Luca de' Medici

ESRF – Grenoble

Reverse-engineering electronic correlations in Iron-based superconductors

Probing and Understanding Exotic Superconductors and Superfluids

ICTP - Trieste 29.10.2014

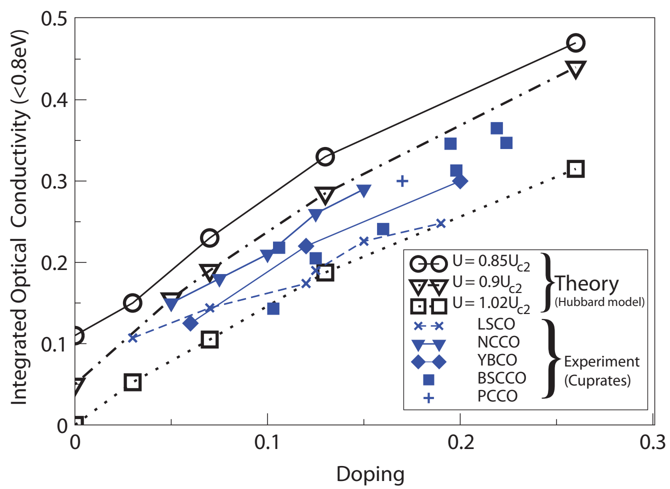
Collaborators

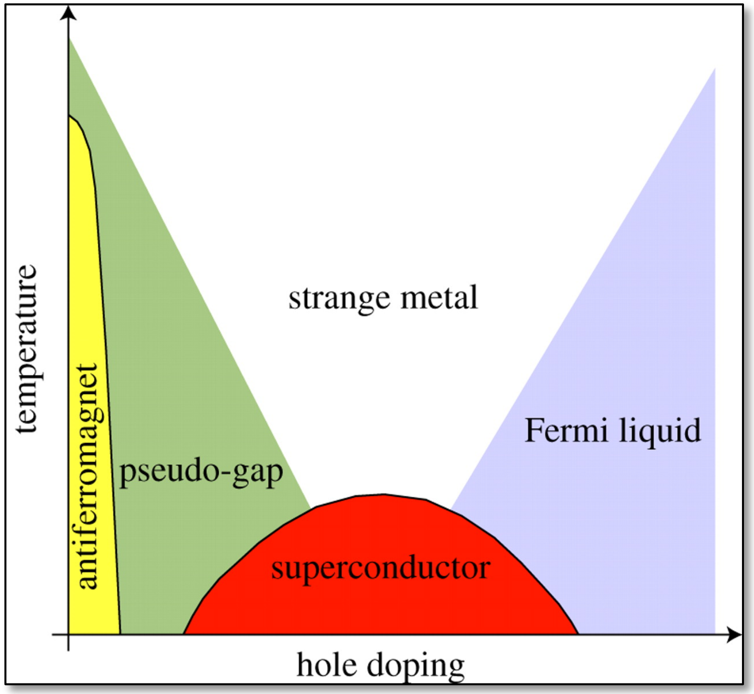
Massimo Capone

Gianluca Giovannetti

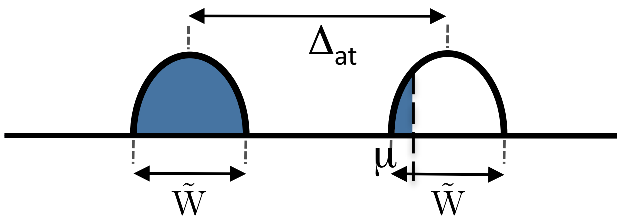
Cuprates: Mottness

Comanac et al. Nat.Phys. 2008





'Mottness'



Spectrum of charge excitations

The proximity to a Mott state strongly affects the properties of a system:

- reduced metallicity (Z~x)
- mass enhancement
- transfer of spectral weight from low to high energy (e.g. in optical response)
- tendency towards magnetism
- …

Cuprates: Pseudogap as Selective Mottness

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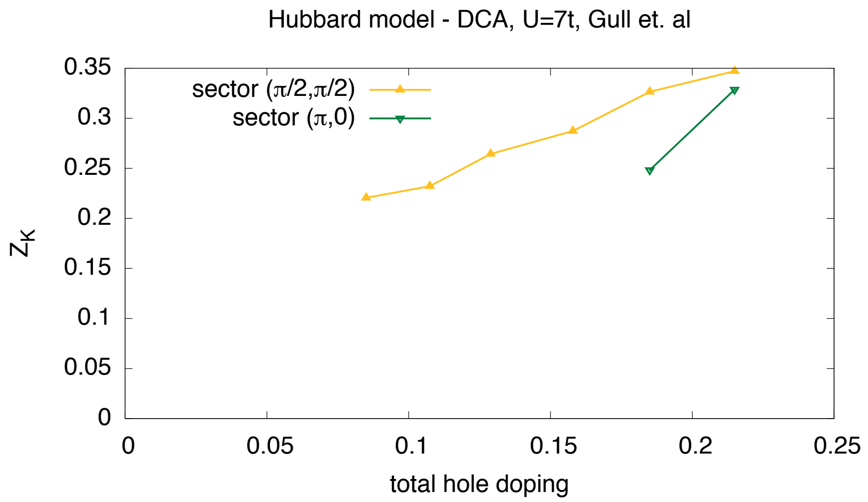
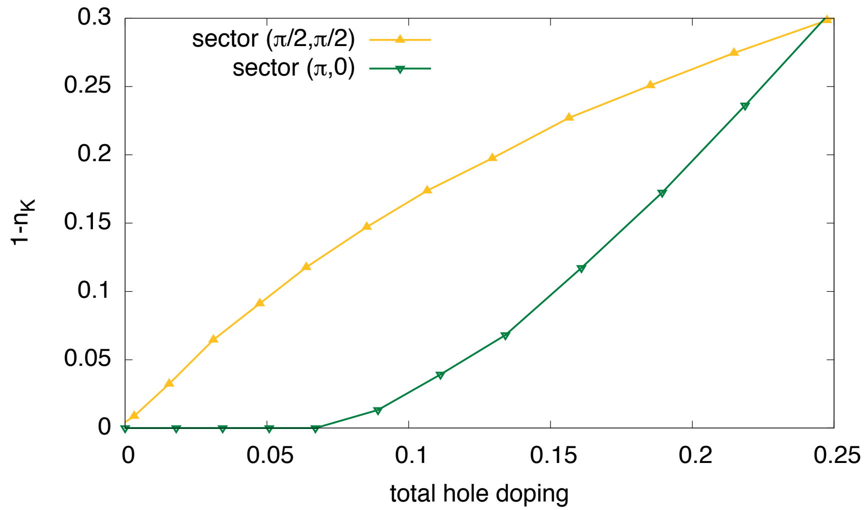
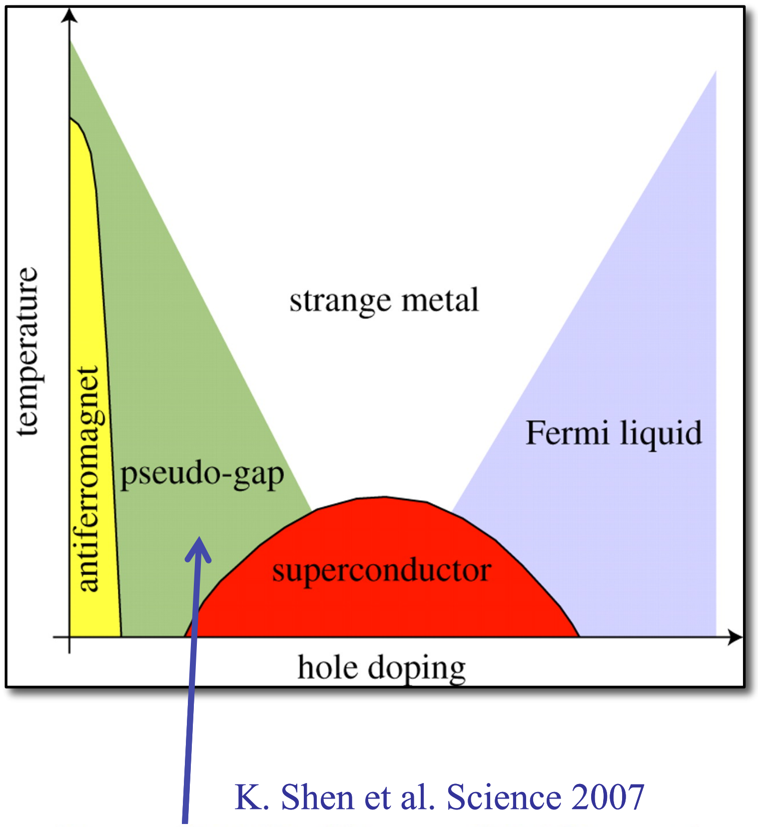
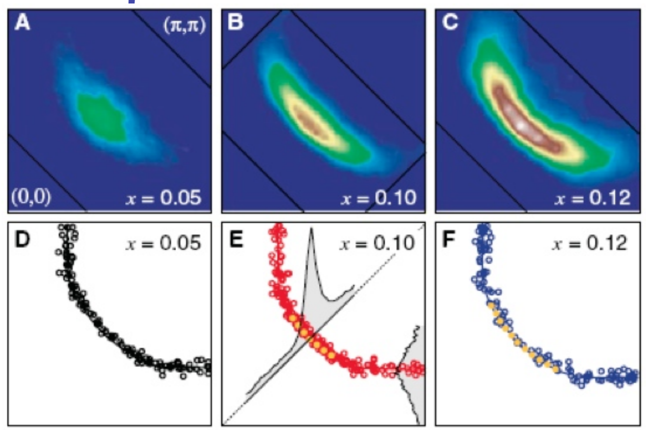




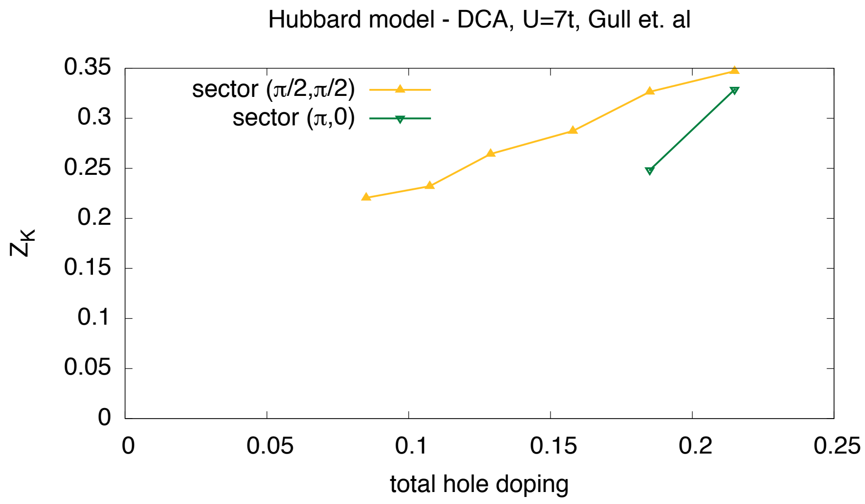
DCA calculation from: Gull et al.
Phys Rev. B 82, 155101 (2010)

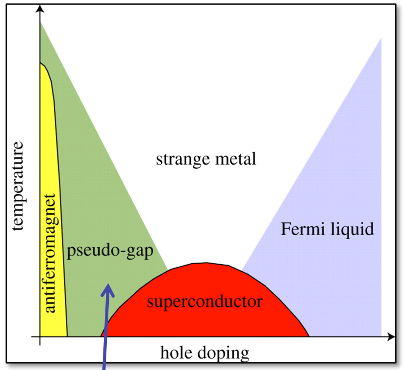


K. Shen et al. Science 2007



Cuprates: Pseudogap as Selective Mottness





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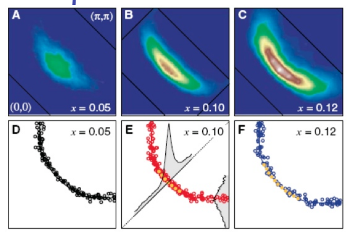

