Iron superconductors: Correlations, magnetism and optical conductivity

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Outline

- Introduction to correlations in iron superconductors
- Orbital differentiation in the magnetic state of iron superconductors
- Optical conductivity and correlations. Interband transitions and doping dependence.

How correlated are the iron superconductors?

Iron superconductors

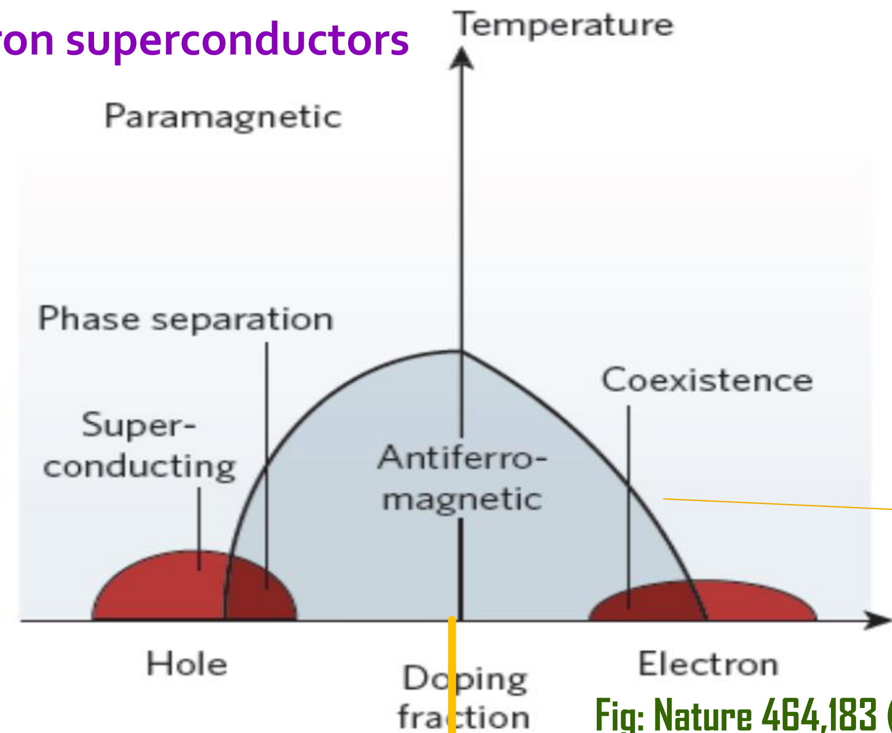
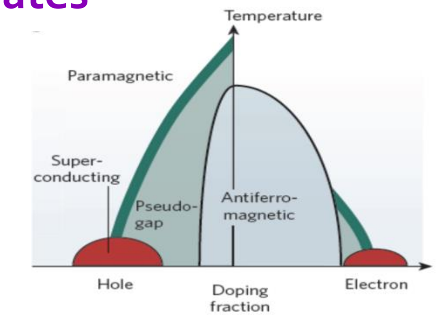


Fig: Nature 464,183 (2010)

Cuprates



As in cuprates, in iron superconductors superconductivity emerges when antiferromagnetism is suppressed

Contrary to what happens in cuprates the antiferromagnetic phase of undoped iron pnictides is metallic

Does this mean that iron superconductors are not correlated?

How correlated are the iron superconductors?

Weak correlations

Fermi liquid & quasiparticle bands
(quasiparticle weight Z~1,
small mass enhancement)

Localized electrons

Mott physics & localized spins
(quasiparticle weight Z~0,
large mass enhancement)

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)

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

How correlated are the iron superconductors?

Weak correlations — Localized electrons

Weak correlations
Fermi liquid & quasiparticle bands
(quasiparticle weight Z~1,
small mass enhancement)

Localized electrons
Mott physics & localized spins
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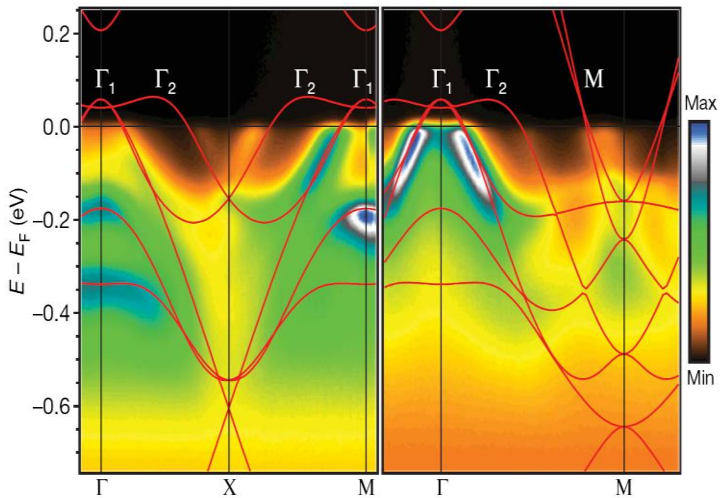
large mass enhancement)

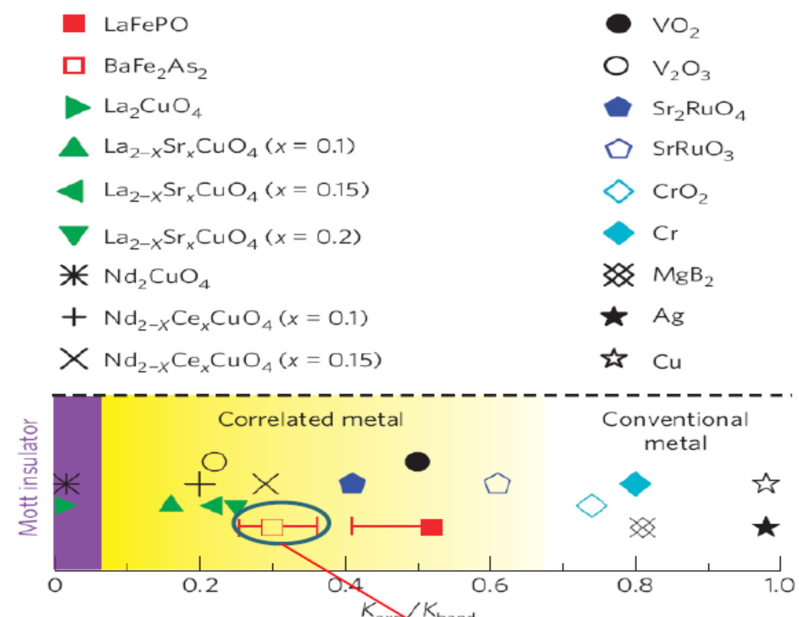
ARPES



Quasiparticle bands are observed
But mass enhancement ~3 (FeAs)
~2 (FeP)

Fig:Lu et al, Nature 455, 81 (2008)

Optical conductivity

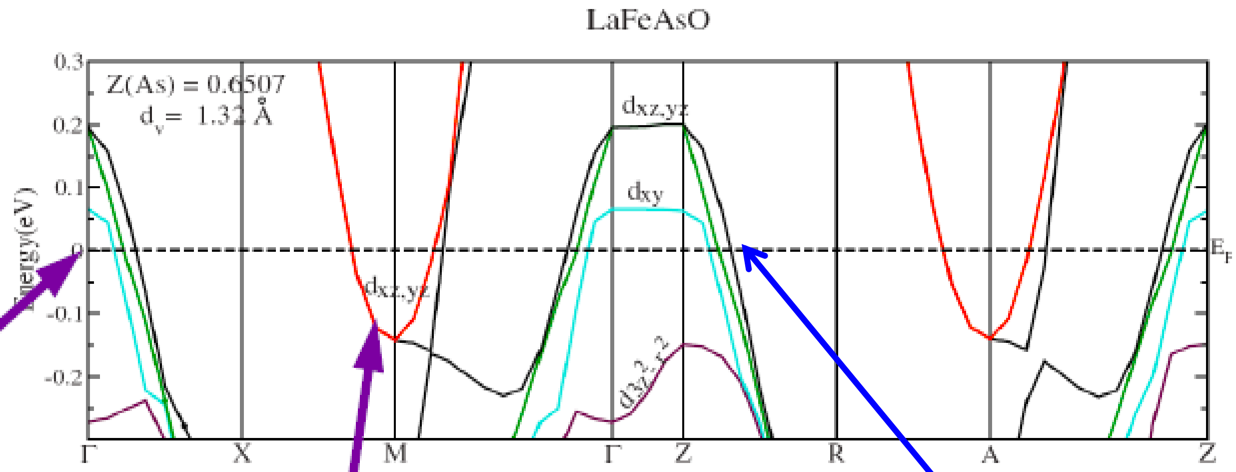


Chalcogenides (Se/Te)
seem more correlated
than pnictides (As)

