New perspectives in superconductors

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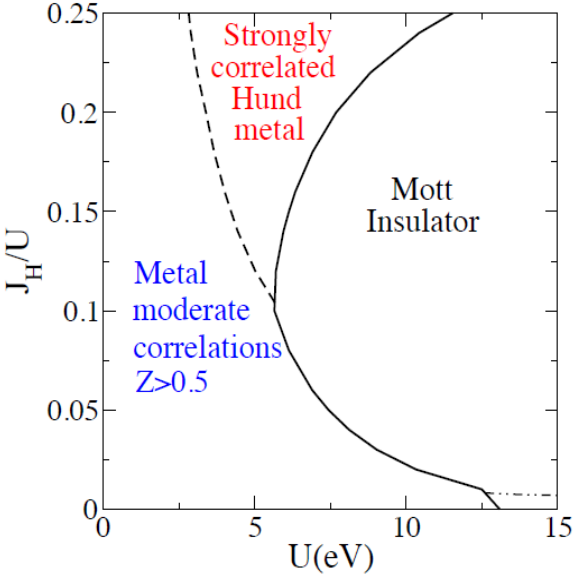
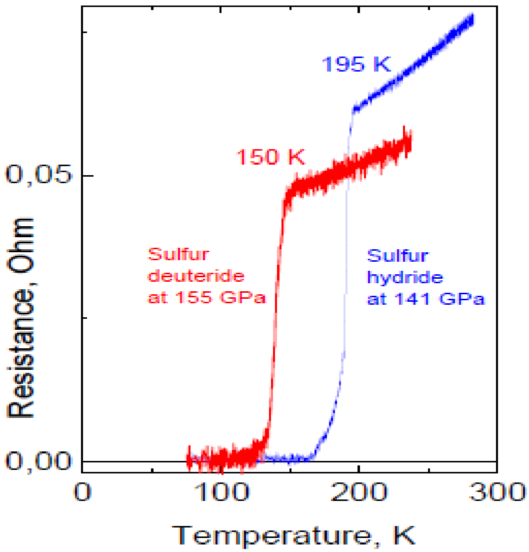




Outline

- Talk I: Correlations in iron superconductors
  - Introduction to correlations in single orbital systems and cuprates.
  - Superconductivity in iron superconductors
  - Correlations in multiorbital systems.
    - Equivalent orbitals. The Hund metal
    - Unequivalent orbitals. Iron superconductors
  - The magnetic state phase diagram
  - Comparison with experiments. Iron superconductors in a (U,J_H) phase diagram
- Talk II: A few new superconducting materials
  - Superconductivity and competing phases
    - CrAs and MnP
    - Ti-oxypnictides. Superconductivity emerging from a nematic state?
  - New quasi-1D superconductors
  - Hydrides. A new record for high-Tc?

A bit of history

1911. Resistivity vanishes below Tc. Discovery of superconductivity

1933. Superconductors expel magnetic fields. Meissner effect

1950. Ginzburg-Landau phenomenological theory

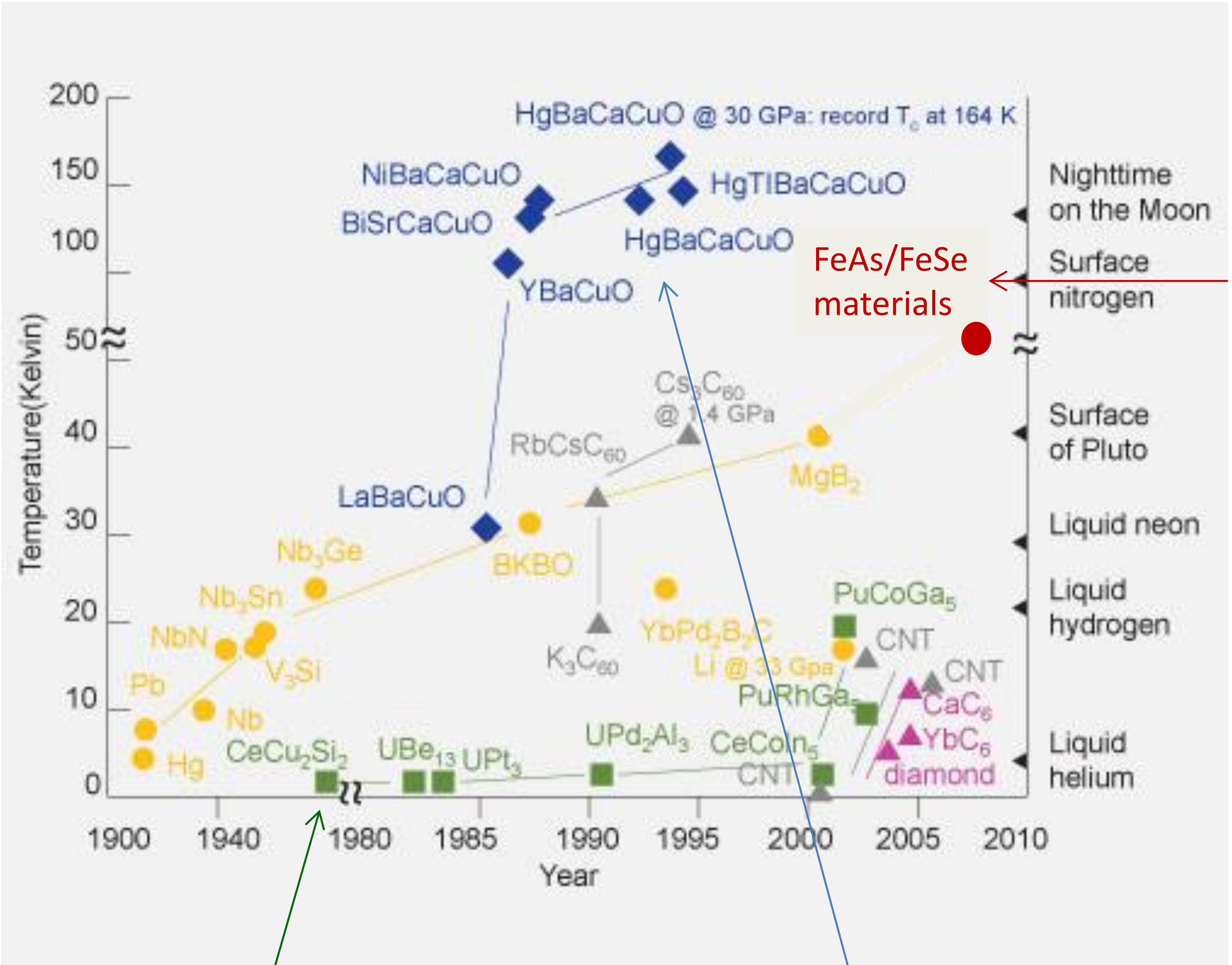
1957. BCS theory. Cooper pairs and electron-phonon interaction

1957-59. Vortices

1962. Josephson effect

In the '70s many superconductors were known (T_c < 25 K)
and people thought that superconductivity was understood

High-Tc superconductivity in iron materials



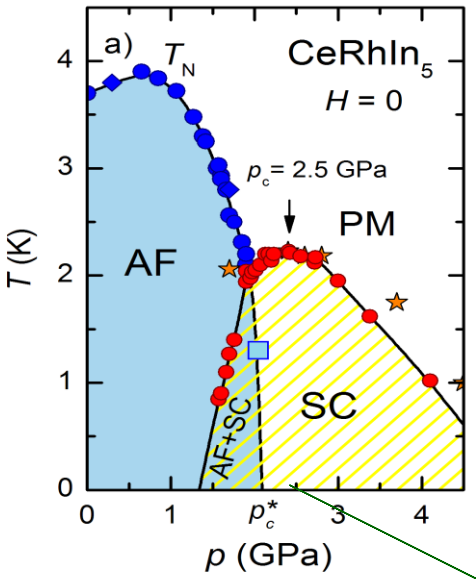
2008. Iron superconductors
The second family of
high Tc superconductors

1979. Superconductivity in
Heavy Fermion compounds

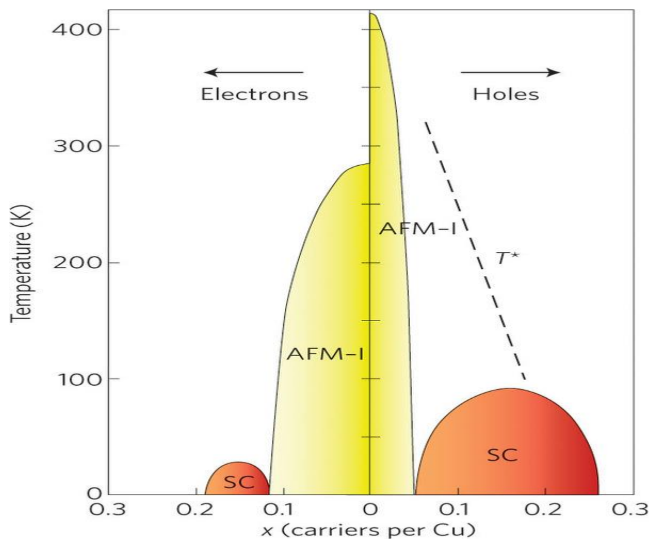
1986. Cuprates. High-Tc
superconductivity

Unconventional superconductivity in correlated systems

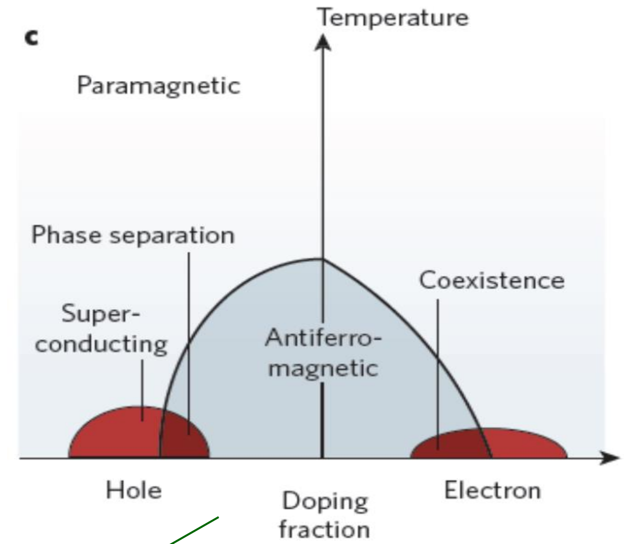
Heavy Fermions



Cuprates



Iron superconductors

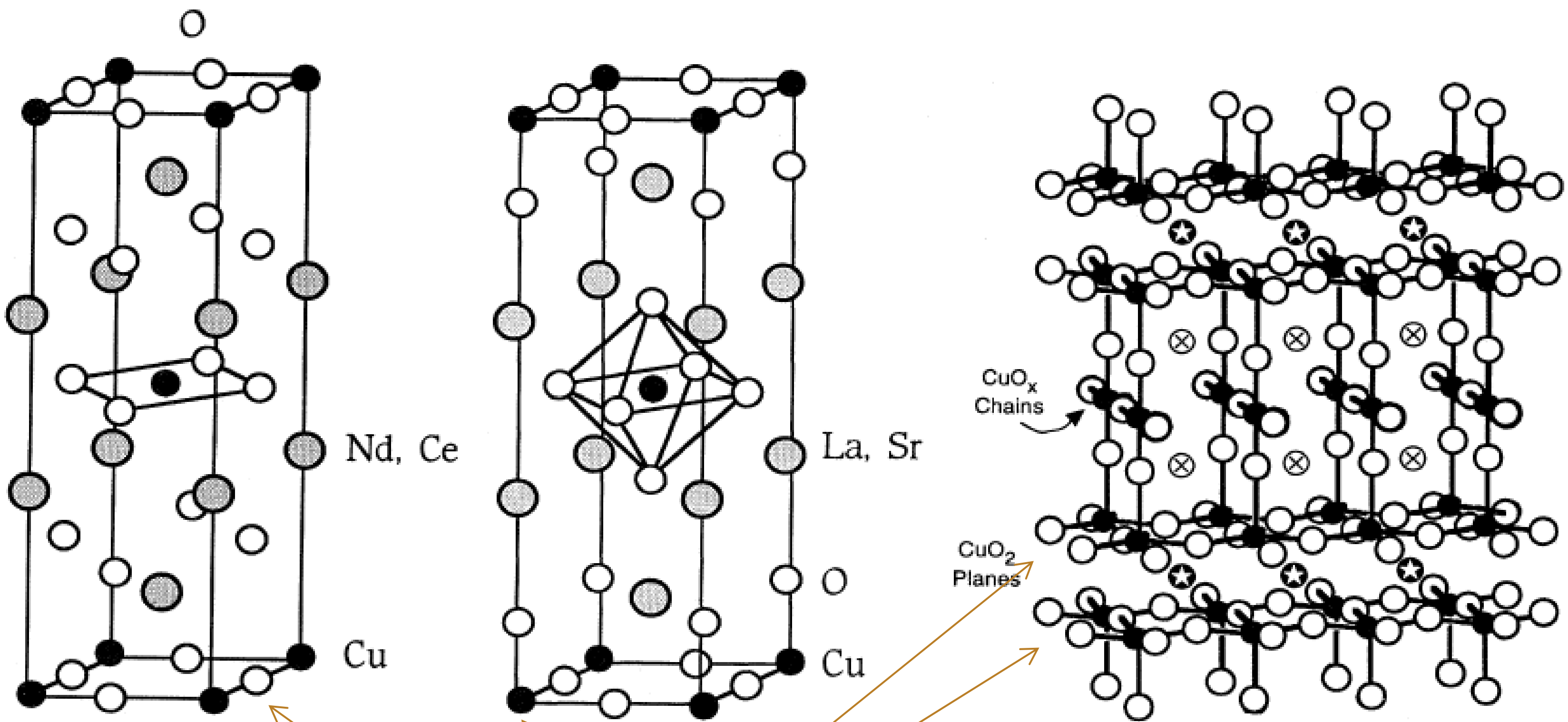


Magnetically mediated superconductivity?

Superconductivity not due to electron-phonon interaction

Cuprates and Mott physics

$NdCuO_4$ $LaCuO_4$ YBa_2CuO_{6+x}



Several families
CuO_2 Planes

Fig: Dagotto, RMP 66, 763 (1993)

The electronic properties are controlled by these planes

Cuprates and Mott physics

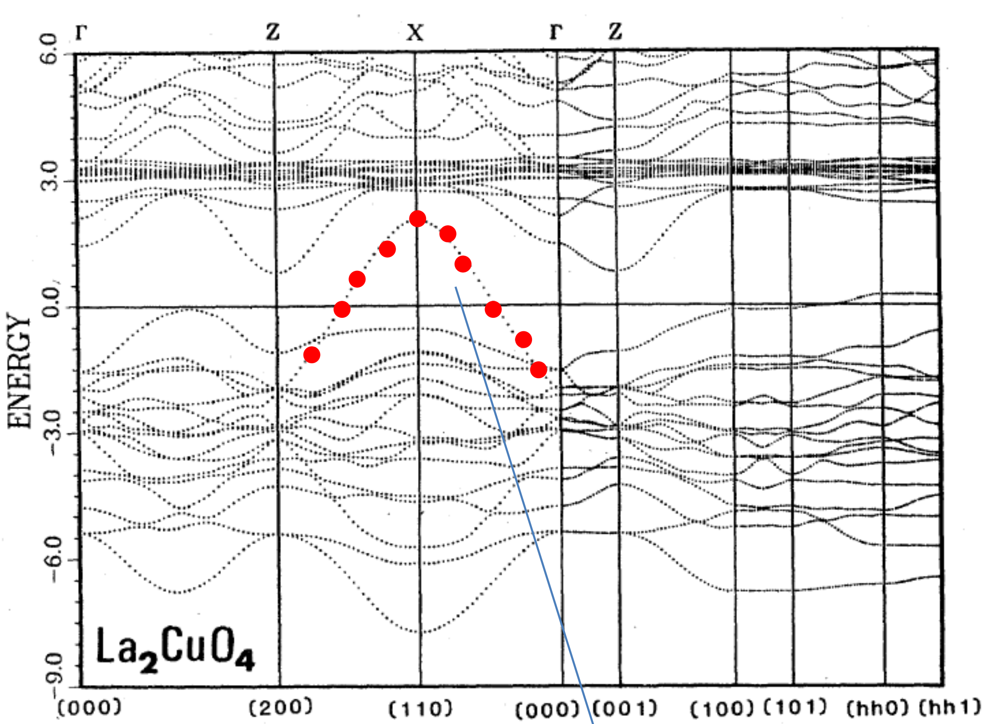


Fig: Pickett, RMP 61, 433 (1989)

CuO$_2$ band

LaCuO$_4$

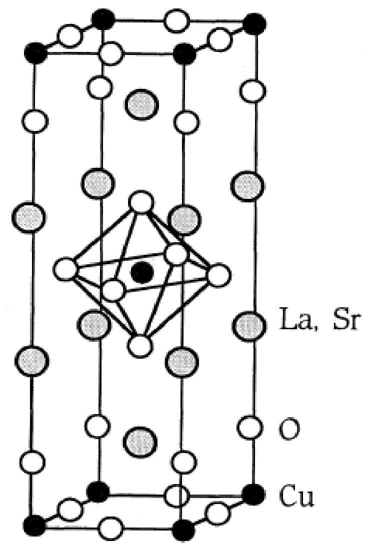
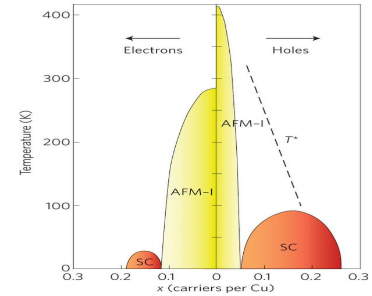


Fig: Dagotto, RMP 66, 763 (1993)



Expected to be metallic, but it is an insulator.

