Electronic correlations in iron superconductors: status, consequences and opportunities

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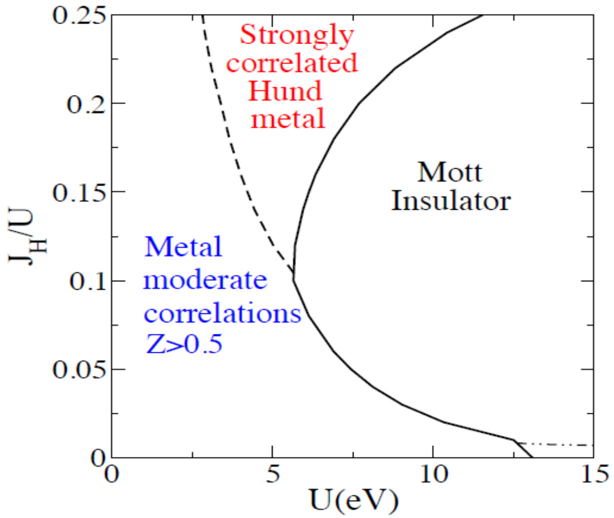
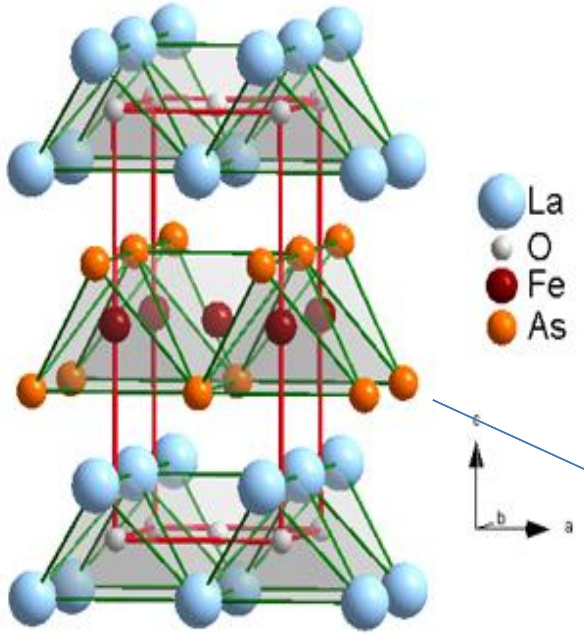


In 2008 it starts the iron age



The iron age

February 2008. **Superconductivity at 26 K in $LaF_xO_{1-x}FeAs$**

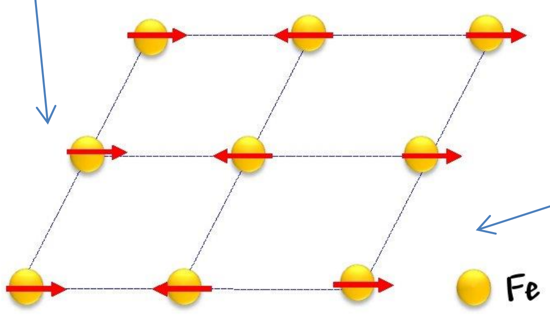
FeAs layer
(also in systems with
FeSe layer)

Short after their discovery it was clear that superconductivity in iron based materials could not be explained by the electron-phonon mechanism

Kamihara et al , JACS 130, 3296 (2008)
(Hosono's group)

Iron superconductors: High-Tc superconductivity, magnetism and nematicity

Ferromagnetic in Y direction



Antiferromagnetic in X direction

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

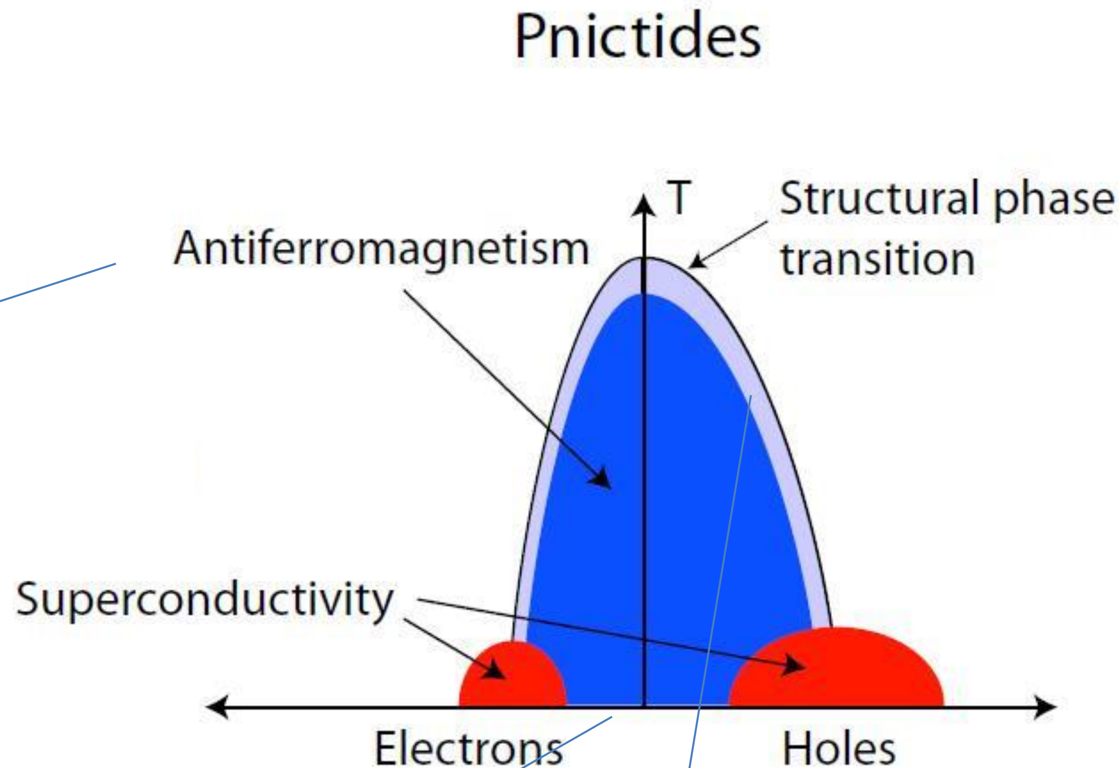


Fig: Lanzara's webpage

Undoped system
(6 electrons per Fe)

Nematic state
(anisotropic in plane)

In many systems the superconductivity also appears if the magnetic phase is suppressed by pressure (a few Gpa)

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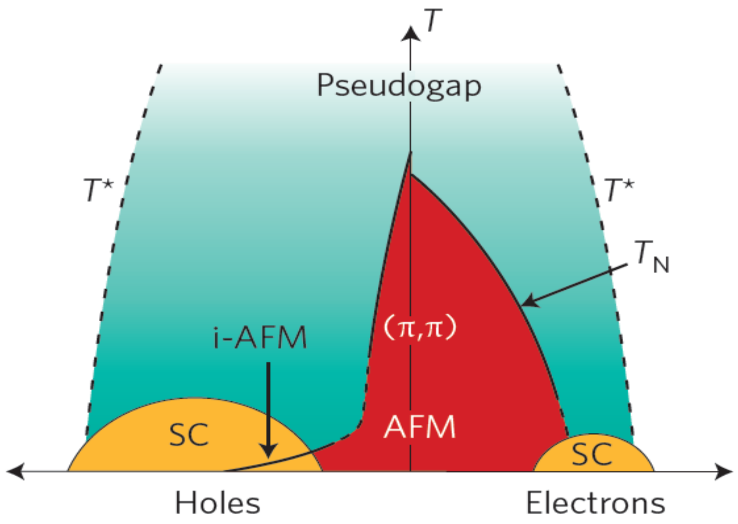
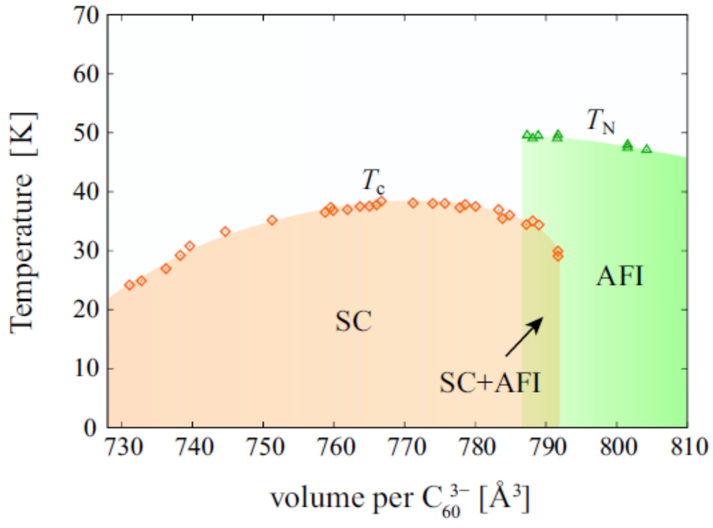
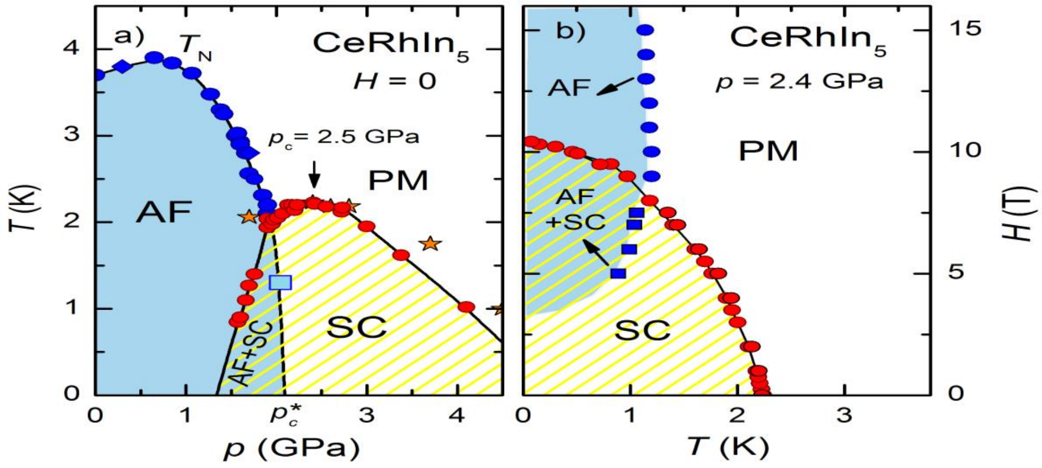
Similarity with the phase diagram of other non-conventional superconductors