We are here Z~0.3

Qazilbash et al, Nat. Phys. 5, 647 (2009)

Iron superconductors are multi-orbital systems



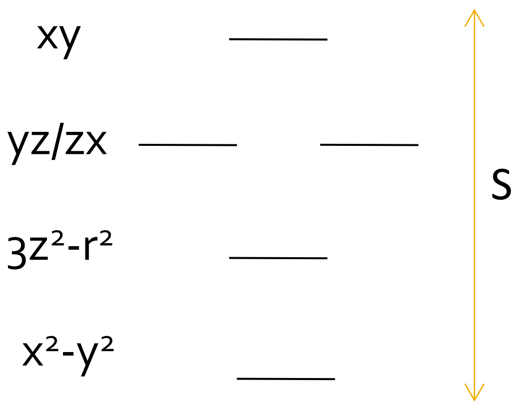
Hole pockets

Electron pockets

Vildosola et al, PRB 78, 064518 (2008)

Several Fe bands cross the Fermi level

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



Small crystal field

Undoped compounds

Compensated FeAs layer

6 electrons in 5 Fe orbitals

In contrast to cuprates

1 electron in 1 orbital

How correlated are the iron superconductors?

Weak correlations

Fermi liquid & quasiparticle bands
(quasiparticle weight Z~1,
small mass enhancement)

Localized electrons

Mott physics & localized spins
(quasiparticle weight Z~0,
large mass enhancement)

Effect of Hund's coupling in determining the correlations
Hund metal

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)

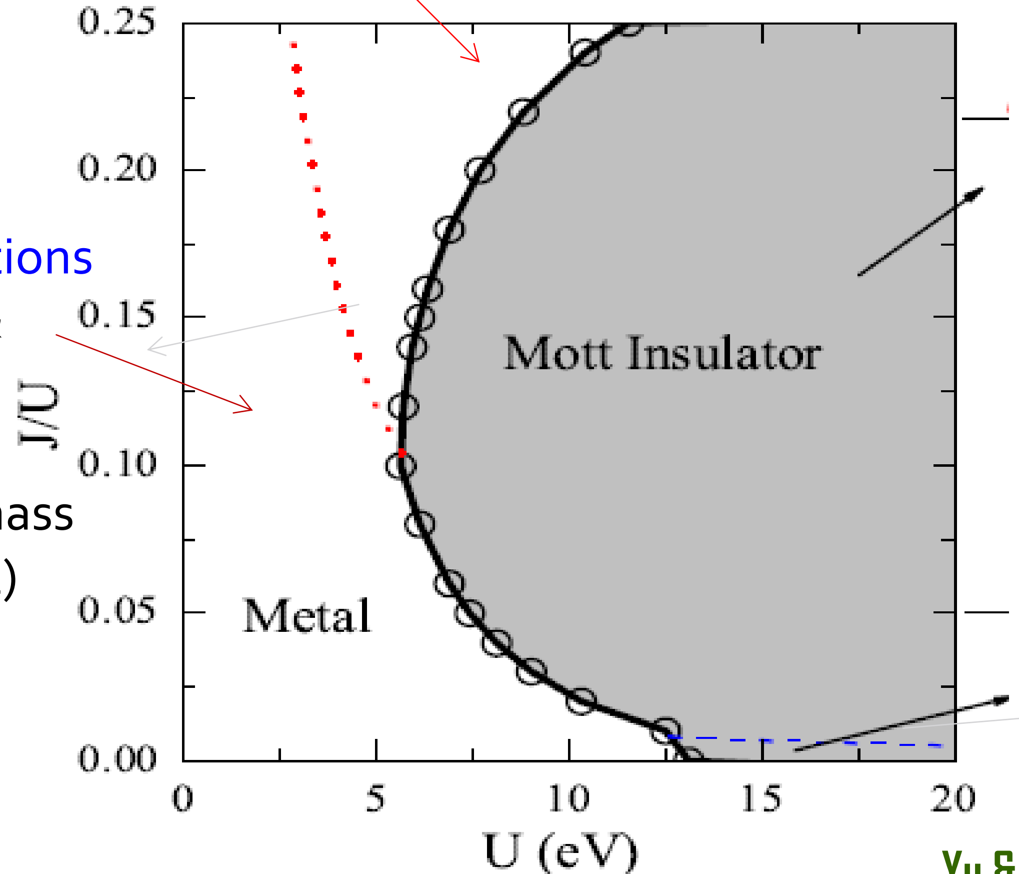
Different correlations in inequivalent orbitals even leading to an effective description with coexisting **localized and itinerant** electrons (**OSMT**)

Yin et al, Nature Materials 10, 932 (2011)
Misawa et al, PRL 108, 177007 (2012)
Yi et al, PRL 110 067003, (2013)
de Medici et al, PRL 112,177001 (2014)

How correlated are the iron superconductors?

Strongly correlated metal at intermediate and large Hund's coupling J/U

Weak correlations
Fermi liquid &
quasiparticle
bands
(Z~1, small mass
enhancement)



Localized electrons
Mott physics &
localized spins Z~0,

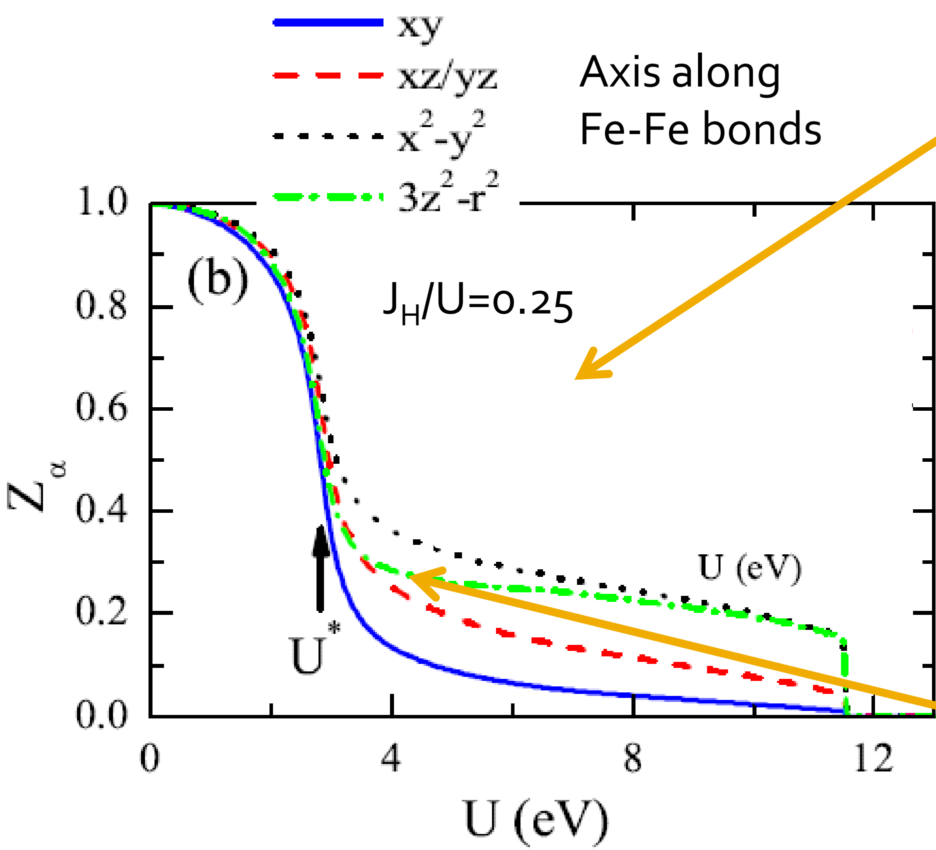
Yu & Si, PRB 86, 085104 (2012)