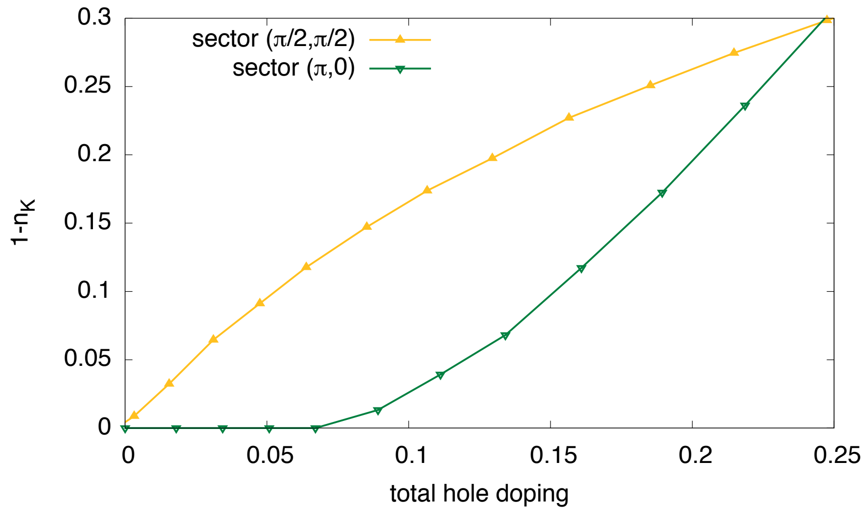

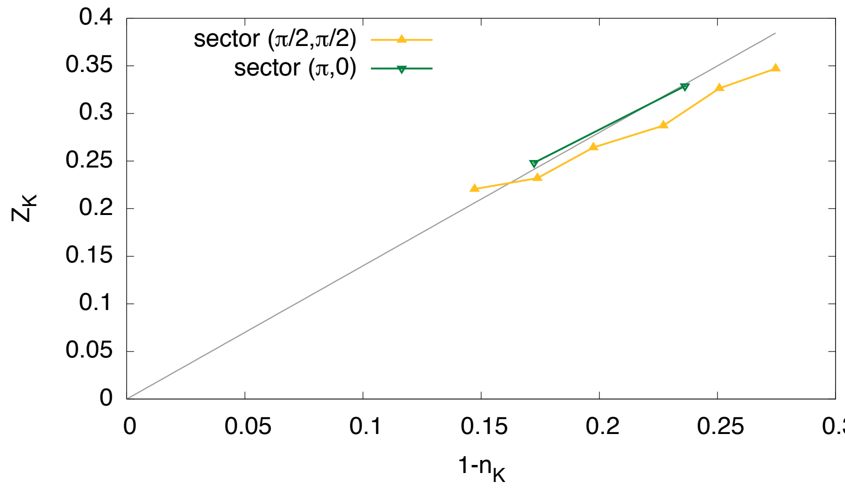

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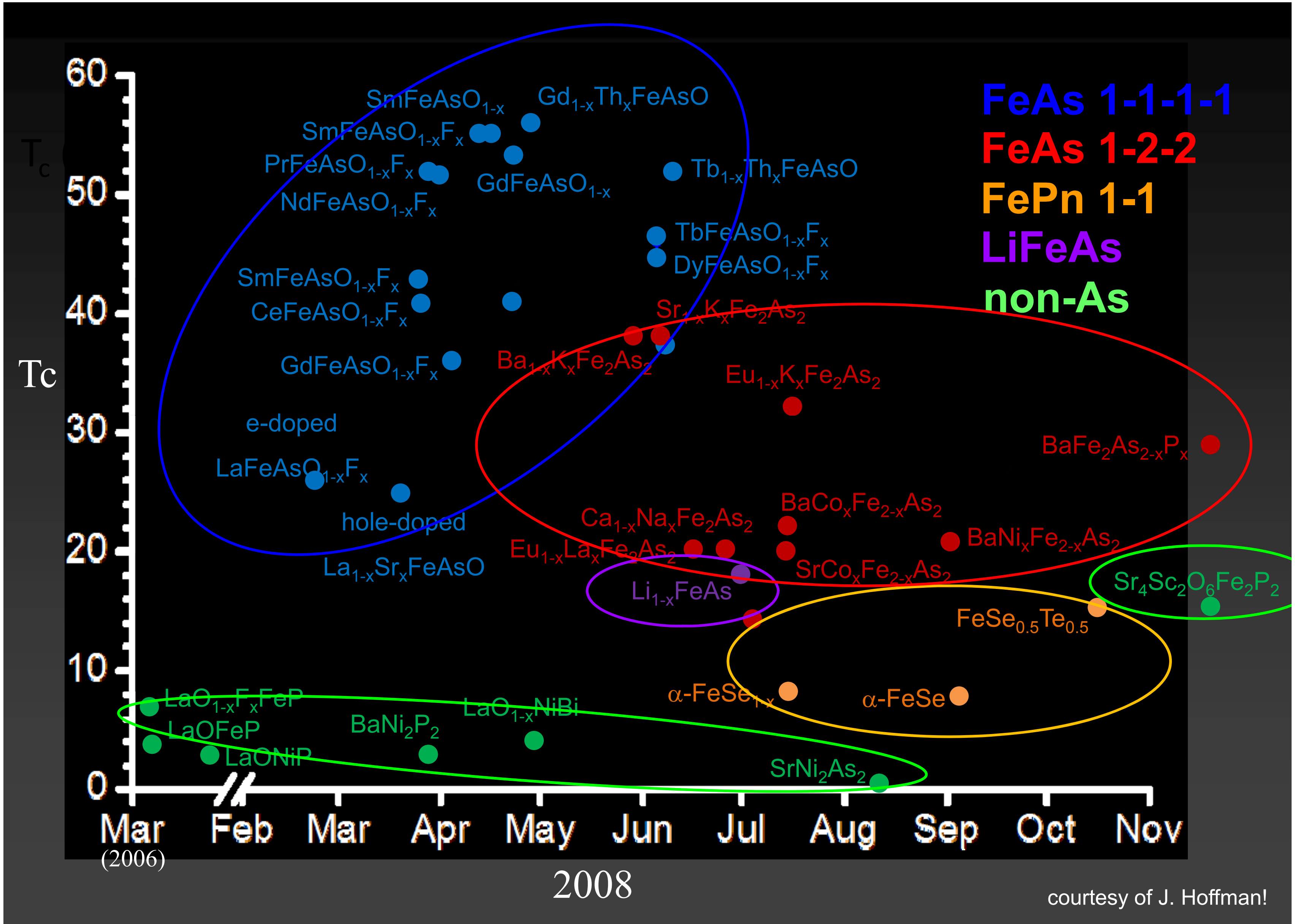
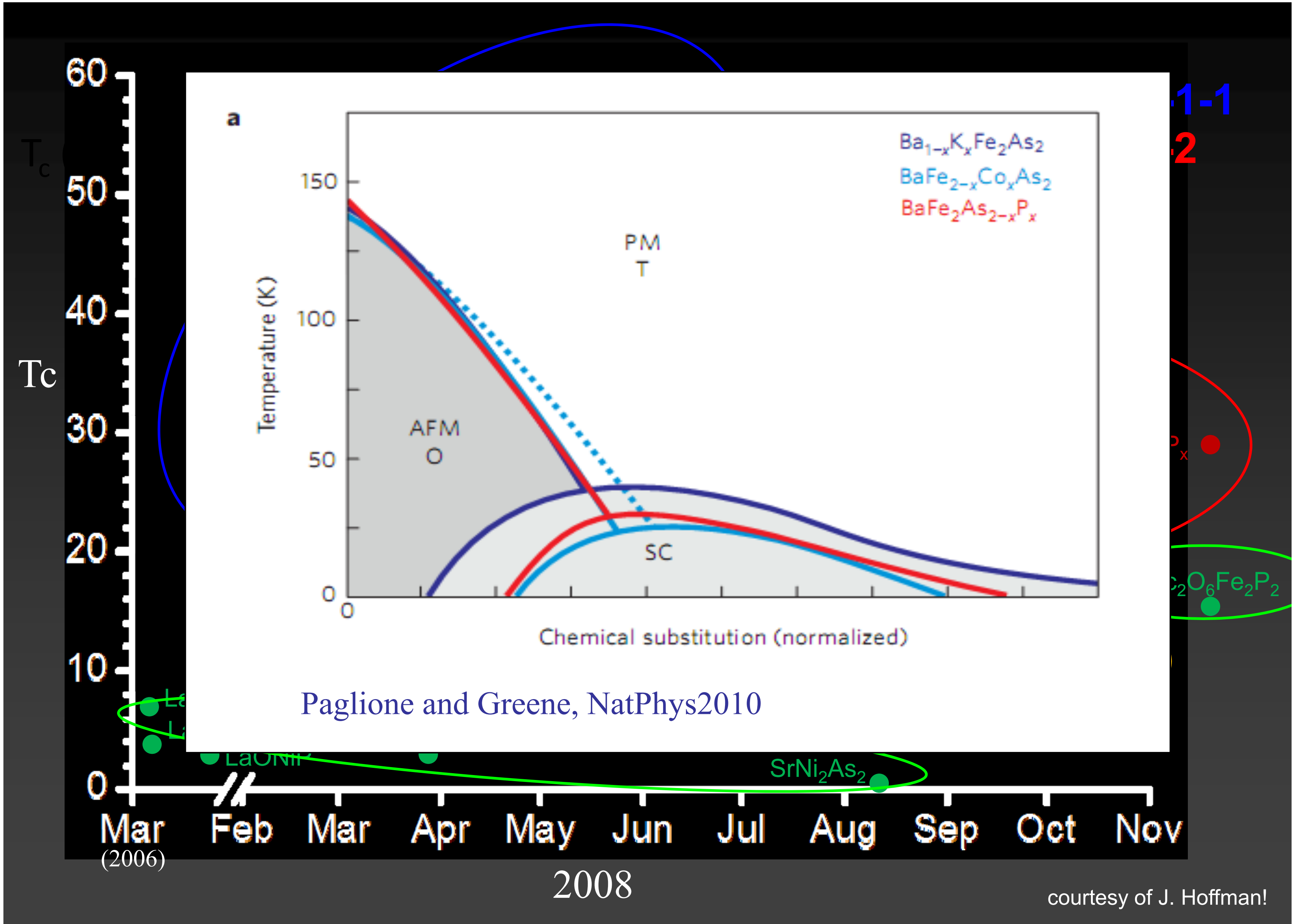

FeAs 1-1-1-1
FeAs 1-2-2
FePn 1-1
LiFeAs
non-As
Tc
60
50
40
30
20
10
0
Mar
(2006)
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
2008
SmFeAsO$_{1-x}$
Gd$_{1-x}$Th$_x$FeAsO
SmFeAsO$_{1-x}$F$_x$
PrFeAsO$_{1-x}$F$_x$
GdFeAsO$_{1-x}$
Tb$_{1-x}$Th$_x$FeAsO
NdFeAsO$_{1-x}$F$_x$
TbFeAsO$_{1-x}$F$_x$
DyFeAsO$_{1-x}$F$_x$
SmFeAsO$_{1-x}$F$_x$
CeFeAsO$_{1-x}$F$_x$
Sr$_{1-x}$K$_x$Fe$_2$As$_2$
GdFeAsO$_{1-x}$F$_x$
Ba$_{1-x}$K$_x$Fe$_2$As$_2$
Eu$_{1-x}$K$_x$Fe$_2$As$_2$
e-doped
BaFe$_2$As$_{2-x}$P$_x$
LaFeAsO$_{1-x}$F$_x$
hole-doped
Ca$_{1-x}$Na$_x$Fe$_2$As$_2$
BaCo$_x$Fe$_{2-x}$As$_2$
BaNi$_x$Fe$_{2-x}$As$_2$
Eu$_{1-x}$La$_x$Fe$_2$As$_2$
La$_{1-x}$Sr$_x$FeAsO
SrCo$_x$Fe$_{2-x}$As$_2$
Li$_{1-x}$FeAs
Sr$_4$Sc$_2$O$_6$Fe$_2$P$_2$
FeSe$_{0.5}$Te$_{0.5}$
LaO$_{1-x}$F$_x$FeP
LaO$_{1-x}$NiBi
α-FeSe$_{1-x}$
α-FeSe
LaOFeP
BaNi$_2$P$_2$
LaONiP
SrNi$_2$As$_2$
courtesy of J. Hoffman!


