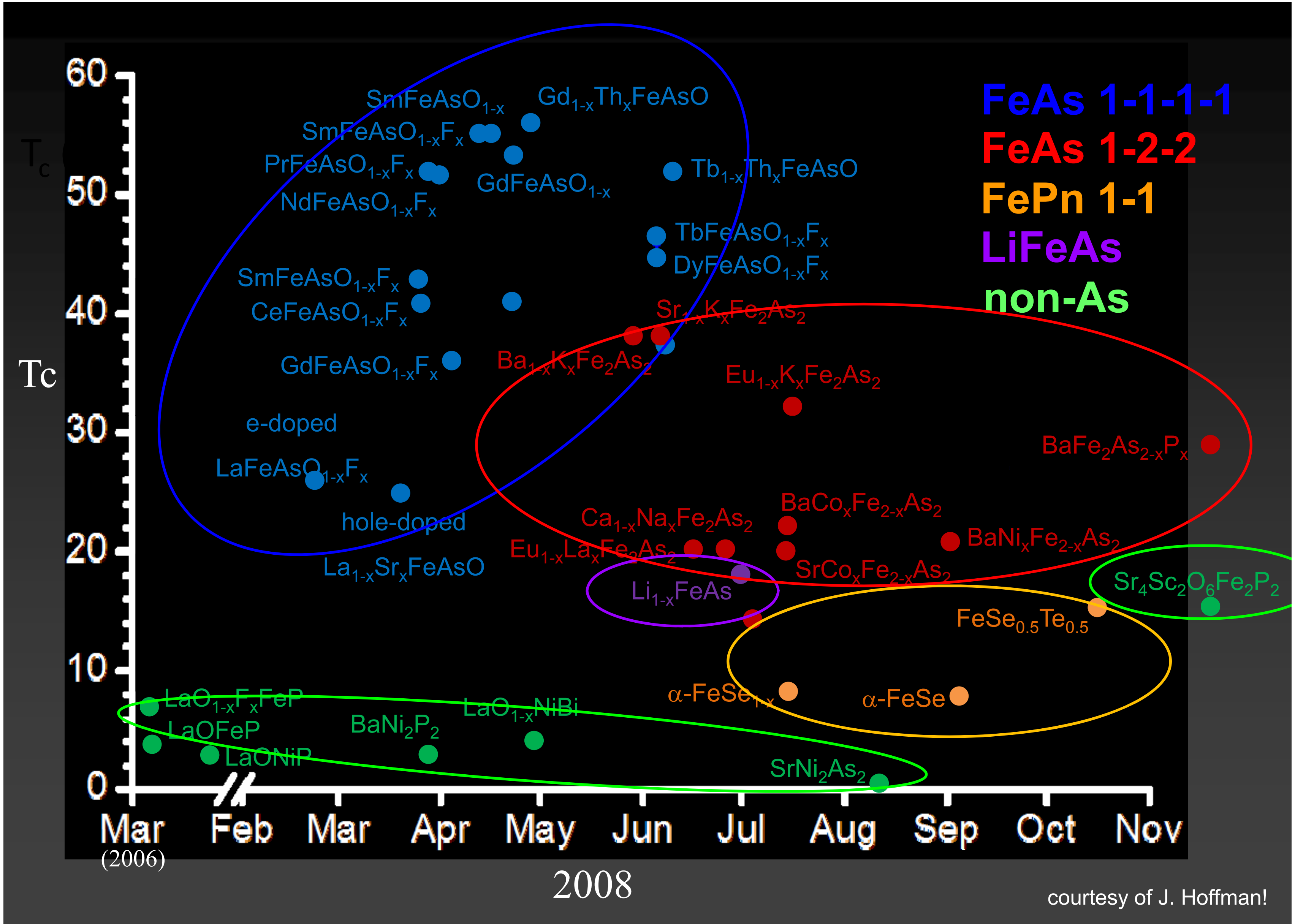
Luca de' Medici

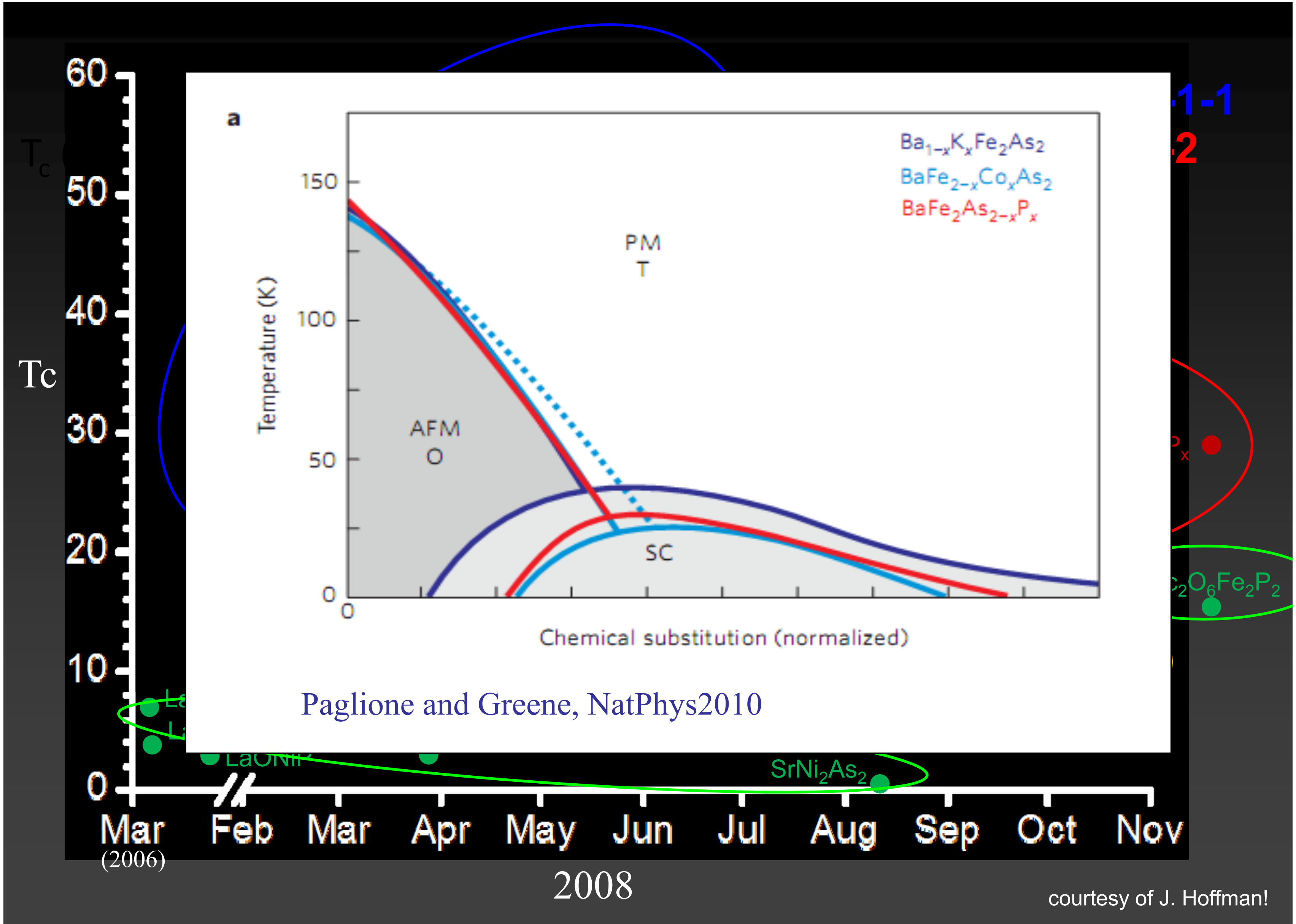
ESRF – Grenoble

Reverse-engineering electronic correlations in Iron-based superconductors

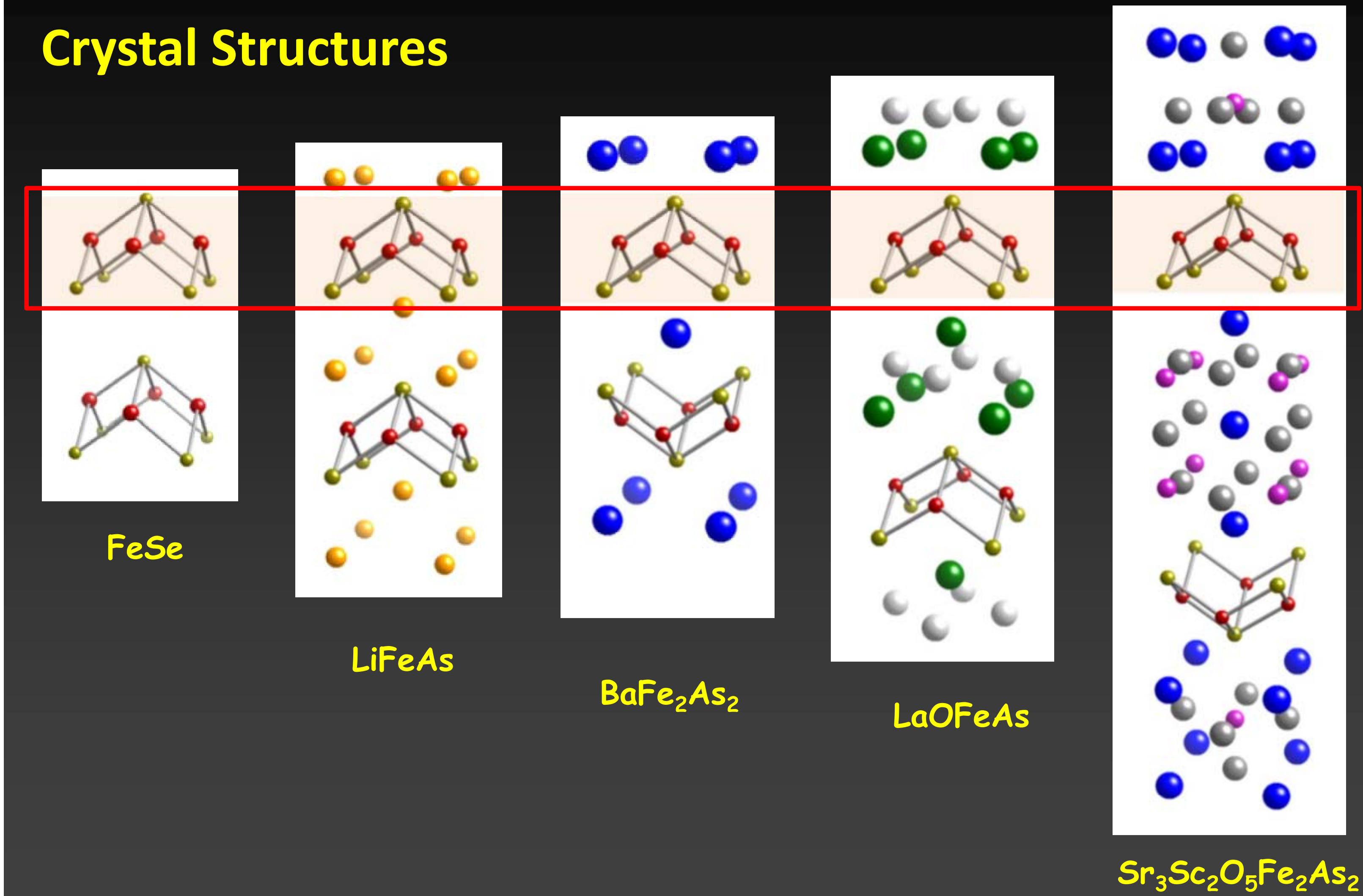
IRONIC14

KITP - UCSB 07.10.2014


FeAs 1-1-1-1
FeAs 1-2-2
FePn 1-1
LiFeAs
non-As
Tc
$SmFeAsO_{1-x}$
$Gd_{1-x}Th_xFeAsO$
$SmFeAsO_{1-x}F_x$
$PrFeAsO_{1-x}F_x$
$GdFeAsO_{1-x}$
$Tb_{1-x}Th_xFeAsO$
$NdFeAsO_{1-x}F_x$
$TbFeAsO_{1-x}F_x$
$DyFeAsO_{1-x}F_x$
$SmFeAsO_{1-x}F_x$
$CeFeAsO_{1-x}F_x$
$Sr_{1-x}K_xFe_2As_2$
$GdFeAsO_{1-x}F_x$
$Ba_{1-x}K_xFe_2As_2$
$Eu_{1-x}K_xFe_2As_2$
e-doped
$LaFeAsO_{1-x}F_x$
$BaFe_2As_{2-x}P_x$
hole-doped
$BaCo_xFe_{2-x}As_2$
$Ca_{1-x}Na_xFe_2As_2$
$BaNi_xFe_{2-x}As_2$
$Eu_{1-x}La_xFe_2As_2$
$La_{1-x}Sr_xFeAsO$
$SrCo_xFe_{2-x}As_2$
$Li_{1-x}FeAs$
$Sr_4Sc_2O_6Fe_2P_2$
$FeSe_{0.5}Te_{0.5}$
$LaO_{1-x}F_xFeP$
$LaO_{1-x}NiBi$
α-$FeSe_{1-x}$
α-FeSe
LaOFeP
$BaNi_2P_2$
LaONiP
$SrNi_2As_2$
60
50
40
30
20
10
0
Mar Feb Mar Apr May Jun Jul Aug Sep Oct Nov
(2006)
2008
courtesy of J. Hoffman!