U(1) Slave Spin calculation for a tight-binding model for iron pnictides

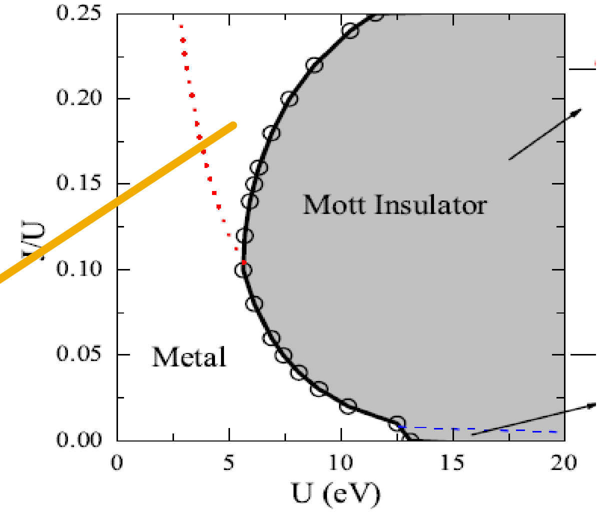
How correlated are the iron superconductors?

Orbital differentiation:

Strength of correlations is different in different orbitals



Axis along Fe-Fe bonds



xy
yz/zx
$x^2-y^2/3z^2-r^2$

Increasing correlations

The values of the quasiparticle weight resemble the experimental ones close to the crossover

U(1) Slave Spin calculation for a tight-binding model for iron pnictides **Yu & Si, PRB 86, 085104 (2012)**

Which is the nature of magnetism?

Weak correlations

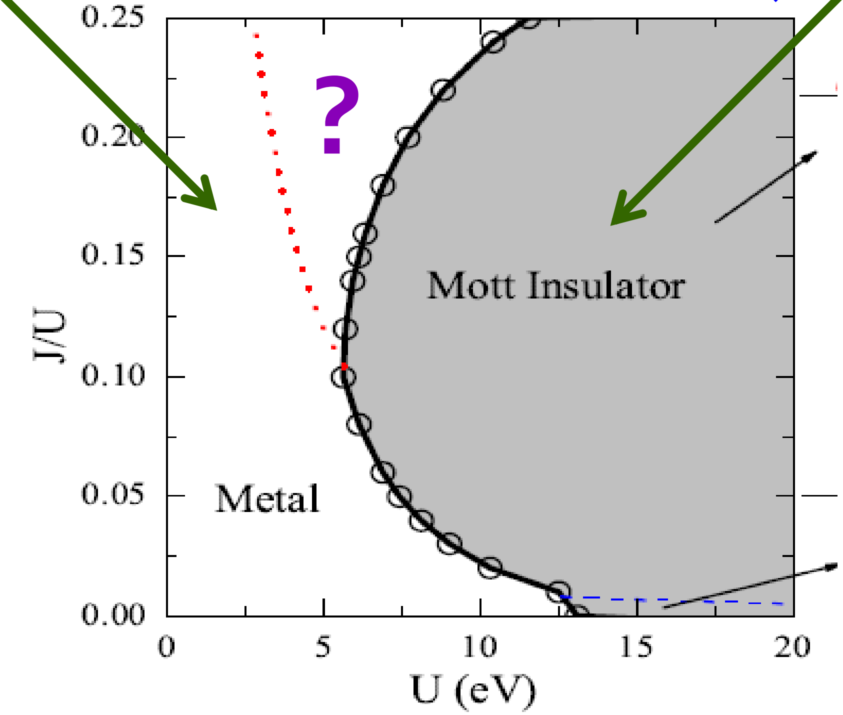
Fermi liquid & quasiparticle bands

Localized electrons

Mott physics & localized spins

Magnetism as a
Fermi surface instability
(nesting)

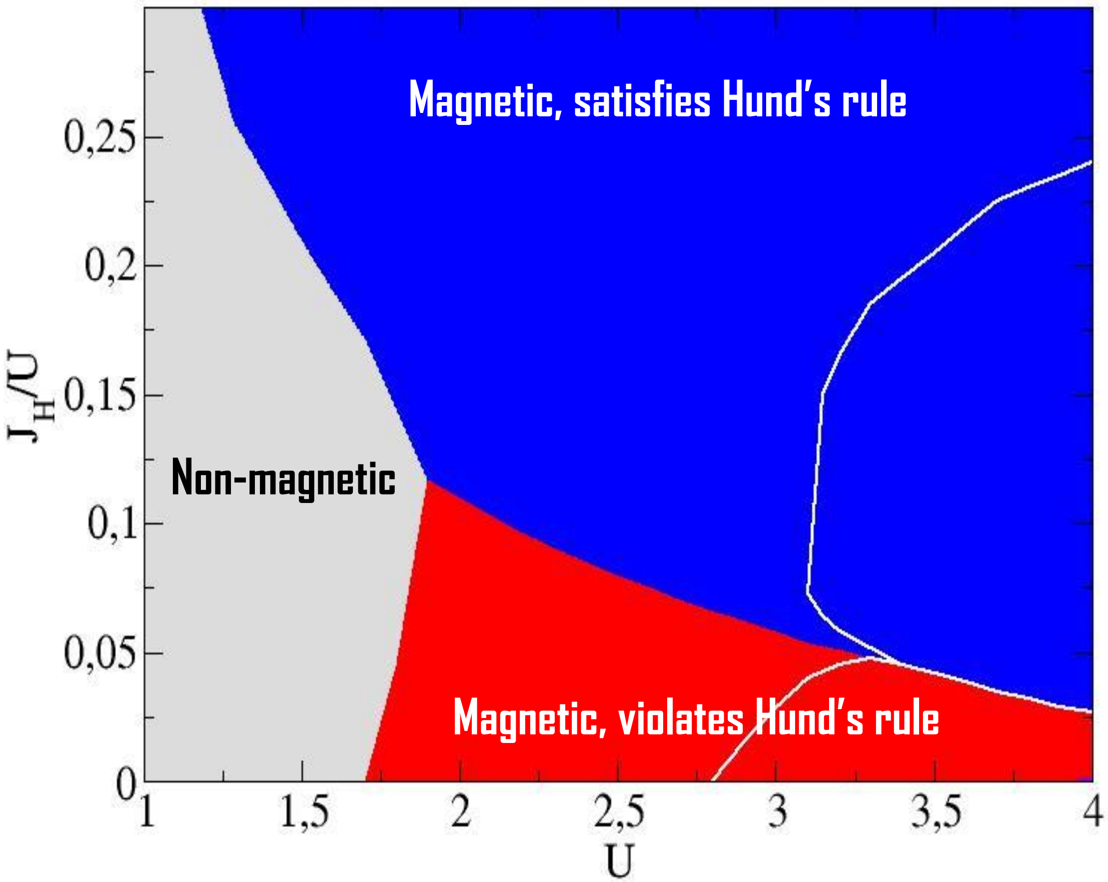
Magnetism due to AF
exchange
between localized spins
(J1-J2 Heisenberg model)



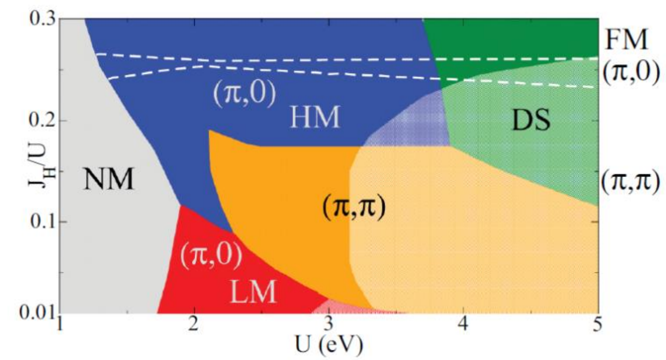
Which is the nature of columnar $(\pi,0)$ magnetism?