Mott insulator: insulating character due to electron-electron interactions

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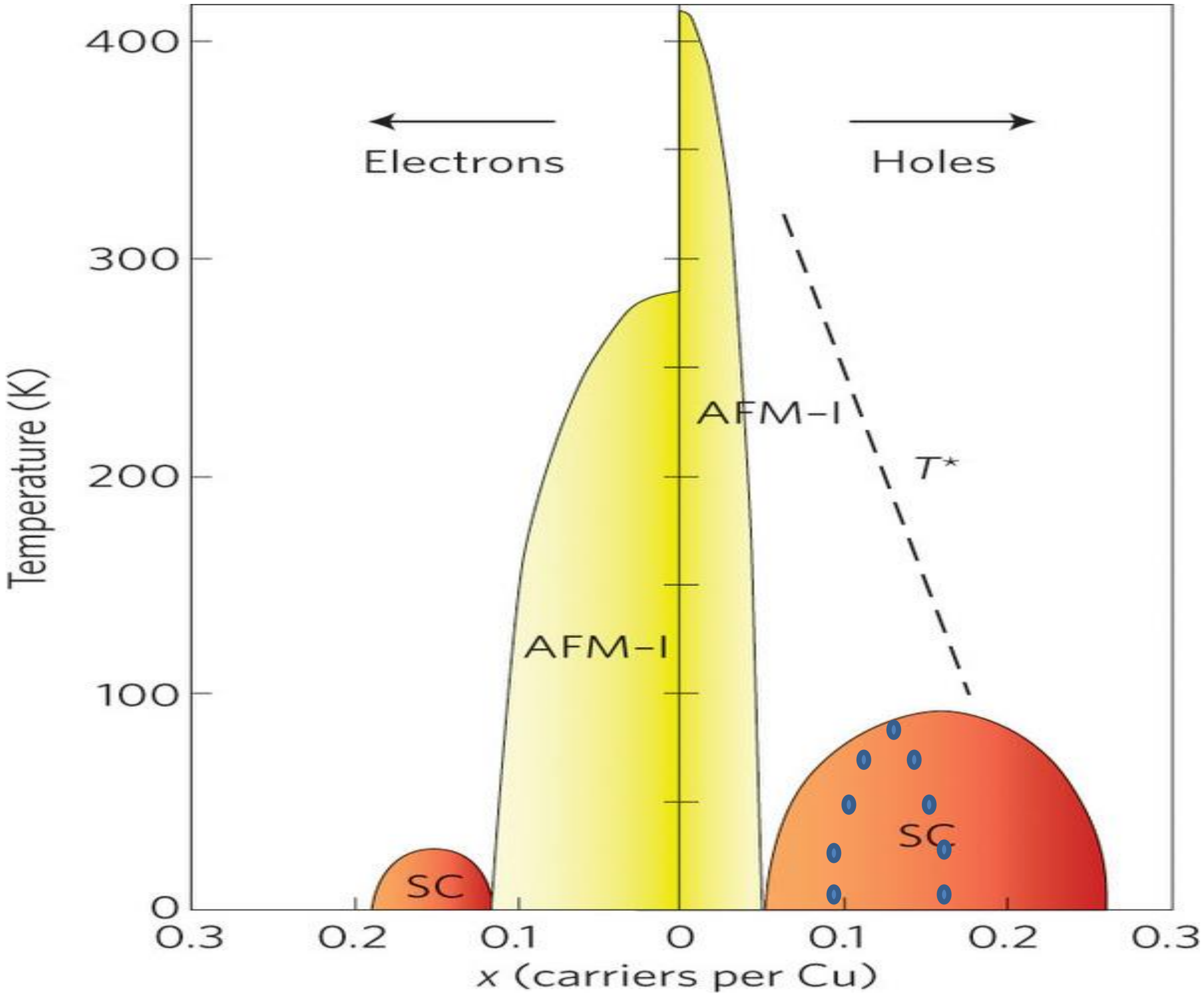
Cuprates and Mott physics



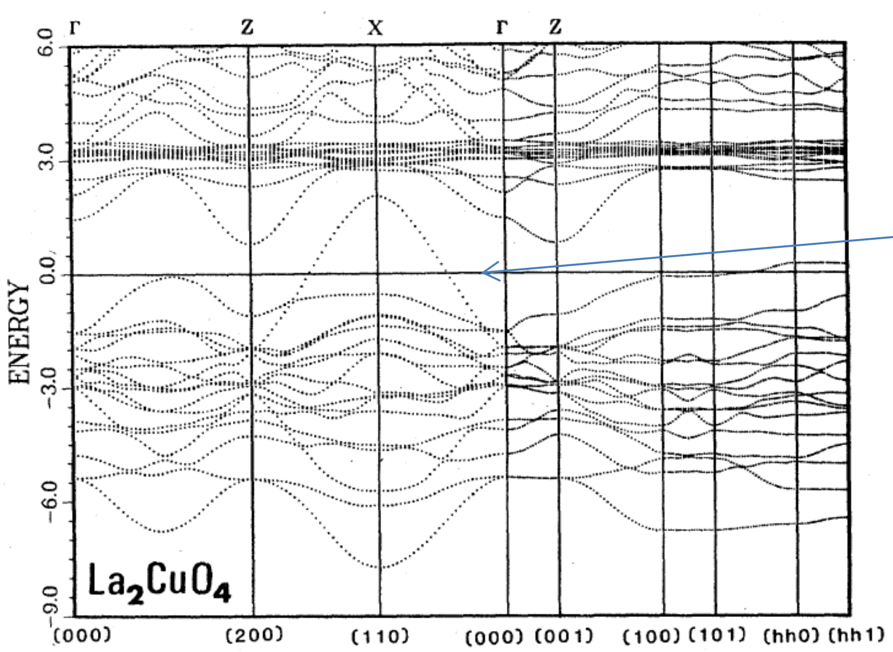
Superconductivity appears when an antiferromagnetic Mott insulator is doped with electrons or holes

Mott insulators. The Hubbard model at half-filling

$$H=\sum_{i,j,\sigma} t\, c^{\dagger}_{i\sigma} c_{j\sigma}$$

Kinetic energy

Atomic lattice with a single orbital per site and average occupancy 1 (half filling)



Simplification for
Band structure

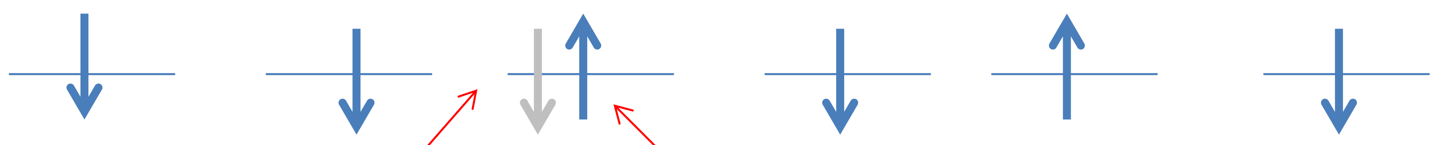
Mott insulators. The Hubbard model at half-filling

$$H=\sum_{i,j,\sigma} t\, c^{\dagger}_{i\sigma}c_{j\sigma} + U\sum_j n_{j\uparrow}n_{j\downarrow}$$

Kinetic energy

Intra-orbital repulsion

Atomic lattice with a single orbital per site and average occupancy 1 (half filling)



Hopping saves energy t

Double occupancy costs energy U

For U >> t electrons localize: Mott insulator
Mott transition at Uc

But away from half-filling the system is always metallic → Correlated metal

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The quasiparticle weight in the single-orbital Hubbard model

Z: a way to quantify the correlations

$$0 \leq Z \leq 1$$

Simple Fermi liquid description:

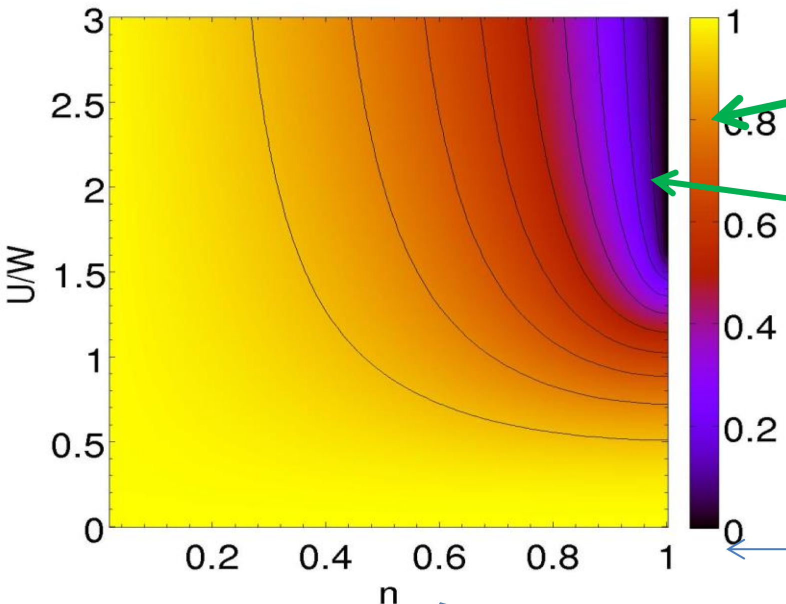
Heavy electron $\quad Z^{-1} \propto m^*/m$

Overlap between the elementary excitations of interacting and non-interacting systems

Z=1 Single-particle picture (U=0)

Z=0 There are no quasiparticles
Breakdown of single-particle picture

Z colour plot for the Hubbard model



Z vanishes at the Mott transition

Correlated metal as U is increased
or half-filled is approached
(only close to the Mott transition).

Half-filling

Electronic filling

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Quasiparticle weight, charge & spin fluctuations in the Hubbard model

Quasiparticle weight Z:

$0 \leq Z \leq 1$

A way to quantify correlations

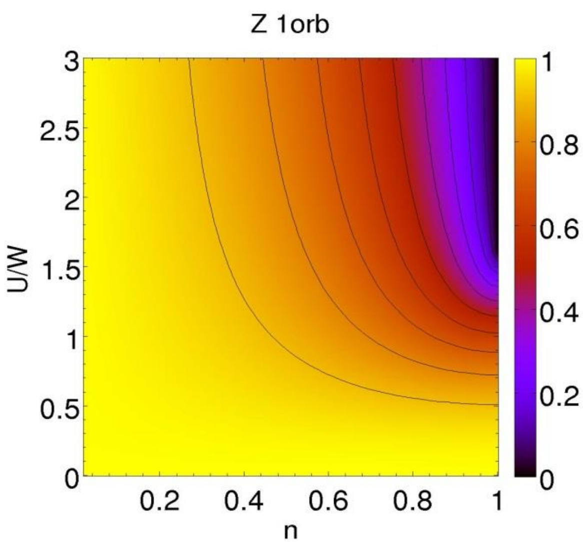
$C_T = \langle n^2 \rangle - \langle n \rangle^2 = \langle (\delta n)^2 \rangle$

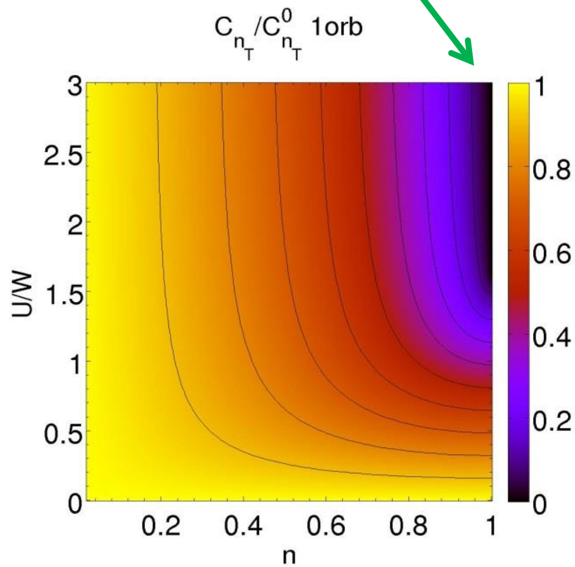
$n = \langle n \rangle + \delta n$

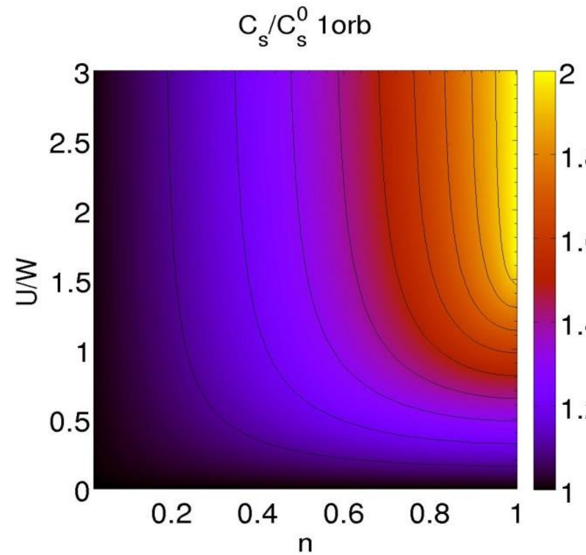
Localization

$C_S = \langle S^2 \rangle - \langle S \rangle^2 = \langle S^2 \rangle$

C_s larger when atoms are spin polarized even if there is no long range order







Mott insulator:

Suppression of charge fluctuations

n= <n>

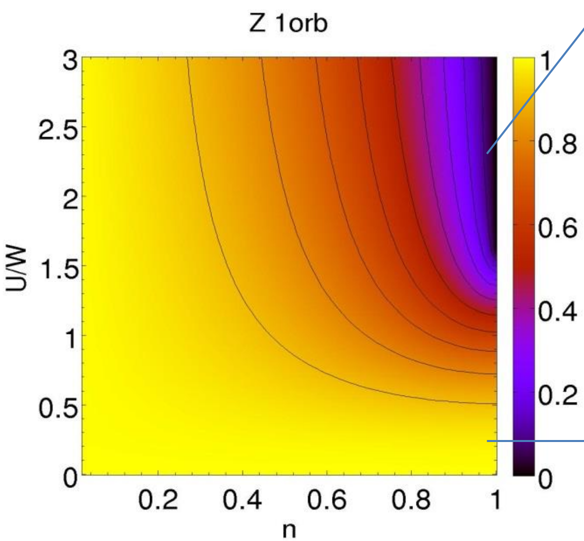
Localized spins at each atomic site

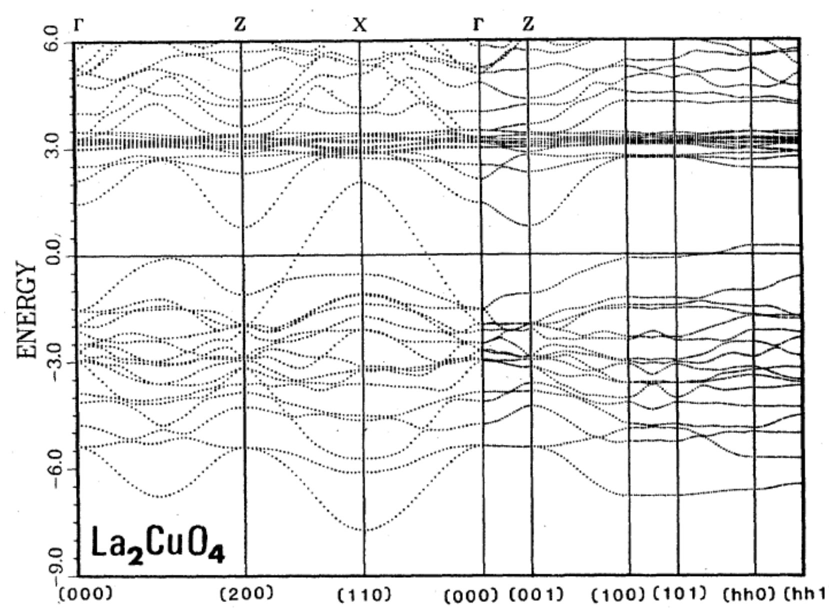
Weakly correlated electrons & localized spins

Quasiparticle weight Z:

$$0 \leq Z \leq 1$$

A way to quantify correlations





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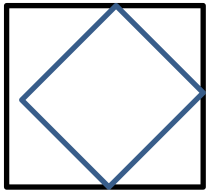
Nature of instabilities: the case of antiferromagnetism

Fermi surface instability

- Delocalized electrons. Energy bands in k-space and Fermi surface good starting point to describe the system.

-The shape of the Fermi surface presents a special feature (nesting)



-In the presence of small interactions antiferromagnetic ordering appears.

- Ordering can be incommensurate

Spin Density Wave
Magnetism driven by interactions

Antiferromagnetic exchange

- Localized electrons. Spins localized in real space

-Kinetic energy favors virtual hopping of electrons ($t^2/\Delta E \sim t^2/\Delta E$).

-Virtual hopping results in interactions between the spins. Magnetic Exchange Spin models

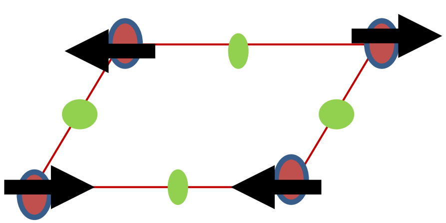
- Magnetic ordering appears if frustration (lattice, hopping, …) does not avoid it.