Cuprates



Fullerides





Heavy fermions

In our way to understand high-Tc superconductors

- Which is the origin of the high-Tc superconductivity?
- Can we find new materials with higher Tc?
- Are the physics of iron superconductors and other non-conventional superconductors, especially cuprates, related?

In our way to understand high-Tc superconductors

- Which is the origin of the high-Tc superconductivity?
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Key issues:

- Correlations in iron superconductors
- Interplay between the spin and orbital degrees of freedom

In our way to understand high-Tc superconductors

- Superconductivity believed to be linked to electronic correlations (maybe magnetic degree of freedom)

- Model containing only electrons

Kinetic energy + Interactions between electrons

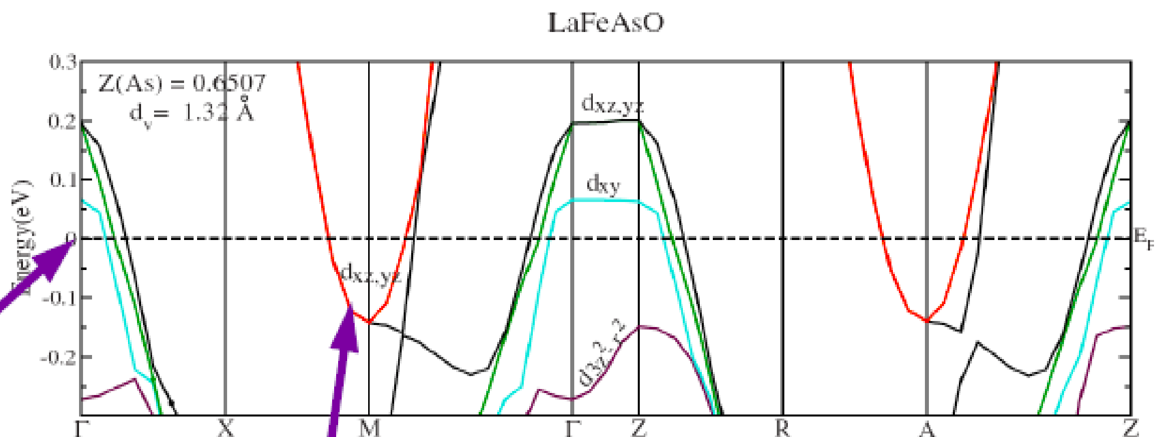
Very often Interactions are restricted to electrons in the same site

- Approximations for the starting limit

A word on correlations

- **Independent-particle description of solids: band theory.**
  - Electrons move in a periodic potential.
  - Electronic states: bands in momentum space, filled following Fermi-Dirac statistics
  - Fermi surface
  - Description via **ab-initio calculations**. Successful in a large number of materials

DFT calculations



Hole pockets

Electron pockets

Vildosola et al, PRB 78, 064518 (2008)

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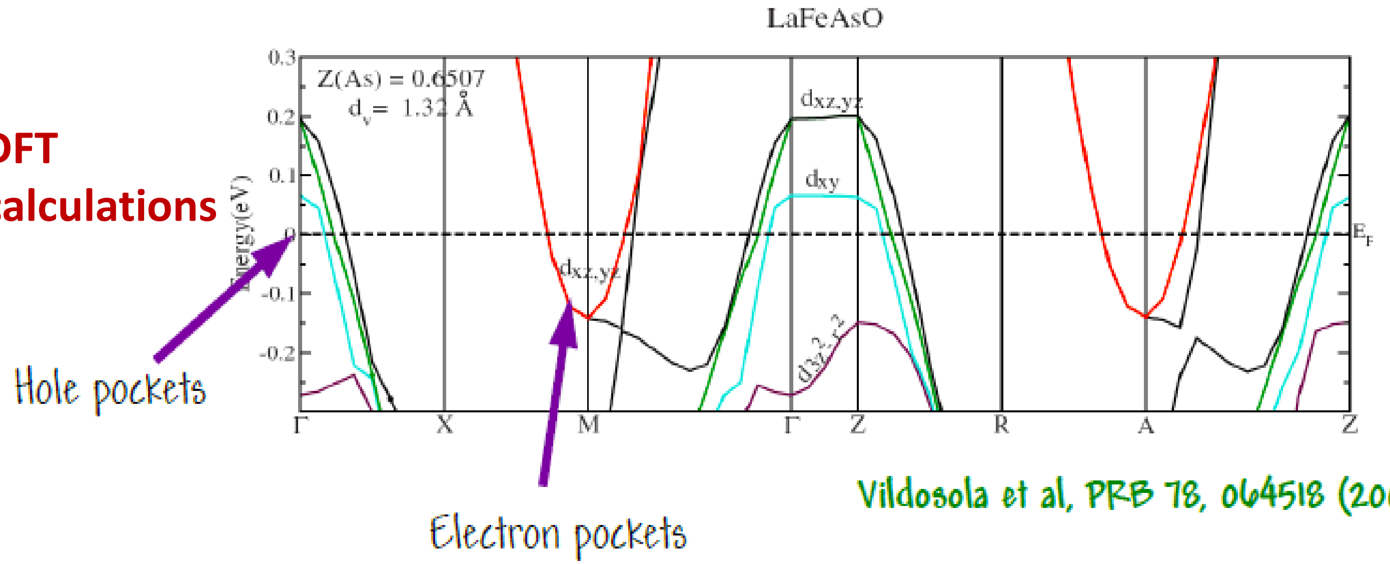


Vildosola et al, PRB 78, 064518 (2008)

Electrons interact: the Fermi sea can be unstable: magnetic ordering, charge ordering …

Weak coupling description of electron interactions

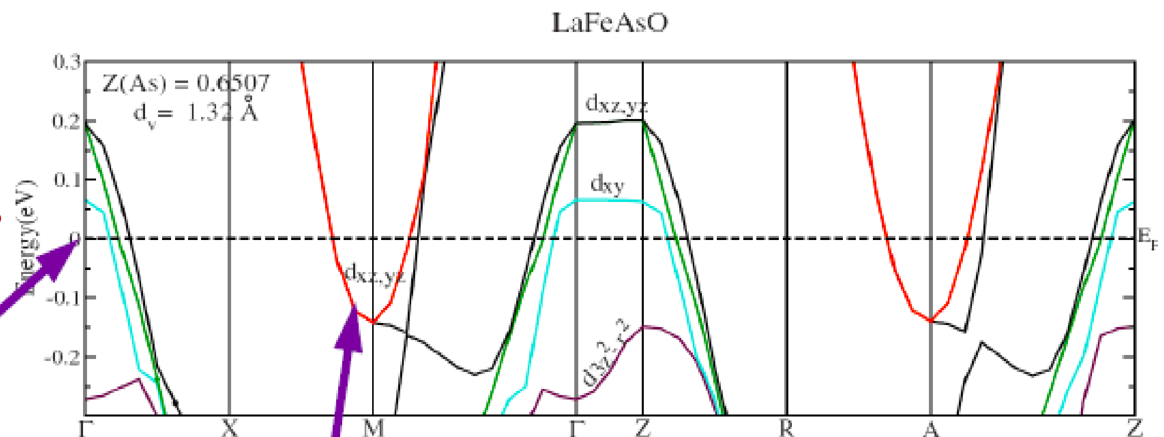
A word on correlations

- **Strong correlations:**

Deviations from ab-initio calculations

- Enhanced mass
- Insulating instead of metallic behavior …

DFT calculations



Hole pockets

Electron pockets

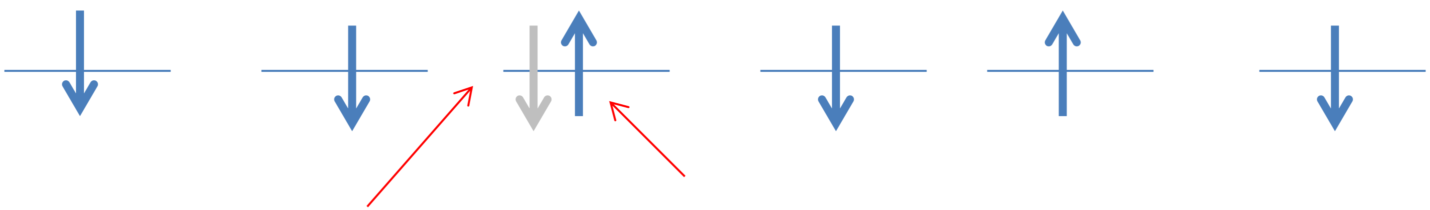
Vildosola et al, PRB 78, 064518 (2008)