$(\pi,0)$ ordering is imposed

Hartree-Fock, 6 electrons in 5-orbital model



$(\pi,0)$ Ferromagnetic in b direction
Antiferromagnetic in a direction



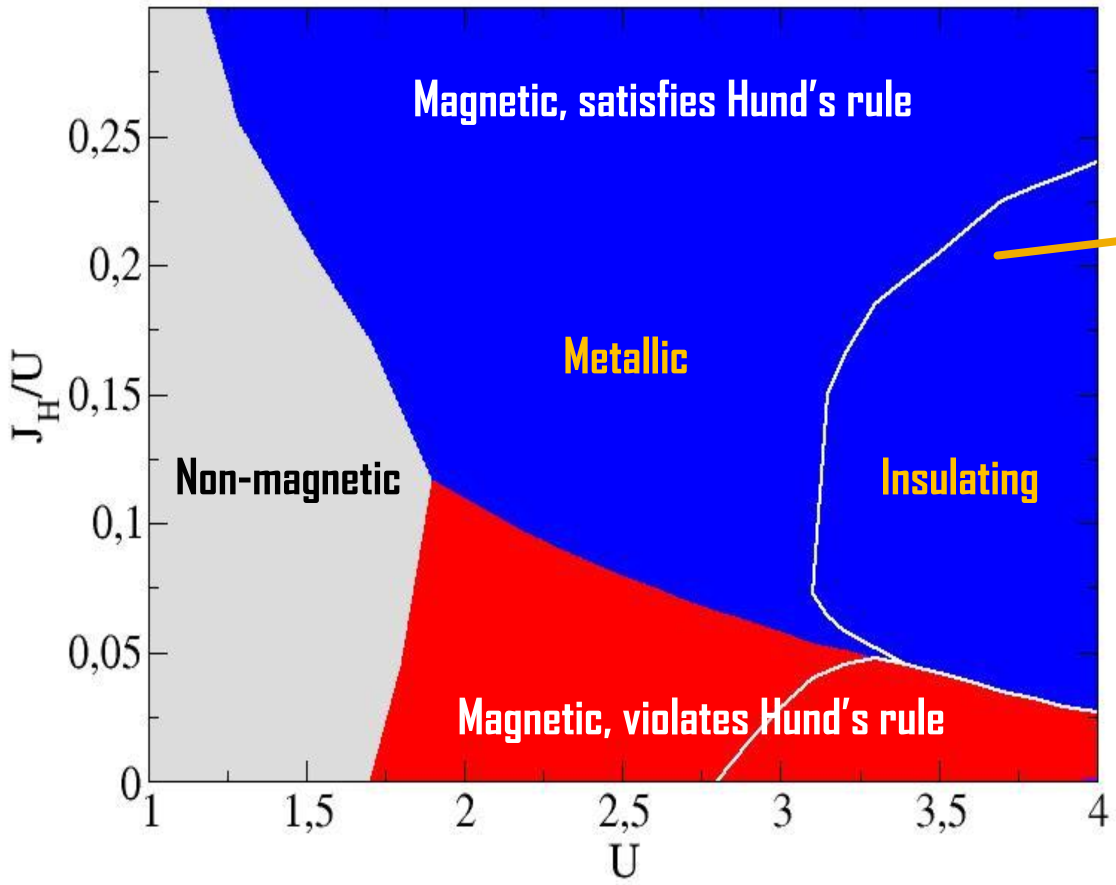
EB, M.J. Calderón, B. Valenzuela, PRL 104, 227201 (2010),
EB, B. Valenzuela M.J. Calderón, PRB 86, 174508 (2012)

M.J. Calderón, G. León, B. Valenzuela, EB, PRB 86, 104514 (2012)

Which is the nature of columnar $(\pi,0)$ magnetism?

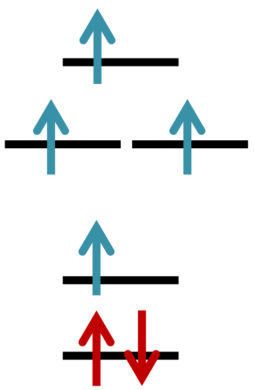
$(\pi,0)$ ordering is imposed

Hartree-Fock, 6 electrons in 5-orbital model



Gap opens at the Fermi level

Deep in the insulating region we find the behavior expected from J_1-J_2 model for localized spins

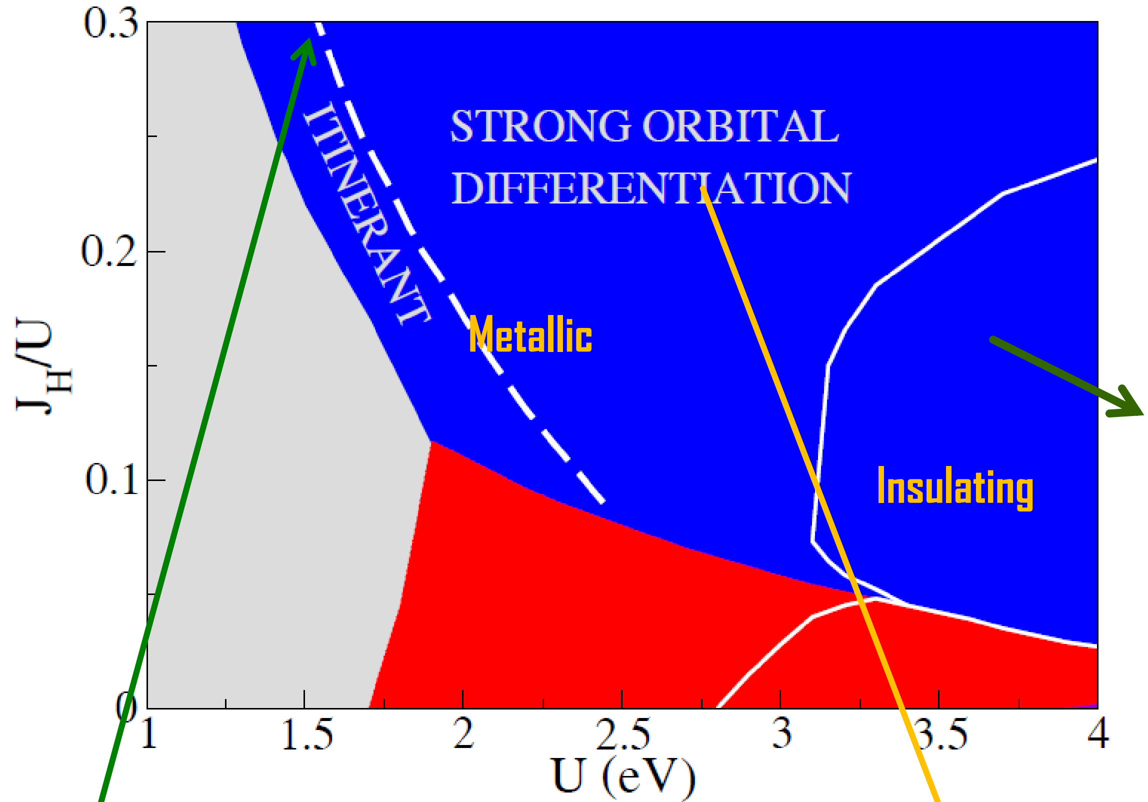


EB, M.J. Calderón, B. Valenzuela, PRL 104, 227201 (2010), EB, B. Valenzuela M.J. Calderón, PRB 86, 174508 (2012)

Which is the nature of columnar (π,0) magnetism?