- Commesurate ordering

Magnetism driven by kinetic energy

Cuprates and Mott physics

Undoped (Cu d^9) dx^2-y^2 orbital is half filled. Mott insulator
Described in terms of a localized electron /spin at each Cu site



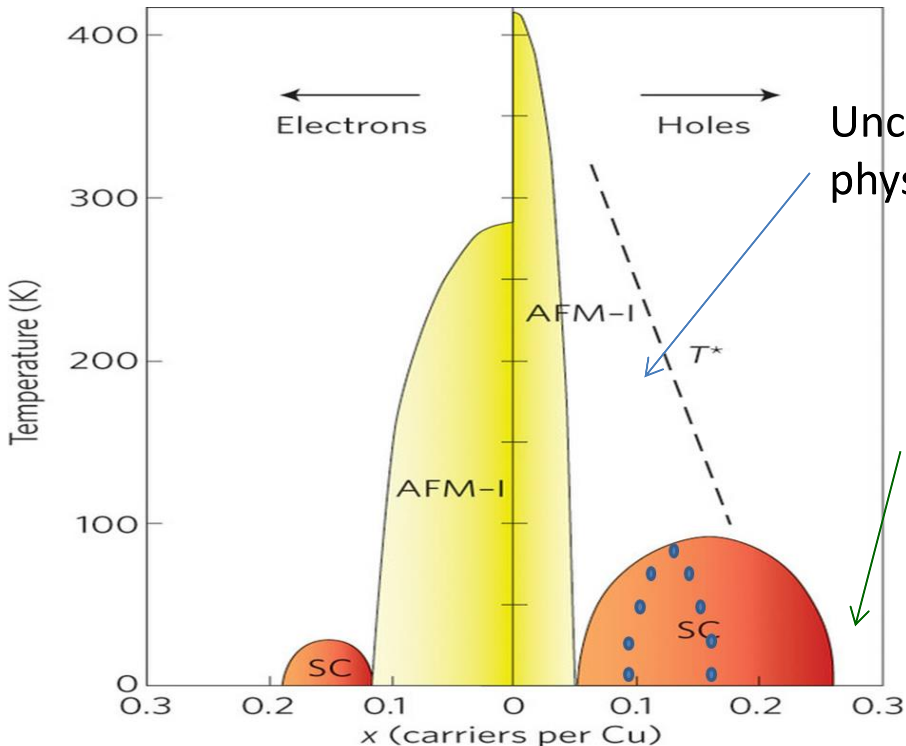
Antiferromagnetic order. Neel state
Interaction between localized spins

Exchange $J \sim t^2/U$

$$H = J S_i S_j$$

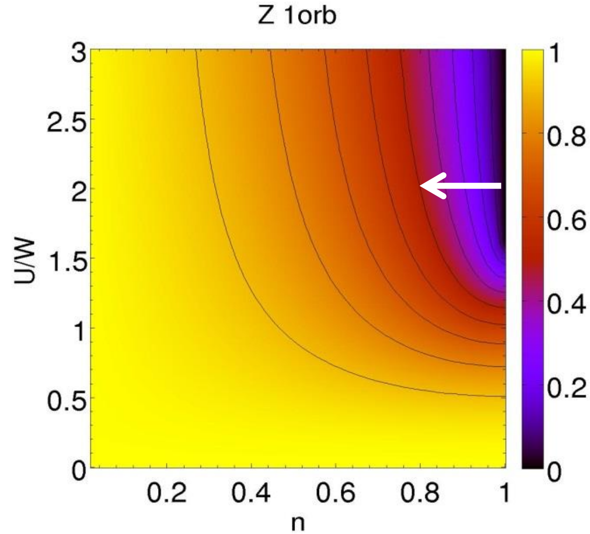
(Heisenberg model)

Cuprates: From a Mott insulator to a high-Tc superconductor



Unconventional physics

Fermi liquid (bands and Fermi surface)

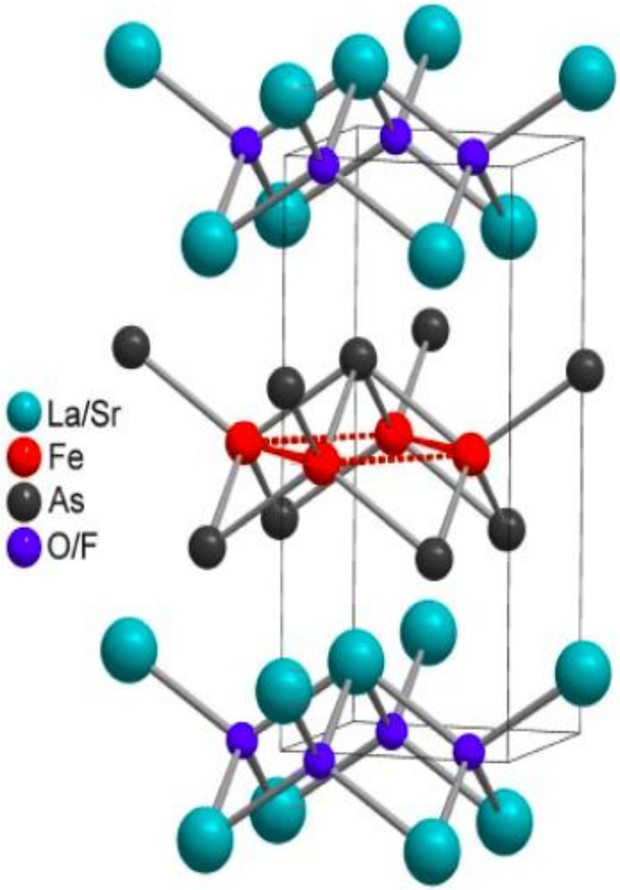


1 electron in 1 orbital:
half-filling
Mott insulator

Antiferromagnetism described in terms of Localized moments

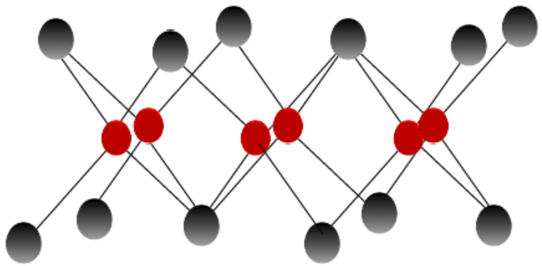
Which is the role of Mott physics
In High-Tc superconductivity?
Do we need localized moments
to explain it?

Fe superconductors: FeAs-FeSe layers

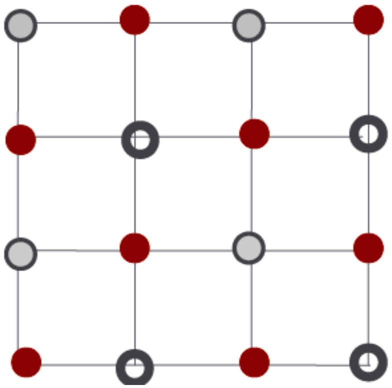


Layered materials

(FeAs/Se planes)



Fe square lattice



Kamihara et al, JACS 130, 3296 (2008)

Fe superconductors: families

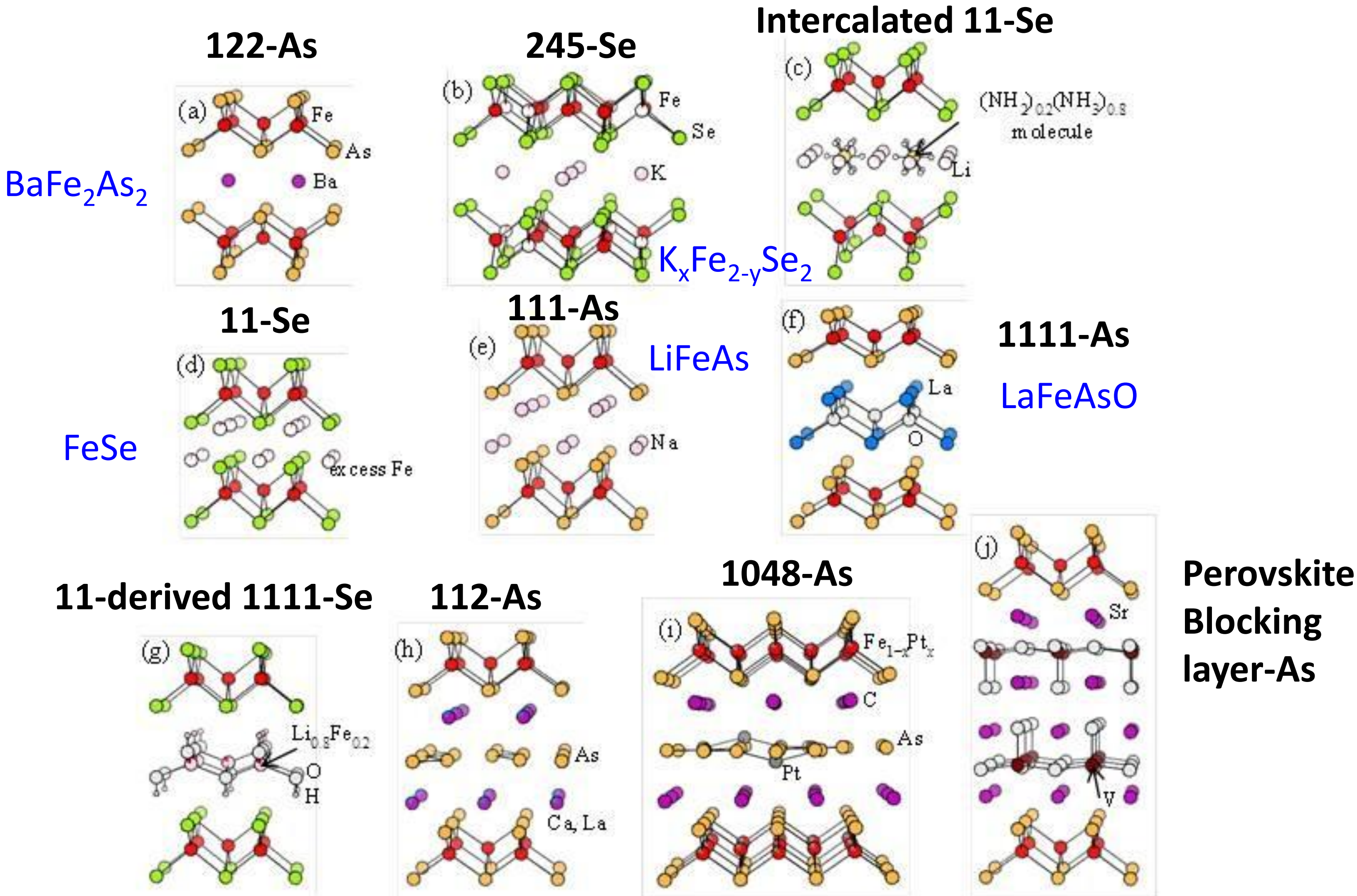
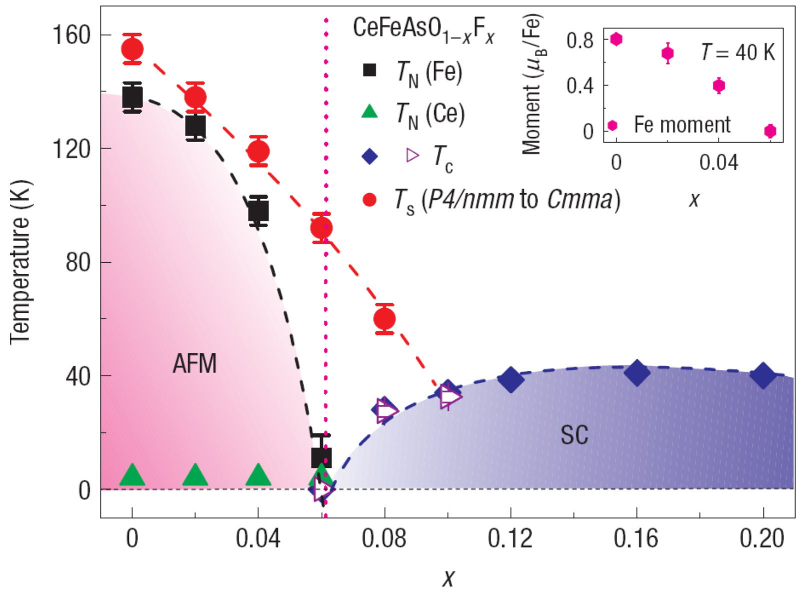


Fig:Hosono & Kuroki, Phys. C (2015), arXiv: 1504.04919

Fe superconductors: phase diagram

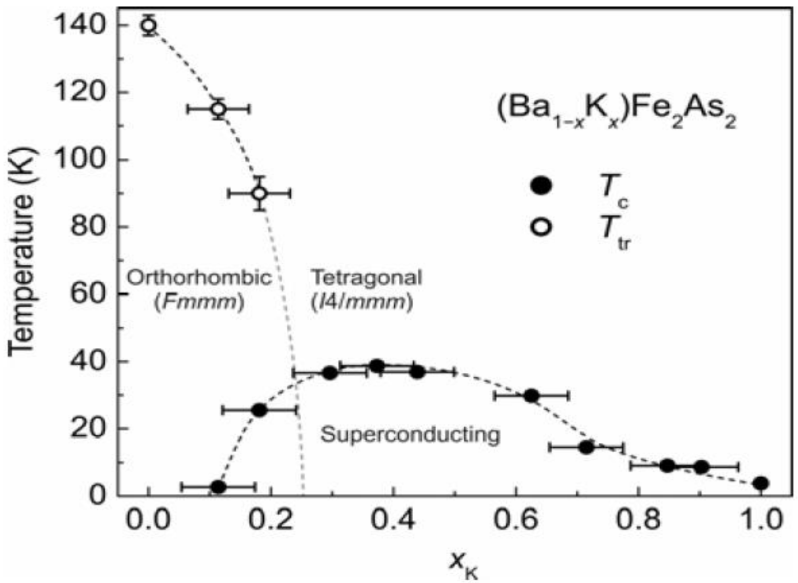
Undoped: 6 e- per Fe

Doping with electrons



Zhao et al, Nat. Mat. 7, 953 (2008),

Doping with holes



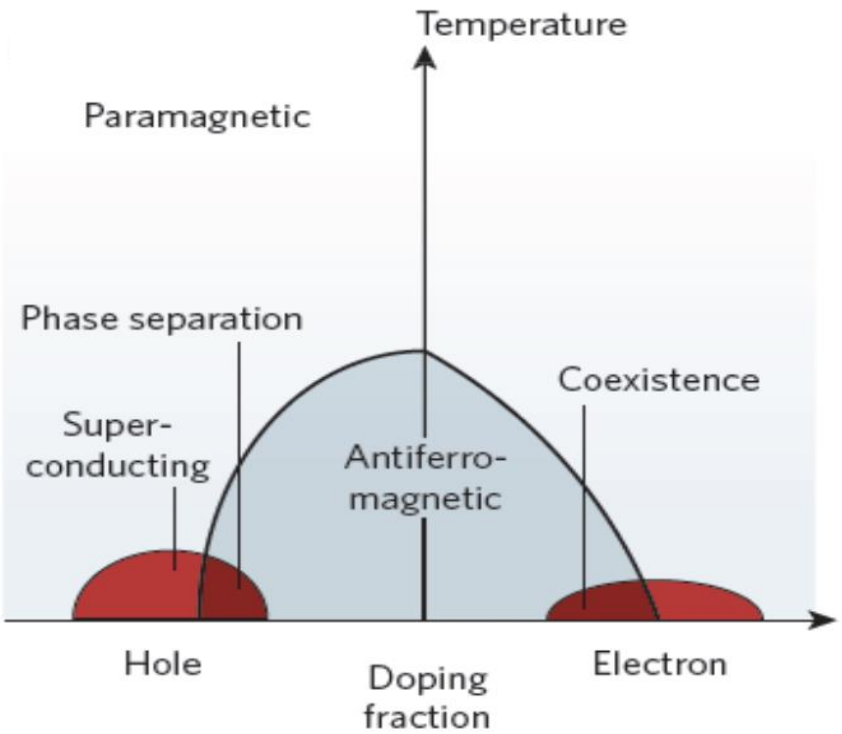
Rotter et al, Angew. Chem. Int. Ed. 47, 7949 (2008)

Undoped iron pnictides/chalcogenides are (not always) AF

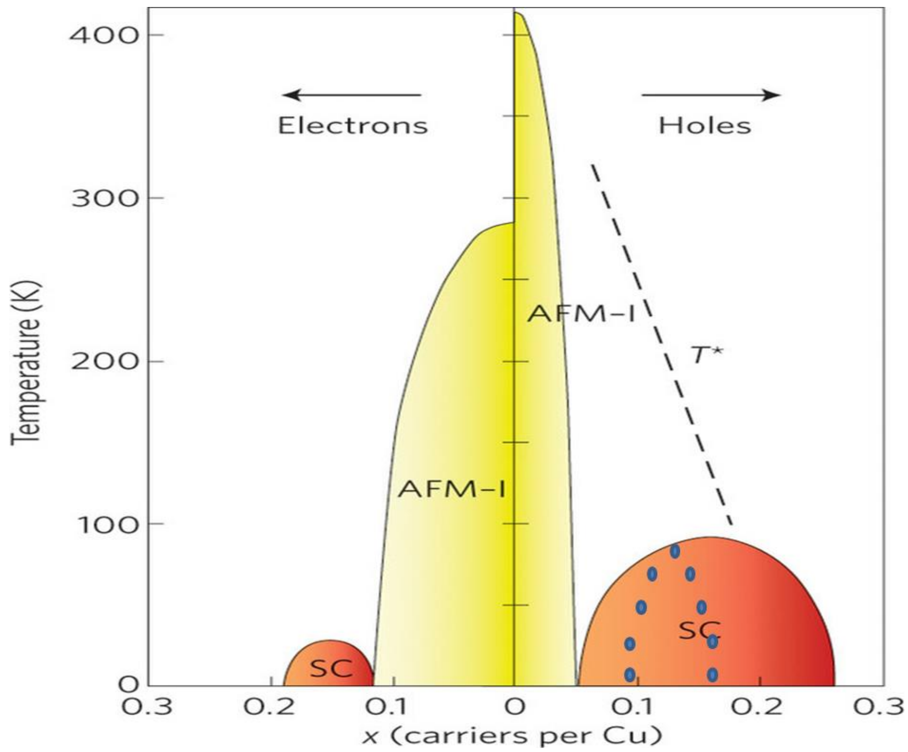
Superconductivity appears when doping with electrons or holes