A word on correlations

- **Local electrons. Mott insulators.**

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

Kinetic energy (t) **+** **Interaction between electrons**
Intra-orbital repulsion (U)



Kinetic energy
(hopping)
saves energy t

Double occupancy
costs energy U

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A word on correlations

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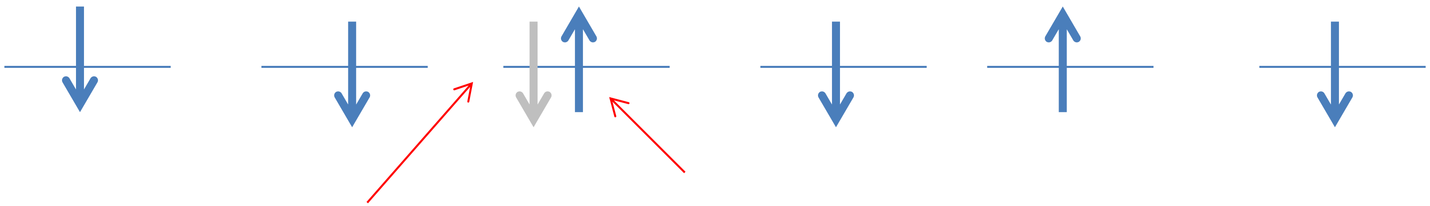

Kinetic energy (hopping) saves energy t

Double occupancy costs energy U

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

Repulsion can drive the system into an insulating state

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

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A word on correlations

- Mott insulator in <u>single orbital systems</u>. The local electrons behave as local spins.

Description in terms of local spins

$$\boxed{H = J \sum_{ij} S_i S_j}$$

Antiferromagnetic Order $J \sim t^2/U$

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A word on correlations

- Mott insulator in <u>single orbital systems</u>. The local electrons behave as local spins.

Description in terms of local spins → $H = J\,\Sigma_{ij}\, S_i S_j$

Antiferromagnetic Order $J \sim t^2/U$

Beyond half-filling (n≠1)

or

for U< Uc (but close to Mott)

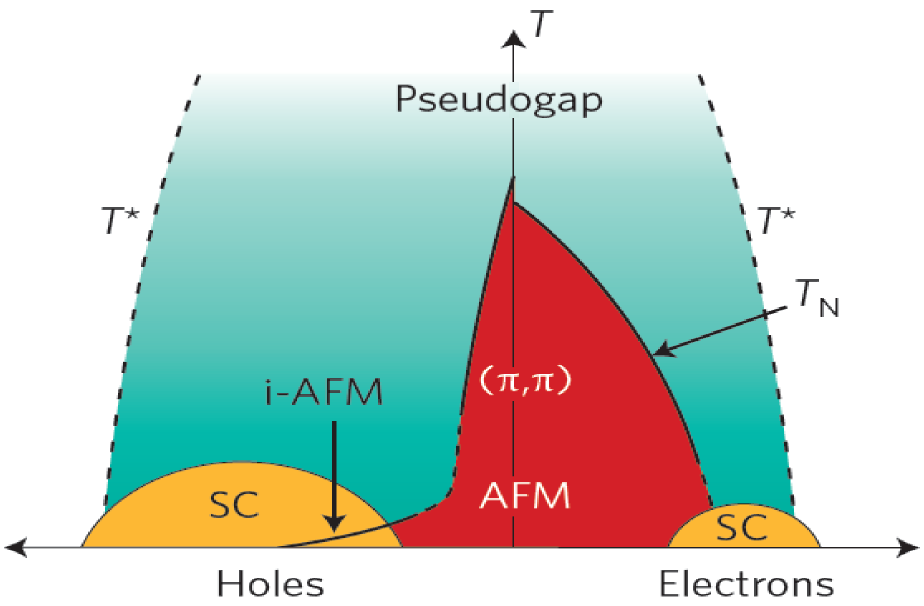
⇒

Metallic system

Behavior and excitations controlled by the local spins

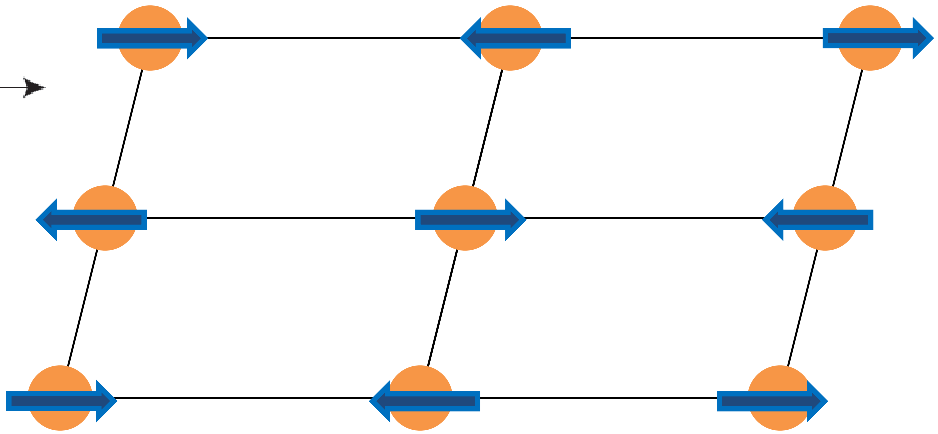
Strong coupling (local) description of the effects of the electron interactions

Undoped cuprates: Mott insulators



Localized electrons described as local spins S=1/2 which interact antiferromagnetically