(π,0) ordering is imposed

Hartree-Fock, 6 electrons in 5-orbital model



Behavior expected from J_1-J_2 model for localized spins

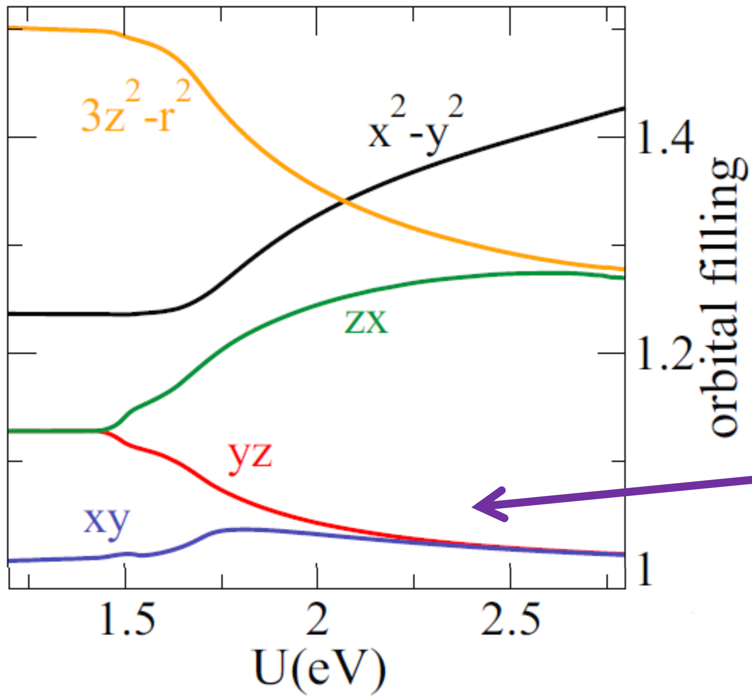
All orbitals itinerant

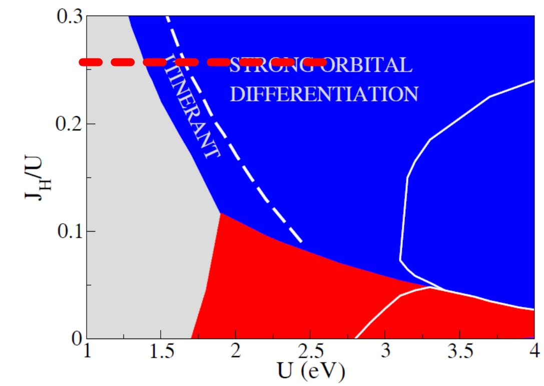
zx, 3z2-r2, x2-y2: itinerant

xy, yz: half-filled gapped orbitals

EB, B. Valenzuela M.J. Calderón, PRB 86, 174508 (2012)

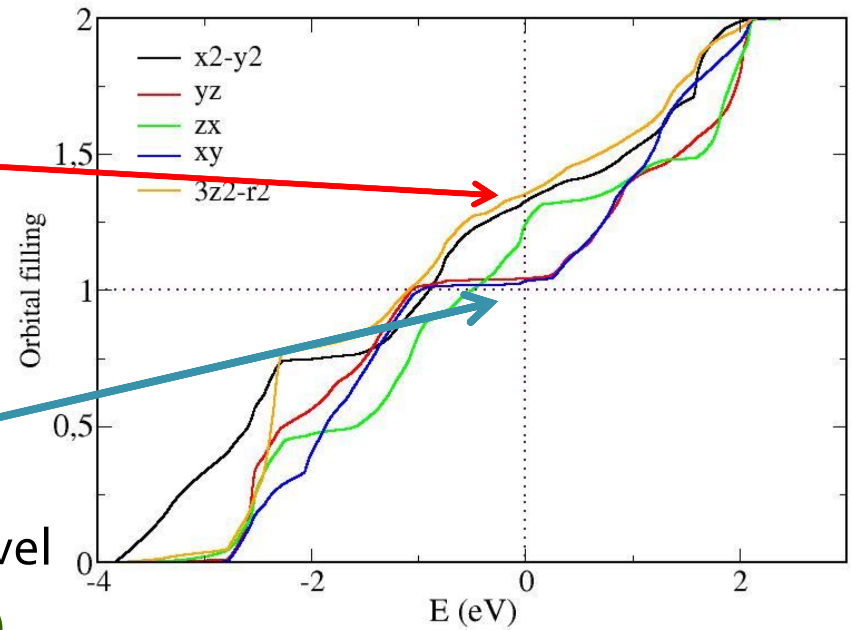
Which is the nature of columnar (π,0) magnetism?





6 electrons

xy & yz go to half-filling
with increasing interactions



zx, 3z²-r², x²-y²
itinerant

U=2.0 eV J/U=0.25

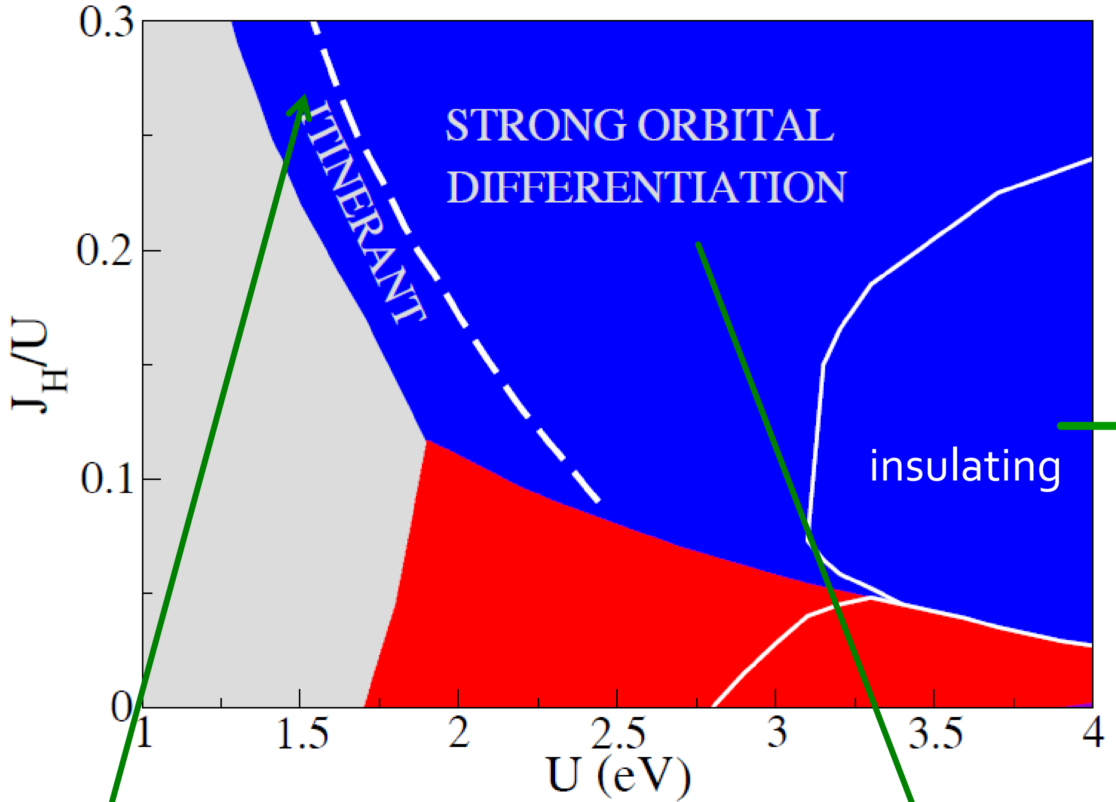
xy, yz
large gap
at the Fermi level

EB, B. Valenzuela M.J. Calderón, PRB 86, 174508 (2012)

Which is the nature of columnar (π,0) magnetism?