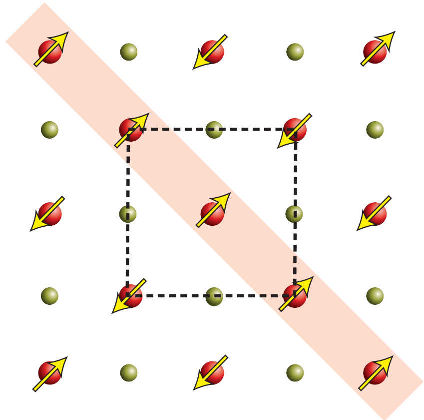

a
Temperature (K)
150
100
50
0
0
Chemical substitution (normalized)
$Ba_{1-x}K_xFe_2As_2$
$BaFe_{2-x}Co_xAs_2$
$BaFe_2As_{2-x}P_x$
PM
T
AFM
O
SC
Paglione and Greene, NatPhys2010
Tc
60
50
40
30
20
10
0
$SrNi_2As_2$
Mar
(2006)
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
2008
courtesy of J. Hoffman!

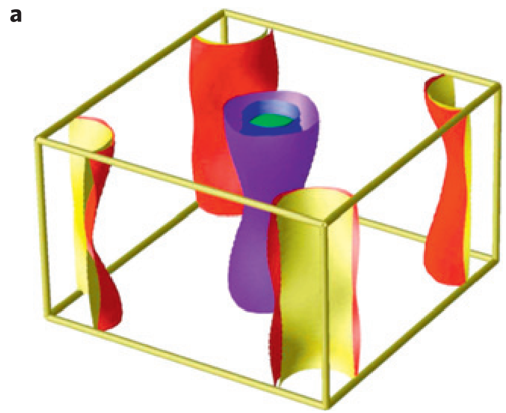
Crystal Structures

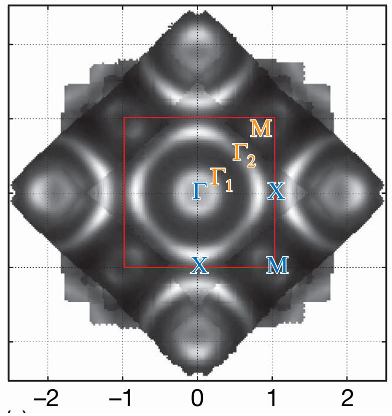


Paglione/Greene review (2010)

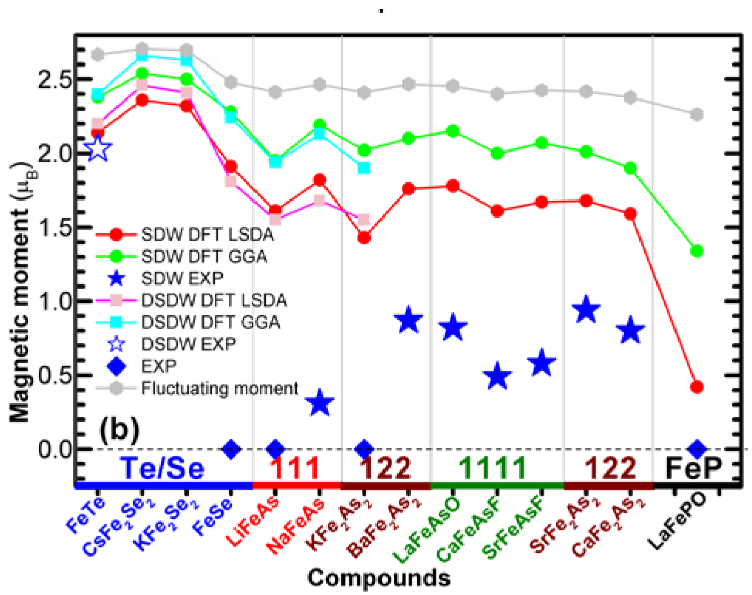
Paglione and Greene, NatPhys2010



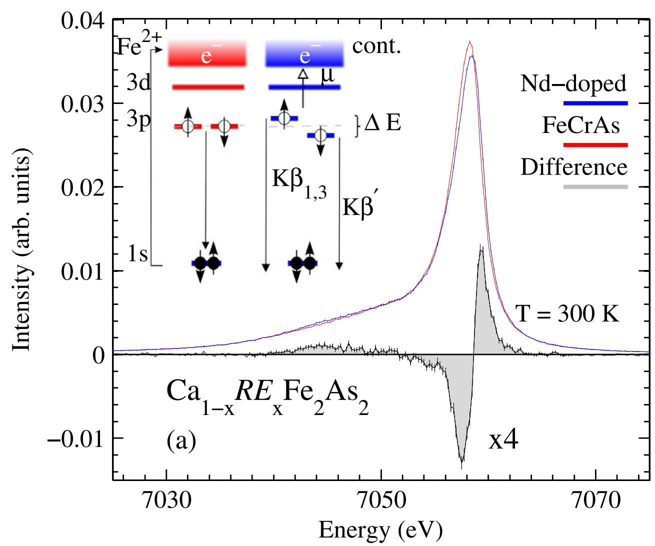




Lu et al. Nature2008



Yin et al. NatMat2011



Gretarsson et al. PRL2013

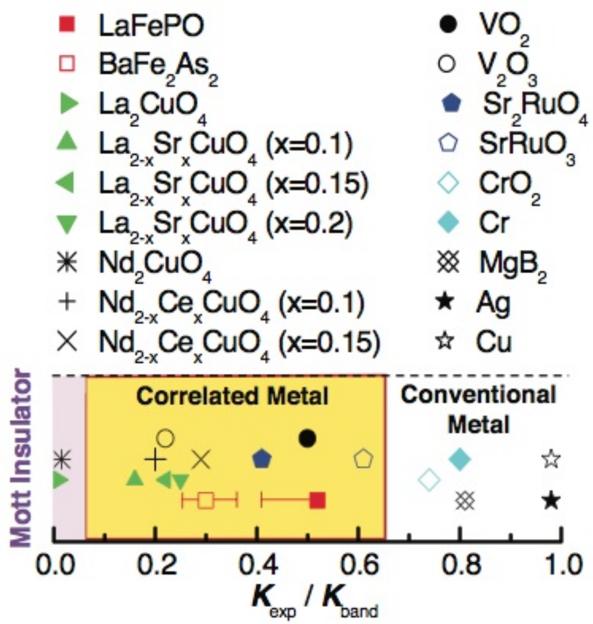
Contrasting evidences for correlation strength

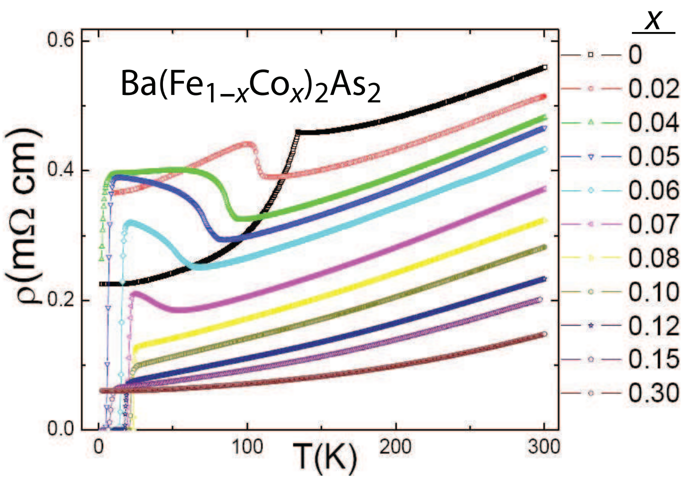
weak
- no Mott insulator in the phase diagram
- no detection of prominent Hubbard bands
- moderate correlations from Optics

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

Weak-coupling vs Strong-coupling scenarios

Qazilbash et al. NatPhys2009





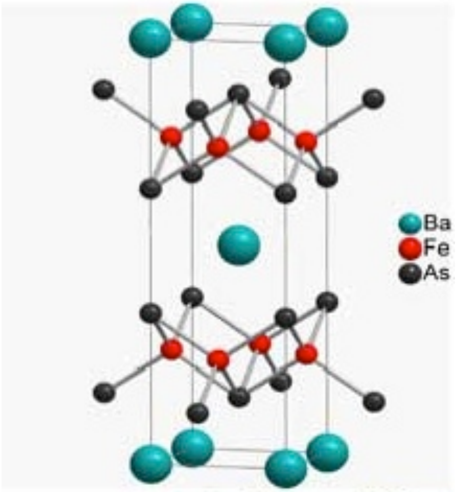
Fang et al. PRB80 (2009)
Rullier-Albenque et al. PRL103 (2009)

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)

Modeling Iron-based superconductors: Hund's coupling

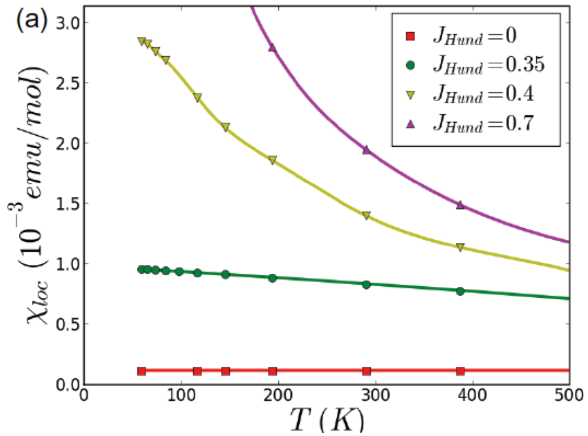


$BaFe_2As_2$

- 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)



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

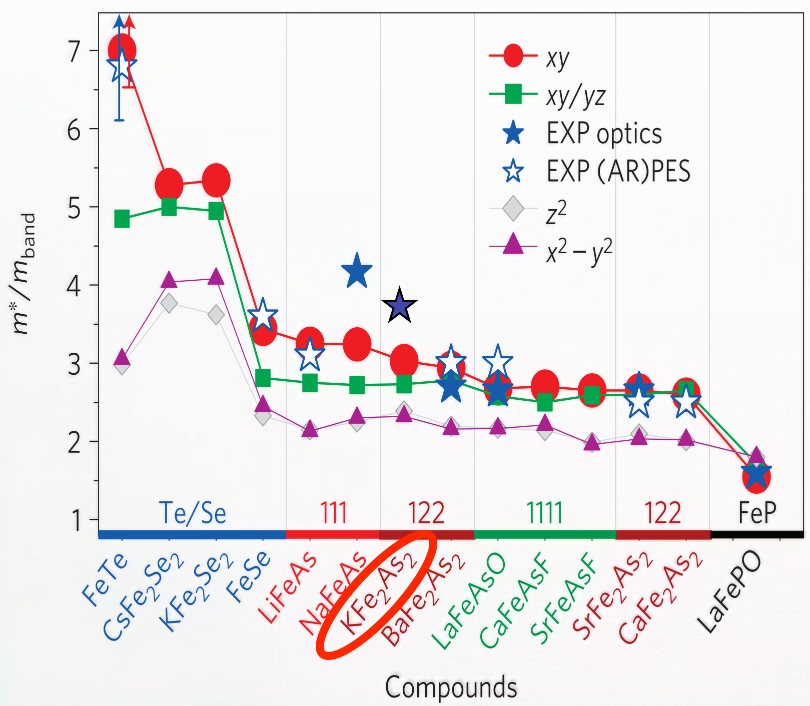
$$+U\sum_{i,m} n_{im\uparrow}n_{im\downarrow} + (U' - \frac{J}{2})\sum_{i,m>m'} n_{im}n_{im'}$$

