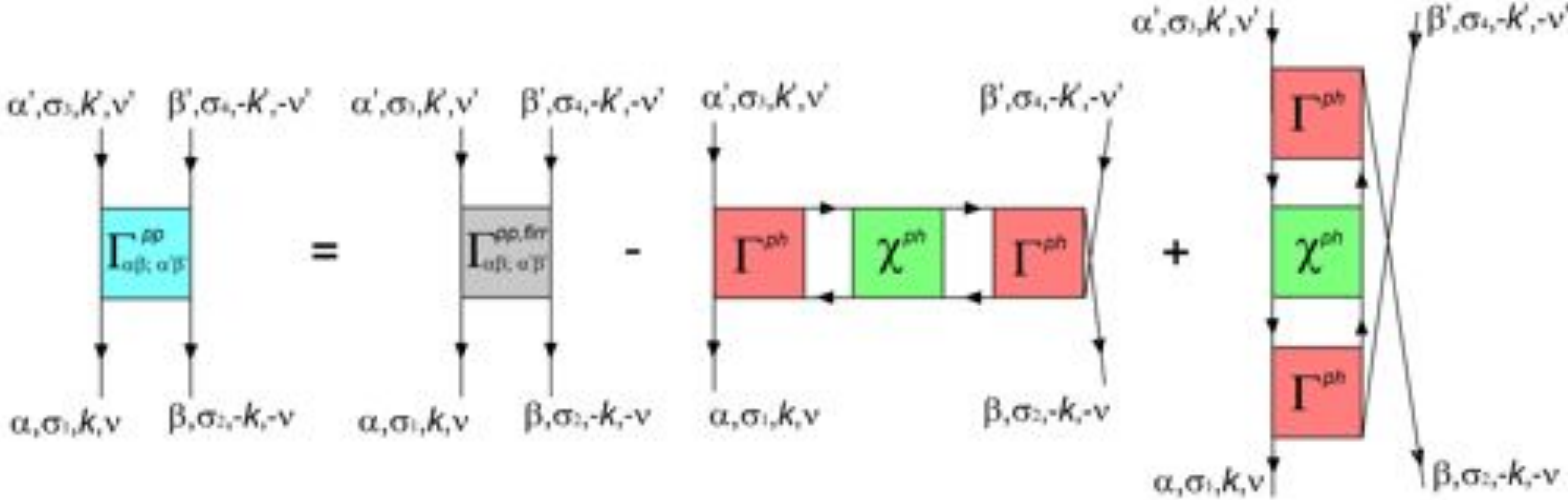

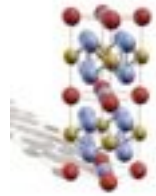

Summary

•Electronic dynamics in Fe superconductors nontrivial because electrons are not well described by localized or itinerant picture: intermediate regime where both the Fermi surface and magnetic exchange play the role.
This regime can be described by LDA+DMFT.

•Mass enhancement due to electronic correlations are significant in Fe superconductors (>~3), exceed 7 in FeTe.

•Electronic correlations are significant because of Hund's coupling, and not because of Hubbard U. New physics of Hund's metals as opposed to Mott insulators!

•Correlations give rise to large fluctuating moment at low energy.

•Magnetic spectrum is very sensitive to details (doping), for superconductivity need significant low energy fluctuating moments and large exchange interaction, which can be found at the intermediate correlation strength.

•Three superconducting symmetries are competing, s+-, d, and novel "orbital-antiphase s+-", which might be the best candidate in LiFeAs.

THANK YOU!