Fe superconductors: phase diagram

Iron superconductors



Cuprates

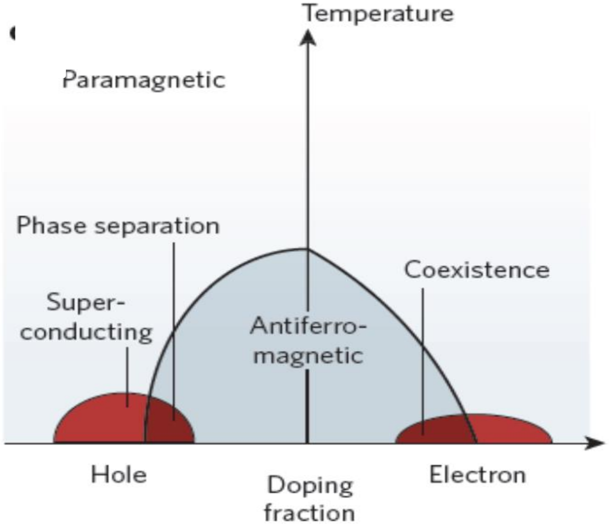


Superconductivity appears when an antiferromagnetic phase is suppressed with electron or hole doping

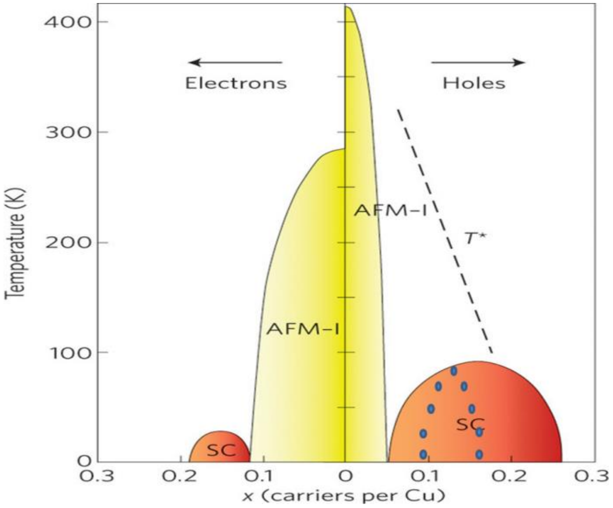
Fig: Nature 464,183 (2010)

Fe superconductors: phase diagram

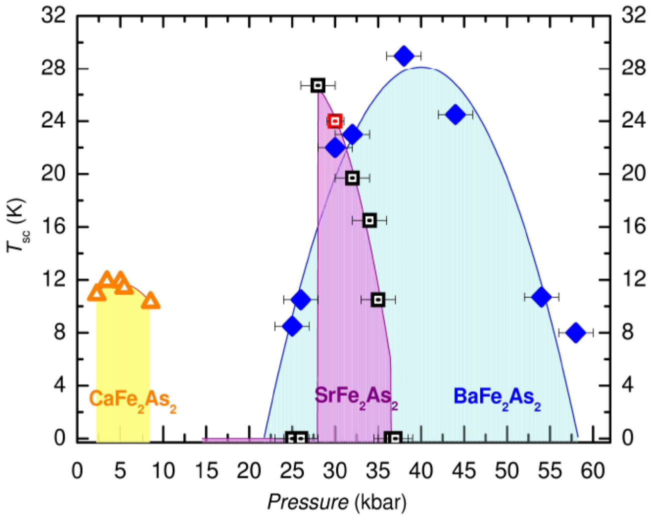
Iron superconductors



Cuprates



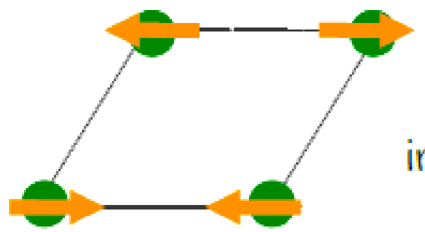
In iron superconductors superconductivity also appears when pressure is applied

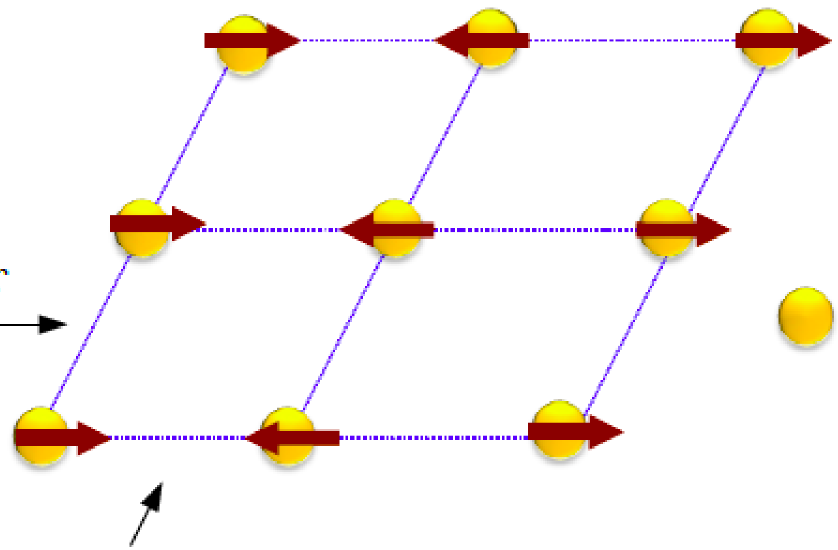


Alireza et al,
J. Phys. Cond. Matt 21, 012208 (2008)

Fig: Nature 464,183 (2010)

Fe superconductors: phase diagram

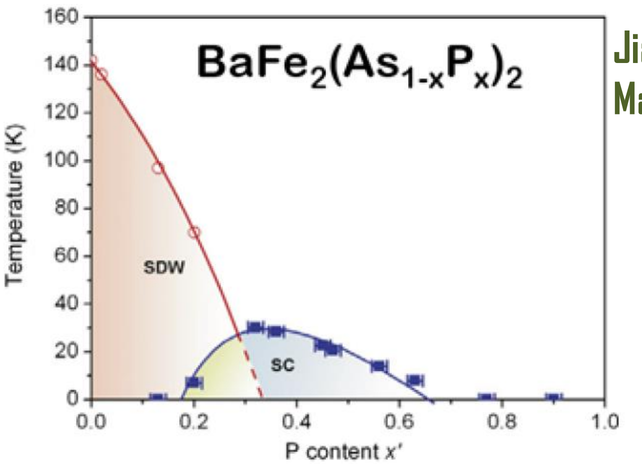




De la Cruz et al, Nature 453, 899 (2008), Zhao et al, Nature Materials 7, 953 (2008)

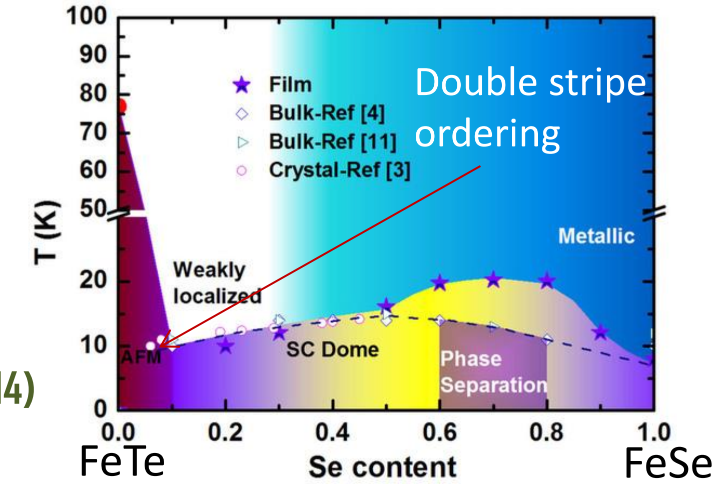
Fe superconductors: phase diagram

Isovalent substitution



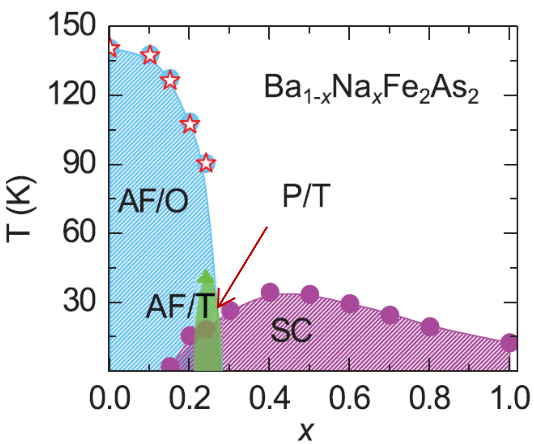
Jiang et al, J. Phys. Cond. Mat. 21, 382203 (2009)

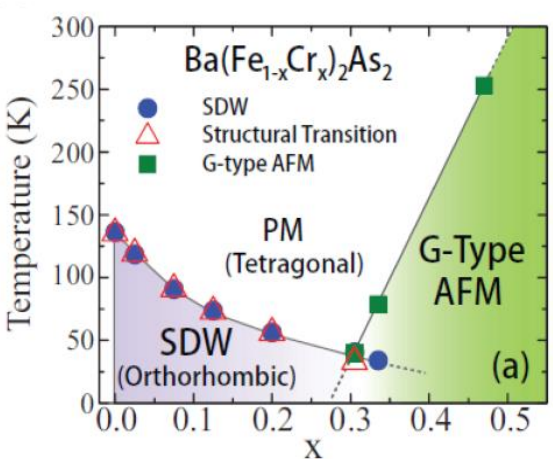
Zhuang et al, Sci. Rep. 4 7273 (2014)

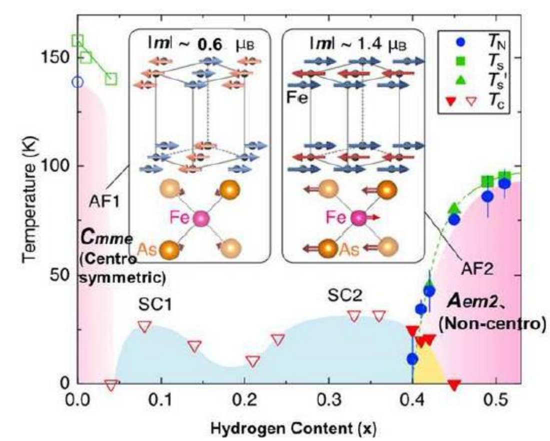


Hole doping

Electron doping







Avci et al, Phys. Rev. B 88, 094510 (2013)

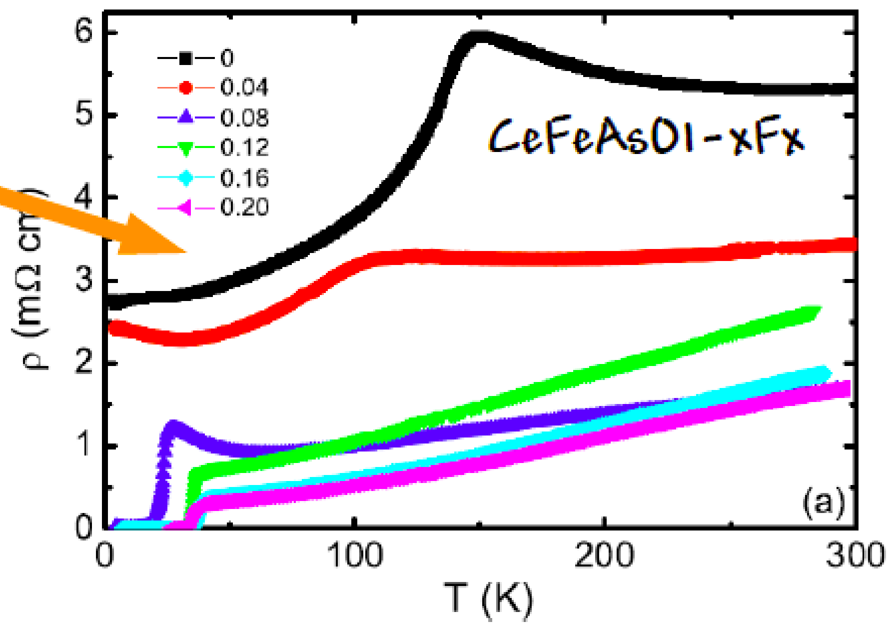
Marty et al, Phys. Rev. B 83, 060509 (2011)

Fujiwara et al, $LaFeAsO_{1-x}H_x$
Phys. Rev. Lett 111, 097002 (2013)

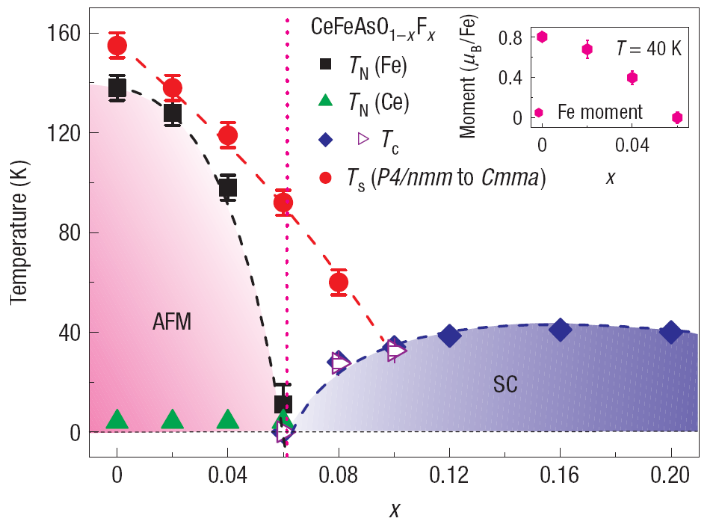
Fe superconductors: Metallicity of parent compounds

Undoped AF pnictides
are metallic

Contrary to cuprates undoped
iron pnictides
are NOT Mott insulators



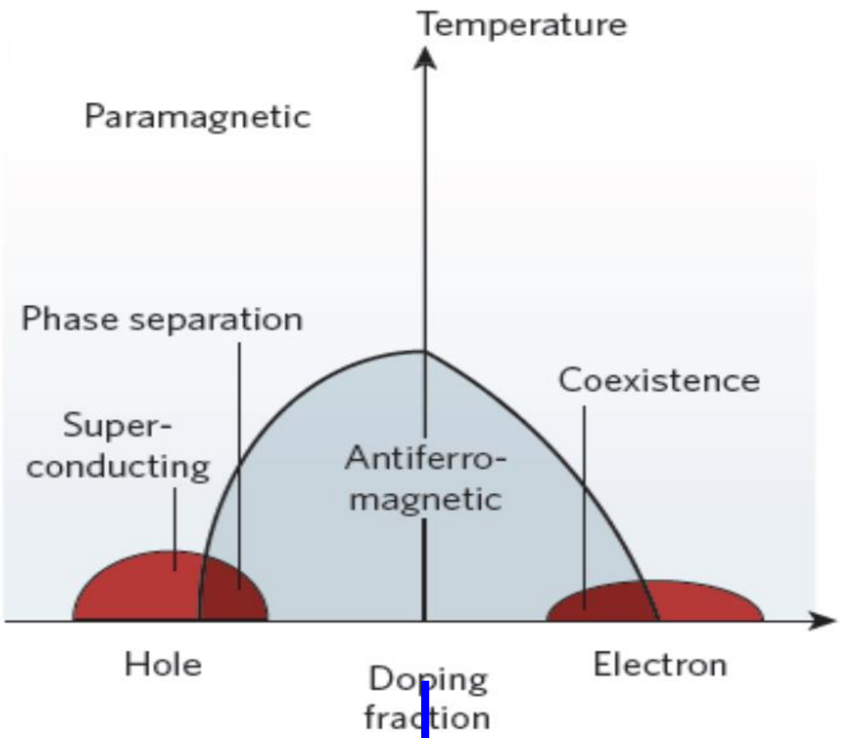
Chen et al, PRL 100, 247002 (2008)



Zhao et al, Nat. Mat. 7, 953 (2008),

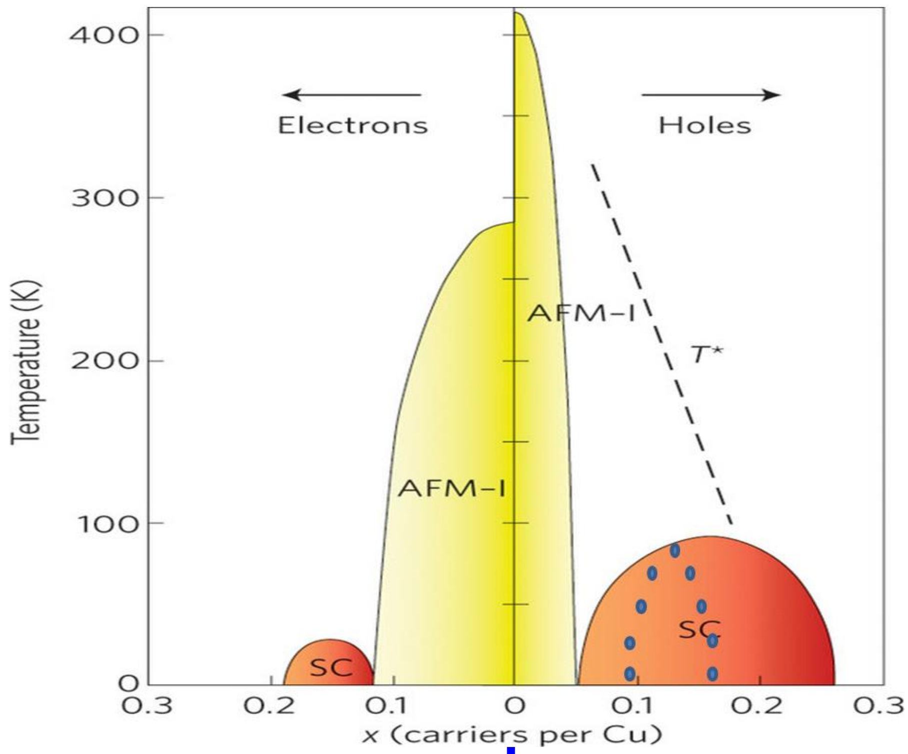
Fe superconductors: Metallicity of parent compounds

Iron superconductors



Antiferromagnetic Metal
Are there local magnetic moments?
Are iron superconductors strongly correlated systems?

Cuprates



AF Mott Insulator
Local magnetic moments
Strongly Correlated Electron System

Can we get high-Tc without local moments?