Tc
60
50
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10
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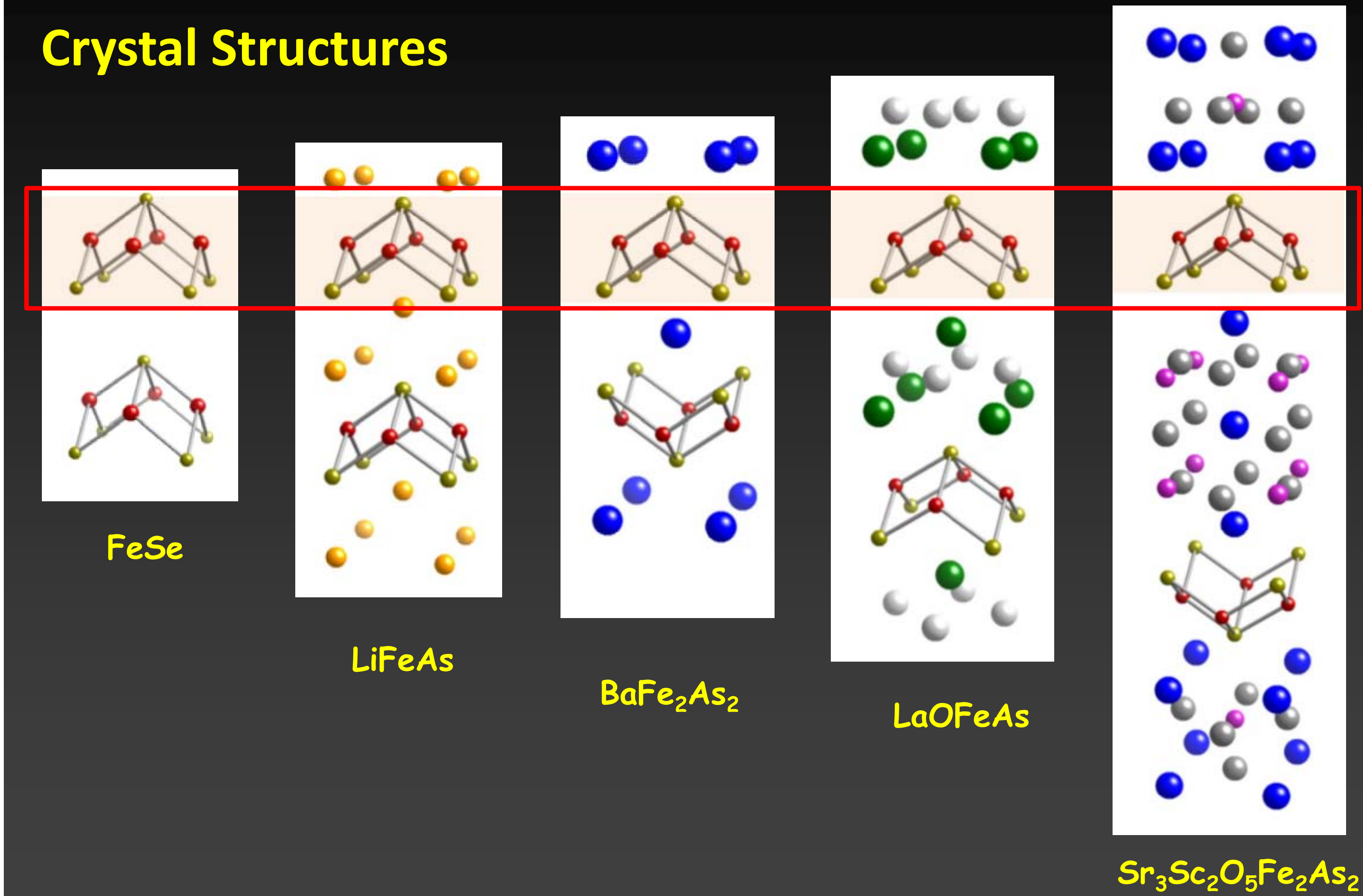
Mar
(2006)
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
2008
SrNi2As2
a
Temperature (K)
150
100
50
0
Ba1−xKxFe2As2
BaFe2−xCoxAs2
BaFe2As2−xPx
PM
T
AFM
O
SC
Chemical substitution (normalized)
Paglione and Greene, NatPhys2010
courtesy of J. Hoffman!

Crystal Structures



Paglione/Greene review (2010)

Iron-based superconductors

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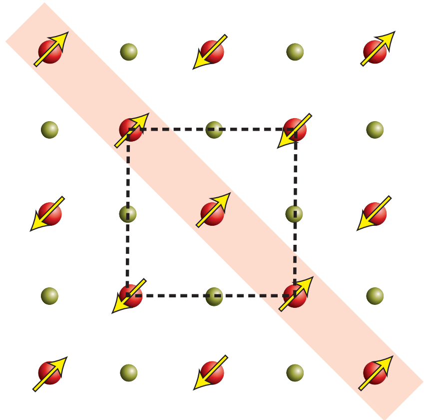
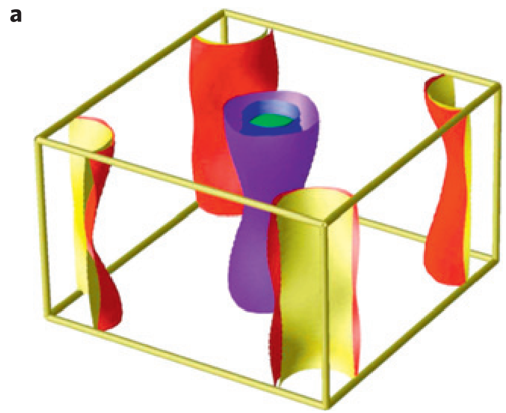
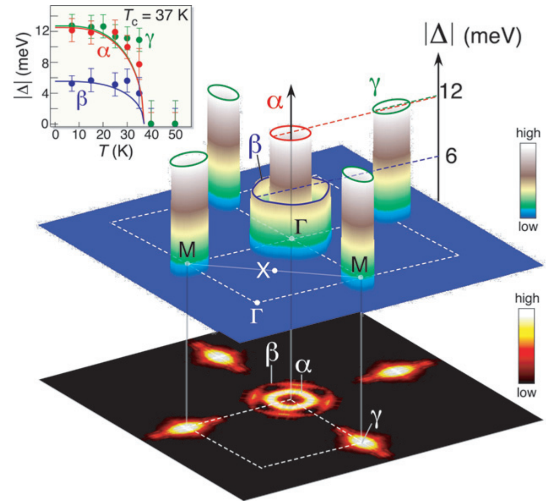
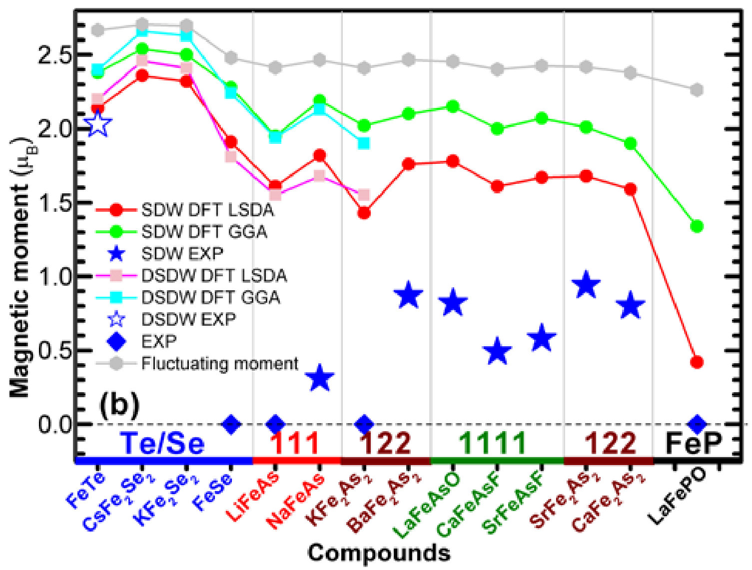
Paglione and Greene, NatPhys2010



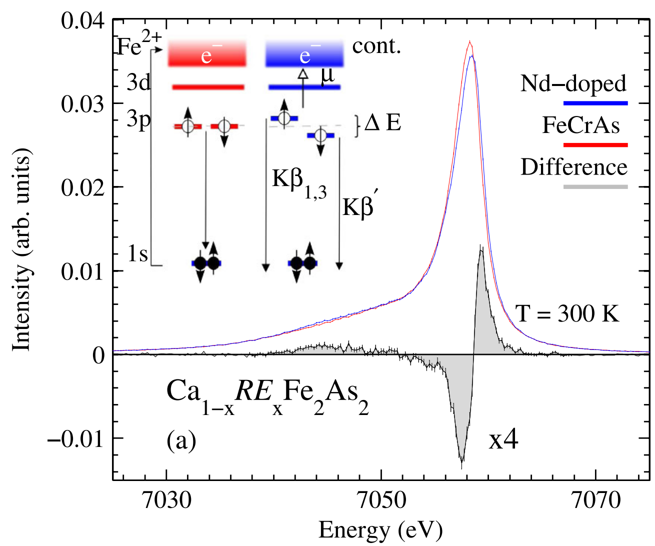




Ding et al. EPL 2008



Yin et al. NatMat2011



Gretarsson et al. PRL2013

Correlations in Iron SC?

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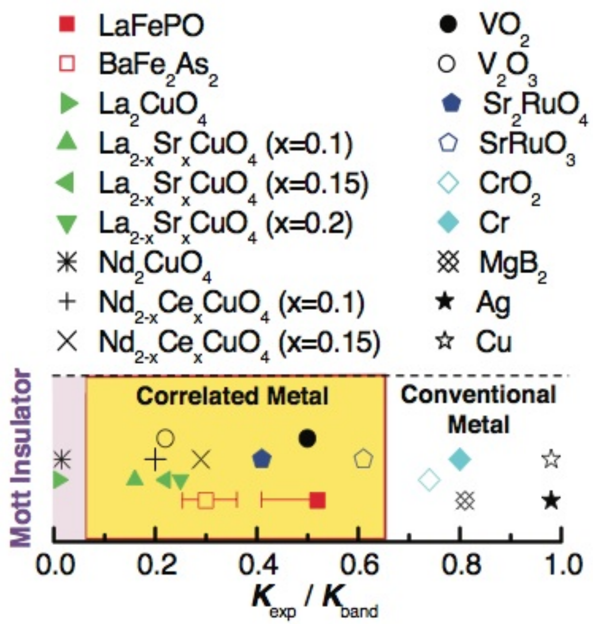
Contrasting evidences for correlation strength

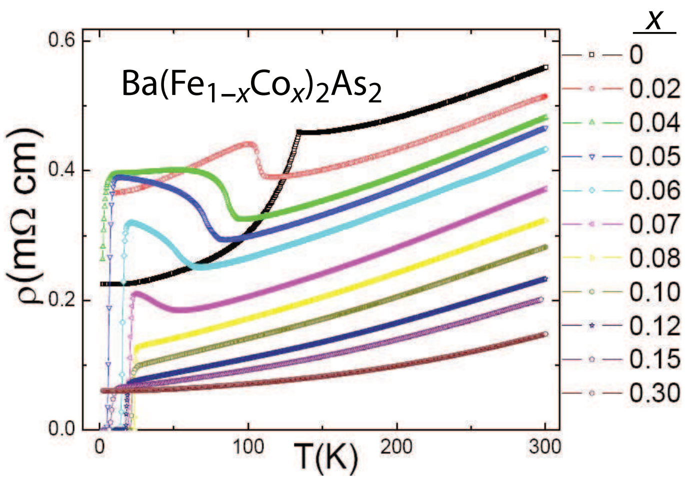
weak {
- no Mott insulator in the phase diagram
- no detection of prominent Hubbard bands
- moderate correlations from Optics

strong {
- bad metallicity
- strong sensitivity to doping
- local vs itinerant magnetism

<u>Weak-coupling vs Strong-coupling scenarios</u>

Qazilbash et al. NatPhys2009

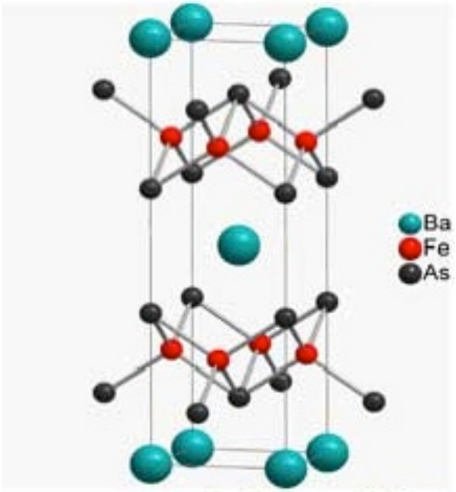




Fang et al. PRB80 (2009)
Rullier-Albenque et al. PRL103 (2009)

Specific heat (mJ/ mol K^2)	
LaFePO	7
$Ba(Co_xFe_{1-x})_2As_2$	15-20
$Ba_{1-x}K_xFe_2As_2$	50
$FeSe_{0.88}$	9.2
KFe_2As_2	69-102
$K_{0.8}Fe_{1.6}Se_2$	6

Review: Stewart, RMP (2011)

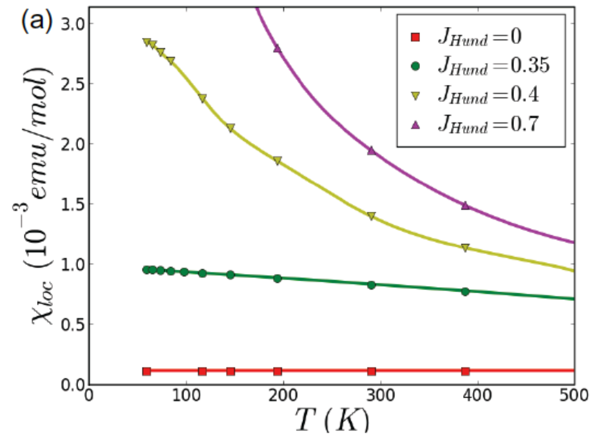


$BaFe_2As_2$

- cubic
- multi-orbital: 5 bands (Fe 3d) at the Fermi level
  n=6 conduction electrons
- Partially lifted degeneracy
- Not a very large U but strong Hund's coupling J
  W~4eV, U~2-4eV, J~0.5eV

Theory:
'Hund's metals'

Haule and Kotliar, NJP 11 (2009)