$$H = J\, S_i S_j$$



Undoped cuprates

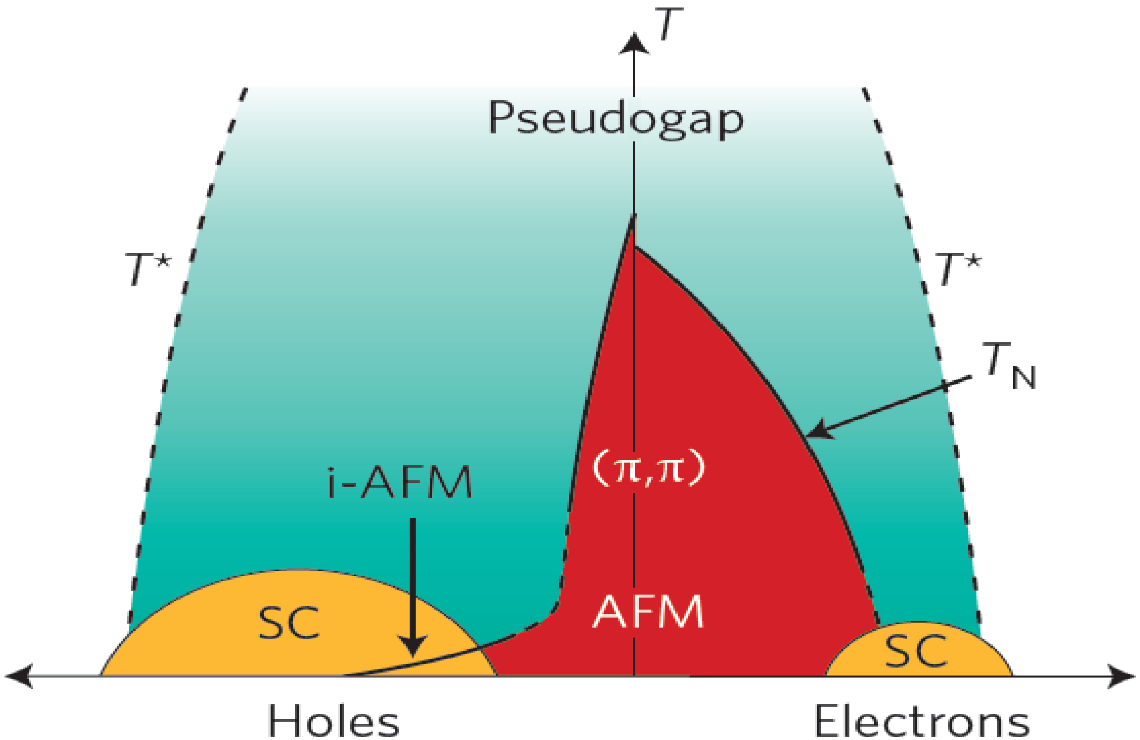
Mott insulator with AF order

Antiferromagnetism due to local moments

Doping a Mott insulator in 2D: high-Tc superconductivity in cuprates

Superconductivity doping with electrons or holes

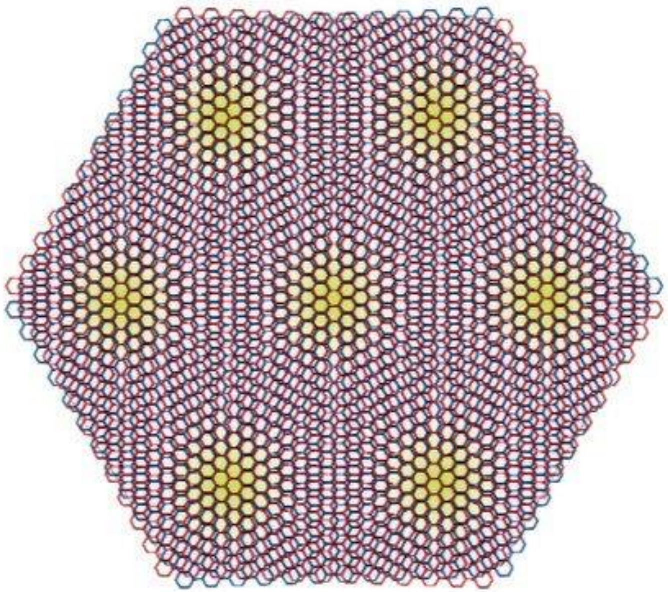
Anomalous behavior in pseudogap state, not well understood

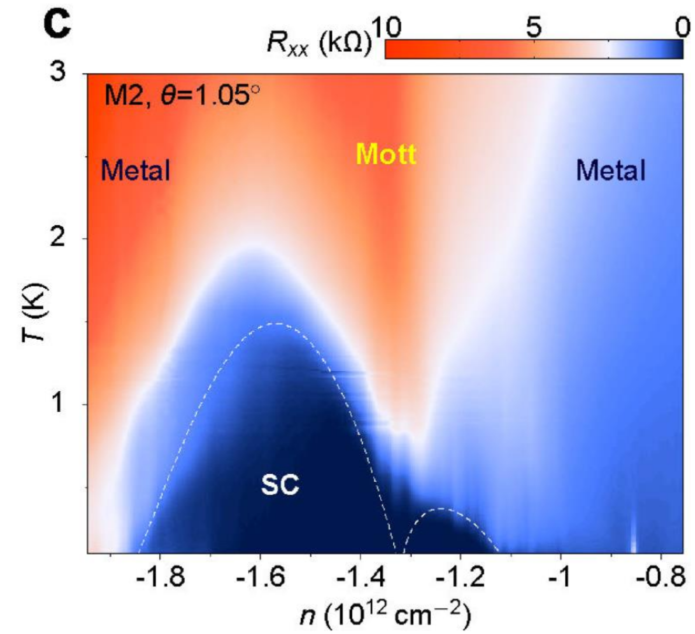


Role of Mott physics in superconductivity?
(superconductivity has been found in models with strong or weak correlations)

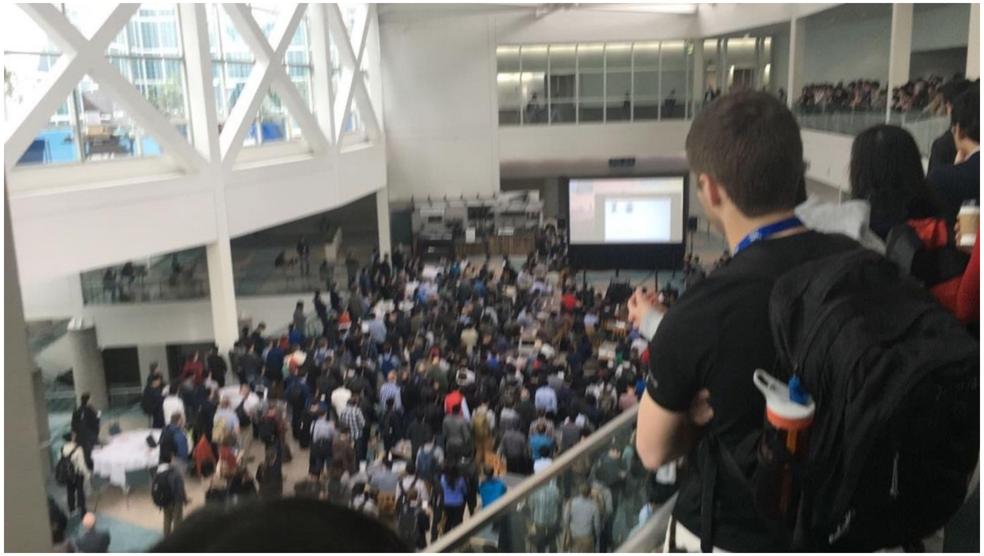
High-Tc from very strong interactions (local electrons)

Superconductivity emerging from a Mott insulator in twisted bilayer graphene?





Cao et al, Nature 556, 43 (2018)
Cao et al, Nature 556, 80 (2018)



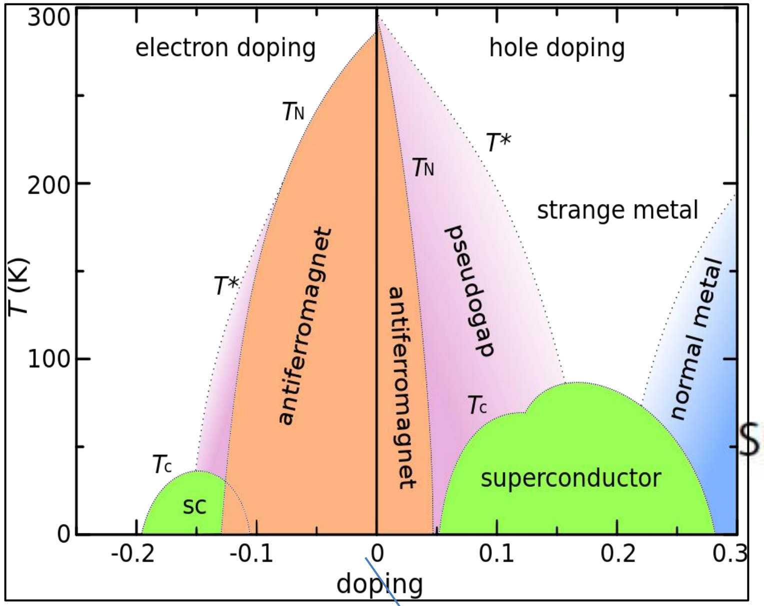
The talk seen ~ 4000 times
in youtube

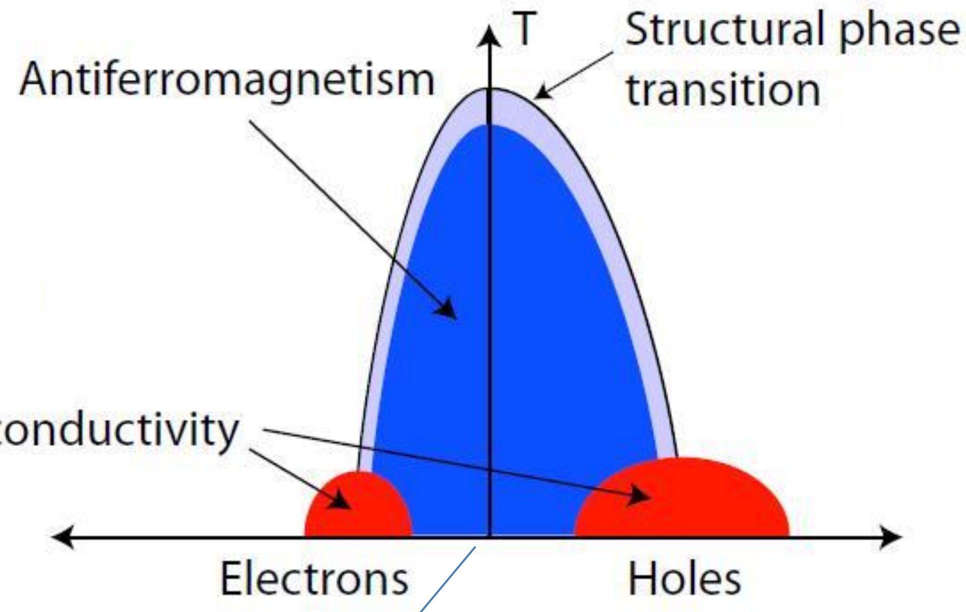
Is there Mott physics in iron superconductors?