Correlations in iron superconductors

Weak correlations

(properties, origin of magnetism and of superconductivity described in terms of **itinerant electrons. Fermi surface physics**)

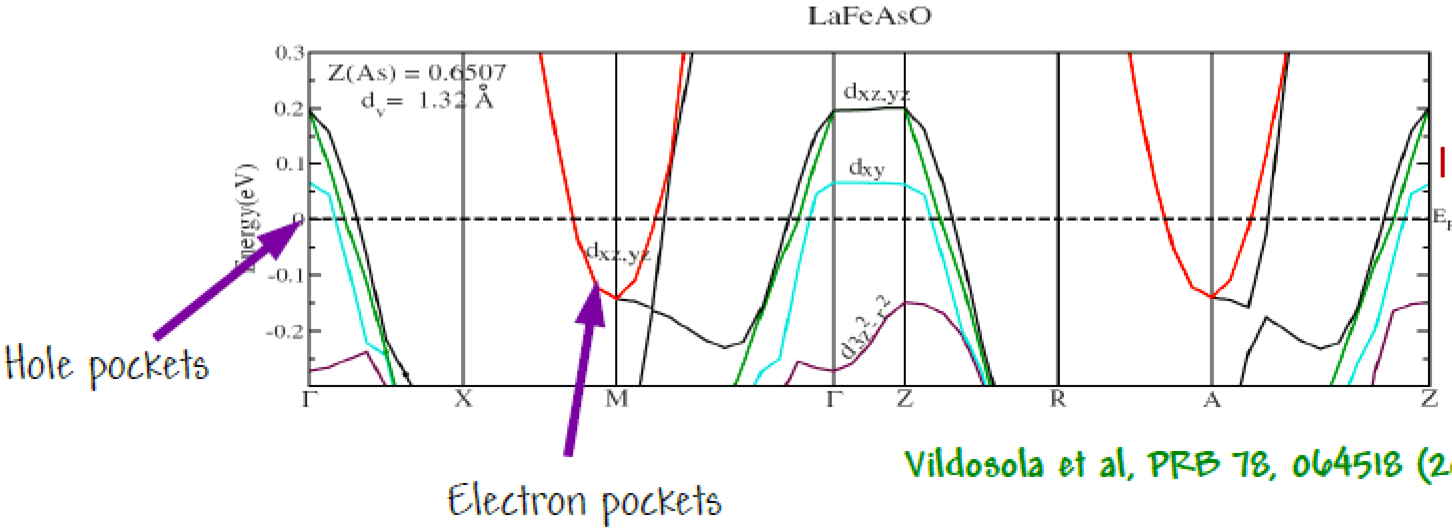
Raghu et al, PRB 77, 220503 (2008),
Mazin et al, PRB 78, 085104 (2008),
Chubukov et al, PRB 78, 134512 (2008),
Cvetkovic & Tesanovic,EPL85, 37002 (2008)

Localized electrons

(properties, origin of magnetism and of superconductivity described in terms of **localized electrons. Spin models**)

Yildirim, PRL 101, 057010 (2008),
Si and Abrahams, PRL 101, 057010 (2008)

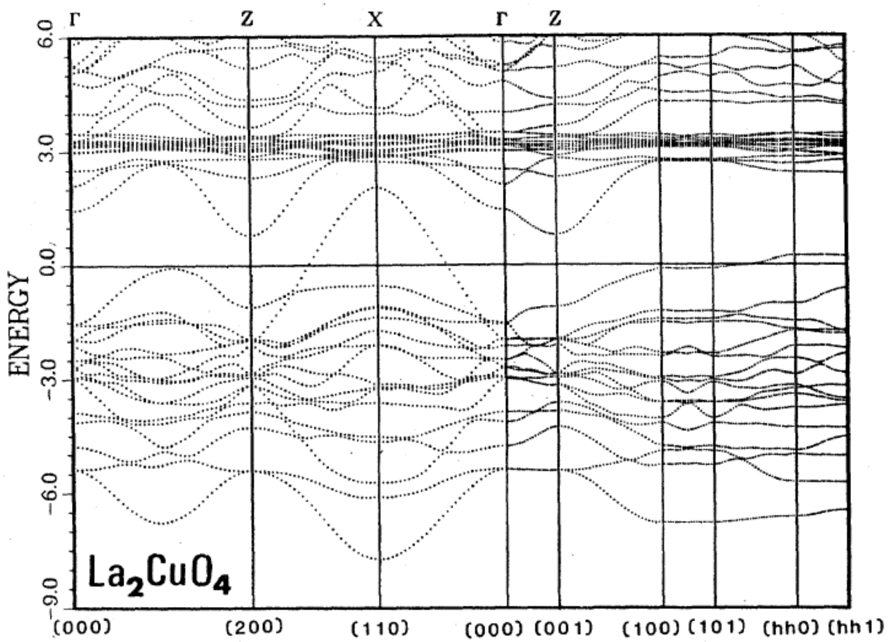
Iron superconductors :multi-orbital character



Iron superconductors

Vildosola et al, PRB 78, 064518 (2008)

Cuprates



LDA: Fe bands at the Fermi level.
Several orbitals involved
Undoped: 6 electrons in 5 orbitals

In cuprates a single band crosses the Fermi level
Undoped: 1 electron in 1 orbital

Fig: Pickett, RMP 61, 433 (1989)

Correlations in iron superconductors

Weak correlations

(properties, origin of magnetism and of superconductivity described in terms of **itinerant electrons. Fermi surface physics**)

Localized electrons

(properties, origin of magnetism and of superconductivity described in terms of **localized electrons. Spin models**)

Hund metal

(Correlations due to Hund's coupling)

Shorikov et al, arXiv:0804.3283

Haule & Kotliar NJP 11,025021 (2009)

Werner et al, PRL 101, 166404 (2008),
de Medici et al, PRL 107, 255701 (2011)

Yu & Si, PRB 86, 085104 (2012)

Fanfarillo & Bascones, arXiv:1501.04607

6 electrons in 5 orbitals
Average doping n=1.2
Like doped Mott insulators

Ishida& Liebsch, PRB 82, 1551006 (2010)

Werner et al, Nature Phys. 8, 331 (2012)
Calderon et al, PRB 90, 115128 (2014)

Correlations can be different for different orbitals leading even to a description in terms of the coexistence of localized and itinerant electrons

Yin et al, Nature Materials 10, 932 (2011)
Bascones et al, PRB 86, 174508 (2012)

Yi et al, PRL 110 067003, (2013)

de Medici et al, PRL 112, 177001 (2014)

Multiorbital character may play an important role

Correlations in iron superconductors

Weak correlations

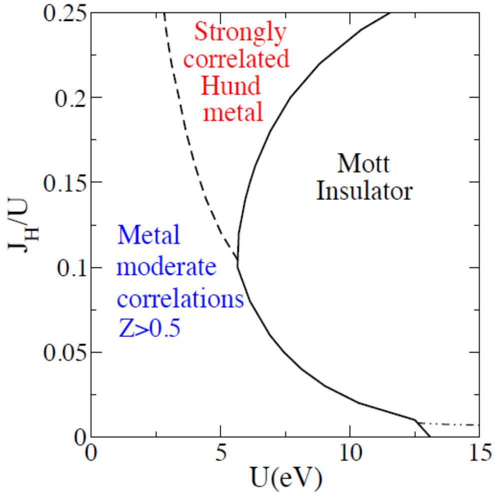
(properties, origin of magnetism and of superconductivity described in terms of **itinerant electrons. Fermi surface physics**)

Localized electrons

(properties, origin of magnetism and of superconductivity described in terms of **localized electrons. Spin models**)

Hund metal

(Correlations due to Hund's coupling)



6 electrons in 5 orbitals

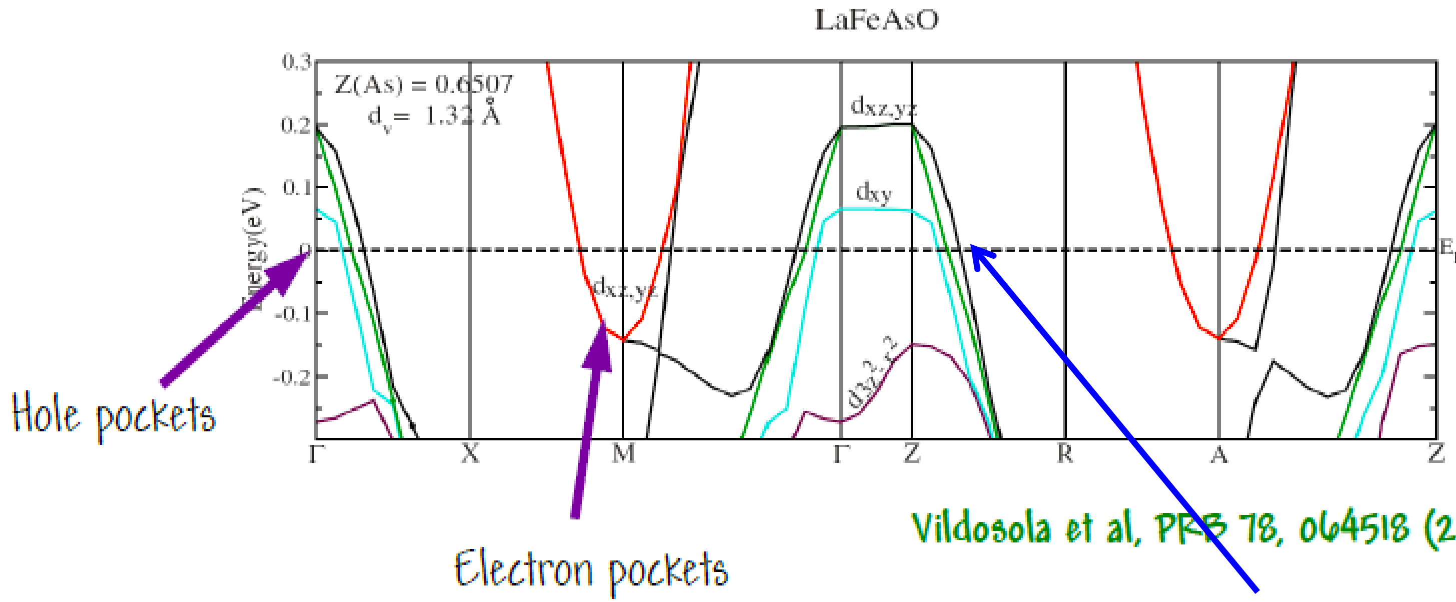
Average doping n=1.2

Like doped Mott insulators

Correlations can be different for different orbitals leading even to a description in terms of the coexistence of localized and itinerant electrons (OSMT)

Review: Bascones et al, arXiv:1503.04223, CRAS in press

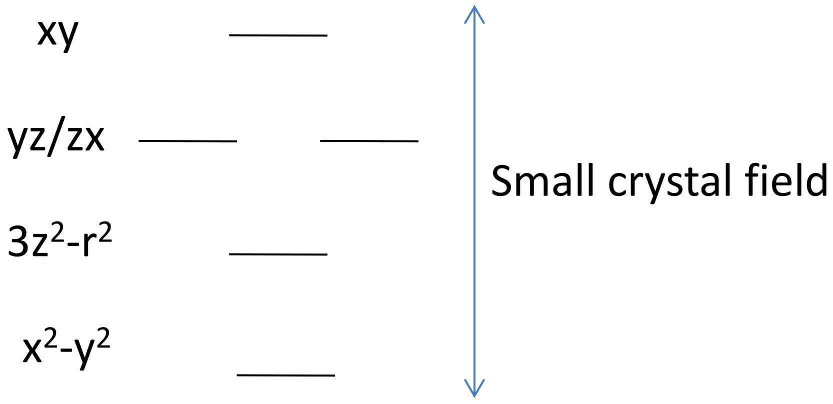
Iron superconductors: multi-orbital systems



Vildosola et al, PRB 78, 064518 (2008)

The 5 Fe d-orbitals are necessary
to describe the electronic properties

Several Fe bands
cross the Fermi level



Undoped compounds

Compensated FeAs layer
6 electrons in 5 Fe orbitals

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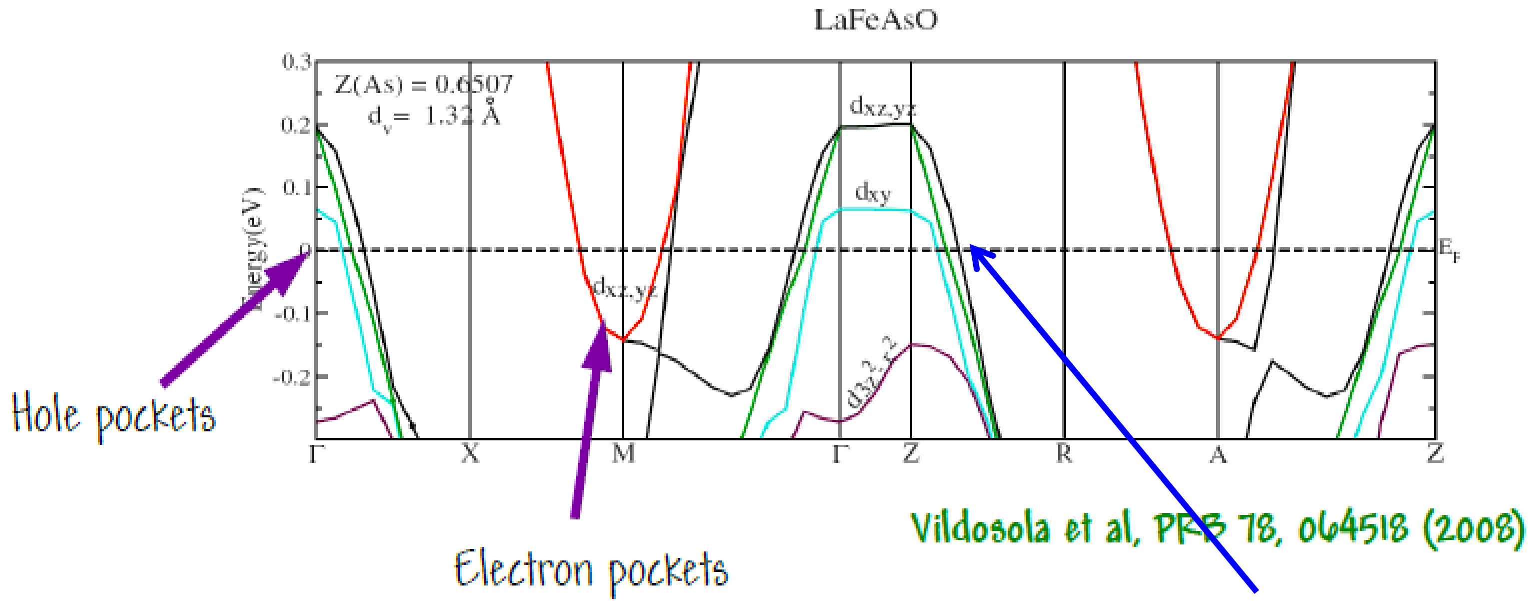

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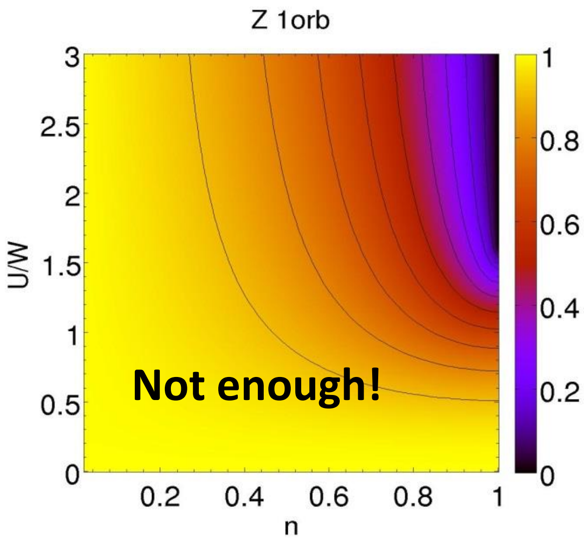


Undoped compounds

Compensated FeAs layer
6 electrons in 5 Fe orbitals

Hubbard-Kanamori Hamiltonian for multi-orbital systems

$$H = \sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^{\dagger} c_{j,\beta,\sigma} + h.c. + U \sum_{j,\gamma} n_{j,\gamma,\uparrow} n_{j,\gamma,\downarrow}$$

Tight-binding (hopping)

Intra-orbital repulsion

$$+ \left(U' - \frac{J_H}{2}\right) \sum_{j,\gamma>\beta,\sigma,\tilde{\sigma}} n_{j,\gamma,\sigma} n_{j,\beta,\tilde{\sigma}} - 2J_H \sum_{j,\gamma>\beta} \vec{S}_{j,\gamma} \vec{S}_{j,\beta}$$

Inter-orbital repulsion

Hund's coupling

$$+ J' \sum_{j,\gamma\neq\beta} c_{j,\gamma,\uparrow}^{\dagger} c_{j,\gamma,\downarrow}^{\dagger} c_{j,\beta,\downarrow} c_{j,\beta,\uparrow} + \sum_{j,\gamma,\sigma} \epsilon_{\gamma} n_{j,\gamma,\sigma} .$$

Pair hopping

Crystal field

$U' = U - 2J_H$ $\quad J' = J_H$

Two interaction parameters: U, J_H

Local Interactions

Hubbard-Kanamori Hamiltonian for multi-orbital systems

$$H_{\rm int} = U\sum_a n_{a\uparrow}n_{a\downarrow} + (U' - J_H)\sum_{a<b,\sigma} n_{a\sigma}n_{b\sigma}$$
$$+ U'\sum_{a\neq b} n_{a\uparrow}n_{b\downarrow} - J_H\sum_{a\neq b} c^\dagger_{a\uparrow}c_{a\downarrow}c^\dagger_{b\downarrow}c_{b\uparrow}$$
$$+ J'\sum_{a\neq b} c^\dagger_{a\uparrow}c^\dagger_{a\downarrow}c_{b\downarrow}c_{b\uparrow}$$

$U' = U - 2J_H$ $\quad J' = J_H$ $\longrightarrow$ $U - 3J_H$ $\longrightarrow$ $J_H/U < 0.33$