Suggested model

Hartree-Fock



All orbitals localized

All orbitals itinerant

xy, yz: localized orbitals
zx, 3z2-r2, x2-y2: itinerant

EB, B. Valenzuela M.J. Calderón, PRB 86, 174508 (2012)

Which is the nature of columnar (π,0) magnetism?

xy, yz: localized orbitals zx, 3z2-r2, x2-y2: itinerant

Decreasing localization

xy — More correlated in non-magnetic DMFT/slave spins/VMC.
Close to half-filling in non-interacting bands.

localized in our description

yz

Intermediate in non-magnetic DMFT/slave spins

zx

Different degree of localization
(AF state)
yz & zx along Fe-Fe bonds

$3z^2$-r^2

x^2-y^2

Less correlated in non-magnetic DMFT/slave spins.
Larger filling in non-interacting bands.

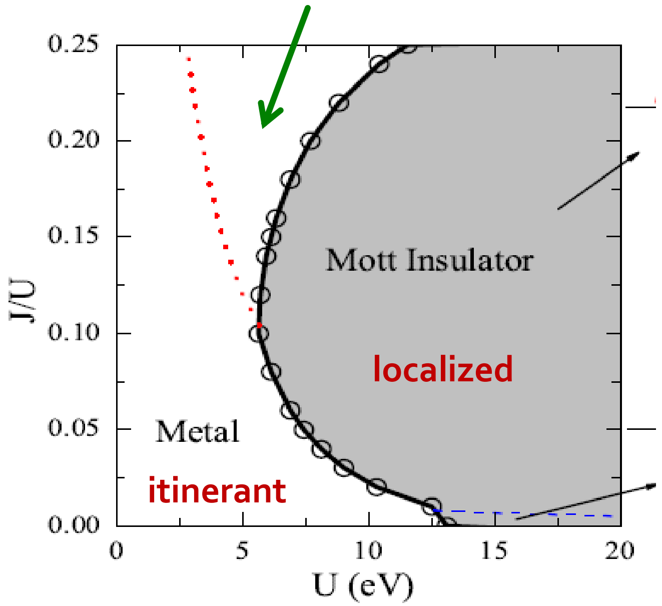
Itinerant in our description

EB, B. Valenzuela M.J. Calderón, PRB 86, 174508 (2012)

How correlated are the iron superconductors?

Non-Magnetic State

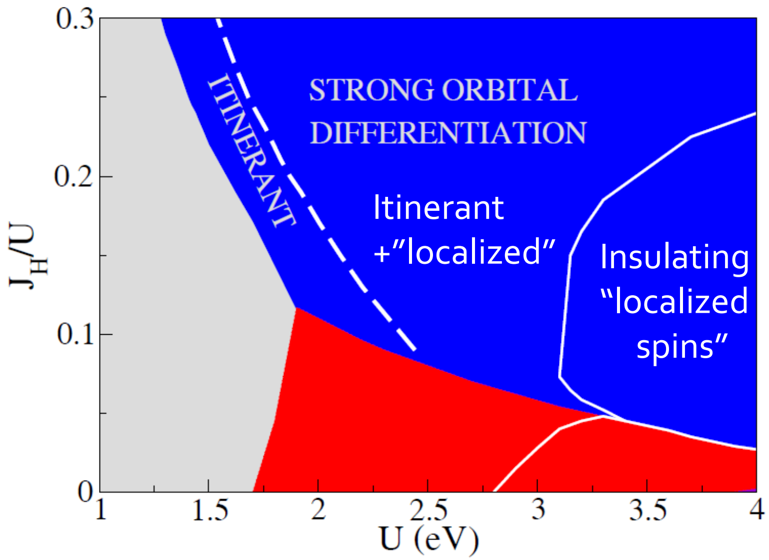
Strongly correlated metal
with orbital differentiation



Yu & Si, PRB 86, 085104 (2012)

U(1) Slave spin

Magnetic State

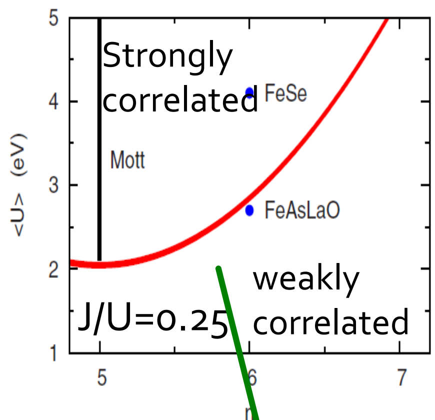


EB, M.J. Calderón, B. Valenzuela
PRB 86, 174508 (2012)

Hartree-Fock

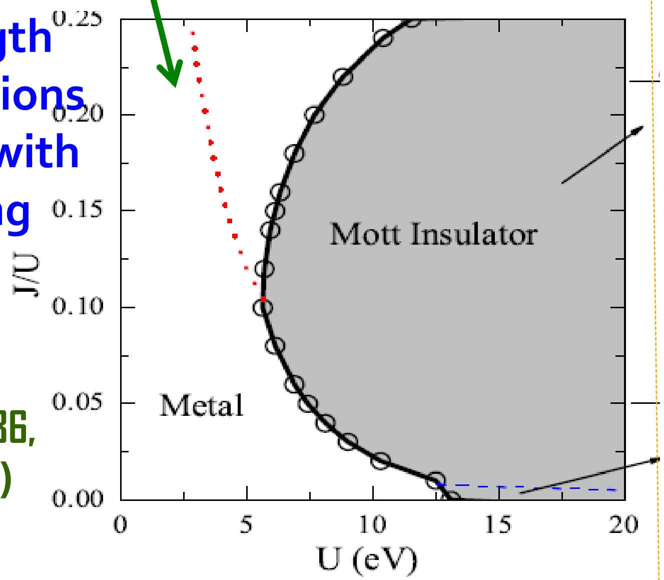
How correlated are the iron superconductors? Doping

Non-Magnetic State



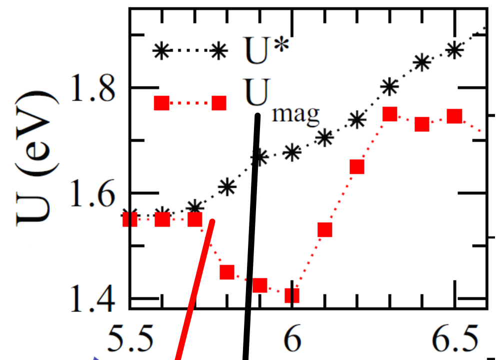
Liebsch & Ishida, PRB 82, 1551006 (2010)

The strength of correlations increases with hole doping



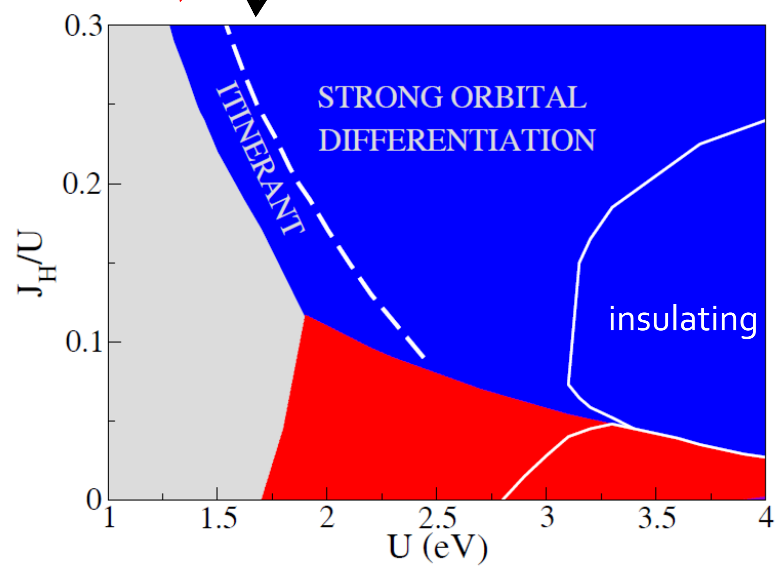
Yu & Si, PRB 86, 085104 (2012)

Magnetic State



EB, M.J. Calderón, B. Valenzuela PRB 86, 174508 (2012)

J/U=0.25



See also: Werner et al, Nature Physics 8, 331 (2012)
Misawa et al, PRL 108, 177007 (2012)

Which is the nature of columnar $(\pi,0)$ magnetism?