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

(U'=U-2J)

DMFT vs experiments

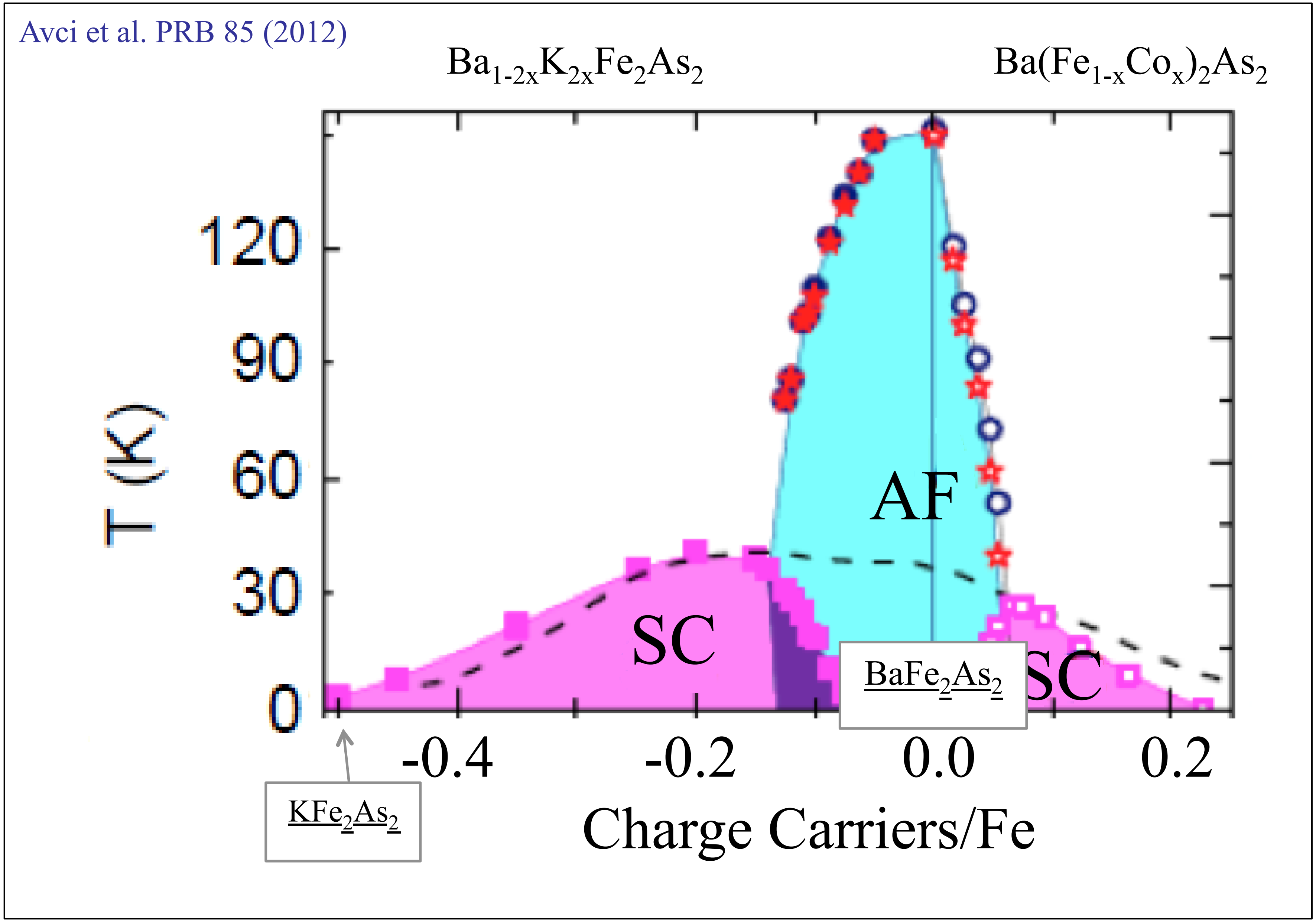
Mass enhancement and maximal Tc



DFT+DMFT accounts for the variations in all families without tuning U and J!

strength (mass enhancement ~ 3)

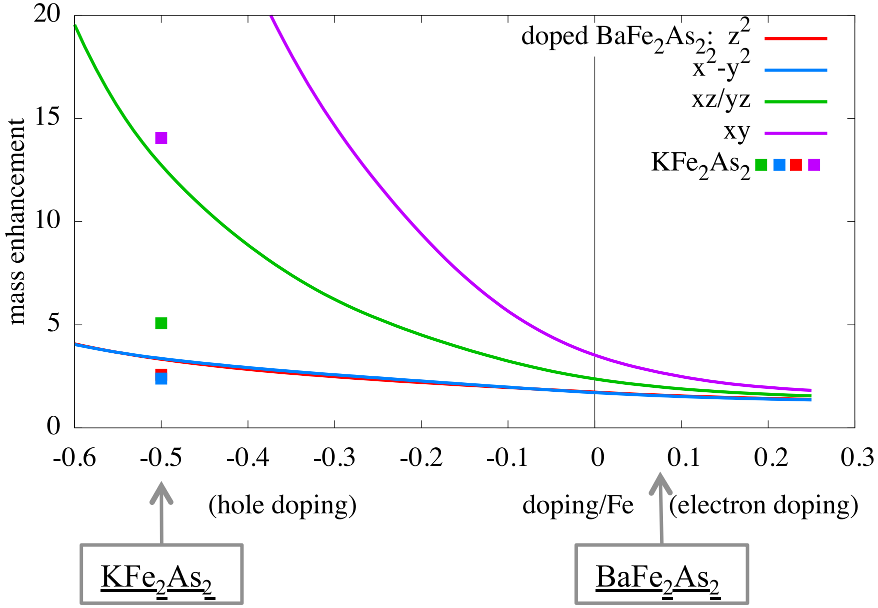
ZPY, K. Haule and G. Kotliar, Nature Materials 10, 932 (2011).


Avci et al. PRB 85 (2012)
$Ba_{1-2x}K_{2x}Fe_2As_2$
$Ba(Fe_{1-x}Co_x)_2As_2$
T (K)
120
90
60
30
0
AF
SC
SC
$BaFe_2As_2$
-0.4
-0.2
0.0
0.2
KFe_2As_2
Charge Carriers/Fe

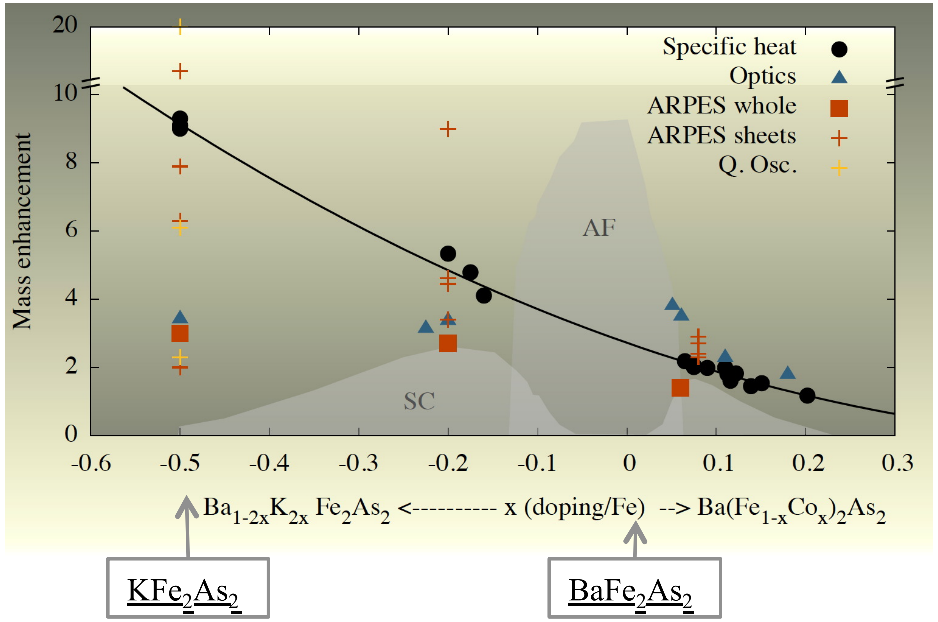
mass enhancements

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

Theory (LDA+Slave-spins)



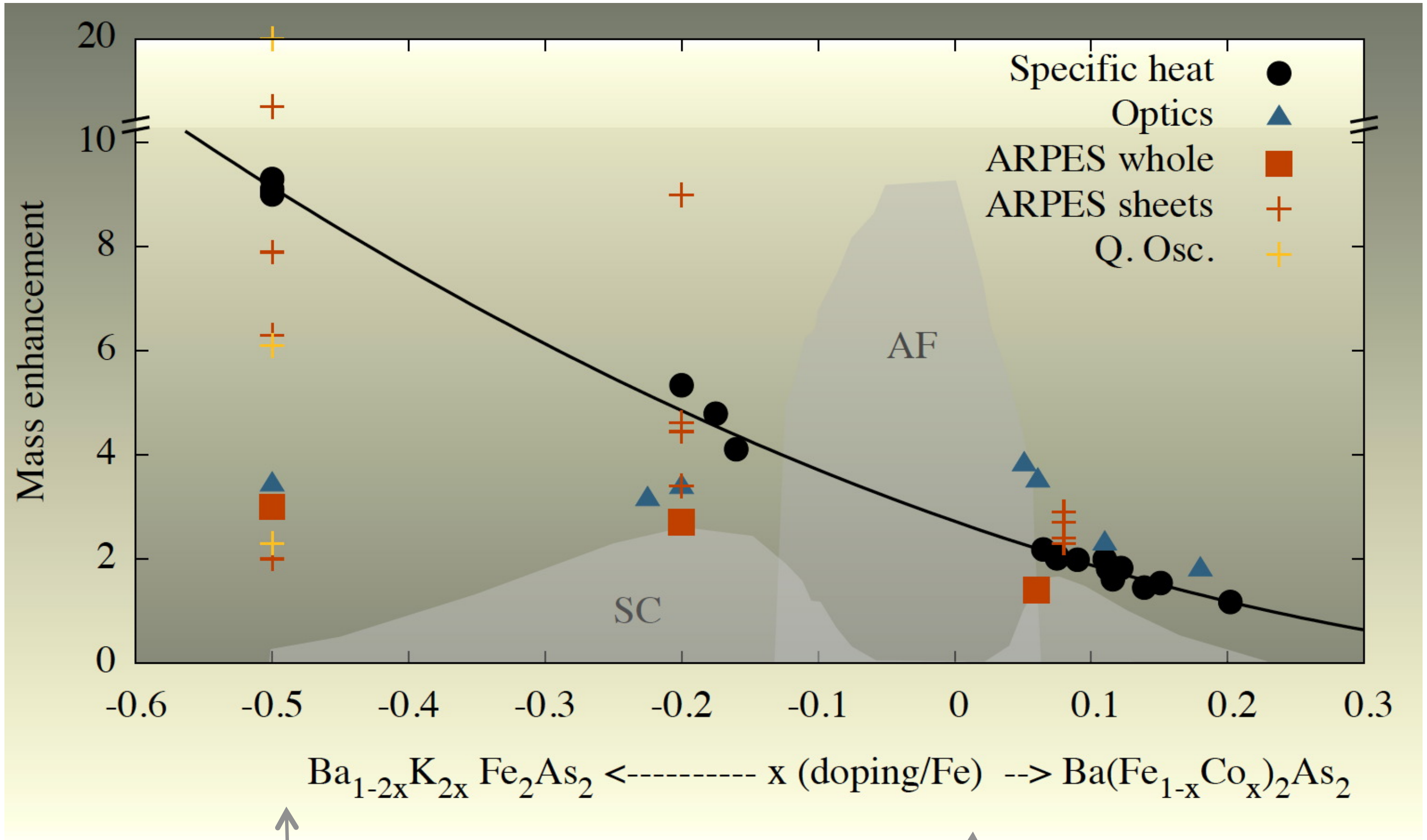
Experimental data
(high-T tetragonal phase)



Selective correlation strength: strongly *and* weakly correlated electrons

Many other theoretical works showing orbital-dependent correlations (DFT+..) : Yin et al., Aichhorn et al., Shorikov et al., Craco, Laad et al., Backes et al. (DMFT), Bascones et al. (Hartree-Fock), Ikeda et al. (FLEX), Yu and 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