Two interaction parameters: U, J_H

Hubbard-Kanamori Hamiltonian for multi-orbital systems

$$
\begin{aligned}
H_{\mathrm{int}} \;=\;& U\sum_{a} n_{a\uparrow}n_{a\downarrow} + (U'-J_H)\sum_{a<b,\sigma} n_{a\sigma}n_{b\sigma} \\
+\;& U'\sum_{a\neq b} n_{a\uparrow}n_{b\downarrow} - J_H\sum_{a\neq b} c^{\dagger}_{a\uparrow}c_{a\downarrow}c^{\dagger}_{b\downarrow}c_{b\uparrow} \\
+\;& J'\sum_{a\neq b} c^{\dagger}_{a\uparrow}c^{\dagger}_{a\downarrow}c_{b\downarrow}c_{b\uparrow}
\end{aligned}
$$

Spin flip

Pair-hopping

Only density-density terms
Included. Hund treated as Ising term

$U'=U-2J_H \qquad J'=J_H$

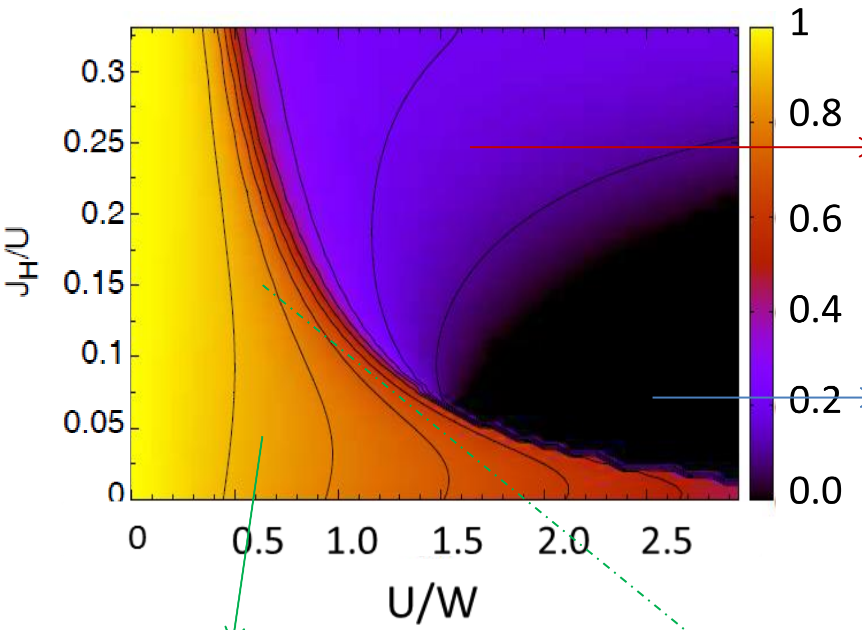
Two interaction parameters: $U,\ J_H$

Equivalent orbitals
No hybridization
No crystal field

Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

Colour plots: **Quasiparticle weight Z**



Hund metal small Z
(strongly correlated, even for small U/W)

n=6 Mott insulator

Weakly correlated metal

Boundary (crossover):
different dependence
on interaction parameters
than the Mott transition

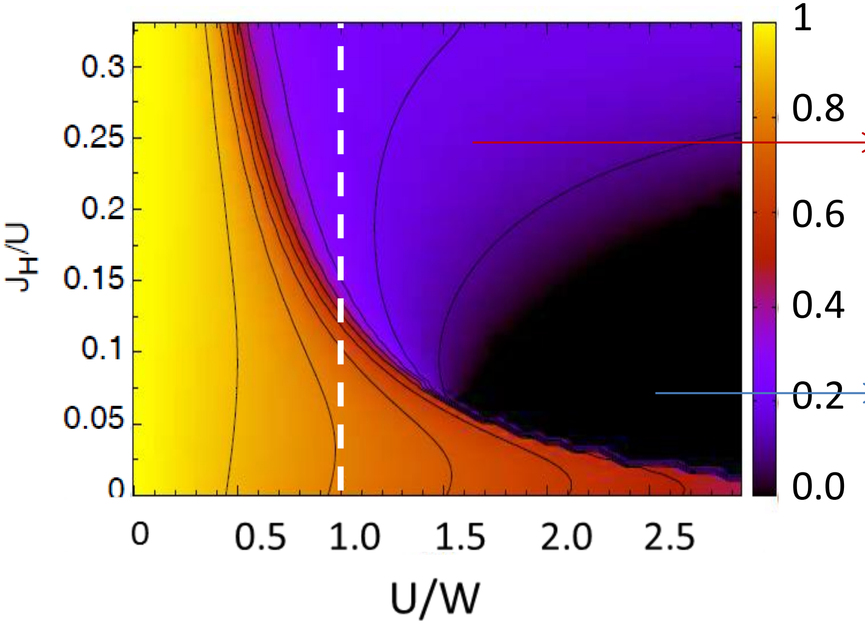
Slave spin. Only density-density terms included

Fanfarillo & EB, arXiv:1501.04607

Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

Colour plots: **Quasiparticle weight Z**

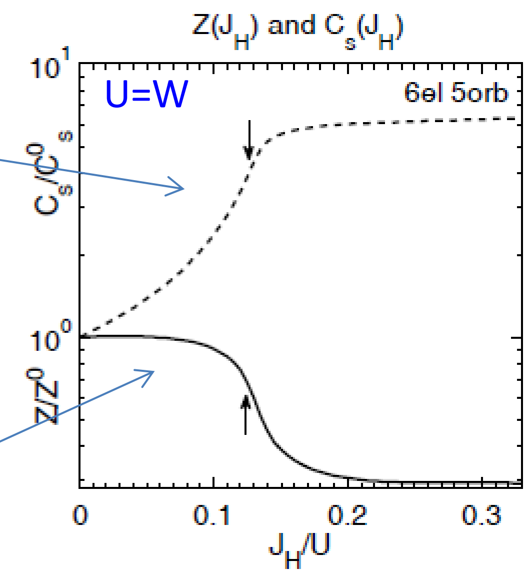


Hund metal

Suppression of Z associated to the atomic spin polarization

n=6 Mott insulator

Enhancement of Spin fluctuations



Loss of kinetic energy to satisfy Hund's rule

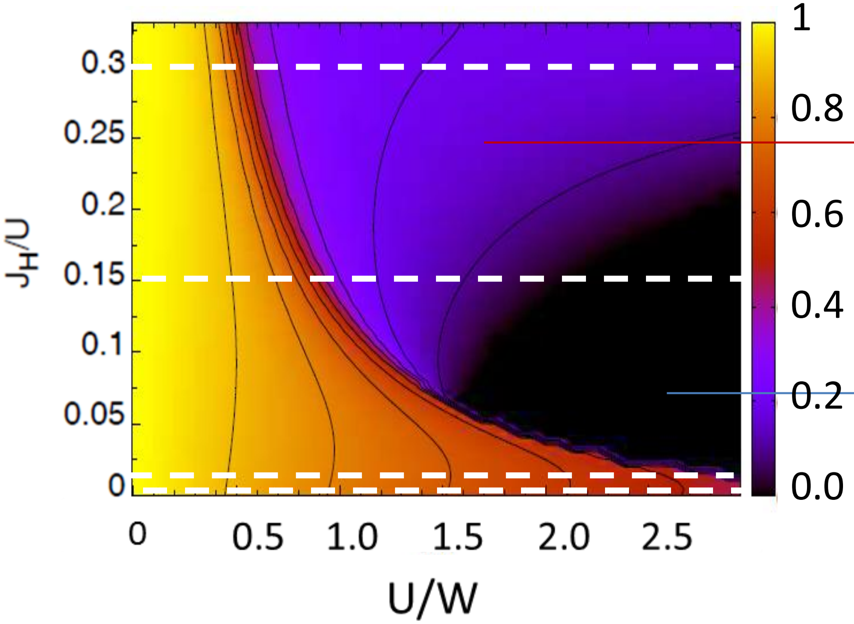
Slave spin. Only density-density terms included

Fanfarillo & EB, arXiv:1501.04607

Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

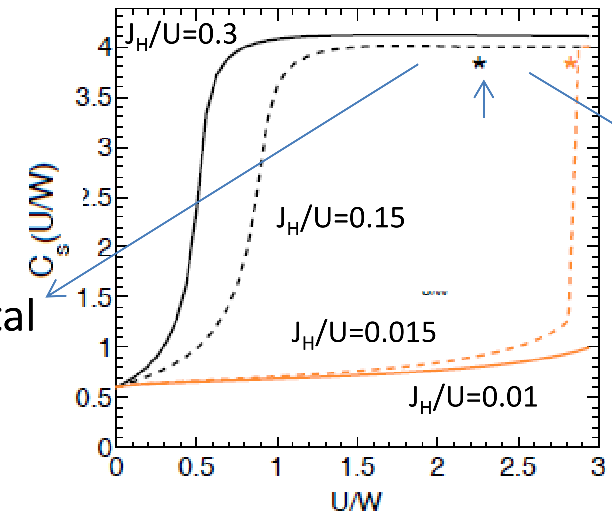
Colour plots: **Quasiparticle weight Z**



Hund metal

n=6 Mott insulator

Suppression of Z associated to the atomic spin polarization



S=2

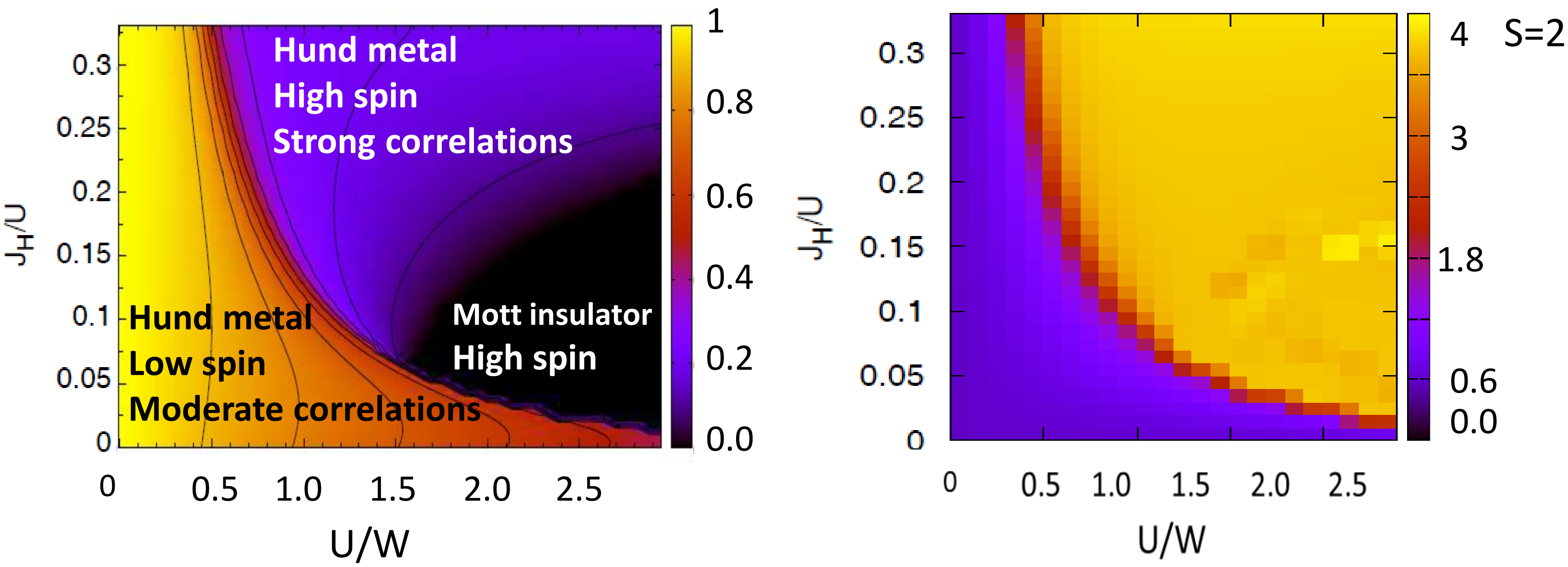
Hund metal

Mott insulator

Slave spin. Only density-density terms included

Fanfarillo & EB, arXiv:1501.04607

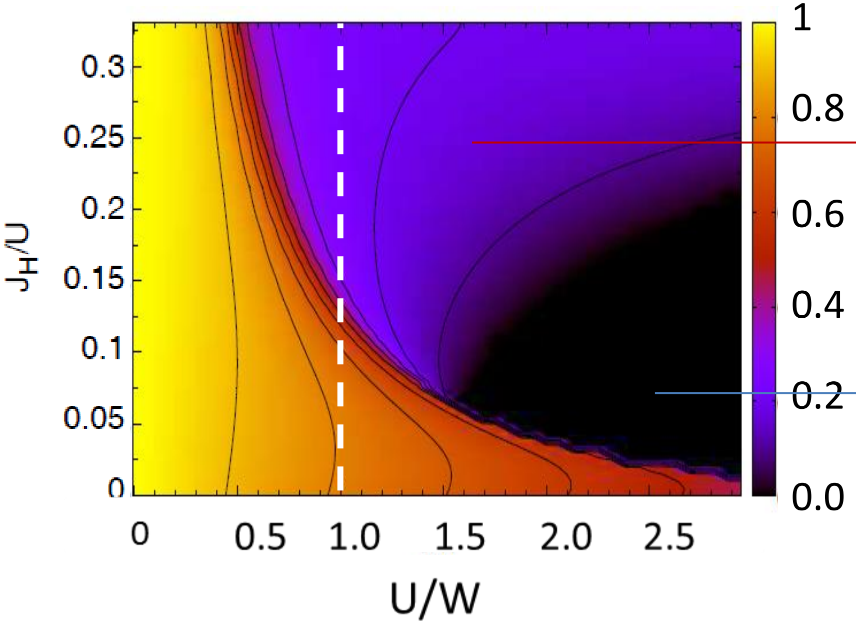
Hund metals: Screening of magnetic moments



Electronic correlations in multi-orbital systems: Hund metals

6 electrons in 5 orbitals

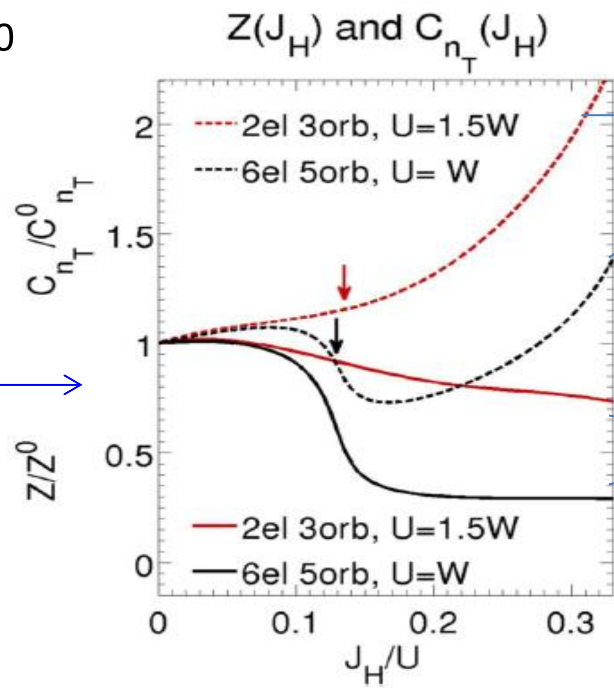
Colour plots: **Quasiparticle weight Z**



Hund metal

n=6 Mott insulator

Fanfarillo & EB, arXiv:1501.04607



Charge fluctuations

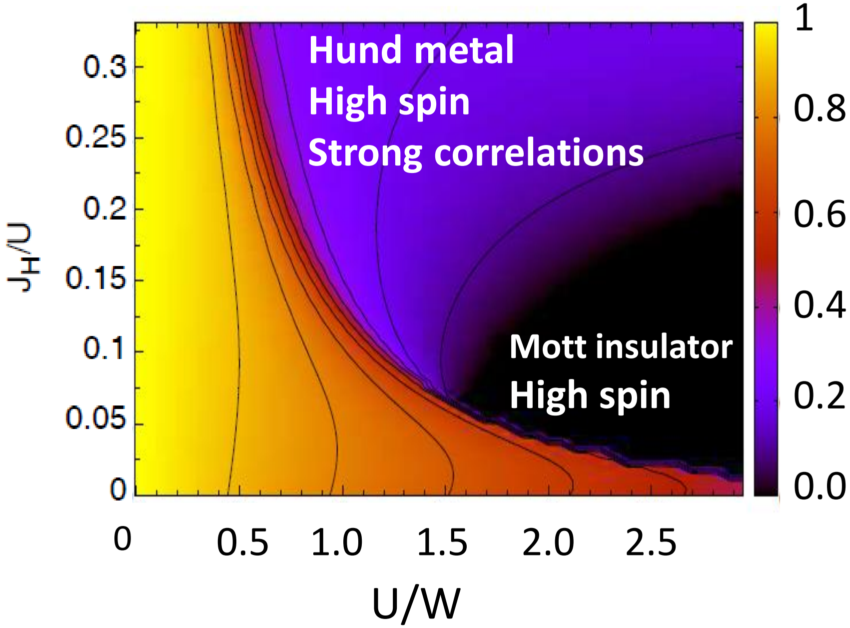
Quasiparticle weight

Different behavior of charge and quasiparticle weight

Slave spin.