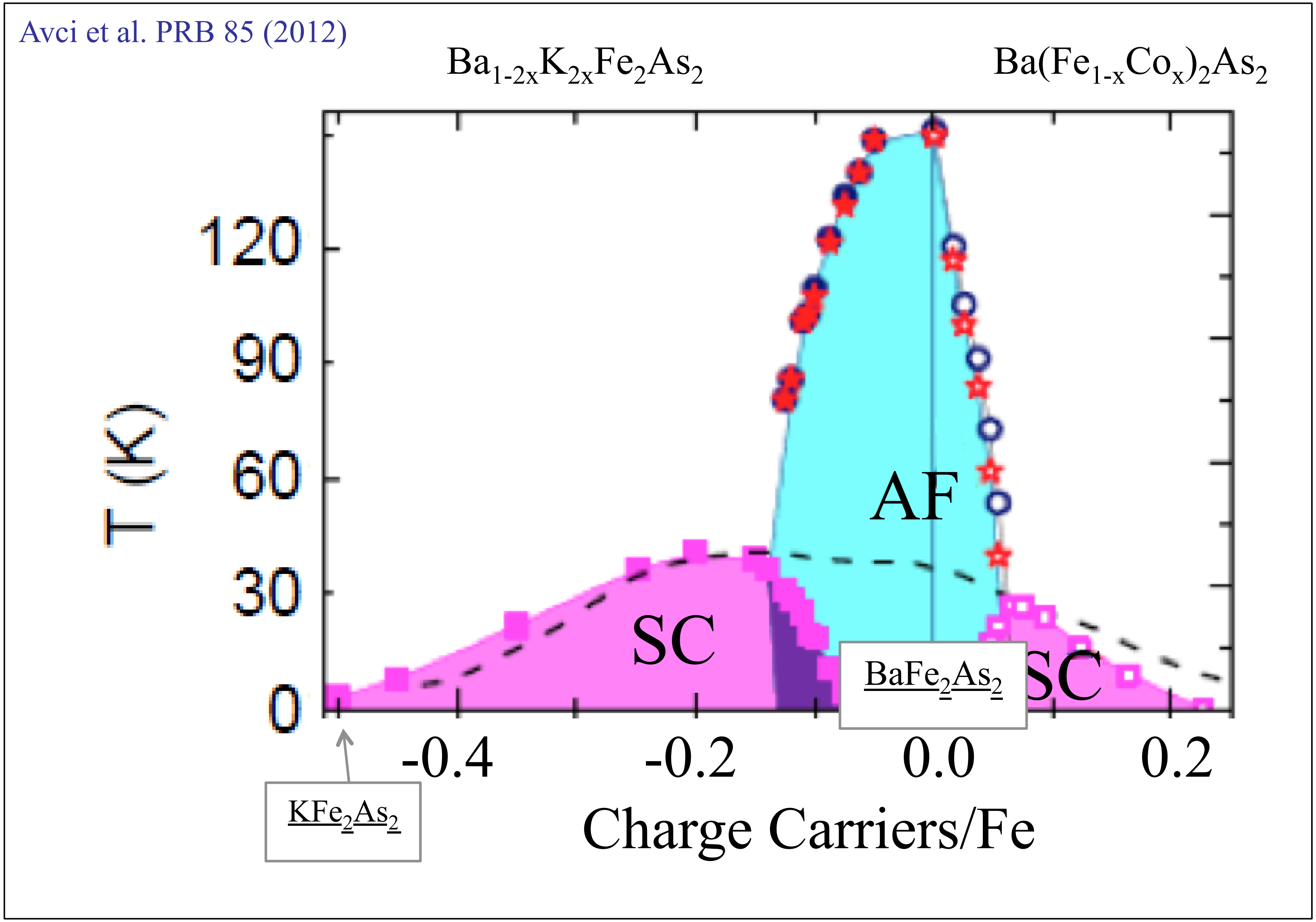
$$H = \sum_k H_k^{DFT}$$

$$+U\sum_{i,m} n_{im\uparrow}n_{im\downarrow} + (U' - \frac{J}{2})\sum_{i,m>m'} n_{im}n_{im'}$$

$$-J\sum_{i,m>m'}\Big[2\mathbf{S}_{im}\cdot\mathbf{S}_{im'} + (d^\dagger_{im\uparrow}d^\dagger_{im\downarrow}d_{im'\uparrow}d_{im'\downarrow} + h.c.)\Big]$$

(U'=U-2J)

Ba-122 Phase diagram

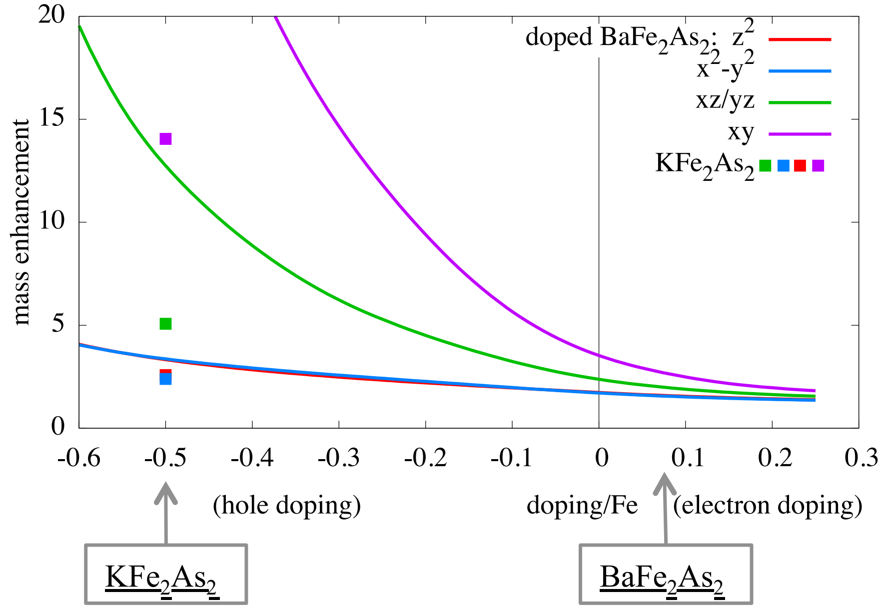


Orbital-dependent correlation strength

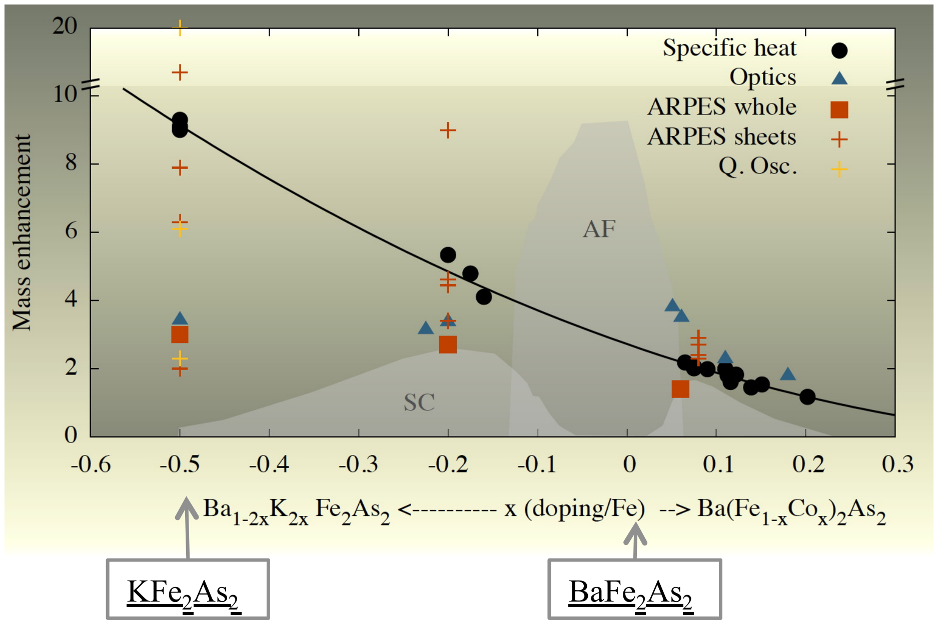
mass enhancements

LdM, G. Giovannetti, M. Capone, PRL 2014

Theory (LDA+Slave-spins)



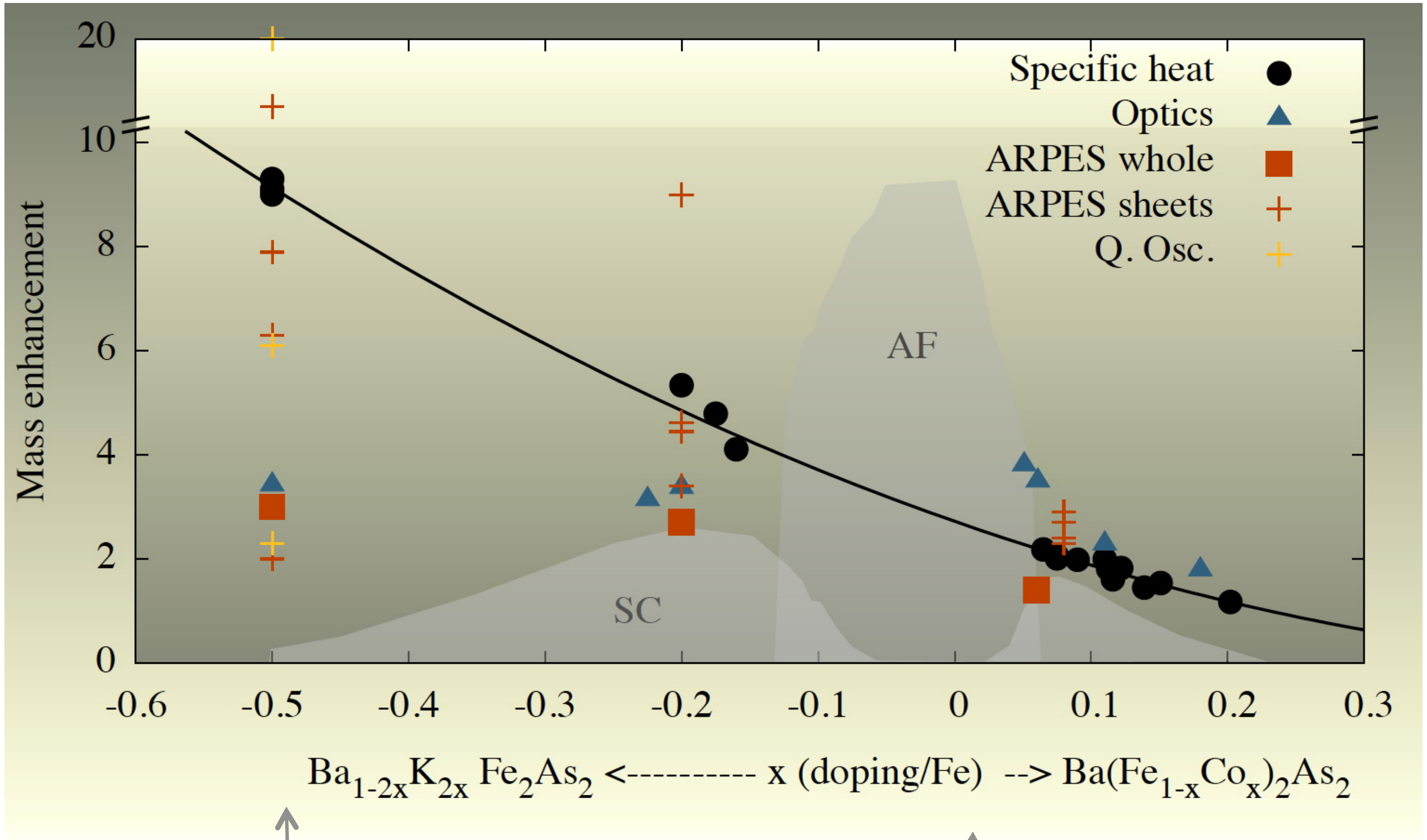
Experimental data
(high-T tetragonal phase)



Selective correlation strength: strongly *and* weakly correlated electrons

Many other theoretical works showing orbital-dependent correlations (DFT+..) : Ishida et al., Aichhorn et al., Shorikov et al., Craco, Laad et al., Werner et al., Yin et al., Backes et al. (DMFT), Misawa Imada (VQMC) Bascones et al. (Hartree-Fock), Ikeda et al. (FLEX), Yu Si (slave spins), Lanatà et al. (Gutzwiller), Calderon et al. (slave-spins), etc.