Phase diagram of early discovered iron based superconductors

Cuprates

Iron Pnictides (FeAs systems)





Mott Insulator

Metallic

Local moments or Fermi surface instability in iron superconductors

Experimentally the system is metallic but with **sizable correlations**

The mass of electrons is enhanced m*~3 with respect to ab-initio

Local moments or Fermi surface instability in iron superconductors

Experimentally the system is metallic but with **sizable correlations**

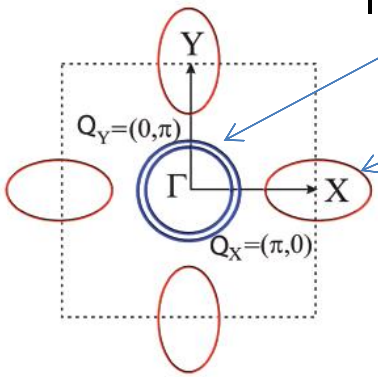
The mass of electrons is enhanced m*~3 with respect to ab-initio),

Approaches to explain magnetism, superconductivity and nematicity

Weakly correlated models
(Electronic bands ,
Fermi surface instability)

Strongly correlated models
(Interactions between local electrons/spins)

Hole pockets



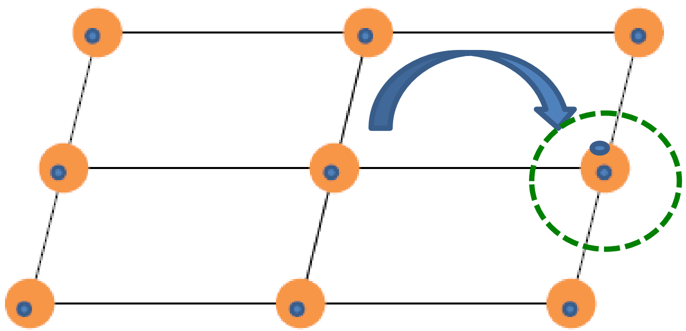
Electron pockets

$$H_{J_1-J_2} = \frac{J_1}{|S|^2}\sum_{\langle i,j\rangle}\vec{S}_i\vec{S}_j + \frac{J_2}{|S|^2}\sum_{\langle\langle i,j\rangle\rangle}\vec{S}_i\vec{S}_j.$$

Not clear which limit works better

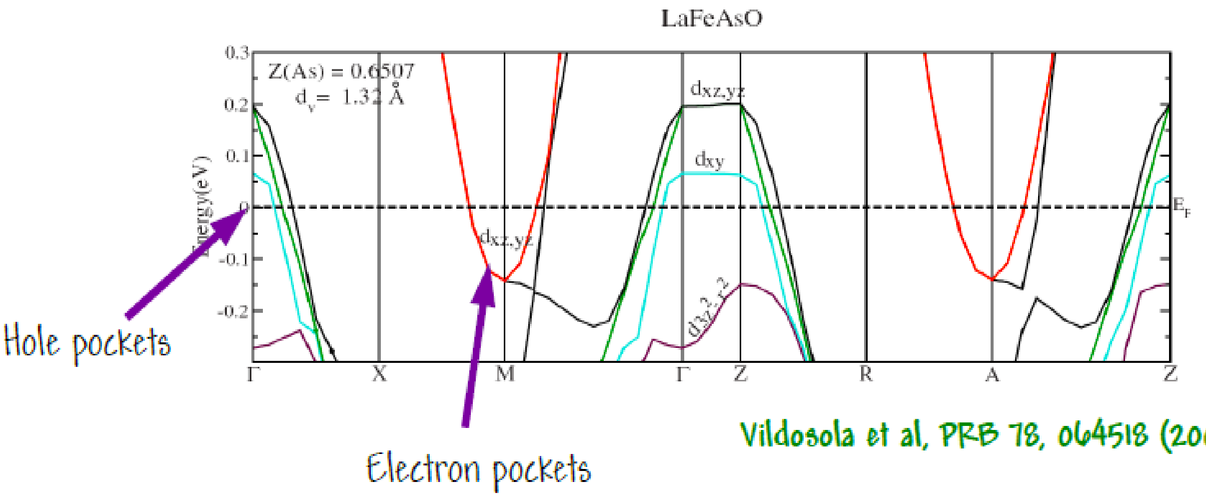
Iron superconductors: Multi-orbital character. Hund coupling

Cuprates: Single-orbital system. Cu lattice. d^9. Undoped: 1 electron in 1 orbital



Cost in energy U

Iron superconductors: Multi-orbital system. Fe lattice. d^6. Undoped: 6electrons in 5orbitals



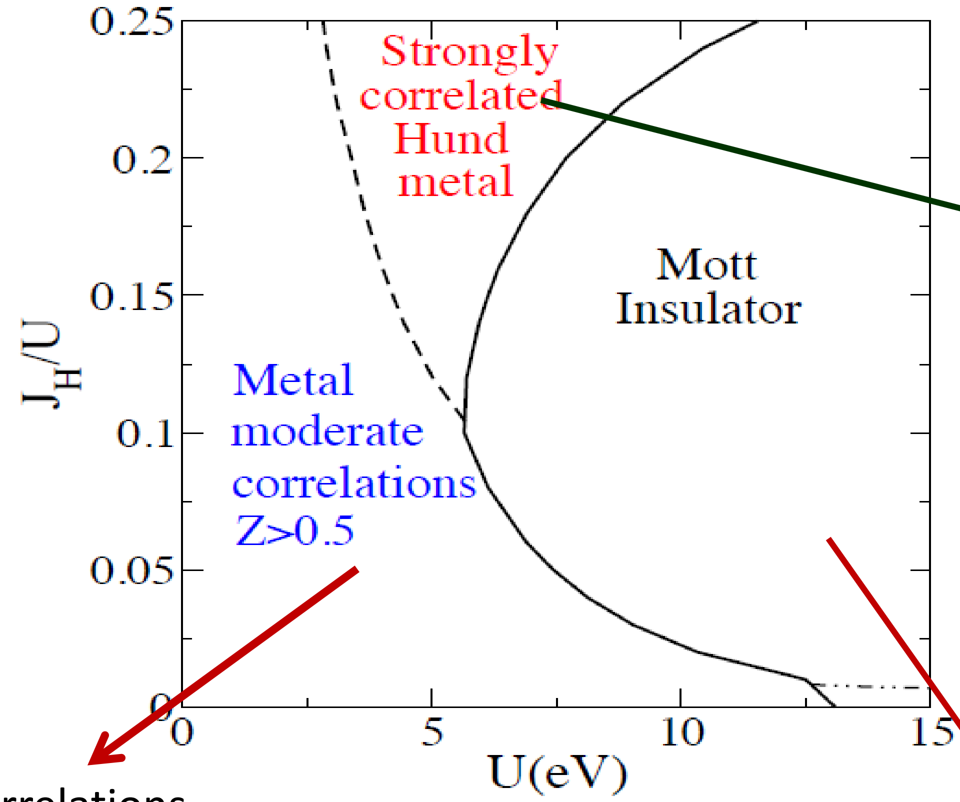
Vildosola et al, PRB 78, 064518 (2008)

Intraorbital interaction: U

Hund's coupling: J_H

Correlations in multi-orbital systems. Hund metals

Correlations diagram for a system with 6 electrons in 5 orbitals (like iron superconductors)



Local spins: electrons forced to have equal spin in each atom due to Hund's coupling **but the charge is not localized. Correlated metal**

Different correlation strengh in different orbitals

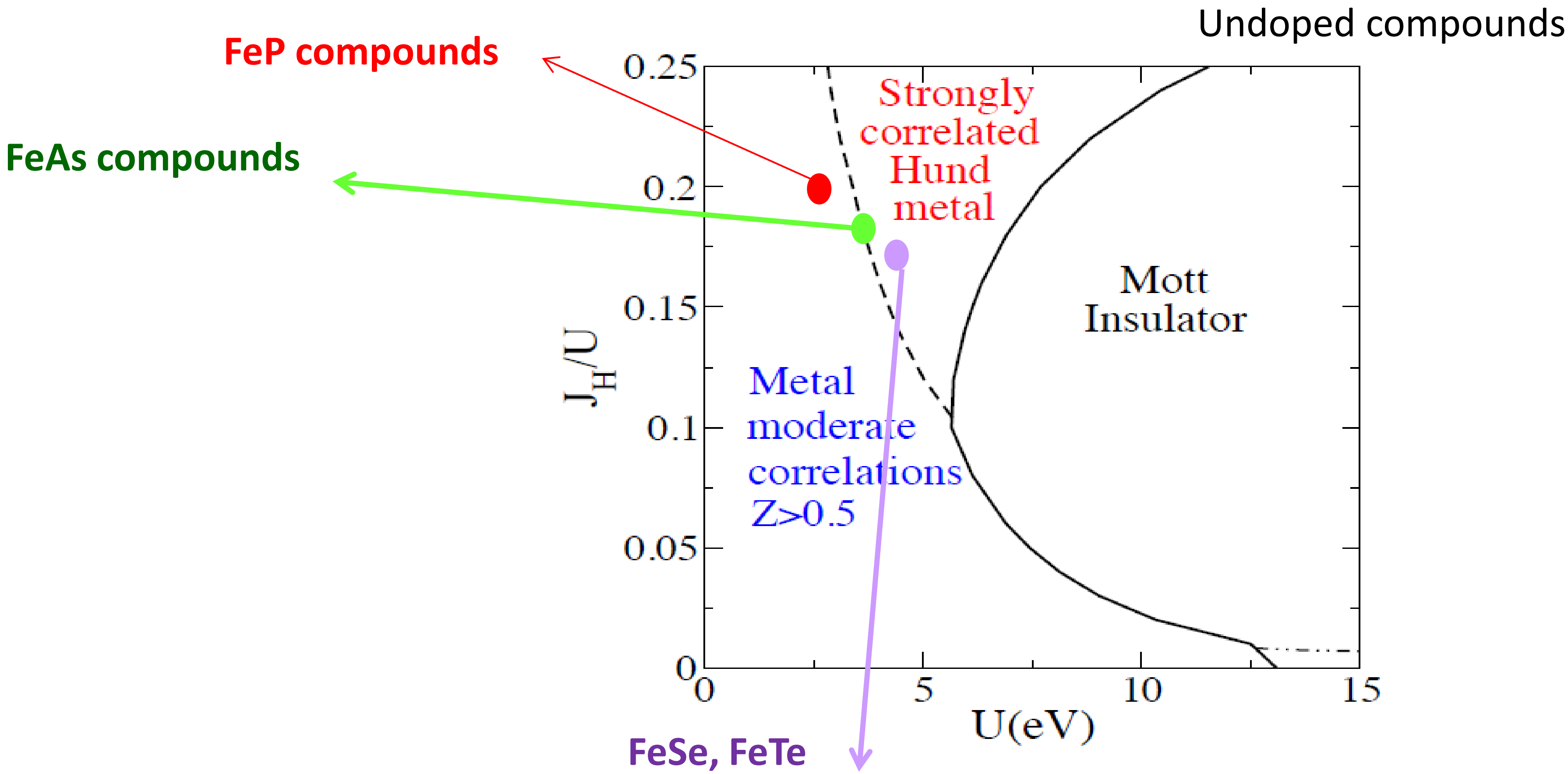
Weak correlations. Description in terms of Electronic bands & Fermi surface instabilities