Model for AF: xy & yz localized and zx, x^2-y^2, $3z^2$-r^2 itinerant

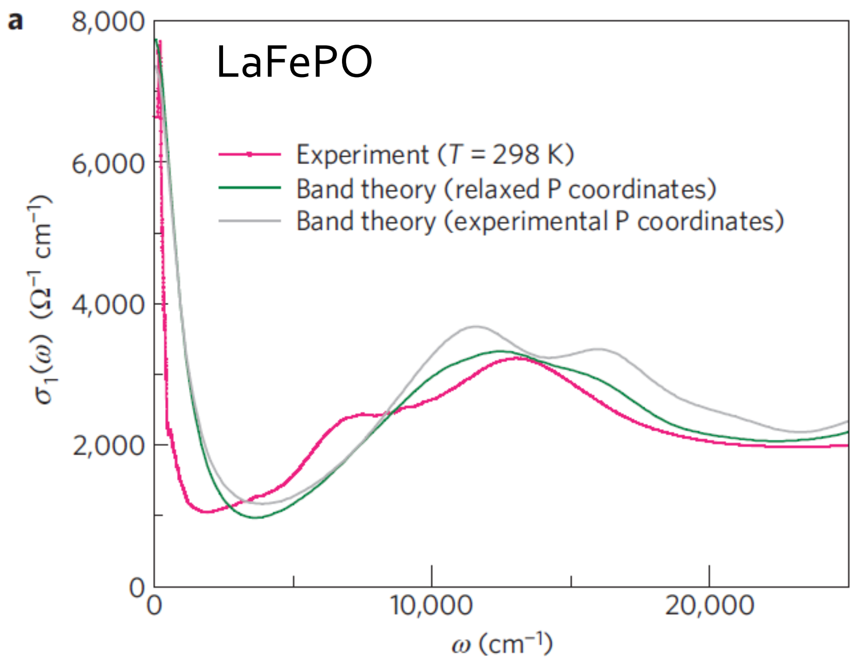
Depending on parameters (Fe-As angle) the localized xy & yz electrons want to be in AF $(\pi,0)$ or $(0,\pi)$ state, due to exchange interactions ($J \sim t^2$)

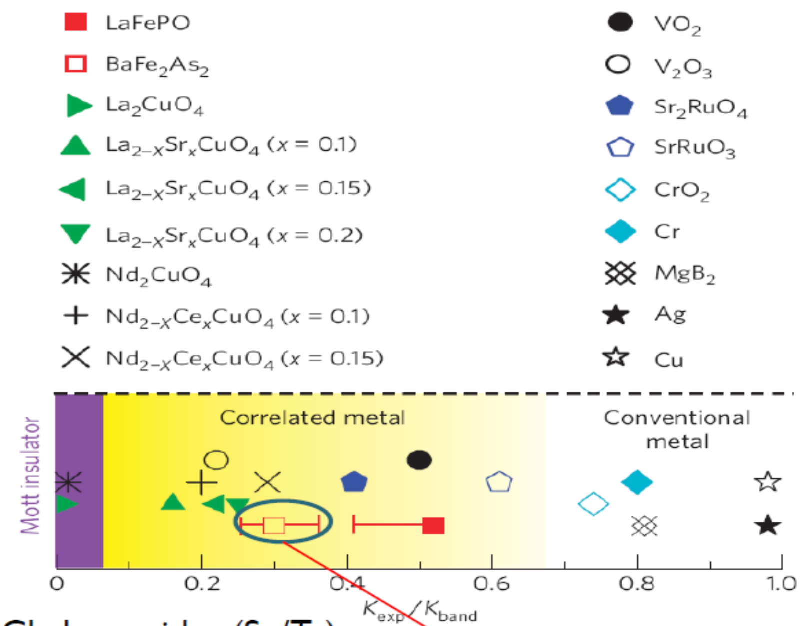
Due to kinetic energy gain the itinerant electrons (4 electrons in 3 orbitals) probably want to be ferromagnetic especially in Y direction (larger hoppings)

The system chooses an AF state with $(\pi,0)$ momentum which has ferromagnetic order along Y direction

EB, B. Valenzuela M.J. Calderón, PRB 86, 174508 (2012)

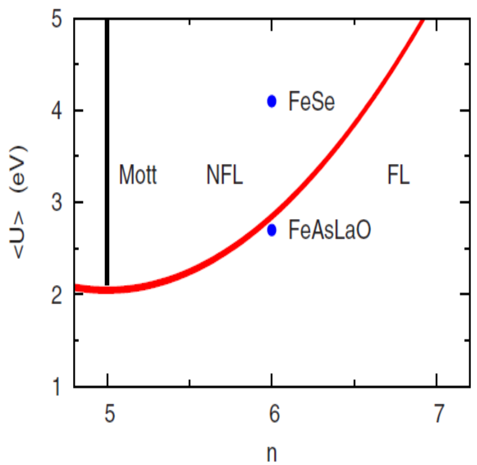
Correlations in optical conductivity: doping





Chalcogenides (Se/Te) seem more correlated than pnictides (As)