Correlations: experimental mass enhancements in Ba-122



KFe_2As_2

$BaFe_2As_2$

(all data in the high-T tetragonal phase)

Sommerfeld coefficient $\gamma \sim N^*(E_F) = \sum_\alpha (m^*/m_b)_\alpha N_b^\alpha(E_F)$

Optics: Drude contribution $D^* = \sum_\alpha (m_b/m^*)_\alpha D_b^\alpha$

References in: LdM, G. Giovannetti, M. Capone, PRL2014

Optics: beware of interband transitions! Calderon et al., PRB2014

Orbital-dependent correlation strength

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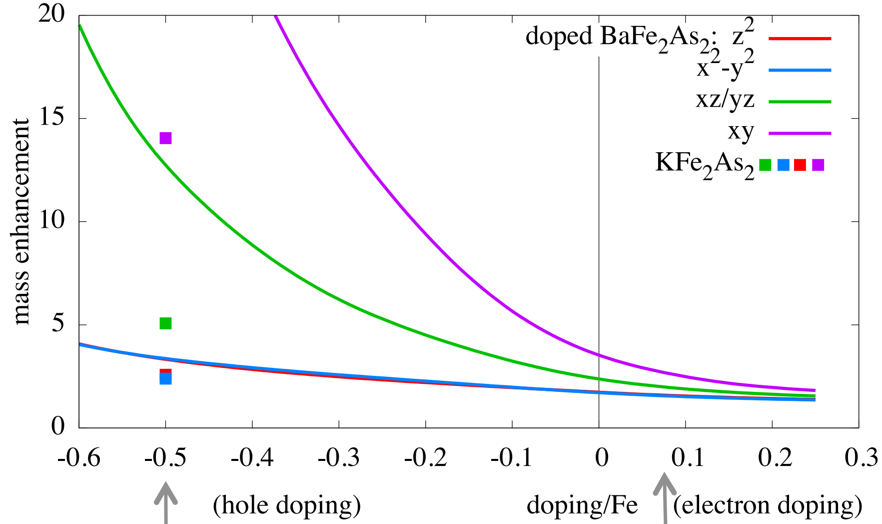
mass enhancements

LdM, G. Giovannetti, M. Capone, PRL 2014

Theory (LDA+Slave-spins)



KFe_2As_2 $BaFe_2As_2$

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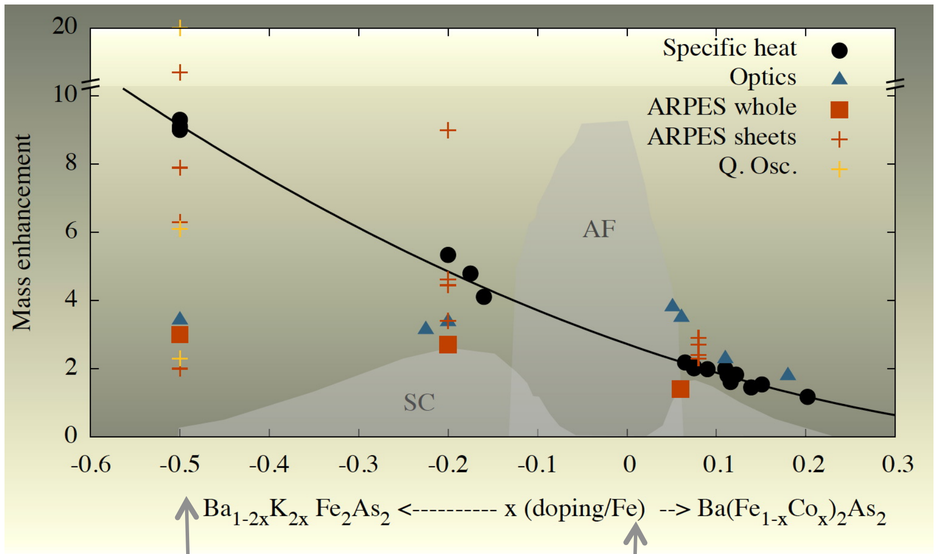
(high-T tetragonal phase)



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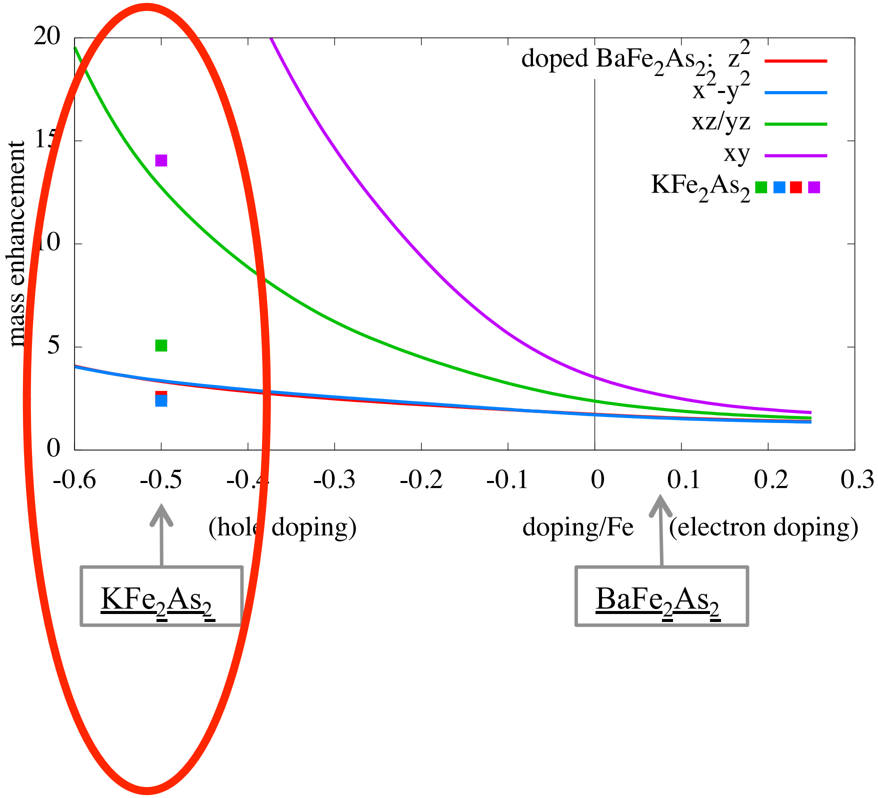
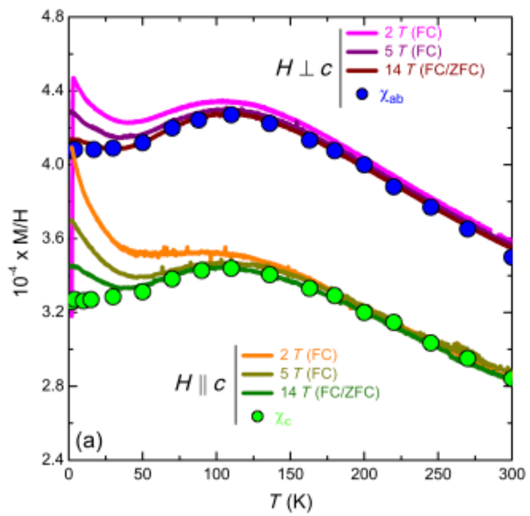


PRL **111,** 027002 (2013) PHYSICAL REVIEW LETTERS week ending 12 JULY 2013

Evidence of Strong Correlations and Coherence-Incoherence Crossover in the Iron Pnictide Superconductor KFe_2As_2

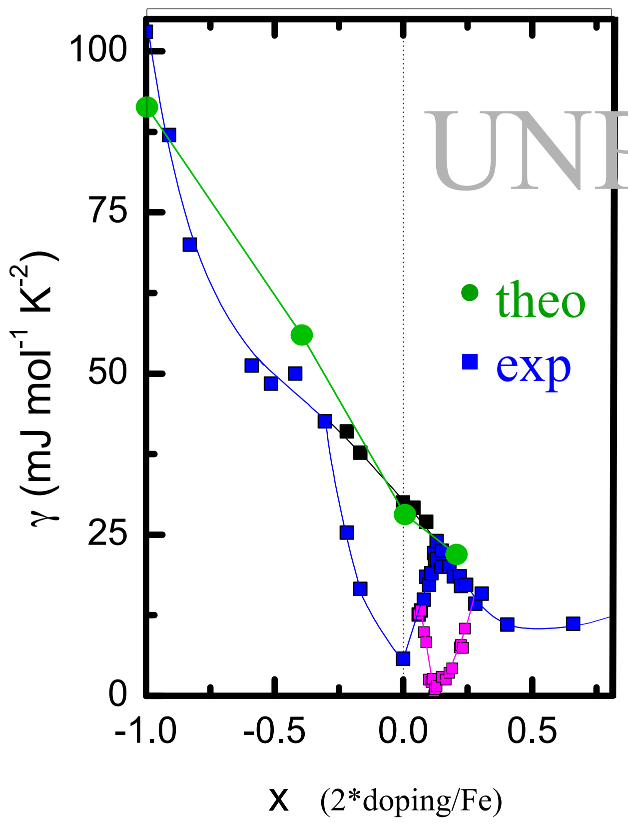
F. Hardy,[1,*] A. E. Böhmer,[1] D. Aoki,[2,3] P. Burger,[1] T. Wolf,[1] P. Schweiss,[1] R. Heid,[1] P. Adelmann,[1] Y. X. Yao,[4] G. Kotliar,[5] J. Schmalian,[6] and C. Meingast[1]
[1]*Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe, Germany*
[2]*INAC/SPSMS, CEA Grenoble, 38054 Grenoble, France*
[3]*IMR, Tohoku University, Oarai, Ibaraki 311-1313, Japan*
[4]*Ames Laboratory US-DOE, Ames, Iowa 50011, USA*
[5]*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*
[6]*Karlsruher Institut für Technologie, Institut für Theorie der Kondensierten Materie, 76128 Karlsruhe, Germany*
(Received 15 January 2013; published 9 July 2013)

Using resistivity, heat-capacity, thermal-expansion, and susceptibility measurements we study the normal-state behavior of KFe_2As_2. Both the Sommerfeld coefficient ($\gamma \approx 103$ mJ mol^{-1} K^{-2}) and the Pauli susceptibility ($\chi \approx 4 \times 10^{-4}$) are strongly enhanced, which confirm the existence of heavy quasiparticles inferred from previous de Haas–van Alphen and angle-resolved photoemission spectroscopy experiments. We discuss this large enhancement using a Gutzwiller slave-boson mean-field calculation, which shows the proximity of KFe_2As_2 to an orbital-selective Mott transition. The temperature dependence of the magnetic susceptibility and the thermal expansion provide strong experimental evidence for the existence of a coherence-incoherence crossover, similar to what is found in heavy fermion and ruthenate compounds, due to Hund's coupling between orbitals.

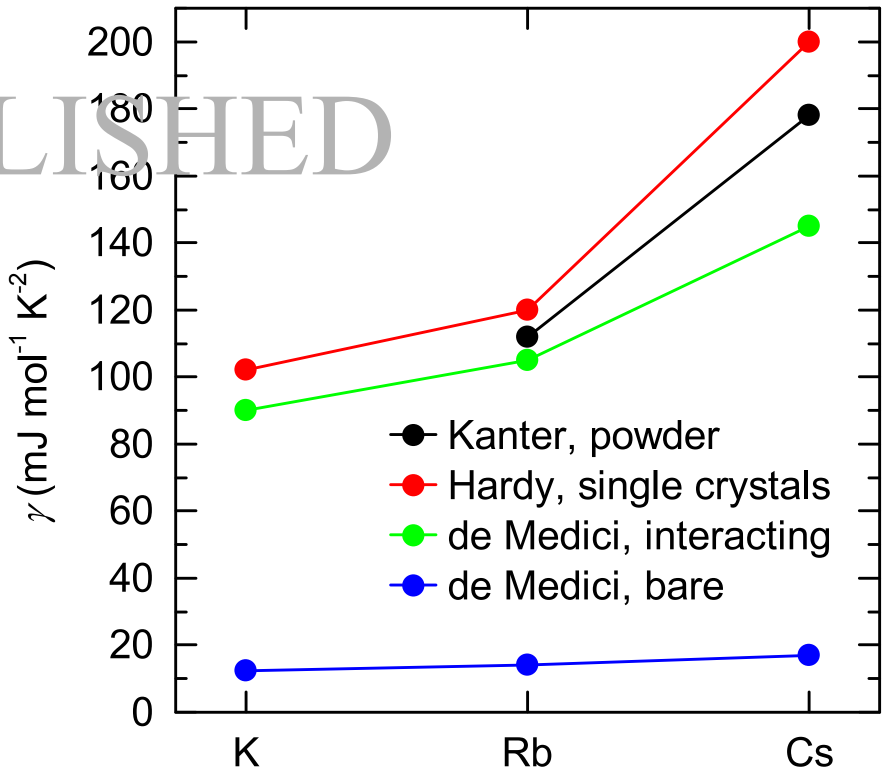


Heavy-fermionic behavior: theory vs experiment

$Ba_{1-x}K_xFe_2As_2$



AFe_2As_2 (A= K, Rb, Cs)