Local electrons: the electronic charge is localized at the atom. Local spins

Yu & Si, PRB 86, 085104 (2012)

Review: Bascones, Valenzuela, Calderón, Comptes Rendus Physique 17, 36 (2016)

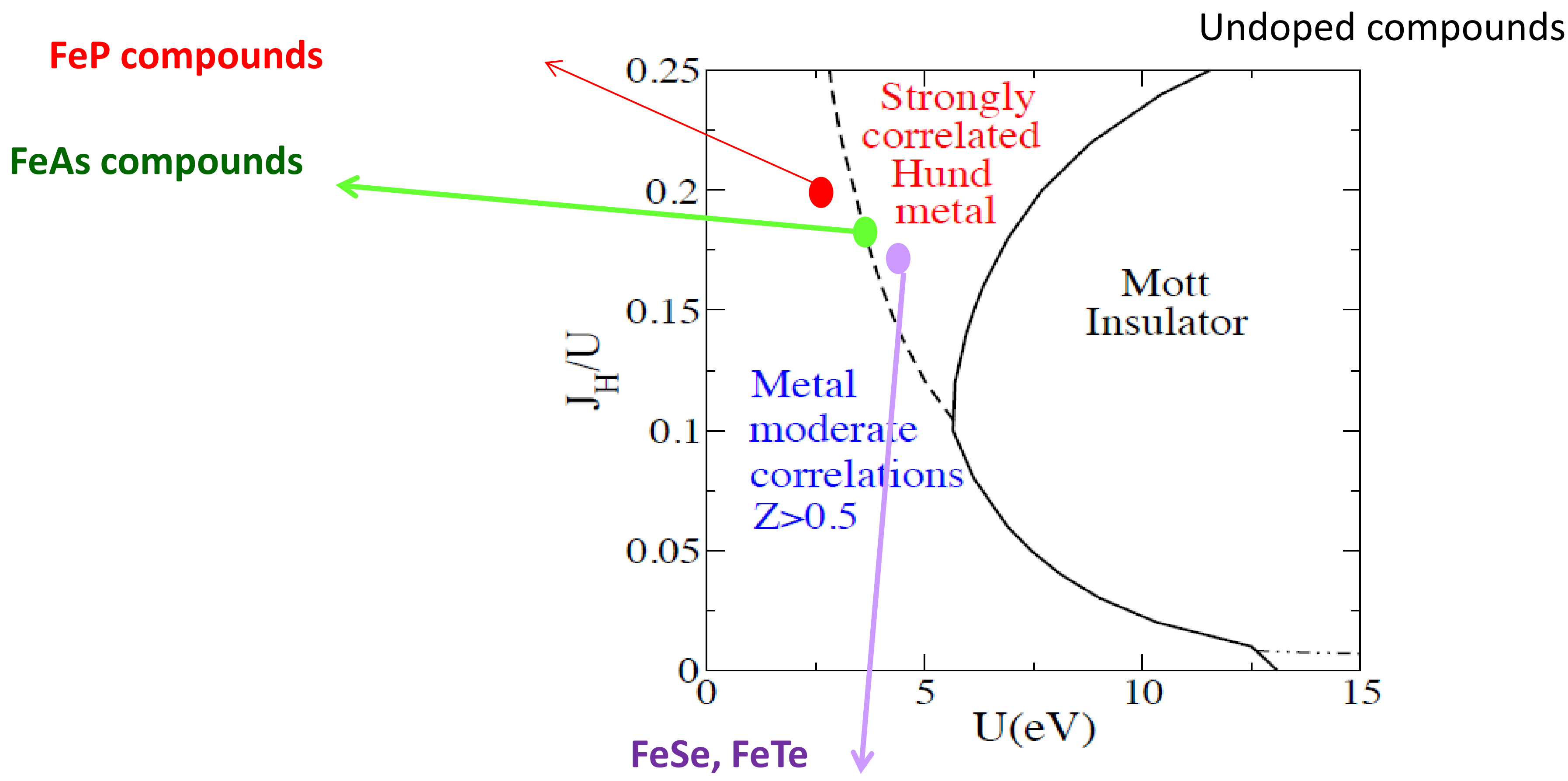
Correlations in iron superconductors: Hund's physics



From analysis of: ARPES,
Xray experiments,
Quantum oscillations, …
Comparison with theory …

Review: Bascones, Valenzuela, Calderón, Comptes Rendus Physique 17, 36 (2016)

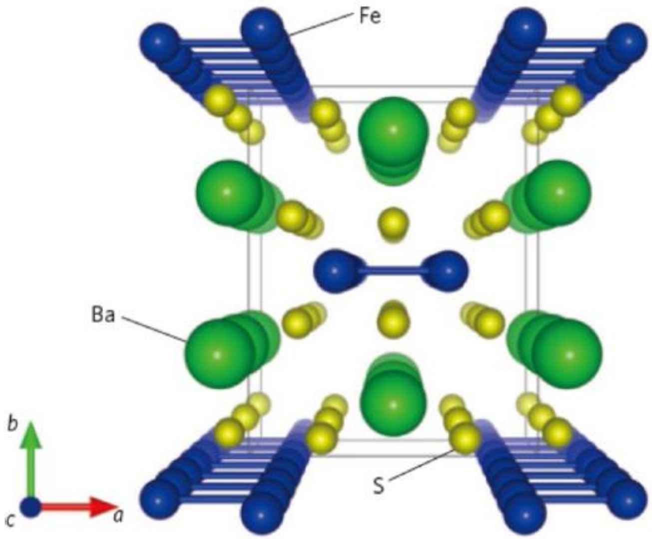
Correlations in iron superconductors: Hund's physics

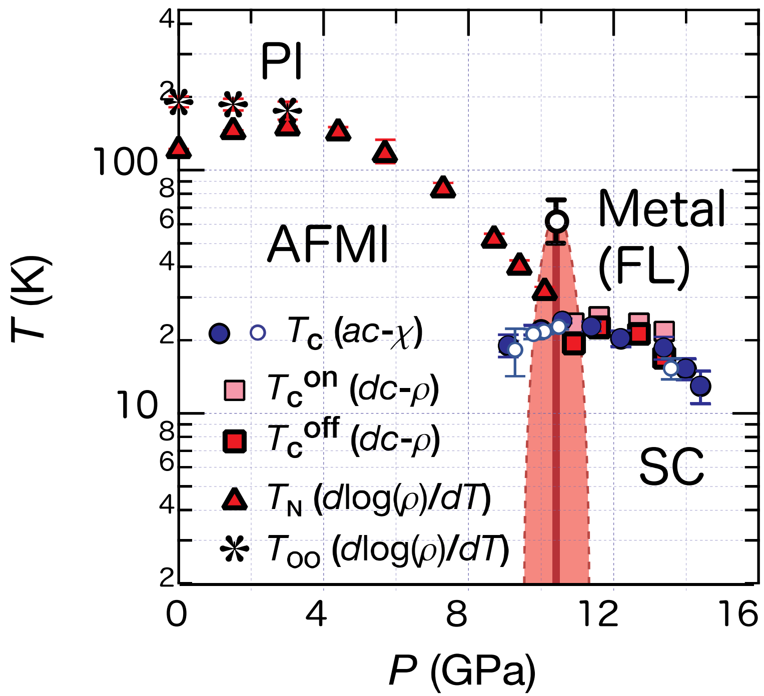


Difficulty to reveal the underlying physics
or intermediate interactions required for high-Tc superconductivity?