We are here

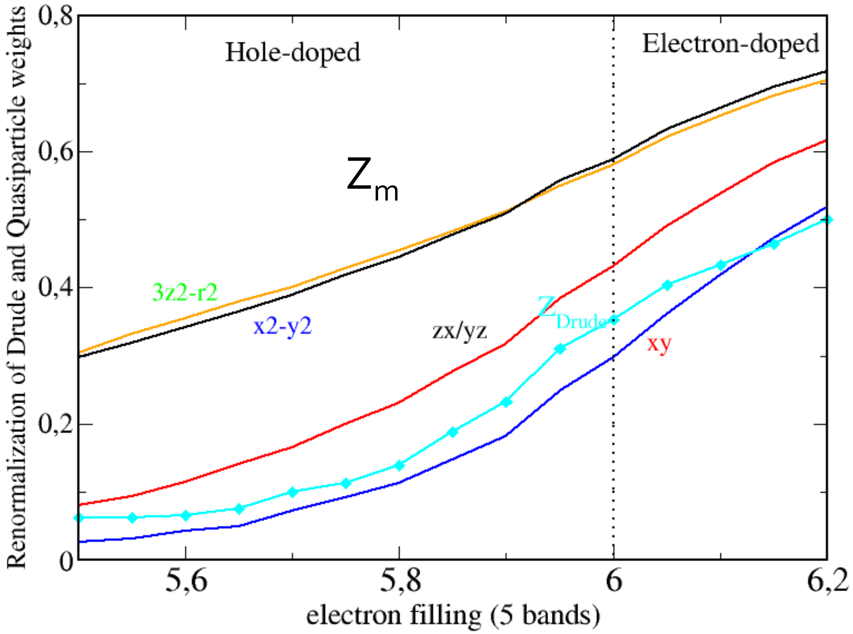


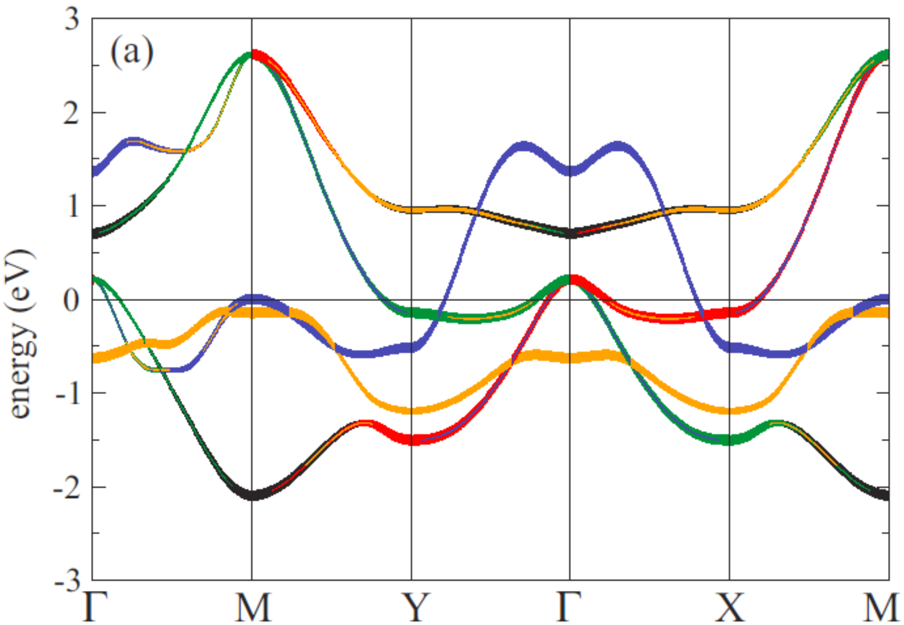
Spectral weight integrated up to 3000 cm^{-1} divided by the Drude weight expected from ab-initio, i.e.
the "renormalization of the Drude Weight"

Liebsch & Ishida, PRB 82, 1551006 (2010)

Qazilbash et al, Nat. Phys. 5, 647 (2009)

Doping dependence of optical conductivity





Non-renormalized tight-binding: **Graser et al, NJP 11, 025016 (2009)**

Quasiparticle weight from Slave Spin Calculations

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

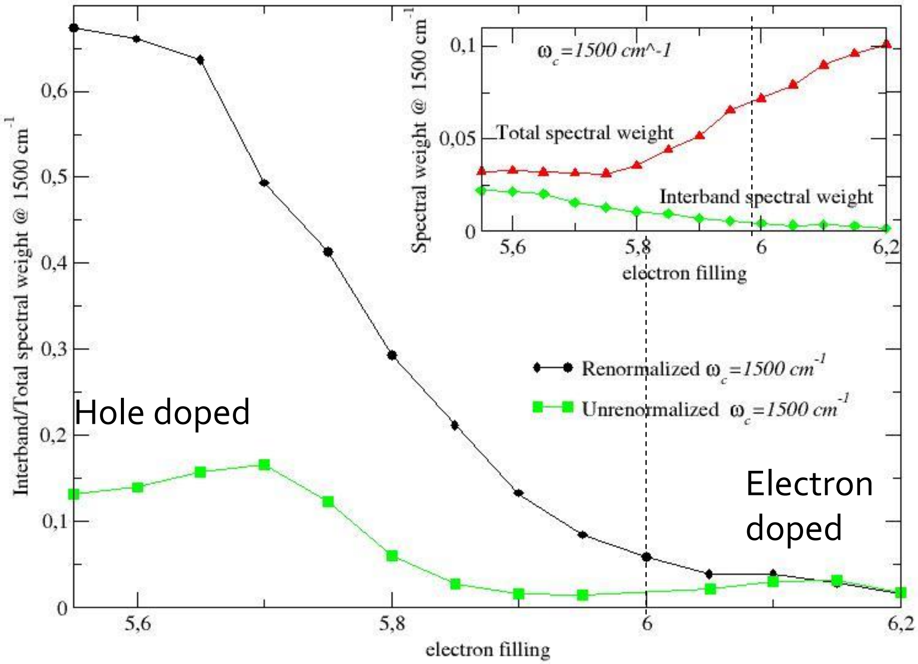
Note: Doping dependence assumes virtual crystal approximation

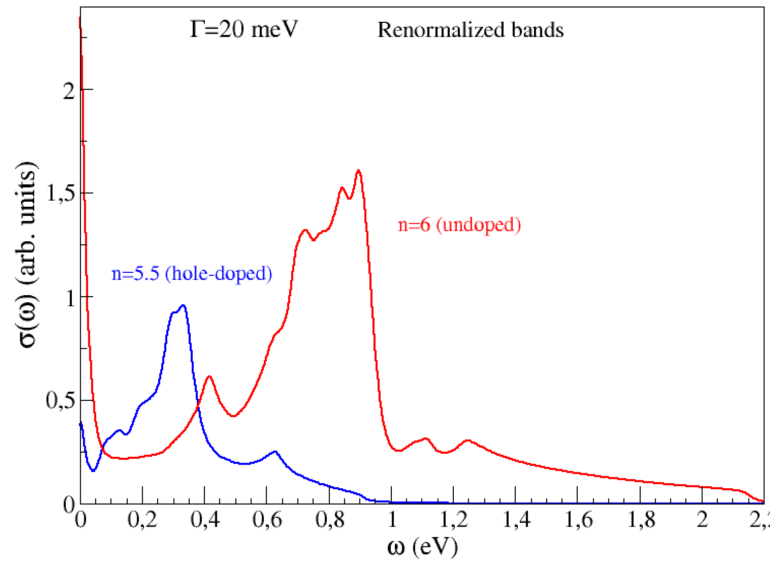
Optical conductivity and Drude Weight calculated with renormalized model using slave spin Z_m and onsite-energies λ_m following

B.Valenzuela, M.J.Calderón, G.León, EB , PRB 87, 075136 (2013)

Calderón, deMedici, Valenzuela, EB (preprint)

Doping dependence of optical conductivity





Many works consider
low energy up to 3000 cm-1

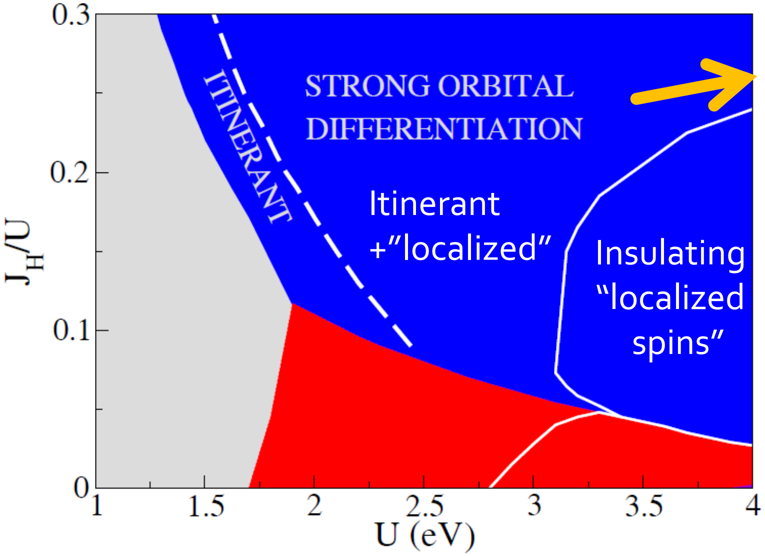
In hole doped samples the coherent contribution to the optical conductivity at intermediate energies is dominated by interband transitions

Note: Doping dependence assumes virtual crystal approximation

Calderón, deMedici, Valenzuela, EB (preprint)

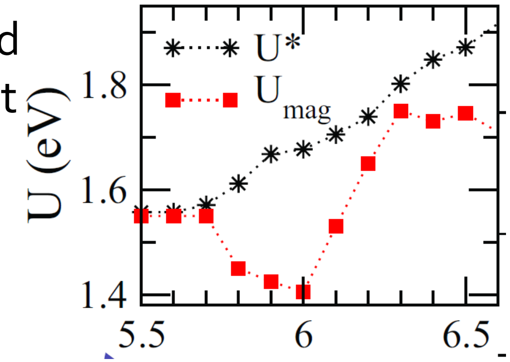
Summary

Magnetic state (Hartree-Fock)



xy & yz half-filled and gapped
Zx, 3z2-r2 and x2-y2 itinerant

Model for itinerant+ localized



Optical conductivity in the non-magnetic state. Doping dependence