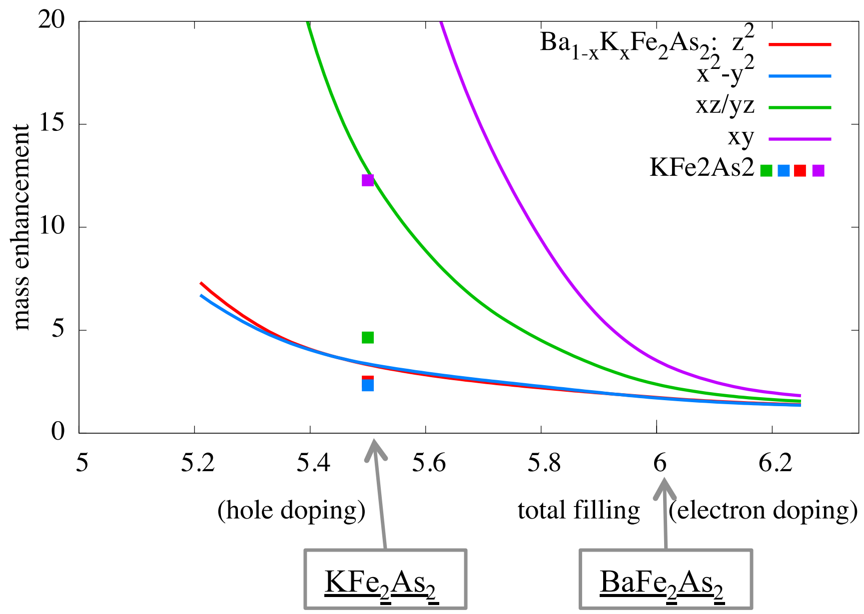


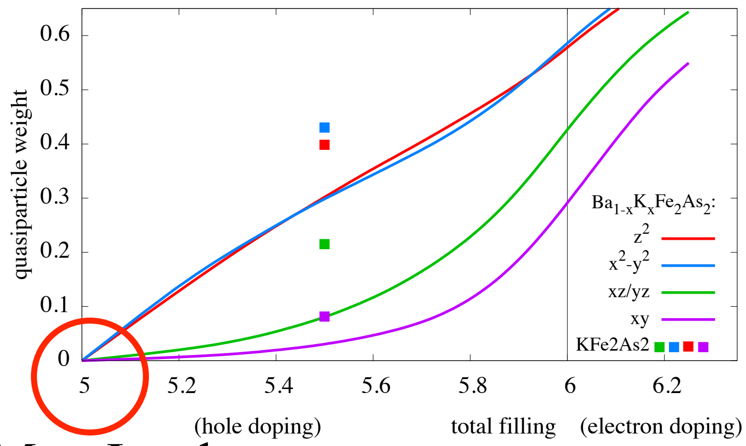
Experiments from Meingast's group in Karlsruhe. F. Hardy et al. unpublished

mass enhancements

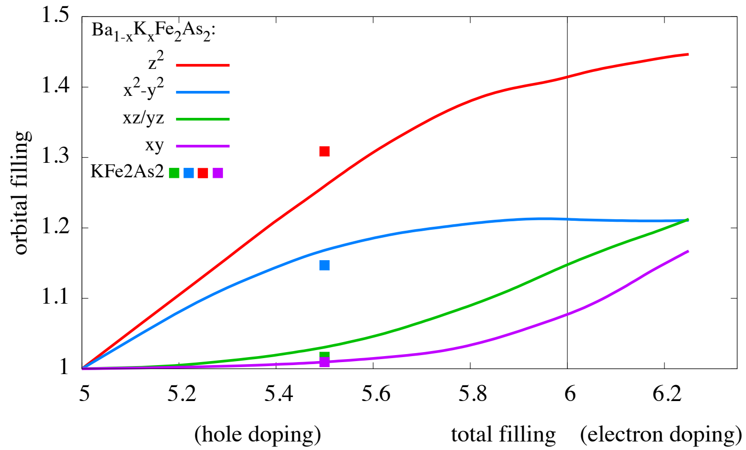
LdM, G. Giovannetti, M. Capone, PRL 2014

Theory (LDA+Slave-spins)

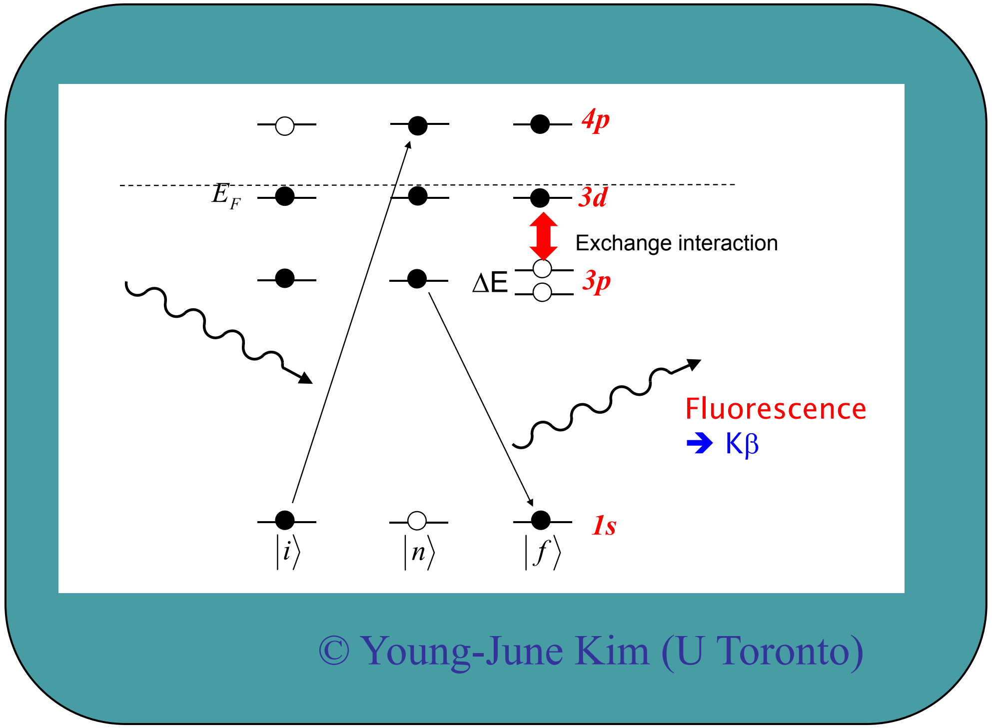


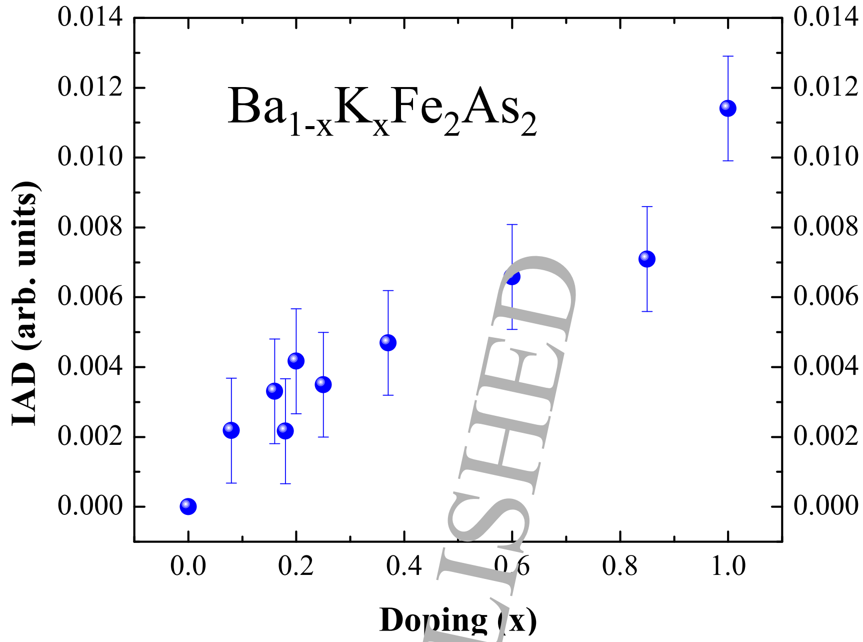


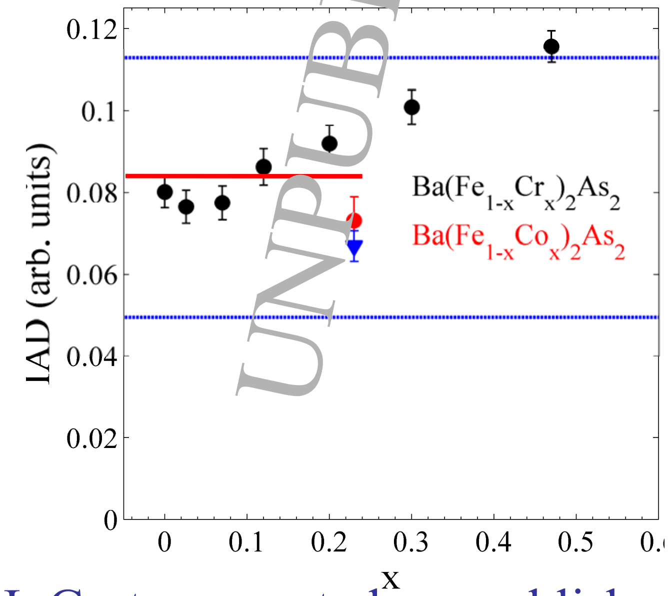
Mott Insulator



Local moments (XES)







Instantaneous local moments building with hole-doping!

S. Lafuerza, H. Gretarsson et al., unpublished

Degenerate 5-band Hubbard model

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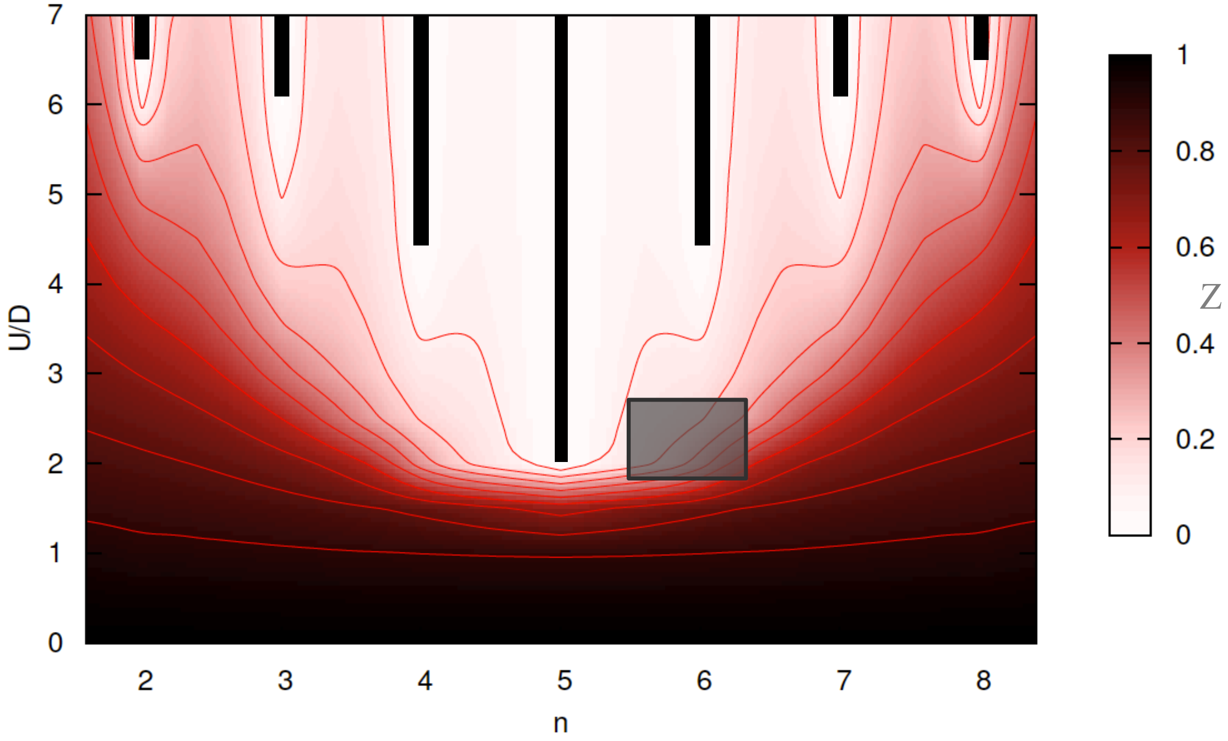
Slave-spin mean field (LdM et al., PRB 72 (2005))

J/U=0.15

J/U=0.20

J/U=0.25



Mott Gap: E(n+1)+E(n-1)-2E(n)

- half-filling: ~U+(N-1)J
- other filling: ~U-3J

LdM, PRB **83** (2011)
LdM, J. Mravlje, A. Georges, PRL **107** (2011)

For a review:
"Strong Correlations from Hunds' Coupling"
A. Georges, LdM, J. Mravlje,
Ann Rev Cond. Mat. 4, 137 (2013)