Review: Bascones, Valenzuela, Calderón, Comptes Rendus Physique 17, 36 (2016)

Superconductivity and magnetism in quasi-1d $BaFe_2S_3$



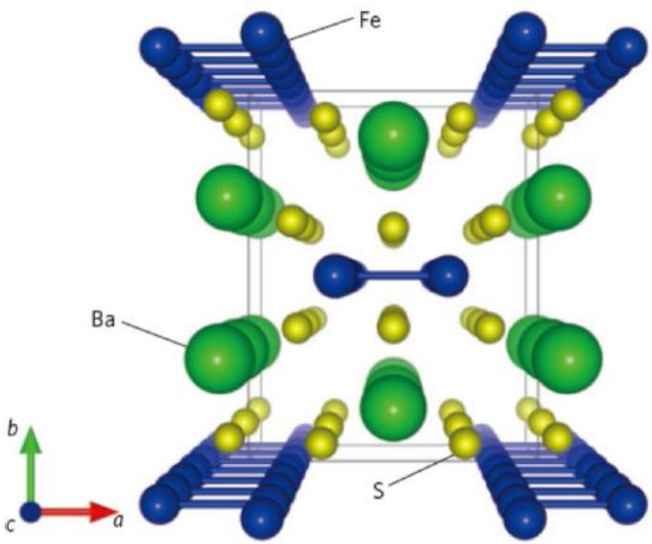


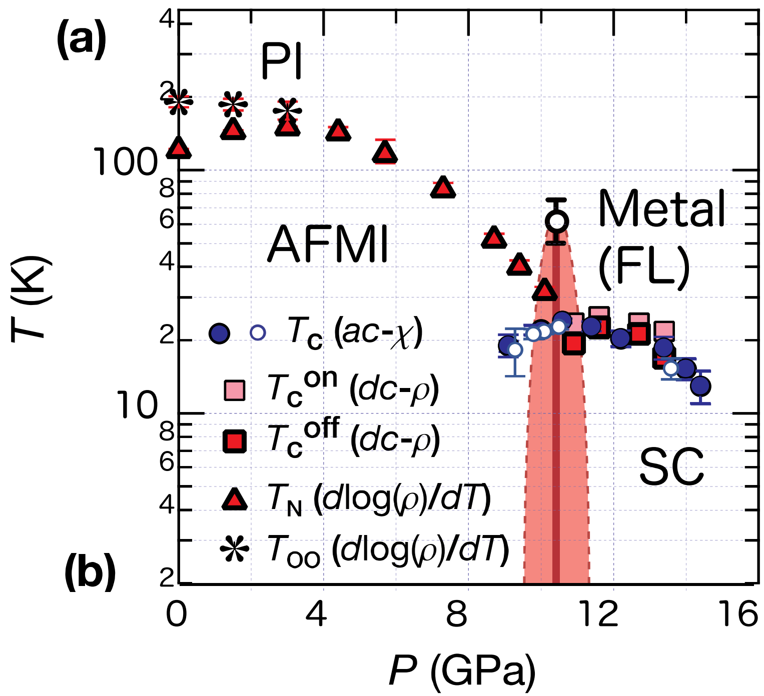
Same electronic filling per Fe
as in undoped iron superconductors

At zero pressure semiconductor Stripe AFM along ladder T_N=120K $\mu=1.2\mu_B$	Under pressure it becomes superconductor T_c up to 24 K @11.6 GPa

Takahashi et al, Nat. Mat. 14, 1008 (2015) **Yamauchi et al, PRL 115, 246402 (2015)**

Superconductivity and magnetism in quasi-1d $BaFe_2S_3$

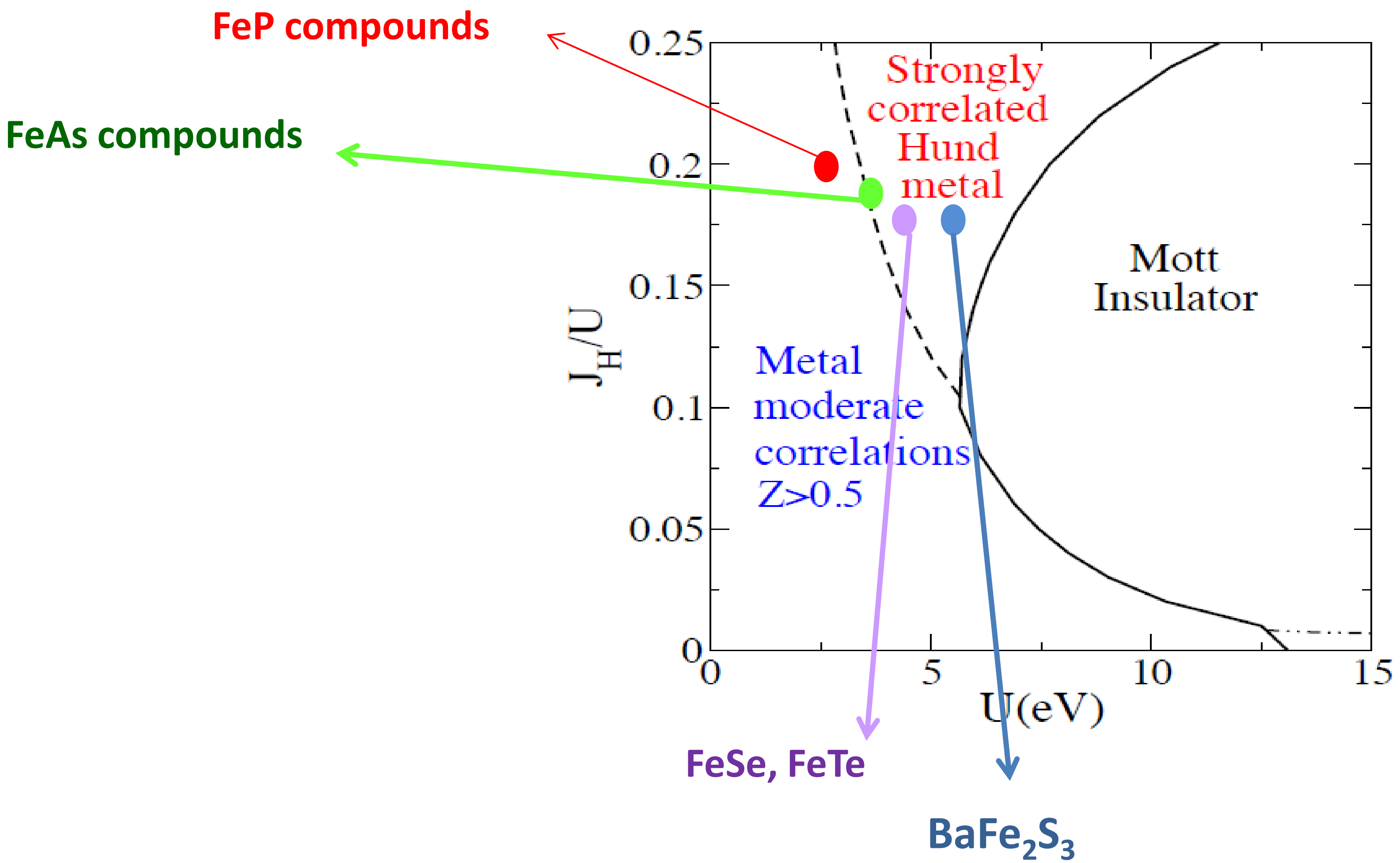




- Is this system a Mott insulator?
- Which is the role of pressure?

Strength of correlations in quasi-1d $BaFe_2S_3$

Undoped compounds



(orbitals with larger weight at the Fermi level extremely correlated)

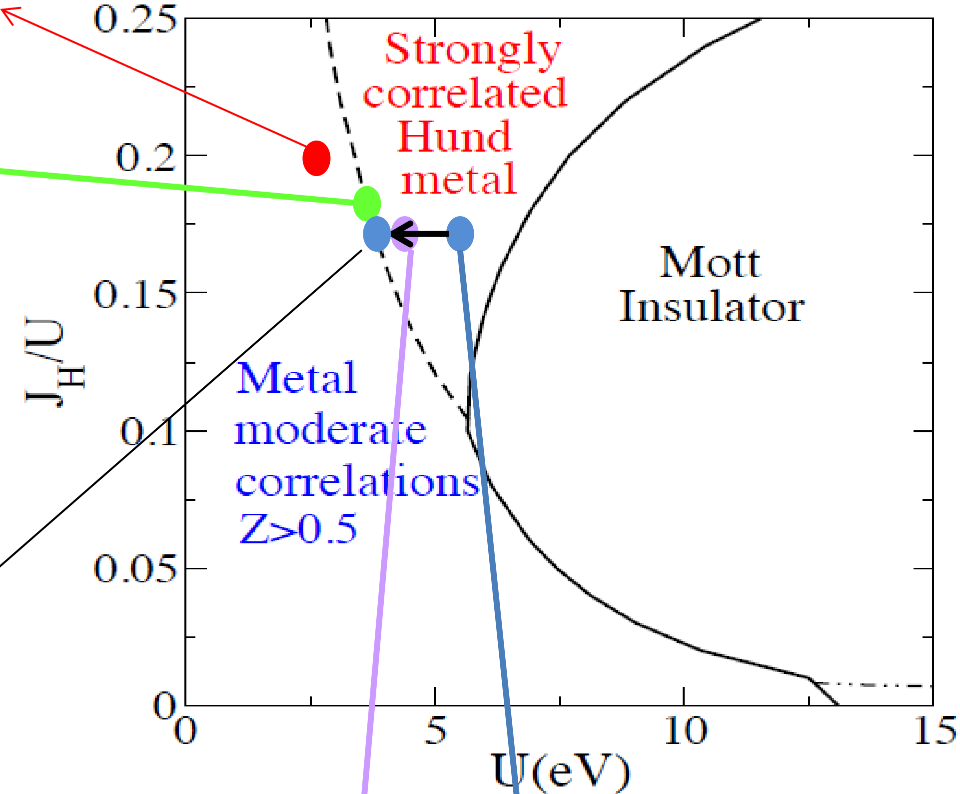
m* ~ 12-15

The role of pressure in quasi-1d $BaFe_2S_3$

Undoped compounds

FeP compounds

FeAs compounds



Suggests optimal interaction

FeSe, FeTe

$BaFe_2S_3$

(orbitals with larger weight at the Fermi level extremely correlated)