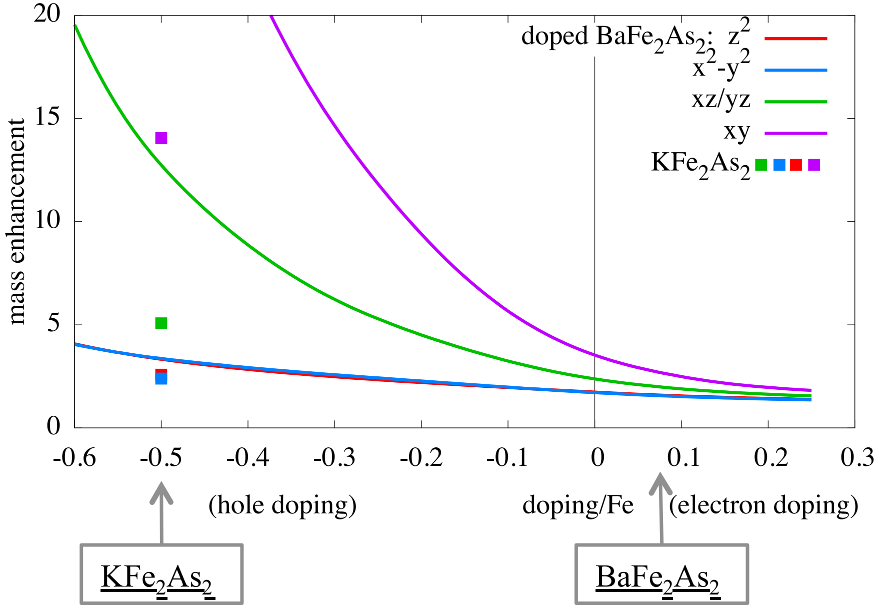
Optics: beware of interband transitions! Calderon et al., PRB2014

Orbital-dependent correlation strength

mass enhancements

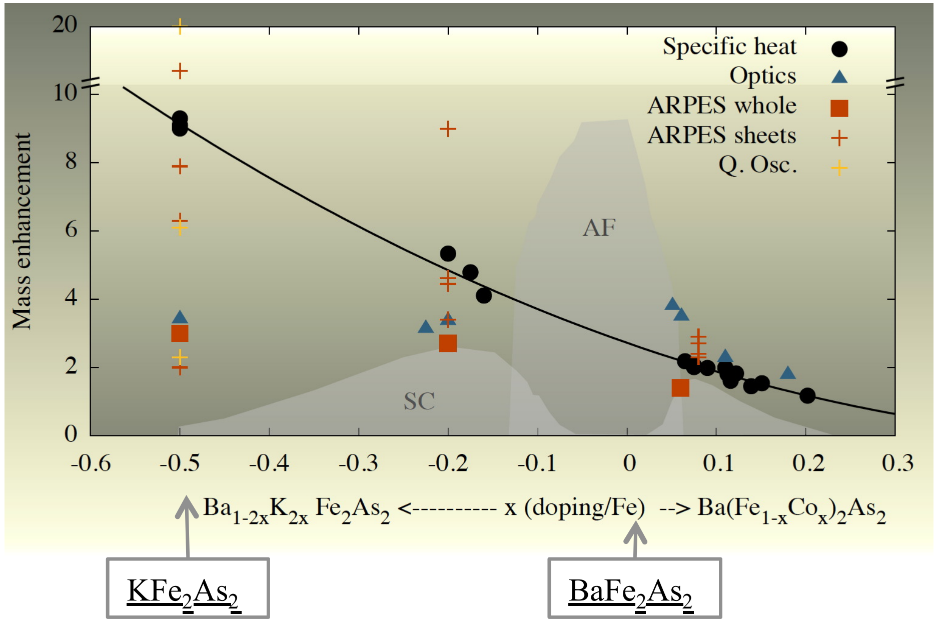
LdM, G. Giovannetti, M. Capone, PRL 2014

Theory (LDA+Slave-spins)



Experimental data

(high-T tetragonal phase)



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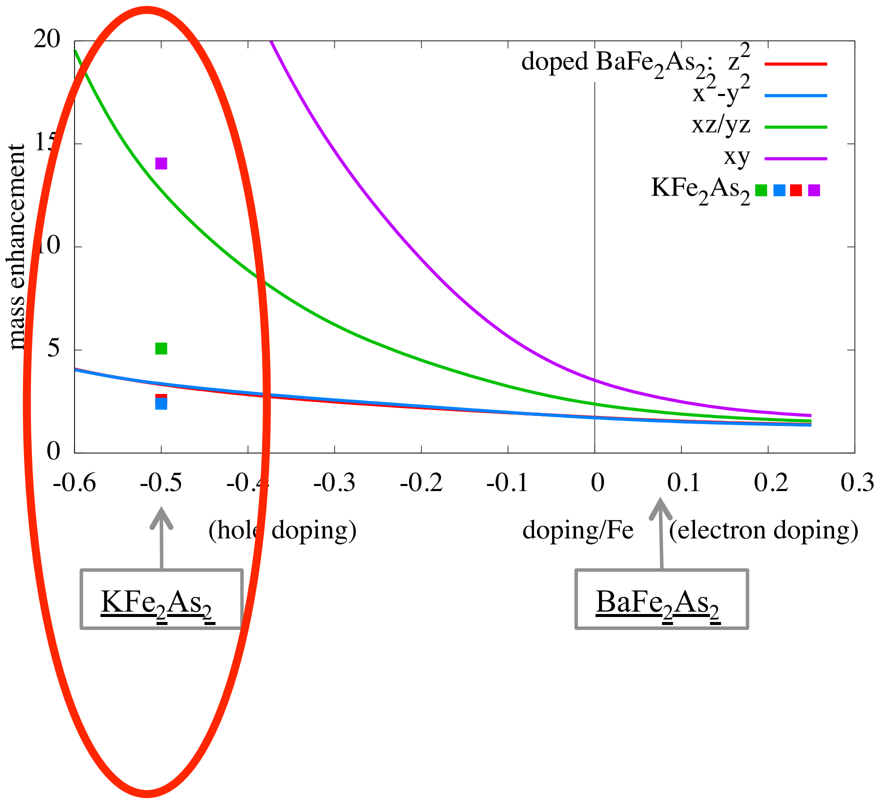
Heavy-fermionic behaviour in KFe_2As_2

Luca de' Medici

mass enhancements

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

Theory (LDA+Slave-spins)



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

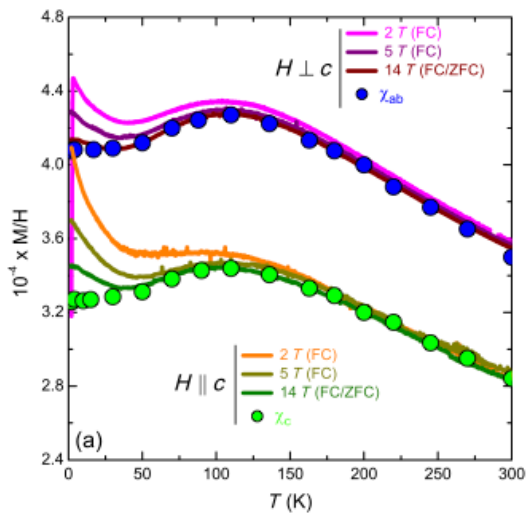
Evidence of Strong Correlations and Coherence-Incoherence Crossover in the Iron Pnictide Superconductor KFe_2As_2

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*

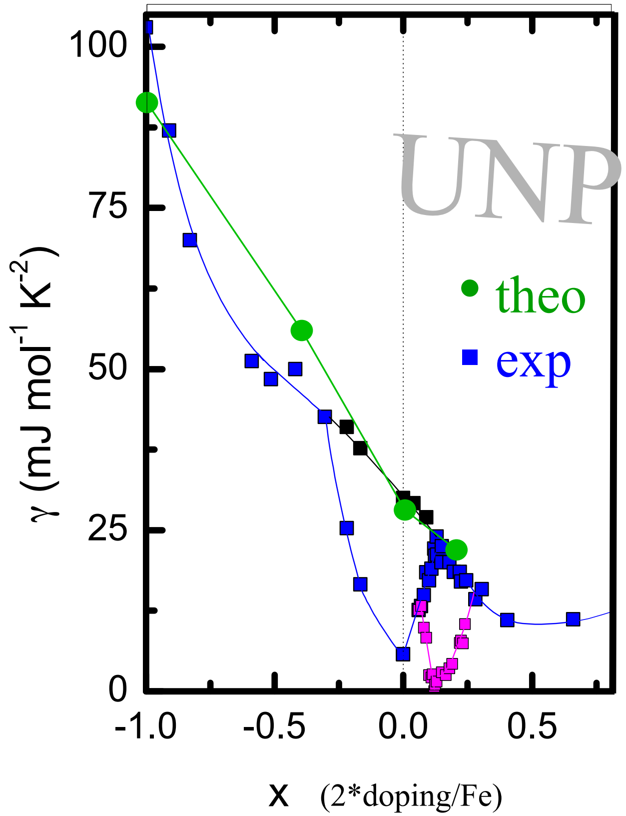
(Received 15 January 2013; published 9 July 2013)

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.

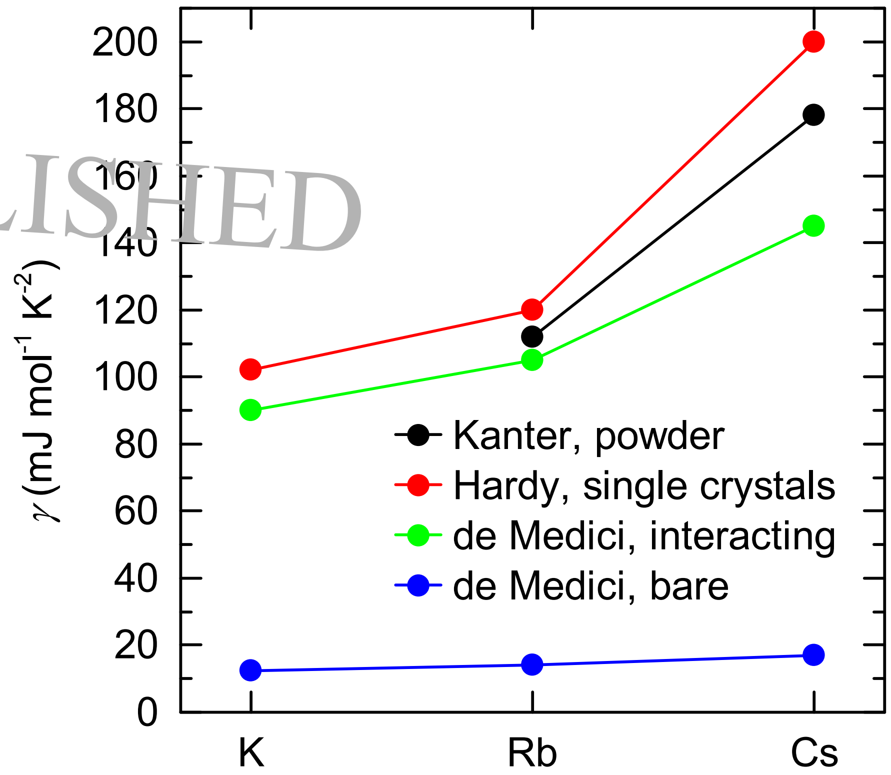


Heavy-fermionic behavior: theory vs experiment

$Ba_{1-x}K_xFe_2As_2$



AFe_2As_2 (A= K, Rb, Cs)