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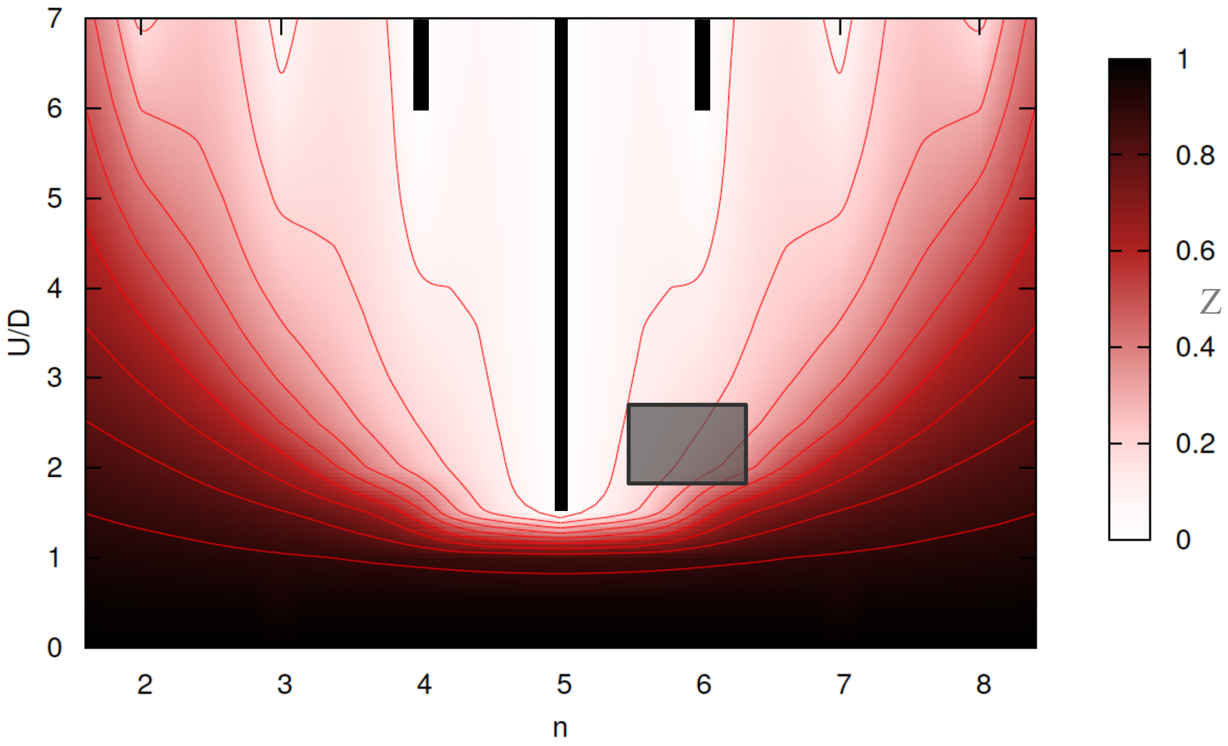

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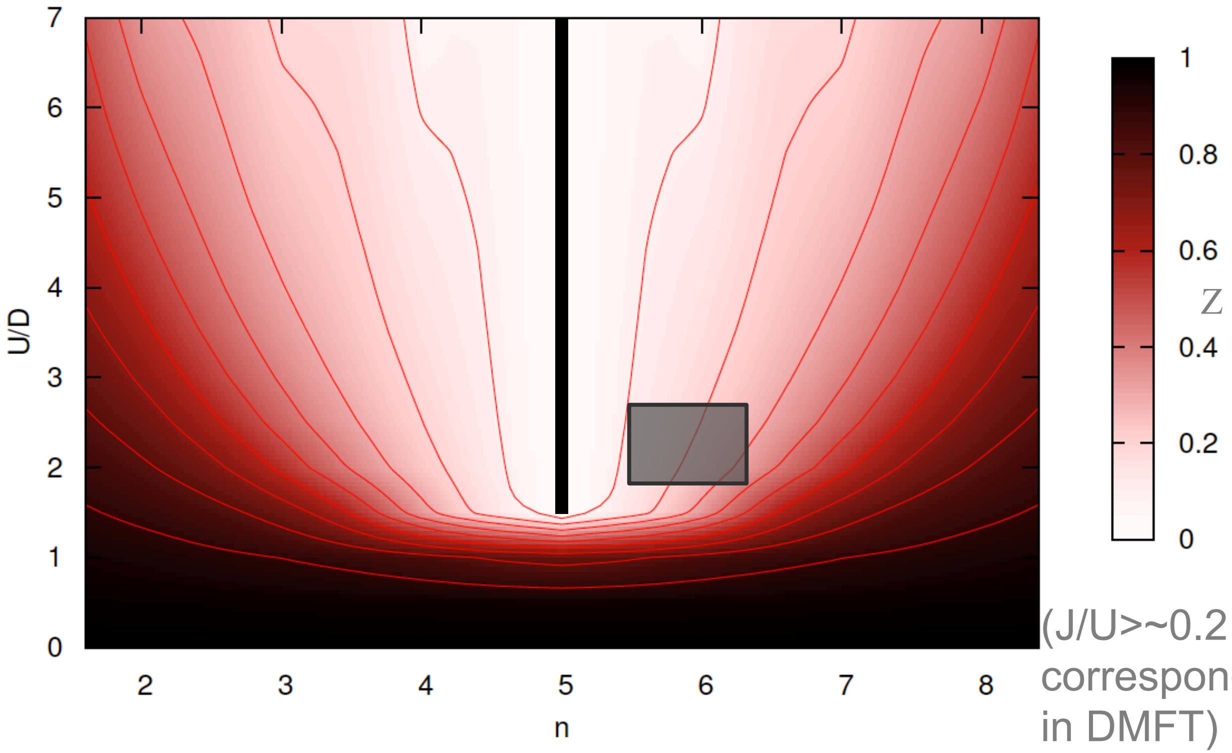

(J/U>~0.2 in Slave-spins corresponds to J/U=0.15 in DMFT)

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Degenerate 5-band Hubbard model

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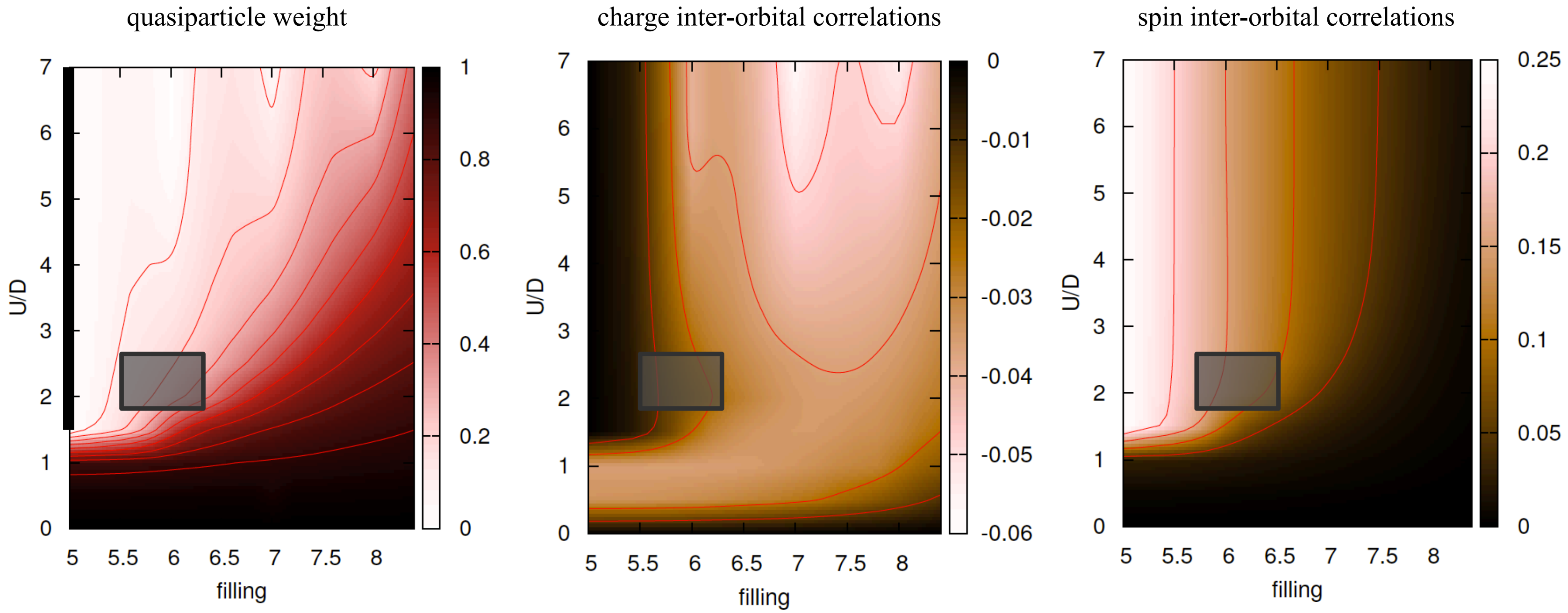
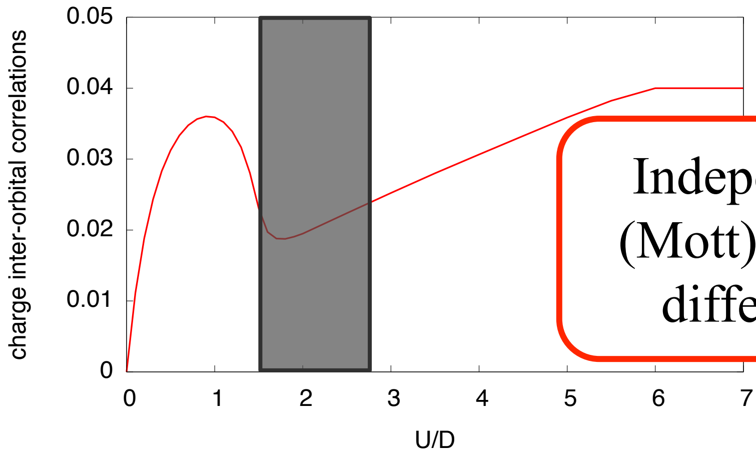
• local inter-orbital spin correlations are enhanced (high-spin locking)

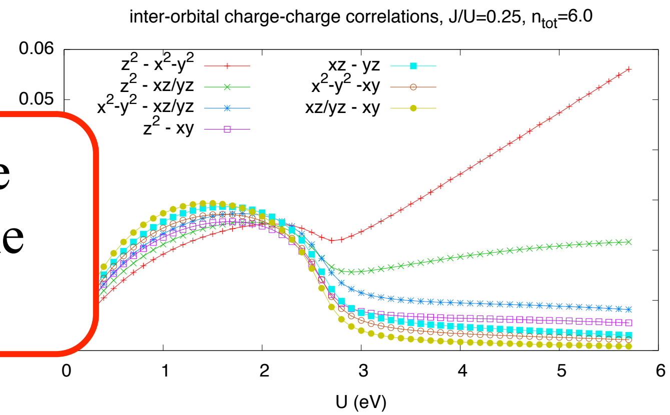
'Near' half-filling:

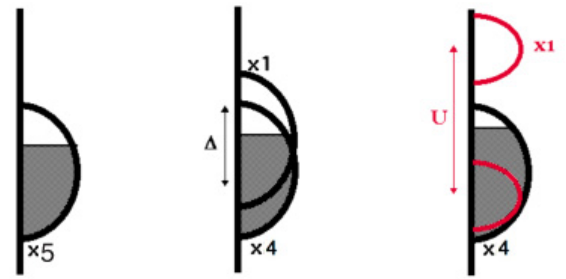


• local inter-orbital charge correlations are suppressed



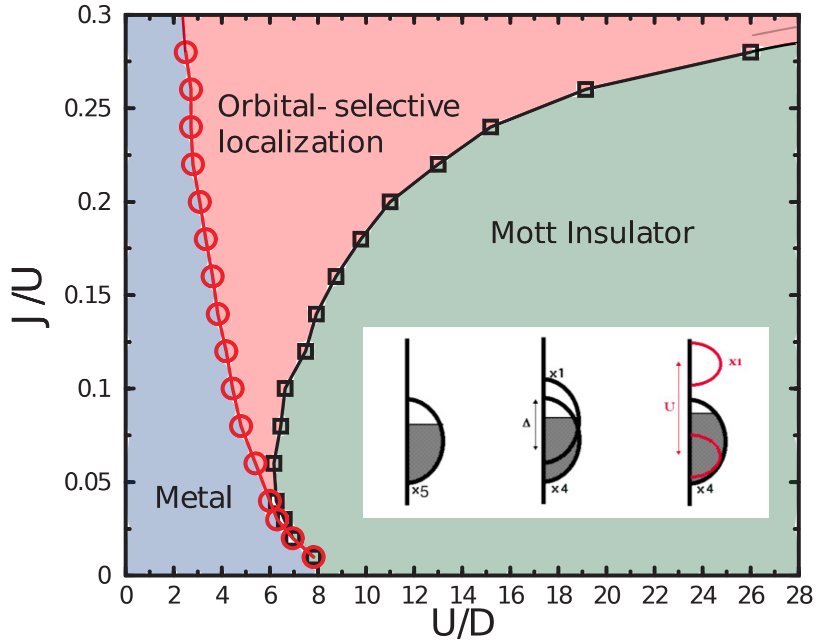
Independent charge (Mott) physics in the different orbitals!