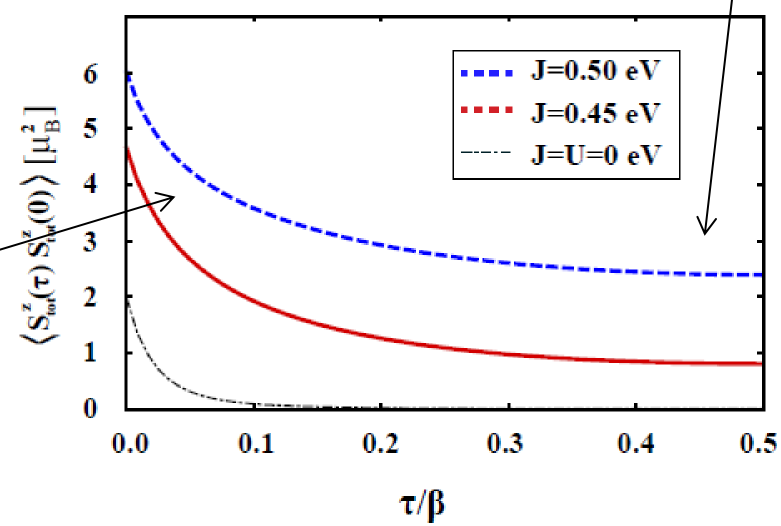
Only density-density terms included

Hund metals: Screening of magnetic moments



Experimental technique
which probes long time scales
(neutron diffraction t~ 10.15 fs)

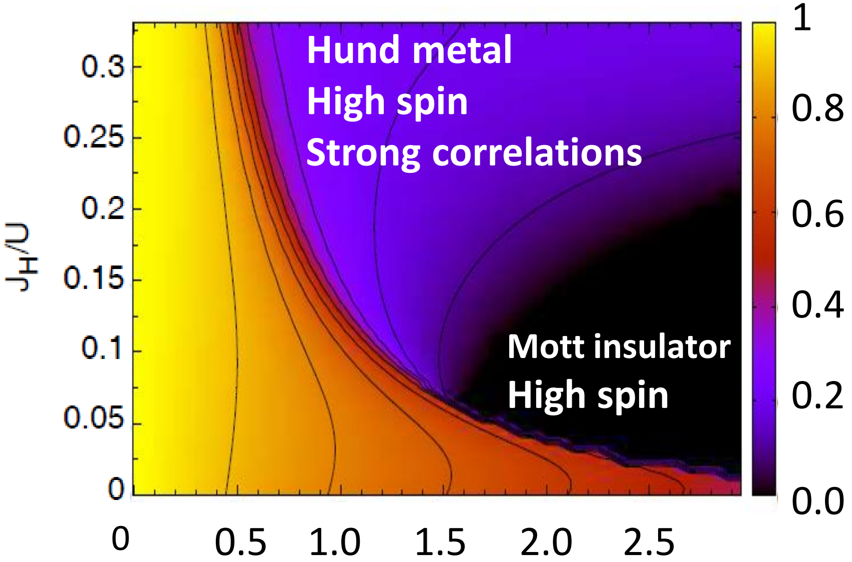
Experimental technique
which probes long time scales
(X-ray PES t~0.1-1 fs)



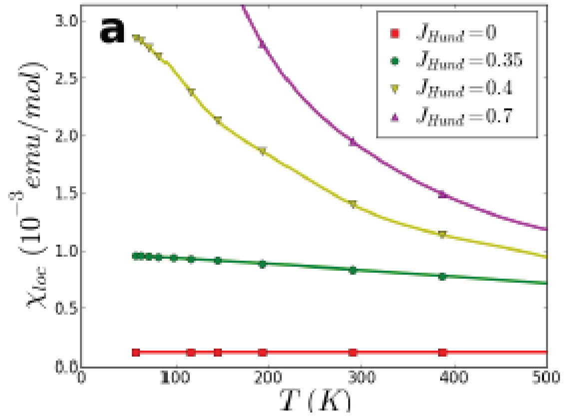
Hansmann et al, PRL 104, 197002 (2010)

Hund metals: Finite temperature behaviour

Quasiparticle weight Z



Spin susceptibility. Spin freezing



Haule & Kotliar, NJP 11, 025021 (2009)

Metal. Small Quasiparticle Weight

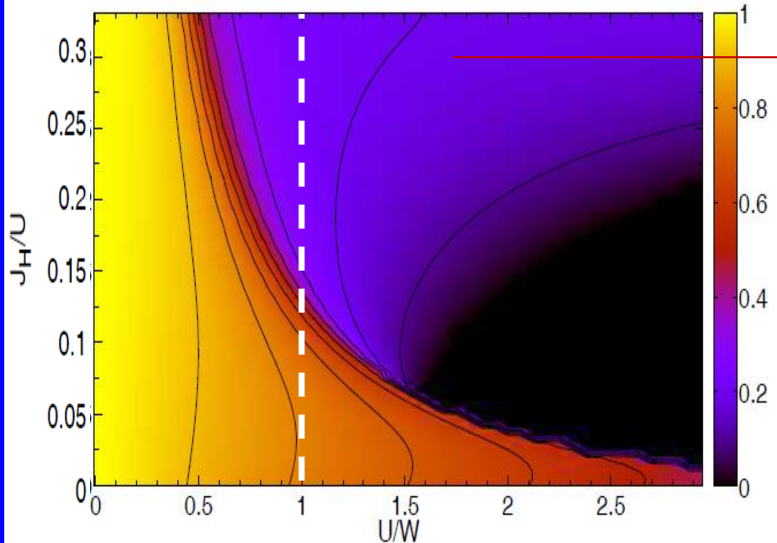
Fermi liquid only at low temperatures (T*)
Incoherent behavior above T*

Spectral weight
in ARPES (Quasiparticle
lost above T*)

Bad metallic behavior
at above T*

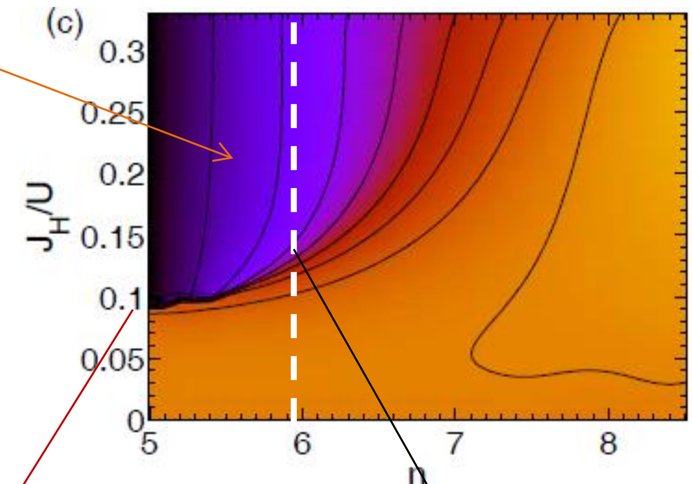
Hund metals: Doping dependence

6 electrons in 5 orbitals



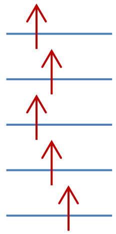
Colour plots: **Quasiparticle weight Z**

Hund metal



Half-filling
Mott insulator

Electron-hole asymmetry
around n=6



Strong correlations
linked to avoiding
double occupancy

Fanfarillo & EB, arXiv:1501.04607

E. Bascones leni@icmm.csic.es

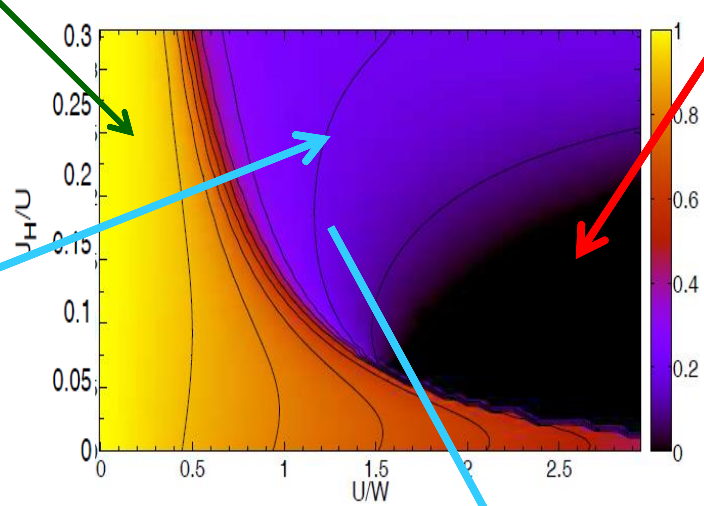
Correlations in multi-orbital systems

Weak correlations

(properties, origin of magnetism and of superconductivity described in terms of **itinerant electrons. Fermi surface physics**)

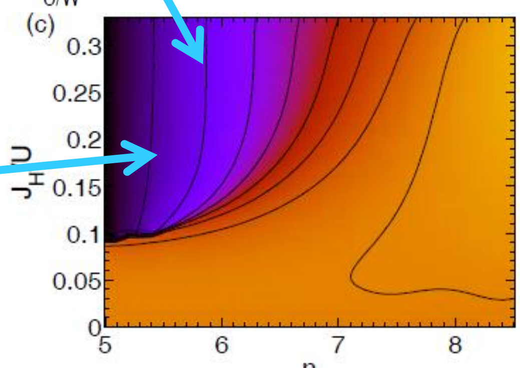
Localized electrons

(properties, origin of magnetism and of superconductivity described in terms of **localized electrons. Spin models**)



Hund metal

(Correlations due to Hund's coupling)



6 electrons in 5 orbitals

Average doping n=1.2

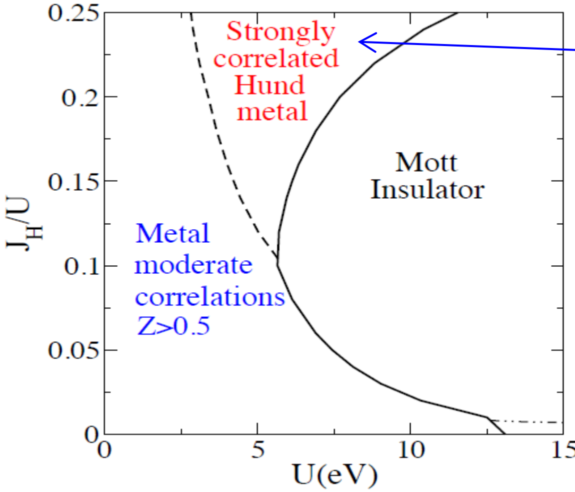
Like doped Mott insulators (note differences with single orbital doped Mott insulator)

Increase of correlations towards half-filling

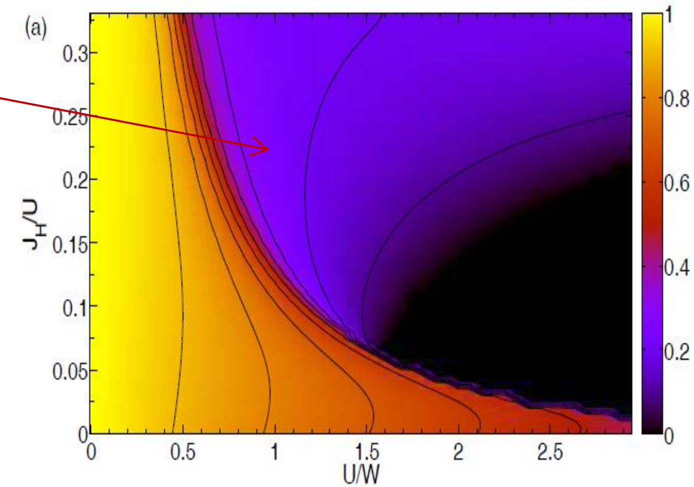
Correlations in iron superconductors

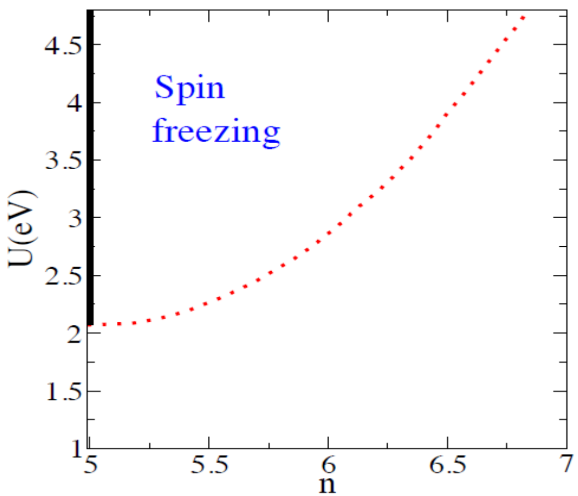
5 band model for iron superconductors

6 electrons (undoped)

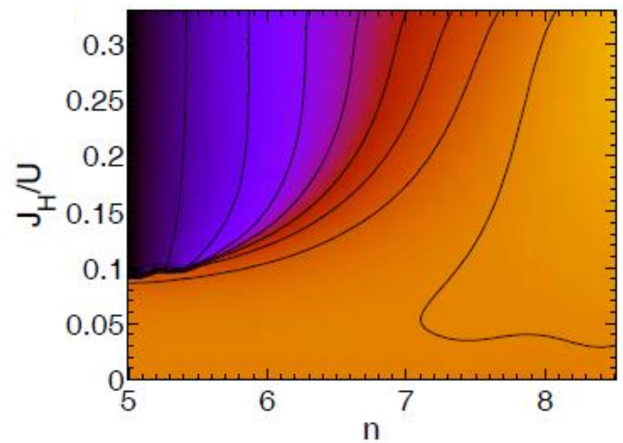


5 band model (Equivalent orbitals)
6 electrons





Correlations enhanced
Towards half-filling
(hole-doping)



Yu & Si, PRB 86, 085104 (2012), Ishida & Liebsch PRB 81, 054513 (2010)   Review: EB et al, arXiv:1503.04223

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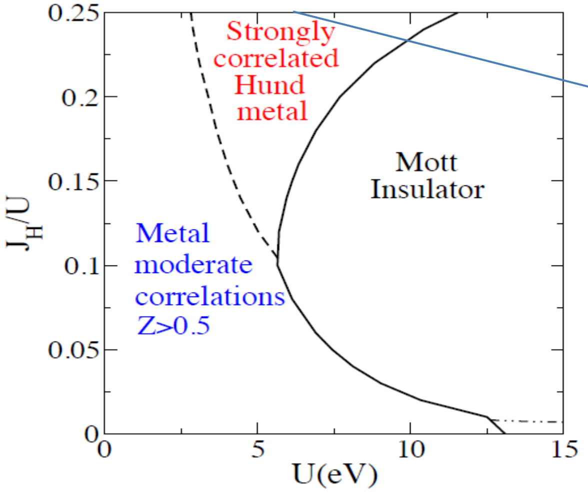

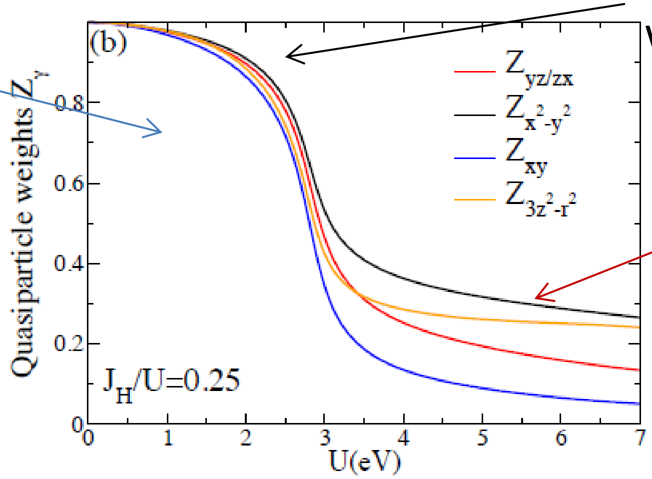

Drop of quasiparticle weight (crossover)

Orbital differentiation (some orbitals more correlated than other)

At finite temperatures the most strongly correlated orbitals can be incoherent while the other ones remain metallic

Figs: Si & Yu, PRB 86, 085104 (2012), Review: EB et al, arXiv:1503.04223

Correlations in iron superconductors

5 band model for iron superconductors

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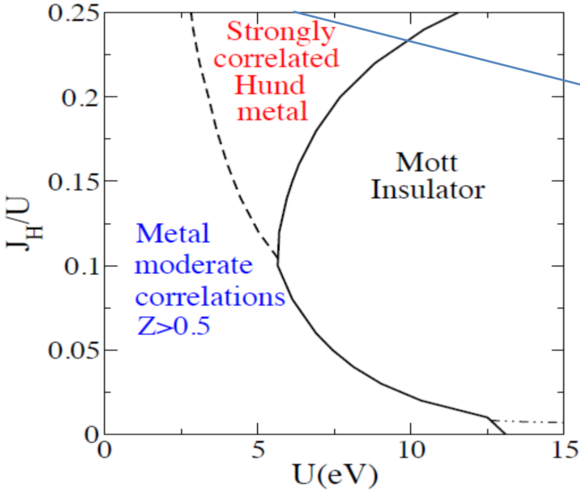

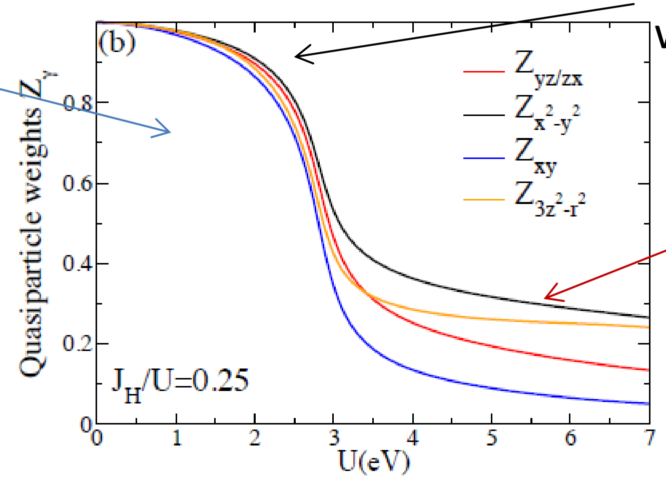

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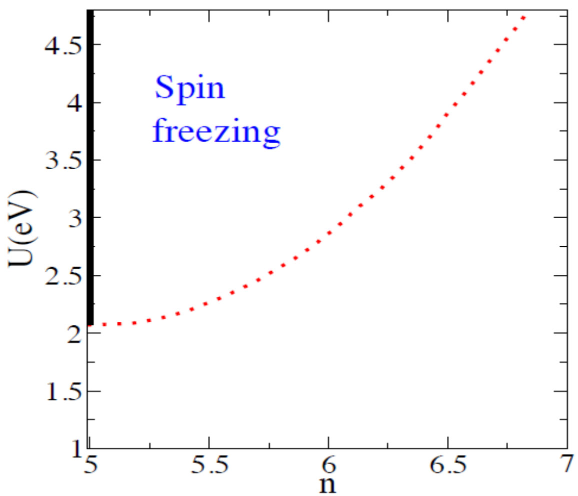
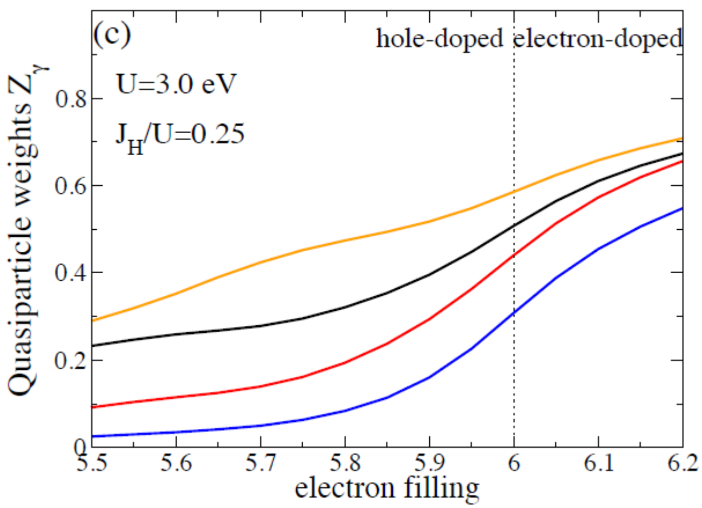