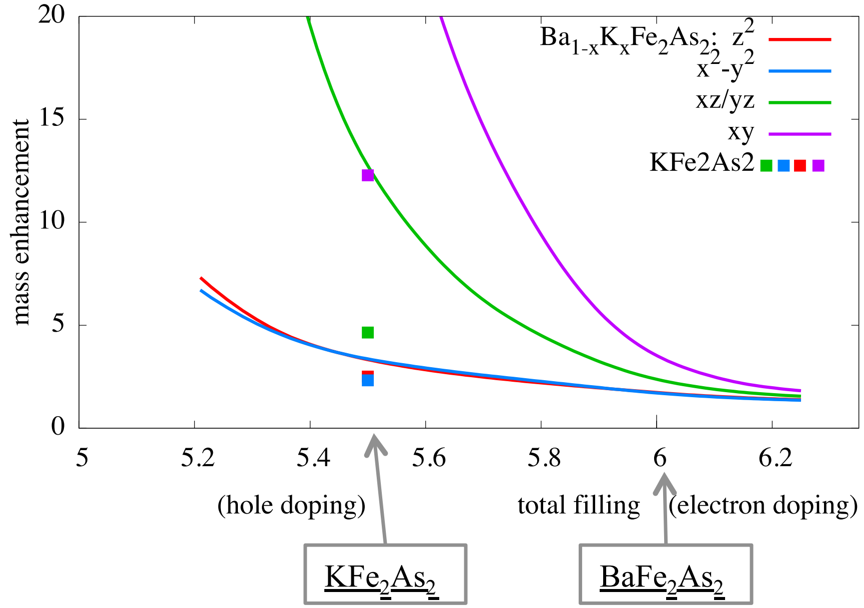
Experiments from Meingast's group in Karlsruhe. F. Hardy et al. unpublished

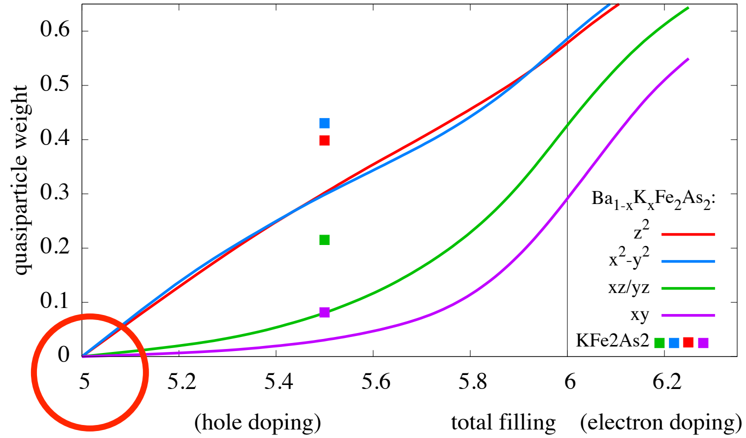
Mott insulating state at half-filling

mass enhancements

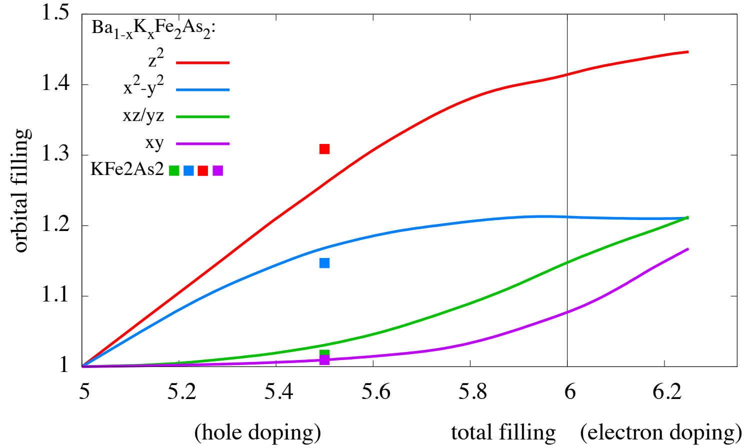
LdM, G. Giovannetti, M. Capone, PRL 2014

Theory (LDA+Slave-spins)

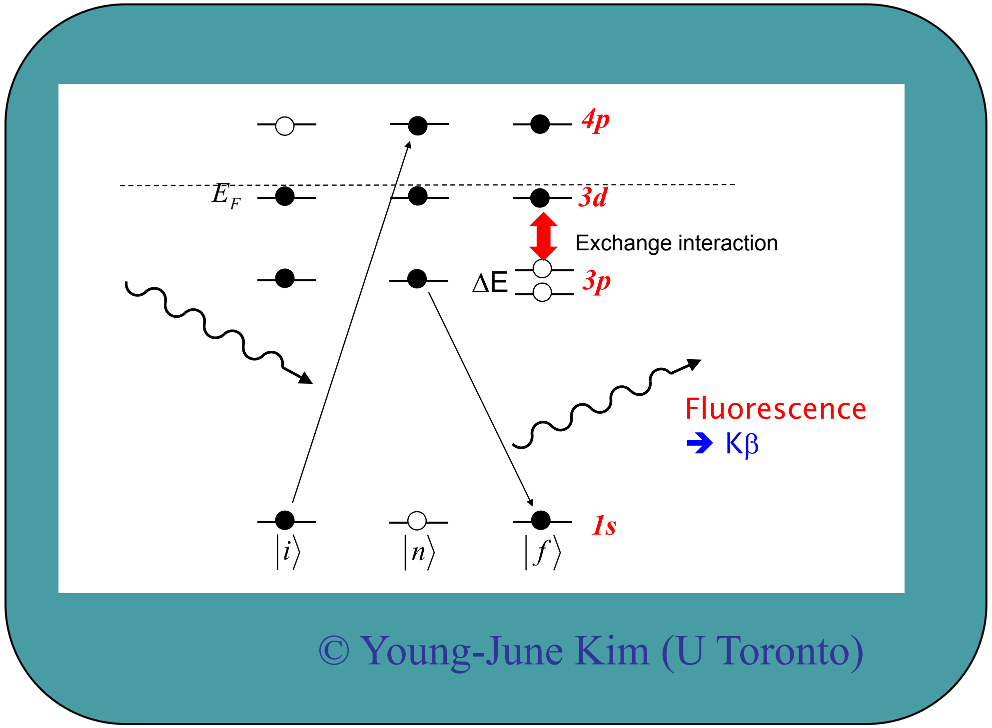


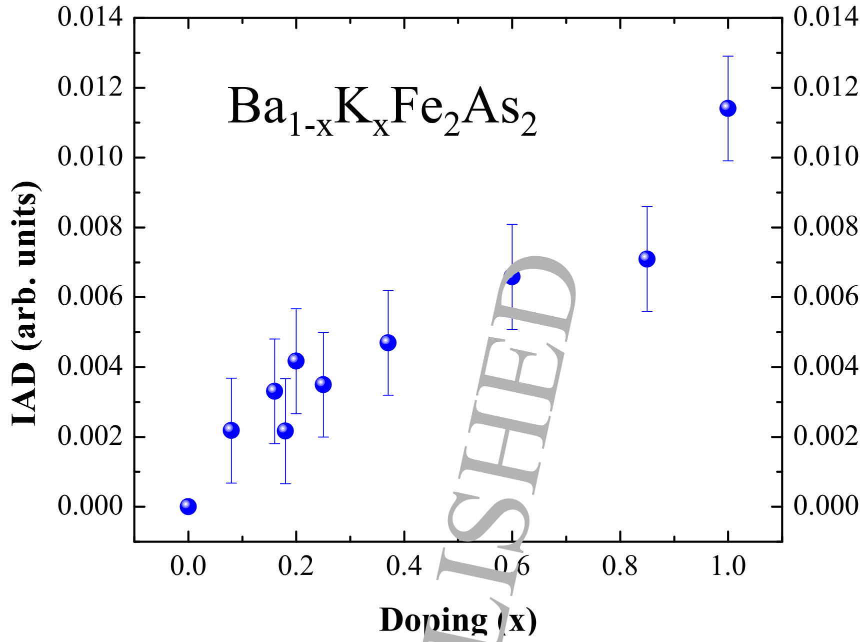


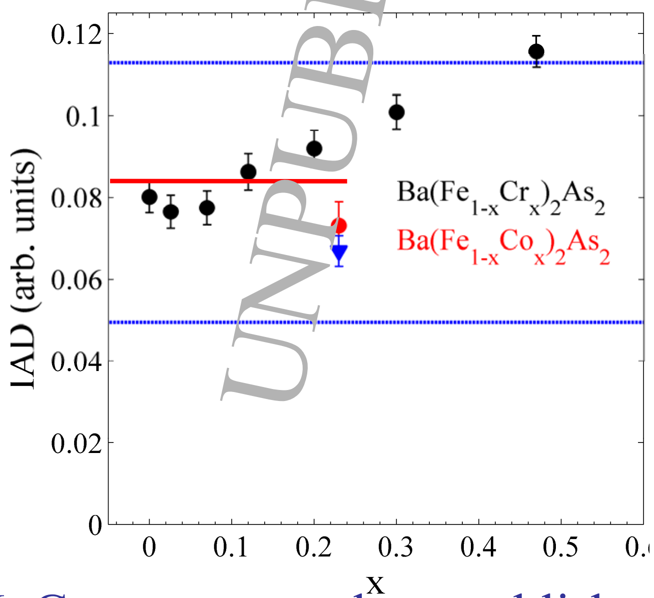
Mott Insulator



Local moments (XES)







Instantaneous local moments building with hole-doping!

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

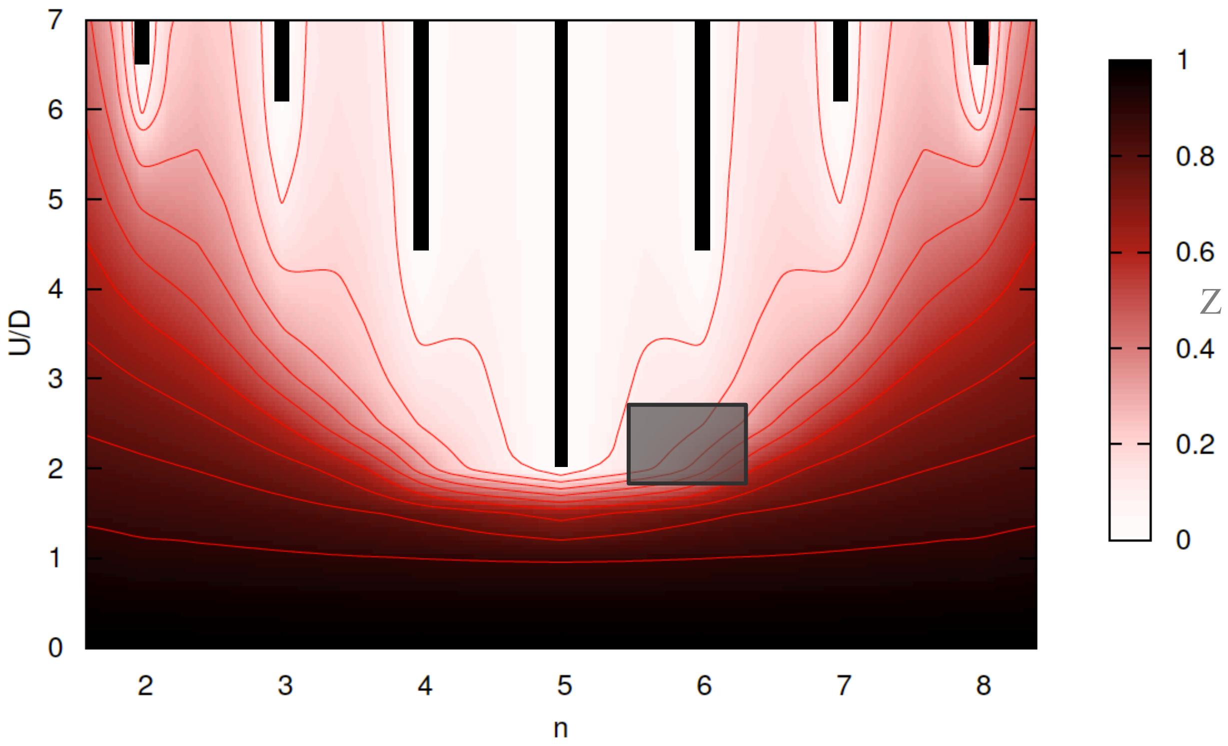
Degenerate 5-band Hubbard model

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)