5 bands of the same width
N=6 (half-filling+1)

Crystal-field (one band up)
+ Hund's coupling



LdM, S.R. Hassan, M. Capone, JSC **22**, 535 (2009)

Orbital-selective Mott transition

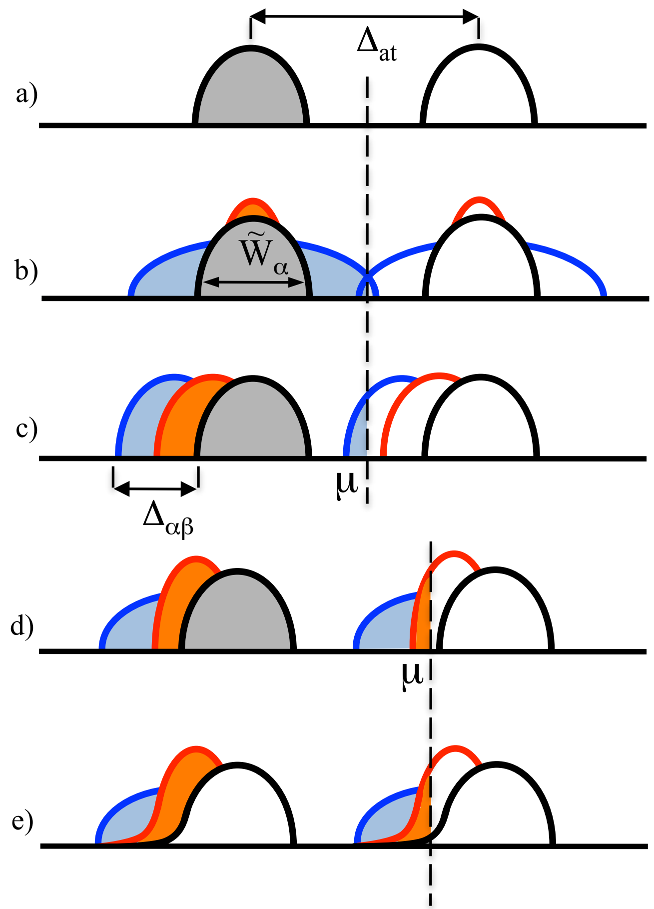
•Coexisting itinerant and localized conduction electrons
• Metallic resistivity and free-moment magnetic response
• non Fermi-liquid physics of the intinerant electrons

Anisimov et al., Eur. Phys. J. B 25 (2002)
Koga et al., Phys. Rev. Lett. 92 (2004)
For a review:
M. Vojta J. Low Temp. Phys. 161 (2010)

J favors the OSMT

(OSMT is the extreme case. More generally J favors a differentiation in the correlation strength for each orbital)

Hund's coupling as an orbital decoupler

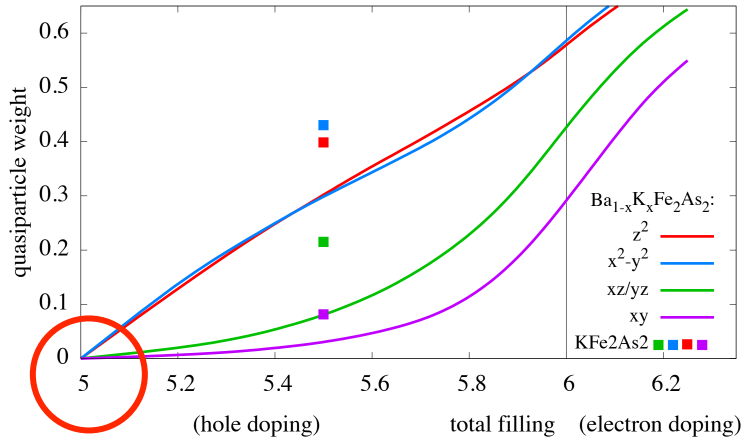


Hund's coupling suppresses the inter-orbital correlations, rendering the charge excitations in the different orbitals independent from one-another, i.e. acting as an **orbital-decoupler for Mott-physics**

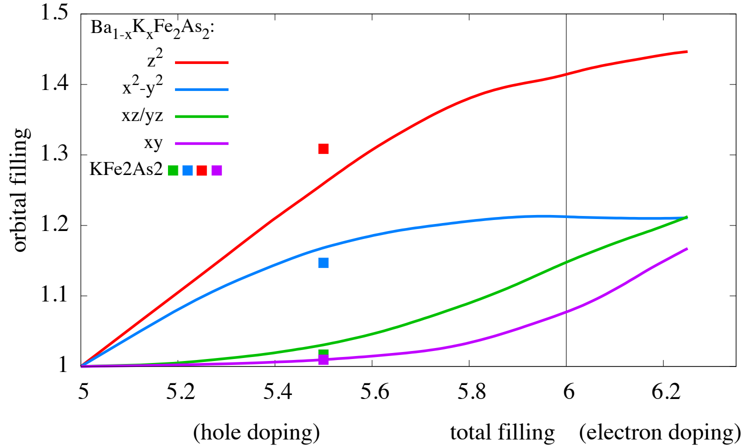
LdM, S.R. Hassan, M. Capone, X. Dai, PRL **102** (2009)
LdM, Phys. Rev. B **83** (2011)
Werner and Millis, Phys. Rev. Lett. **99** (2007)

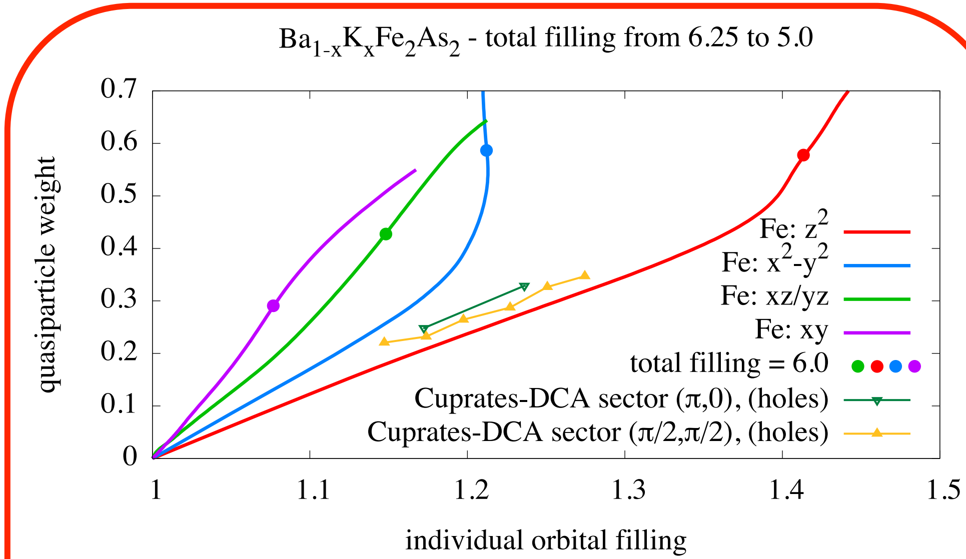
Selective Mottness in iron-SC: doped BaFe2As2 (DFT+SSpins)

Luca de' Medici



Mott Insulator





Strinking linear behaviour, when plotting Z against the individual orbital populations

Same as for cuprates!

Mottness

Orbital-Selective correlation strength

Selective Mottness!

Each orbital behaves as a doped Mott insulator

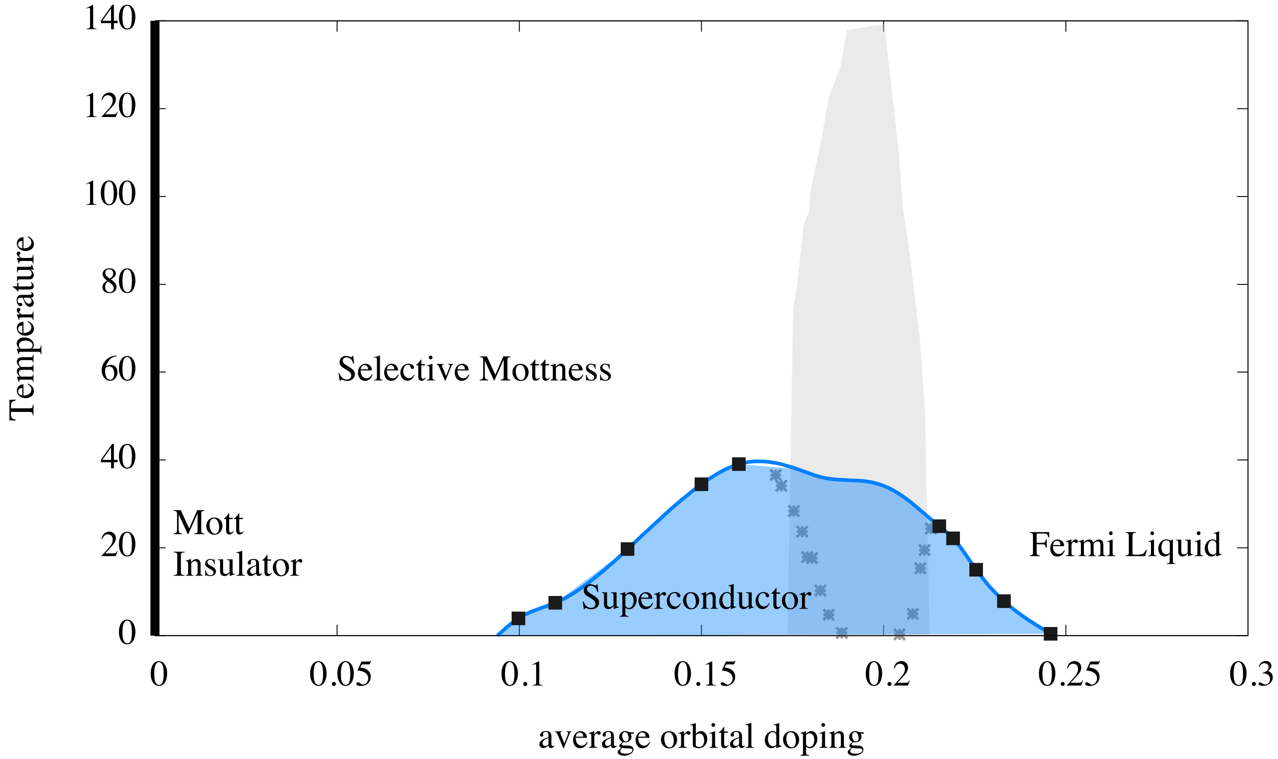
orbital decoupling, and influence of the n=5 Mott insulator

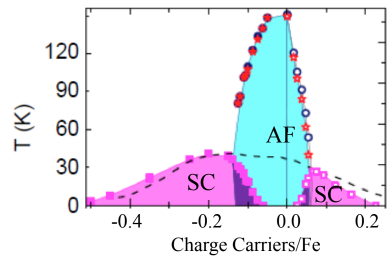
Similar evidences from

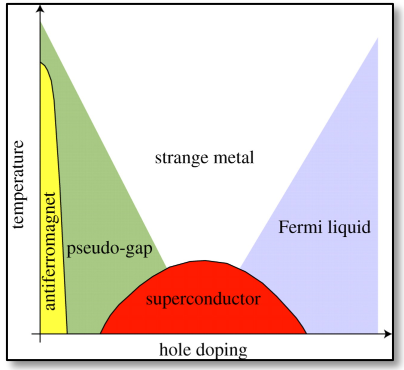
LDA+DMFT: Ishida et al., PRB **81** (2010), Werner et al. NatPhys '12

Variational MC: Misawa et al.,PRL **108** (2012)

Tentative common phase diagram for Cuprates and Iron-SC







When plotted against the average orbital doping the experimental phase diagram of iron-SC closely resembles the one for cuprates! (suppressing magnetism)

- a superconducting dome at 20% doping from a Mott insulator
- a phase with selective Mottness in between the two
- a good Fermi-liquid at higher dopings

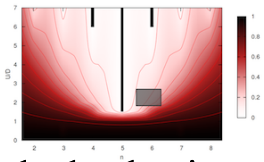
Is then **selective Mottness important for superconductivity?**

A. Hackl and M. Vojta, New J. Phys.11 (2009)
Kou et al. Europhys. Lett. 88 (2009)
Yin W-G et al. Phys. Rev. Lett. 105 (2010)
You Y-Z et al., Phys. Rev. Lett.107 (2011)

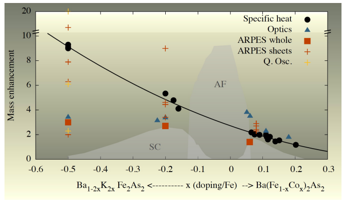
Conclusions:

Luca de' Medici

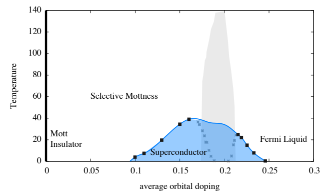
Iron superconductors: Hund's coupling J has a key-role in tuning correlations



- Overall coherence reduced. Mott transition at n=6 pushed far.
- Phase diagram dominated by Mott transition at n=5 (half-filling).
- Filling of the conduction bands is a key variable: correlations increase with hole doping
- J acts as an "**orbital-decoupler**": suppresses inter-orbital charge correlations and favors **orbital selective Mottness**



i.e. coexistence of **strongly *and* weakly correlated** electrons in most of the phase diagram (KFe2As2 heavy fermion)



Analogy with the pseudogap phase in the cuprates

A common phase diagram?

LdM, G. Giovannetti, M. Capone, PRL 112, 177001 (2014)
Perspective in book chapter:
LdM, "Weak *and* strong correlations in Iron superconductors",
in "**Iron-based superconductivity**", eds. W. Yin and G. Xu (BNL) for Springer

LdM, S.R. Hassan, M. Capone, X. Dai, PRL **102**, 126401 (2009)
LdM, S.R. Hassan, M. Capone, JSC **22**, 535 (2009)
LdM, PRB **83**, 205112 (2011)
A. Georges, LdM, J. Mravlje, Annual Reviews Cond. Mat. 4, 137 (2013)