Correlations enhanced Towards half-filling (hole-doping)



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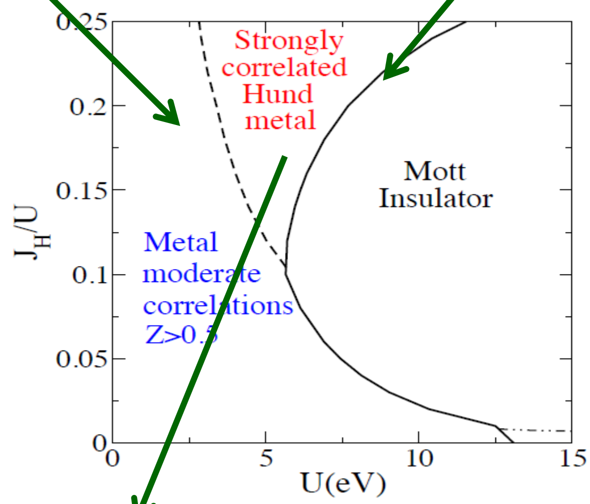


Hund metal

(Correlations due to Hund's coupling)

6 electrons in 5 orbitals

Average doping n=1.2

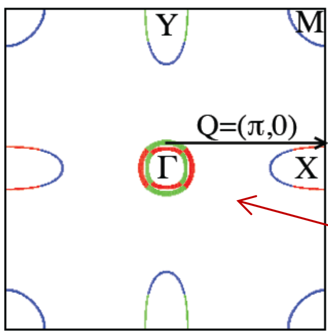
Correlations increase towards Half-filling (hole-doping)

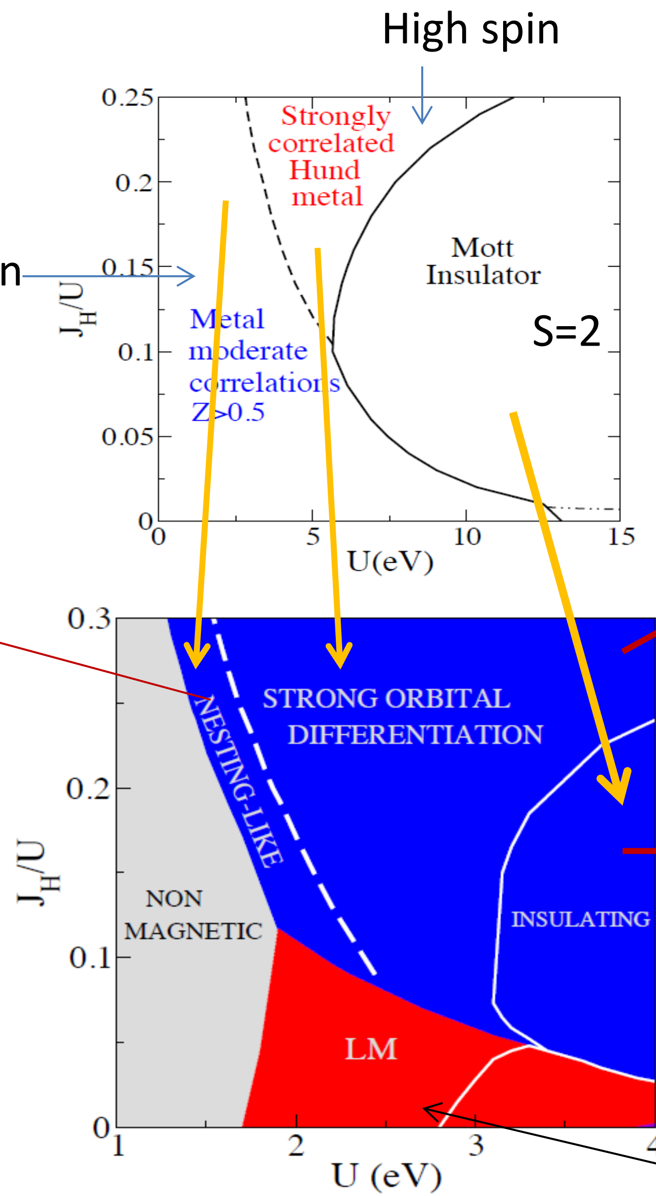
Orbital differentiation

(some orbitals more correlated than others)

Localized+itinerant

The (π,0) magnetic state of iron superconductors





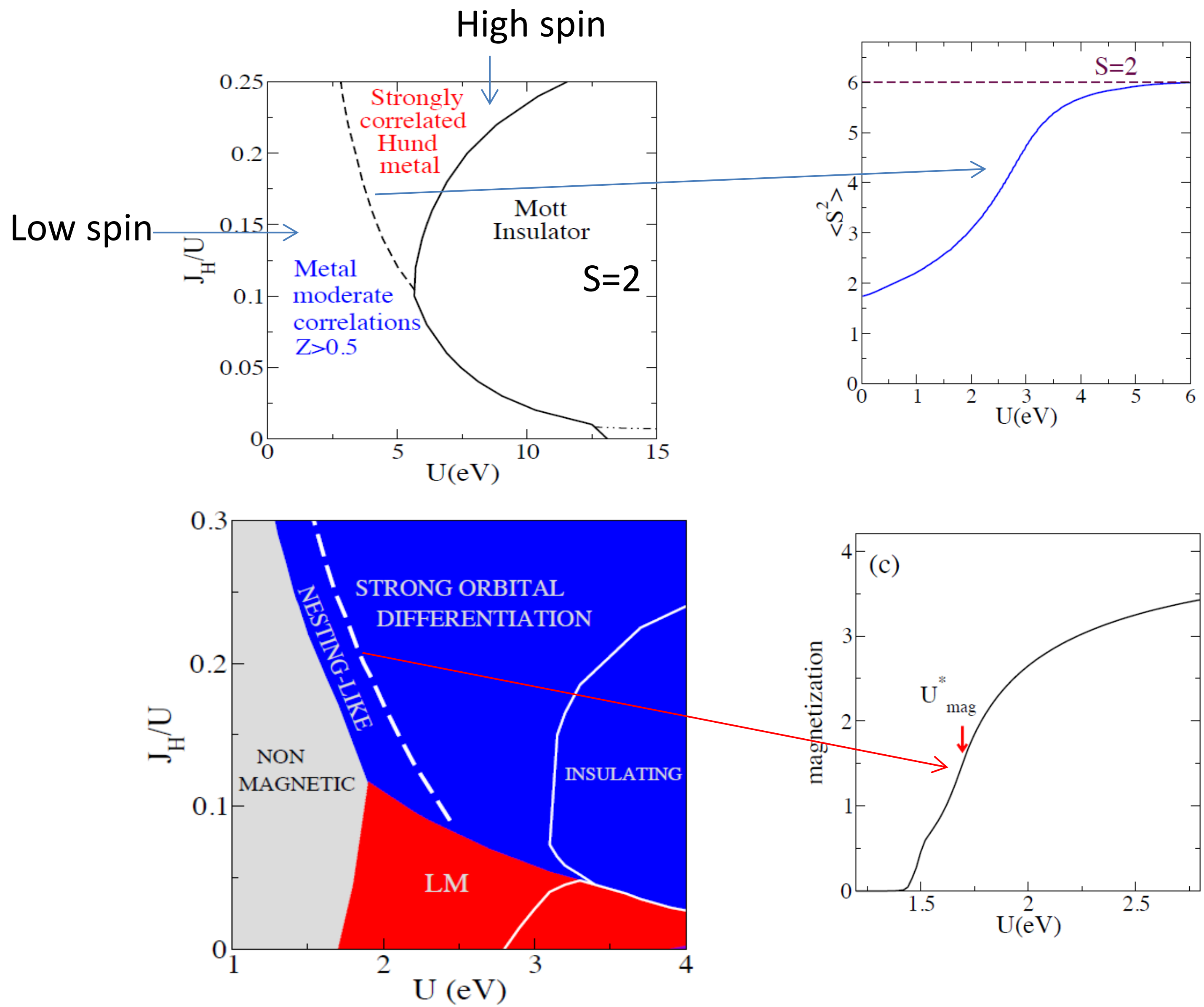
Double exchange-like magnetism with localized (xy and yz) and itinerant (zx, $3z^2$-r^2, x^2-y^2) orbitals

Behavior like J_1-J_2 Heisenberg model (magnetization, orbital filling, competition between different magnetic states)

Violates Hund's rule (low spin)

EB et al, PRB 86, 174508 (2012)

The (π,0) magnetic state of iron superconductors



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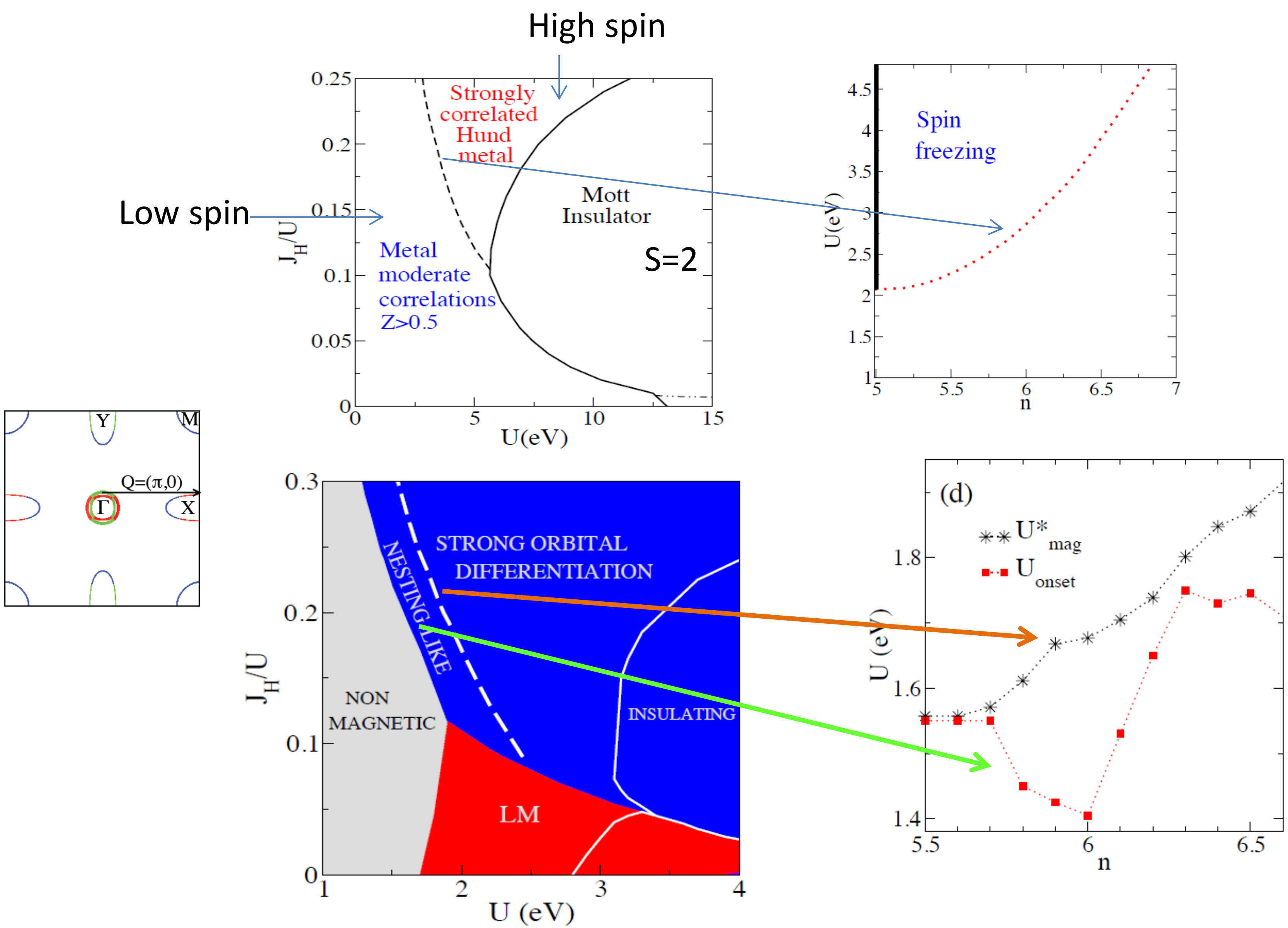


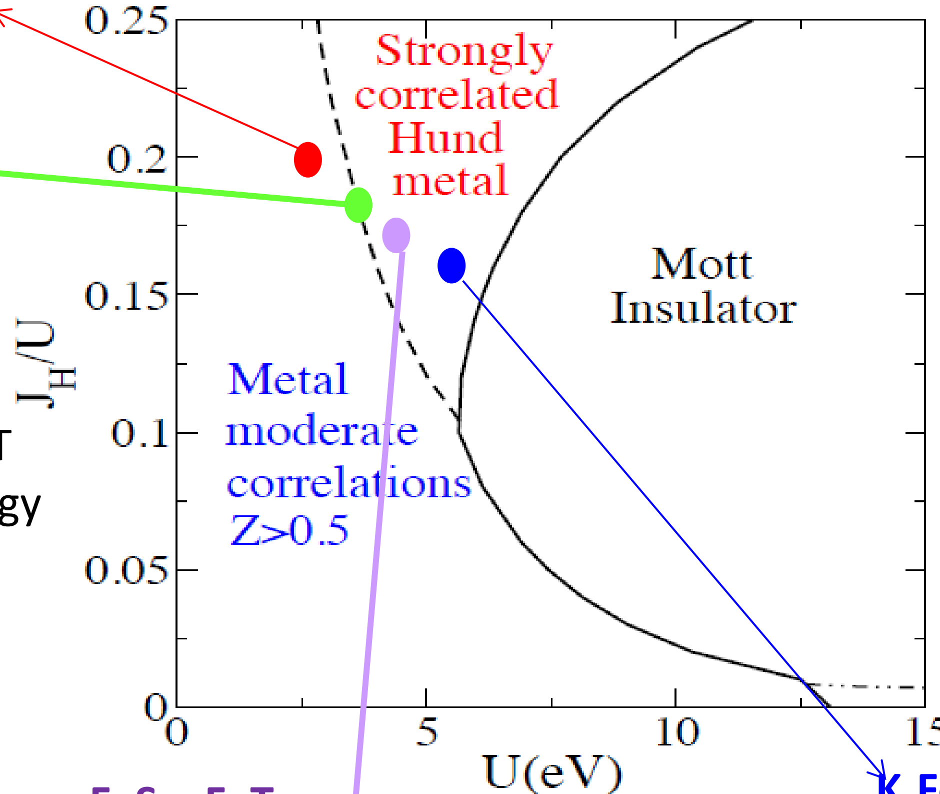
EB et al, PRB 86, 174508 (2012)

Iron superconductors in the (U,J_H) phase diagram

FeP compounds $m^*/m \sim 1.4-2$

FeAs compounds

- $m^*/m \sim 2-3$ (122, 1111)
  up to 5-6 (111)
- $\mu_{ordered} \sim 0.07-1\ \mu_B$
  $\mu_{X\text{-}ray} \sim 1.3-2\ \mu_B$
- Neutrons: Moments at high T & spin waves up to high energy
- Electron-hole asymmetry in correlations (K-Rb-Cs-122 Hund metals)
- χ increases with T
- Sign of resistivity anisotropy not expected from double exchange
- Compatible with ab-initio



FeSe, FeTe

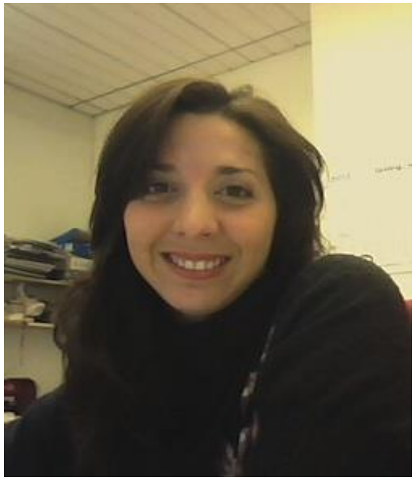
- Double stripe ordering in FeTe not compatible with nesting
- $m^*/m \sim 3.5-7$
- Orbital selective incoherence at finite T
- χ decay with T above T* (180 K-FeSe, 70 K-FeTe)

$K_xFe_{y-x}Se_2$

- $\mu \sim 3\ \mu_B$
- Orbital selective incoherence at finite T

Review: EB et al, arXiv:1503.04223

My collaborators



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María José Calderón
ICMM-CSIC

Belén Valenzuela
ICMM-CSIC

EB et al, PRB 86, 174508 (2012)

Fanfarillo & EB, arXiv:1501.04607

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