Degenerate 5-band Hubbard model

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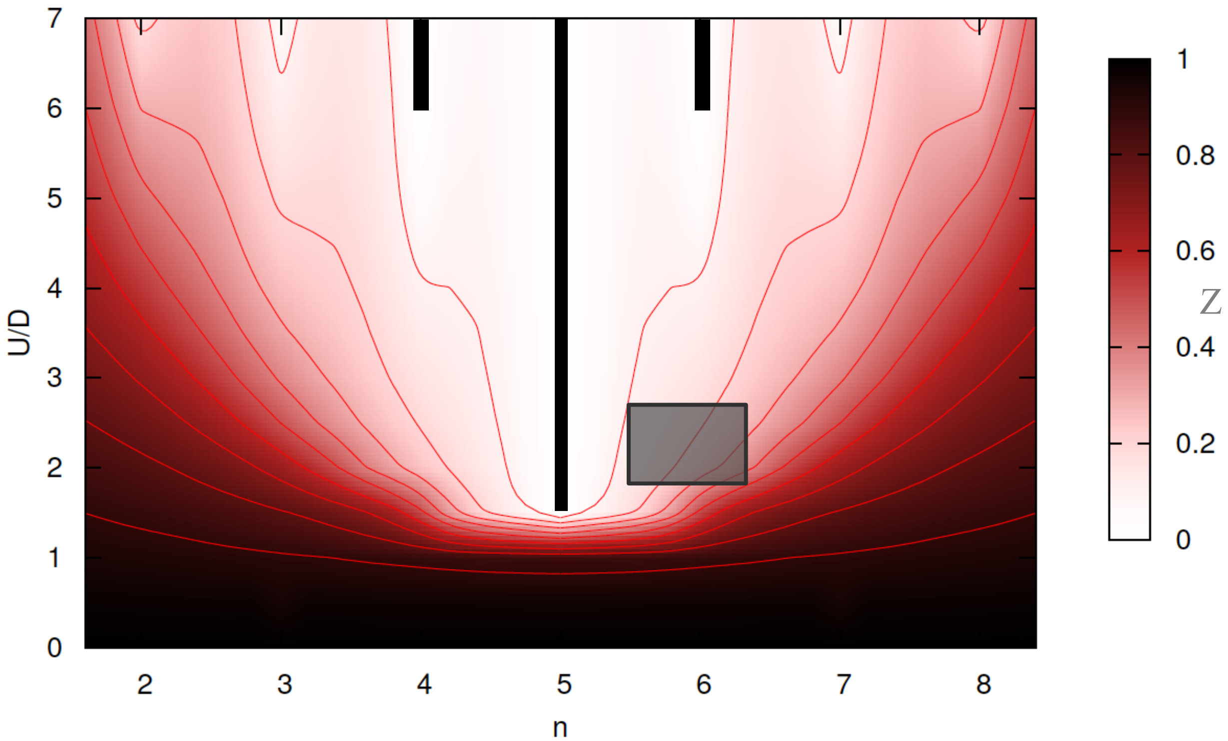

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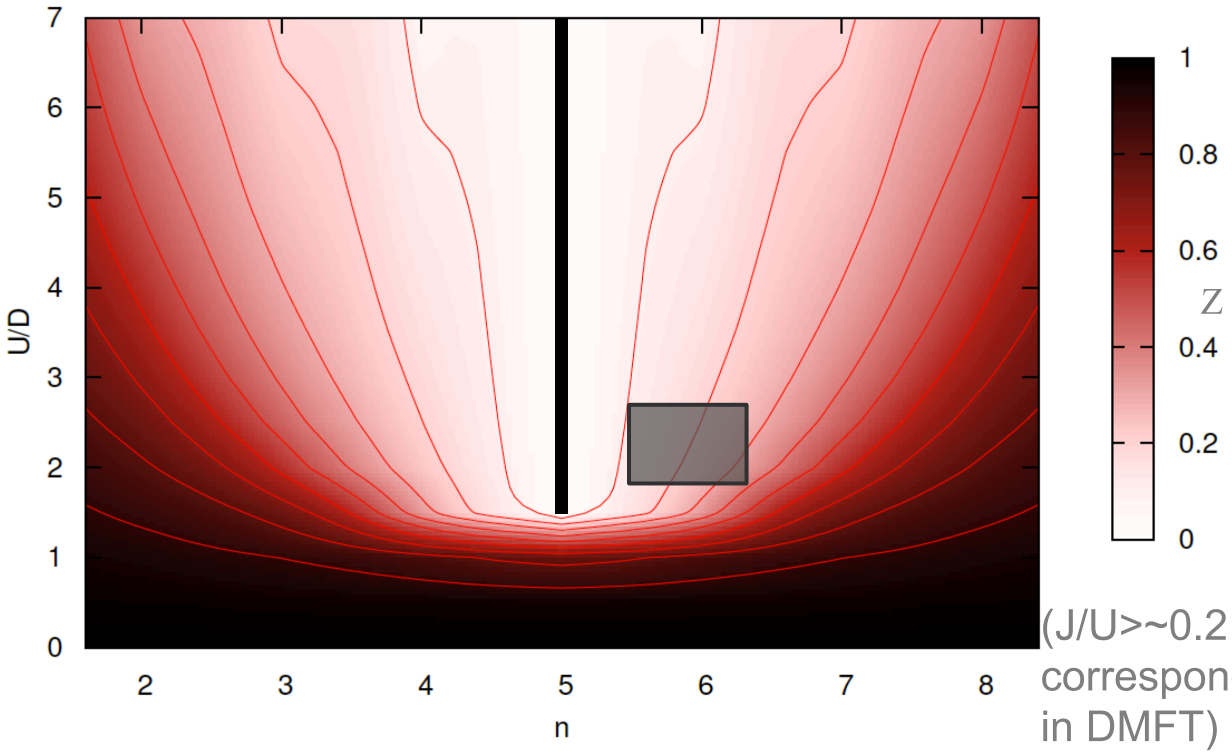

(J/U>~0.2 in Slave-spins corresponds to J/U=0.15 in DMFT)

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)

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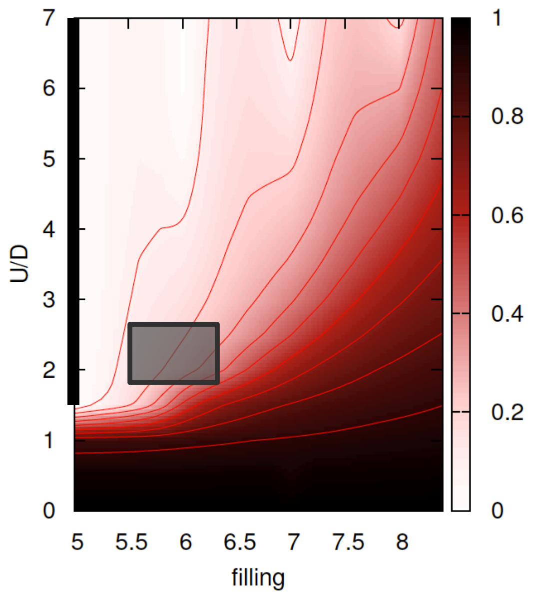
Degenerate 5-band Hubbard model

Luca de' Medici

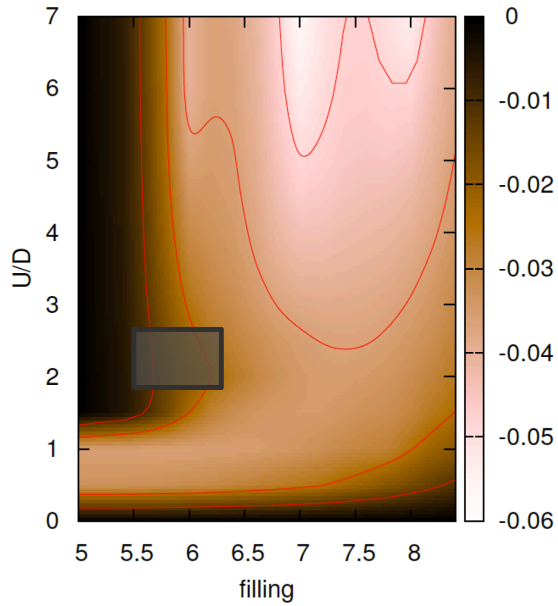
'Near' half-filling:

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

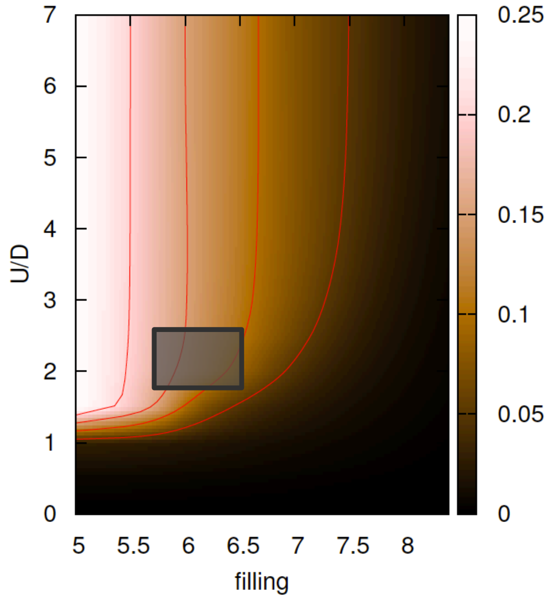
quasiparticle weight



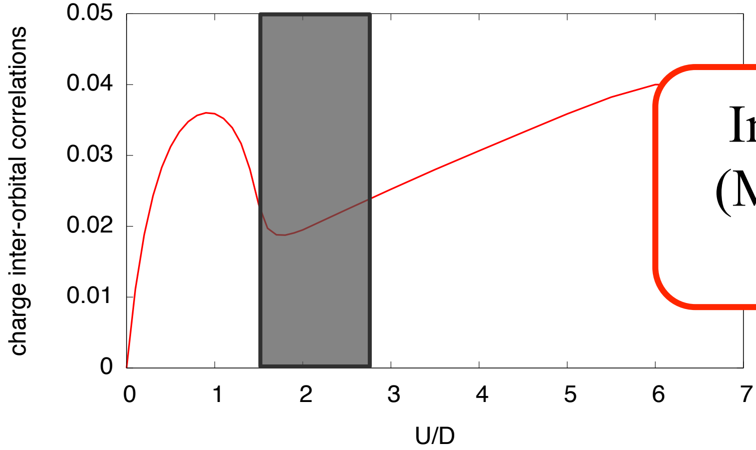
charge inter-orbital correlations



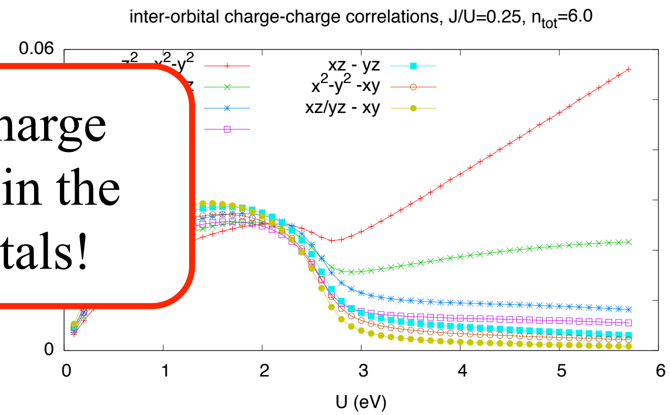
spin inter-orbital correlations



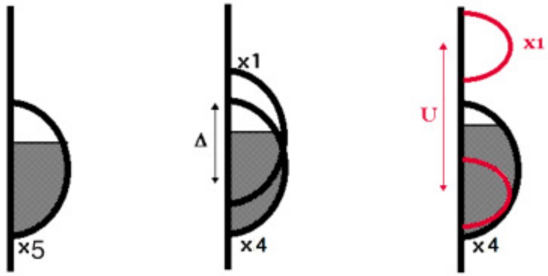
- local inter-orbital charge correlations are suppressed



Independent charge (Mott) physics in the different orbitals!

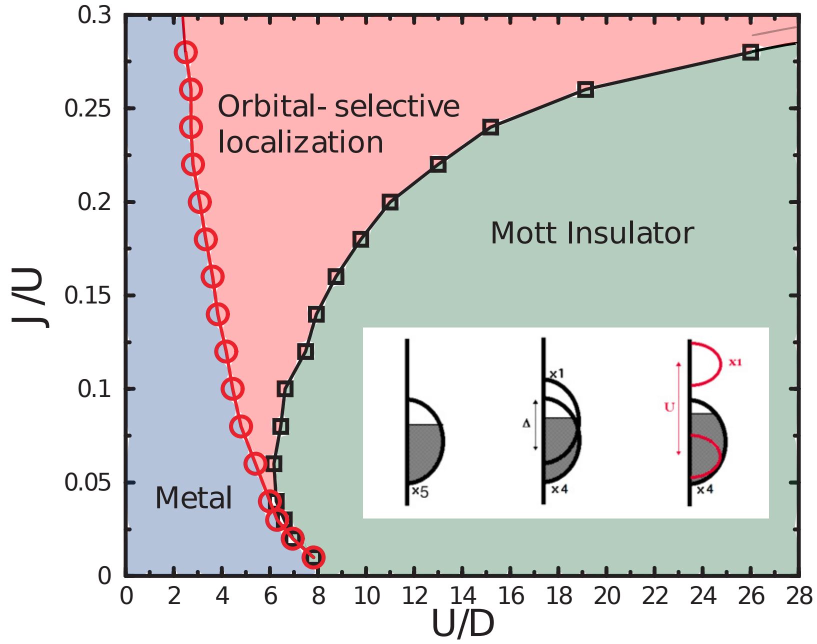


Hund's coupling and Orbital selectivity



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)

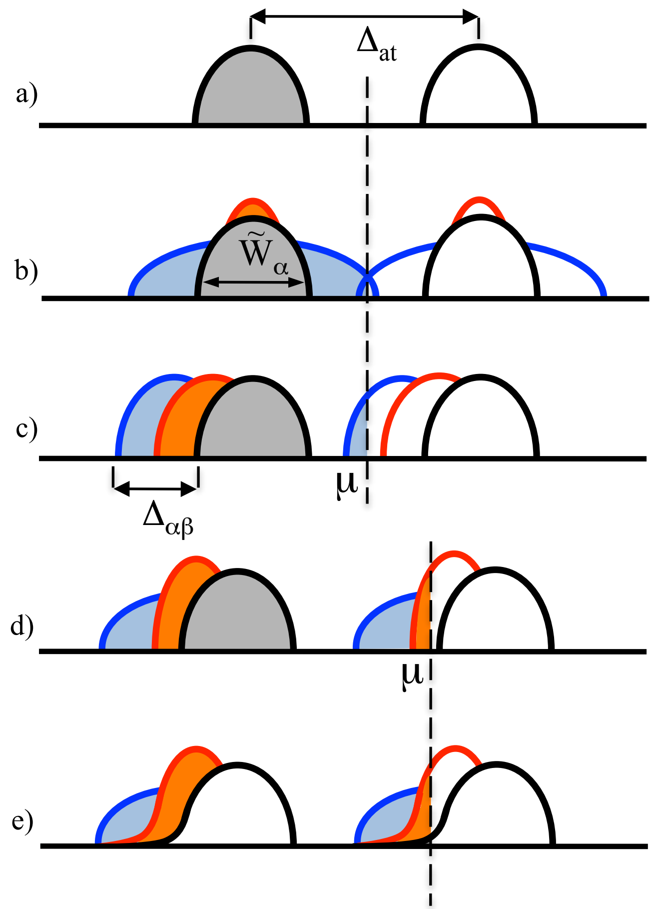
Orbital-selective Mott transition

•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)

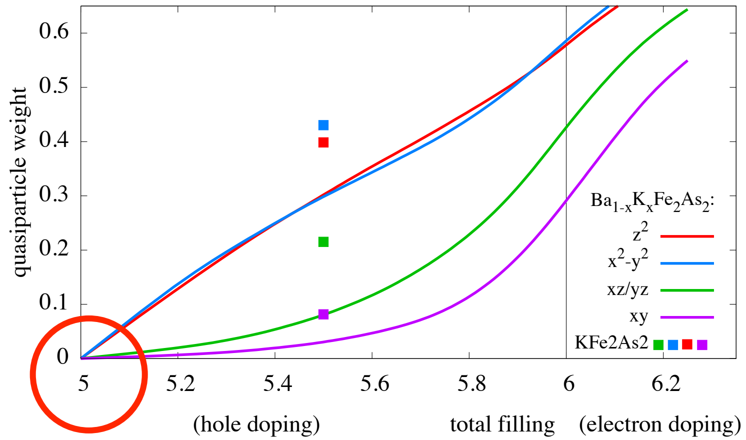


Hund's coupling suppresses the inter-orbital correlations, rendering the charge excitations in the different orbitals independent from one-another, i.e. acting as an **orbital-decoupler for Mott-physics**

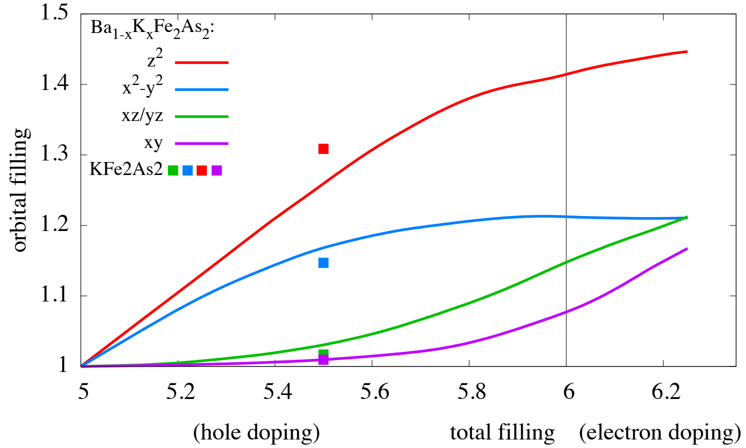
LdM, S.R. Hassan, M. Capone, X. Dai, PRL**102** (2009)
LdM, Phys. Rev. B **83** (2011)
Werner and Millis, Phys. Rev. Lett. **99** (2007)

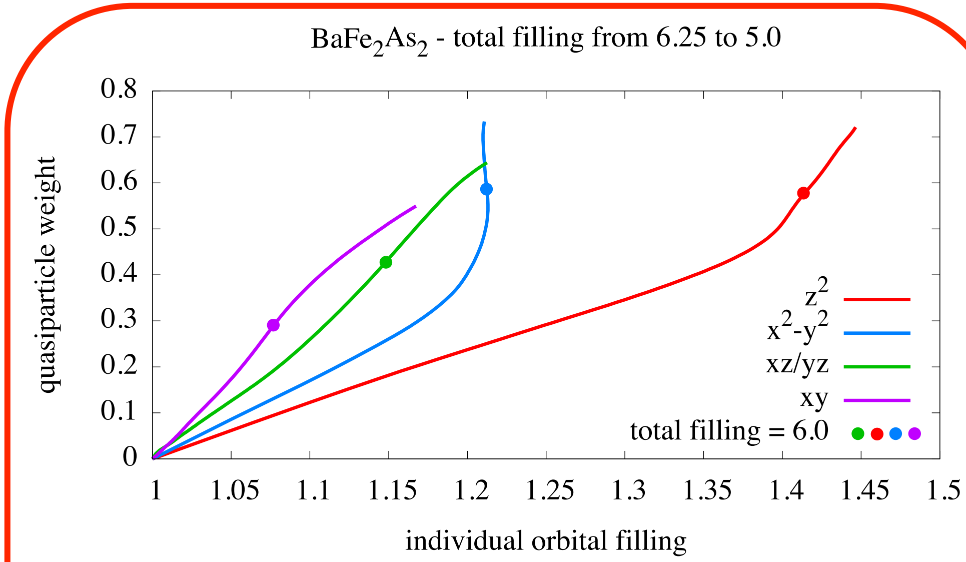
Selective Mottness in iron-SC: doped BaFe2As2 (DFT+SSpins)

Luca de' Medici



Mott Insulator





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

Mottness

Orbital-Selective correlation strength

Selective Mottness!

Each orbital behaves as a doped Mott insulator

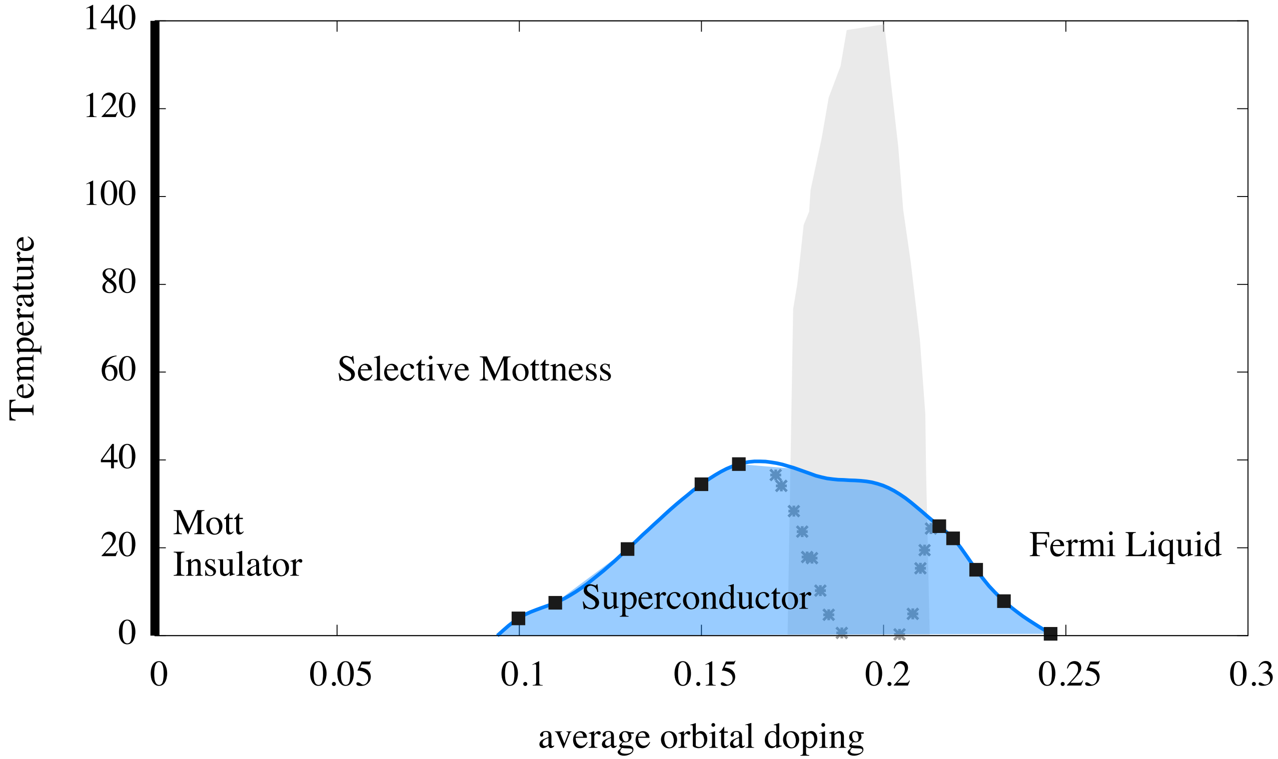
orbital decoupling, and influence of the n=5 Mott insulator

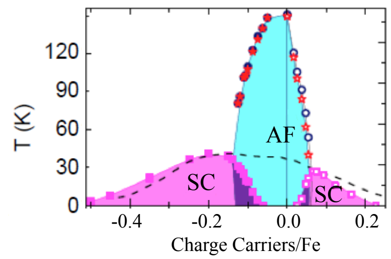
Similar evidences from

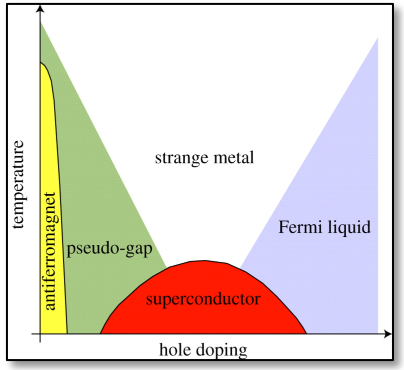
LDA+DMFT: Ishida et al., PRB **81** (2010), Werner et al. NatPhys '12

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)

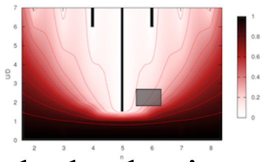
- a superconducting dome at 20% doping from a Mott insulator
- a phase with selective Mottness in between the two
- a good Fermi-liquid at higher dopings

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

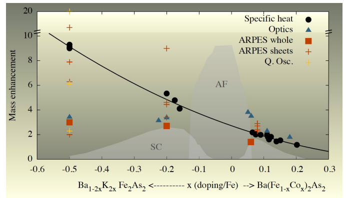
A. Hackl and M. Vojta, New J. Phys.11 (2009)
Kou et al. Europhys. Lett. 88 (2009)
Yin W-G et al. Phys. Rev. Lett. 105 (2010)
You Y-Z et al., Phys. Rev. Lett.107 (2011)

Conclusions:

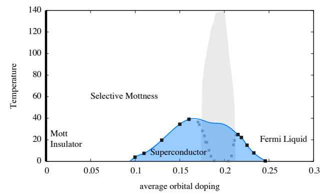
<u>Iron superconductors: Hund's coupling J has a key-role in tuning correlations</u>



- 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 <u>favors **orbital selective Mottness**</u>



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



Analogy with the pseudogap phase in the cuprates

<u>A common phase diagram?</u>

All put in perspective in : 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)
LdM, G. Giovannetti, M. Capone, 'Selective Mottness as a key to Iron superconductors' PRL 112, 177001 (2014)

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<u>G. Giovannetti and M. Capone,</u>
E. Winograd

Cuprates: Pseudogap as Selective Mottness

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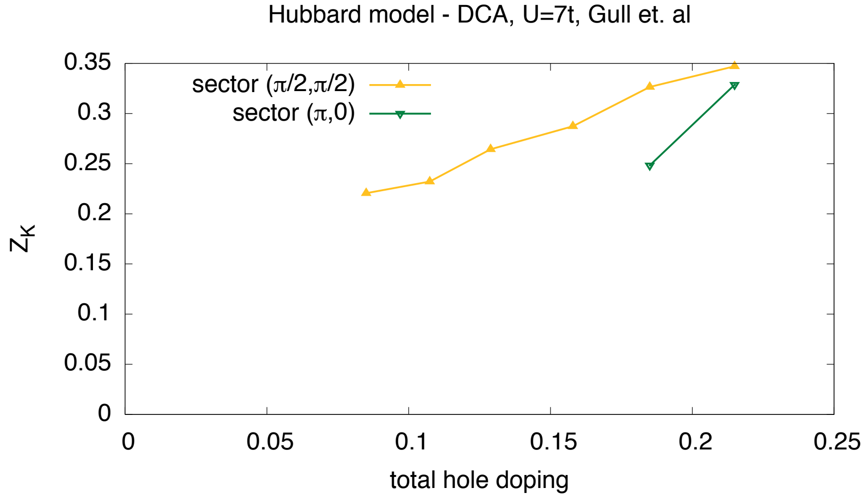
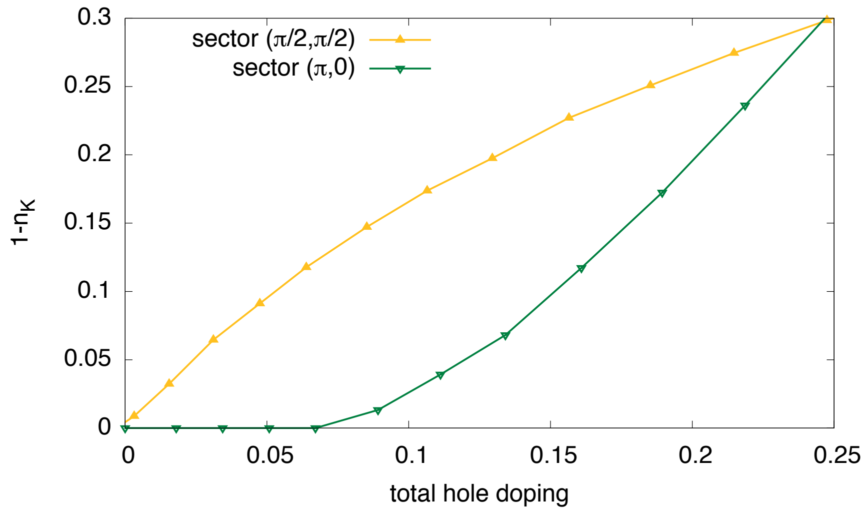
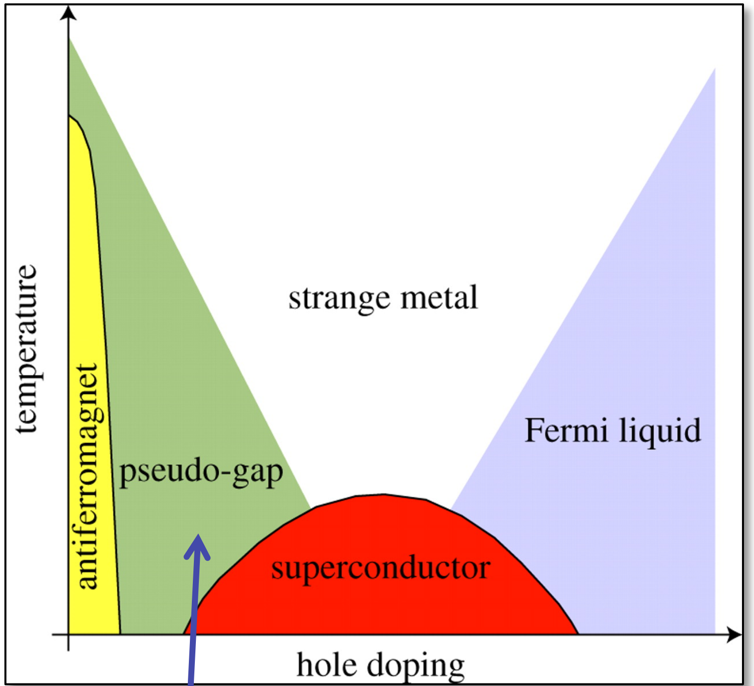
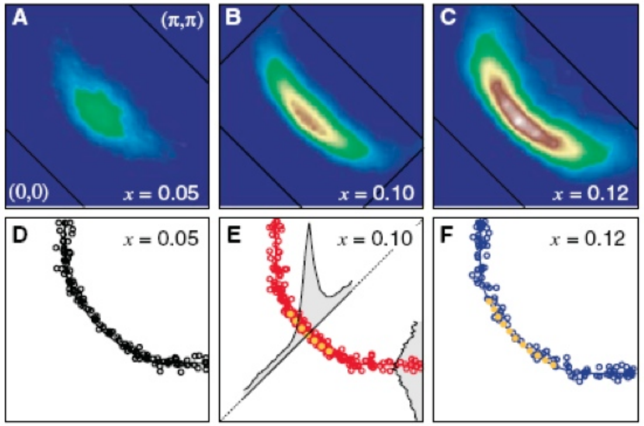




DCA calculation from: Gull et al.
Phys Rev. B 82, 155101 (2010)



K. Shen et al. Science 2007



Cuprates: DCA approach to the 2D Hubbard model

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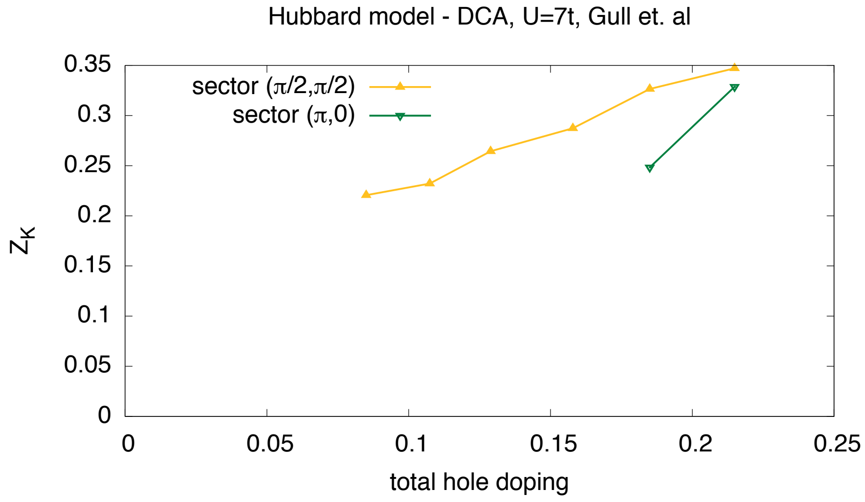

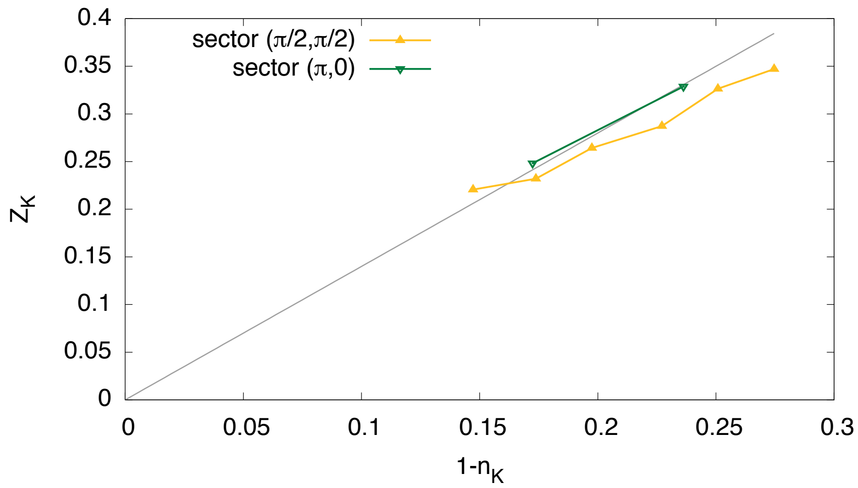

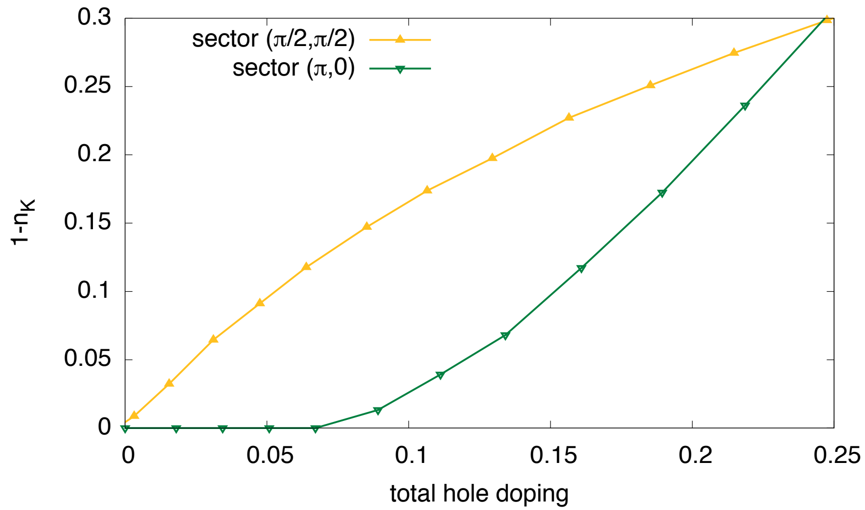

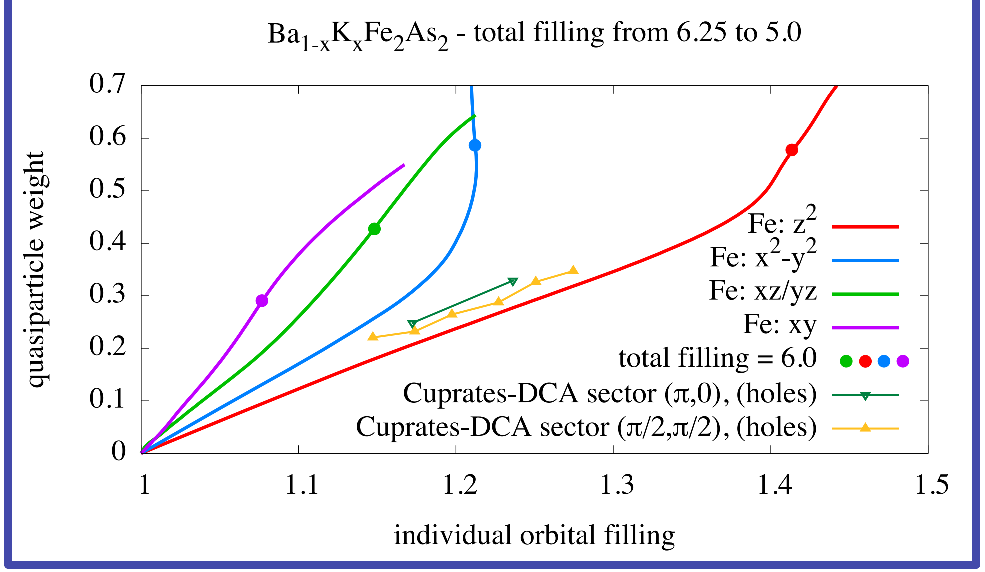

DCA calculation from: Gull et al.
Phys Rev. B 82, 155101 (2010)

Same orbital decoupling!