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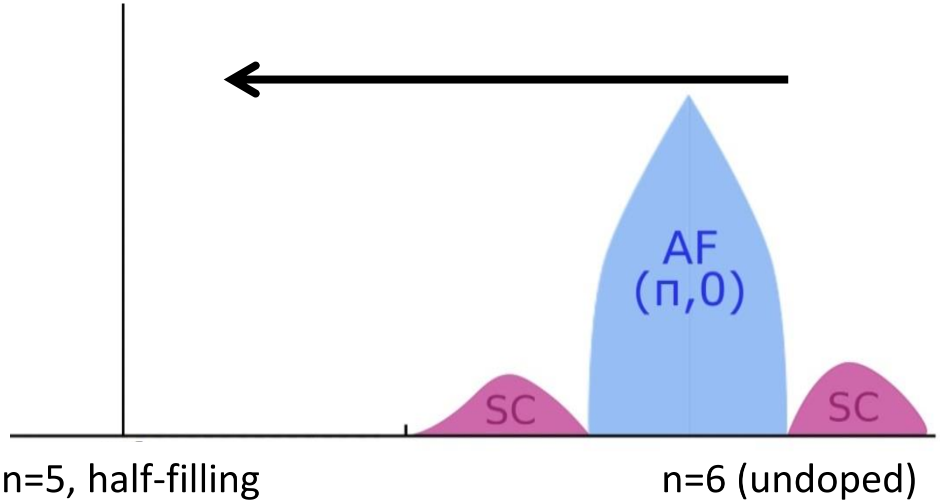
Correlations and electronic filling in iron superconductors

Ishida & Liebsch, PRB 81, 054513 (2010)

Electronic correlations in iron pnictides increase as the system approaches The Mott insulator at half-filling (5 electrons in 5 orbitals),



Confirmed experimentally

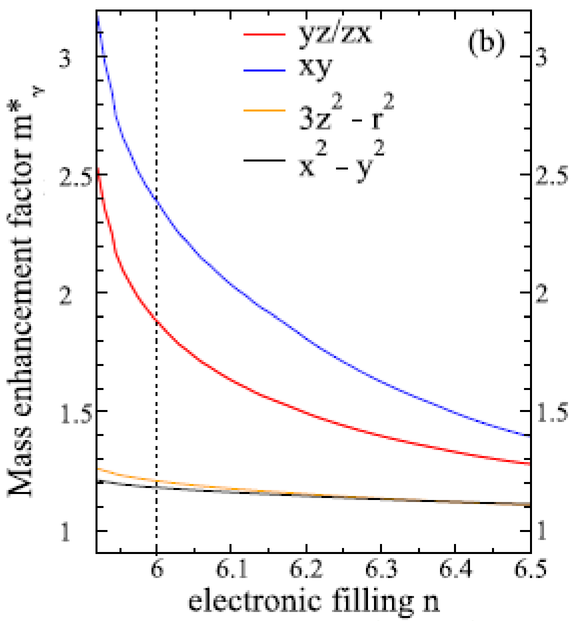


Fig: PRB 95, 075115 (2017)

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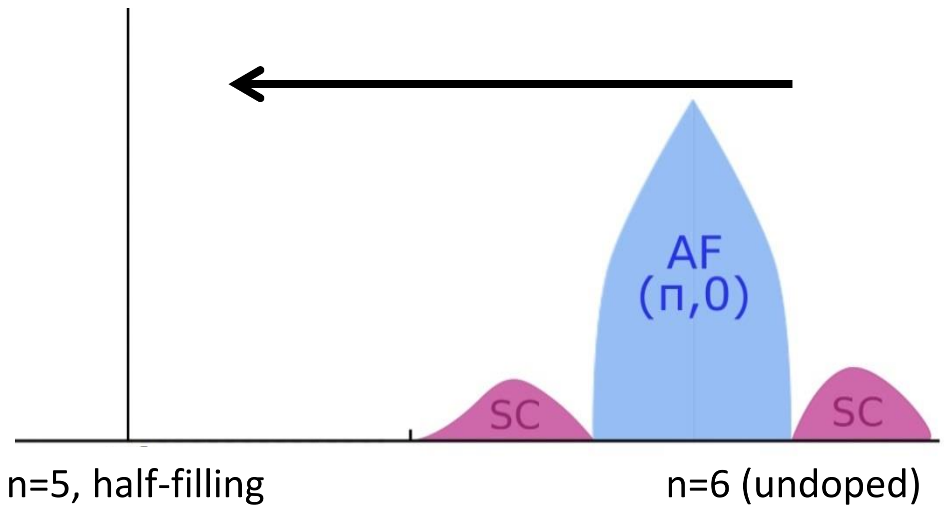
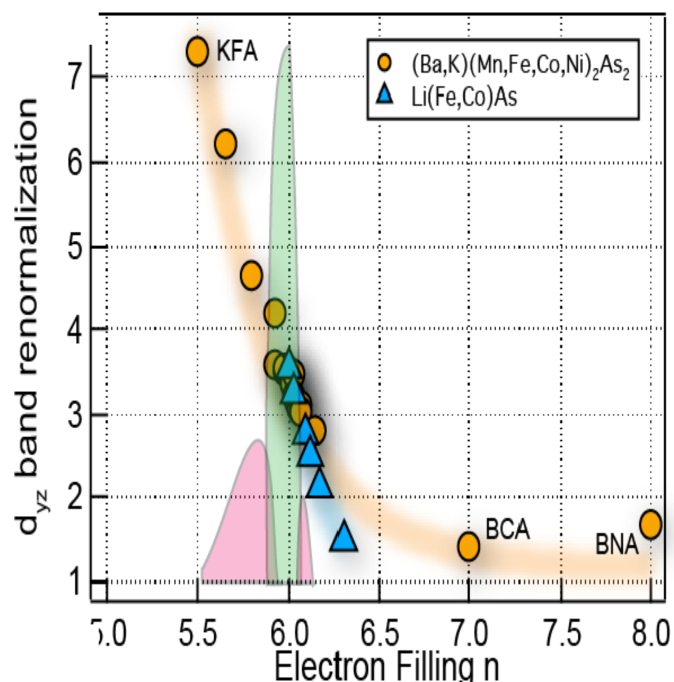


Confirmed experimentally

Fig: Yi et al, NPJ Quantum Materials 2, 57 (2017)



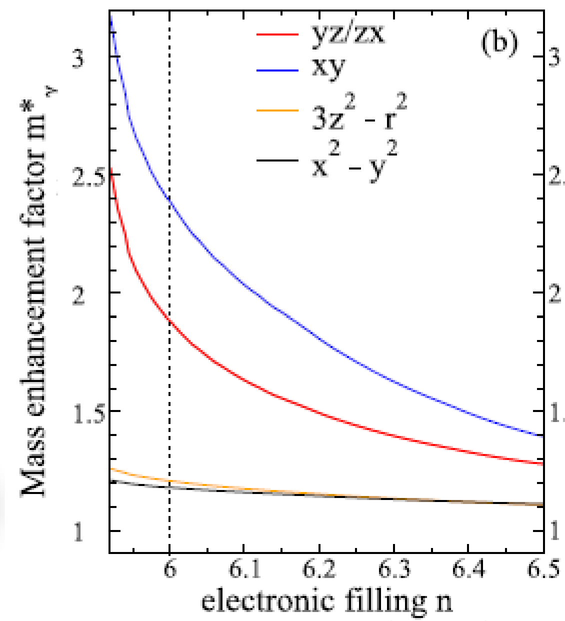


Fig: PRB 95, 075115 (2017)

Hardy et al, PRL 111,027002 (2013)
Nakajima et al, Sci. Rep. 4, 5873 (2014)
McNally et al, PRB 90, 180403 (2014)
Eilers et al, PRL 116, 237003 (2016)
Hardy et al, PRB 94, 205113 (2016)
and others

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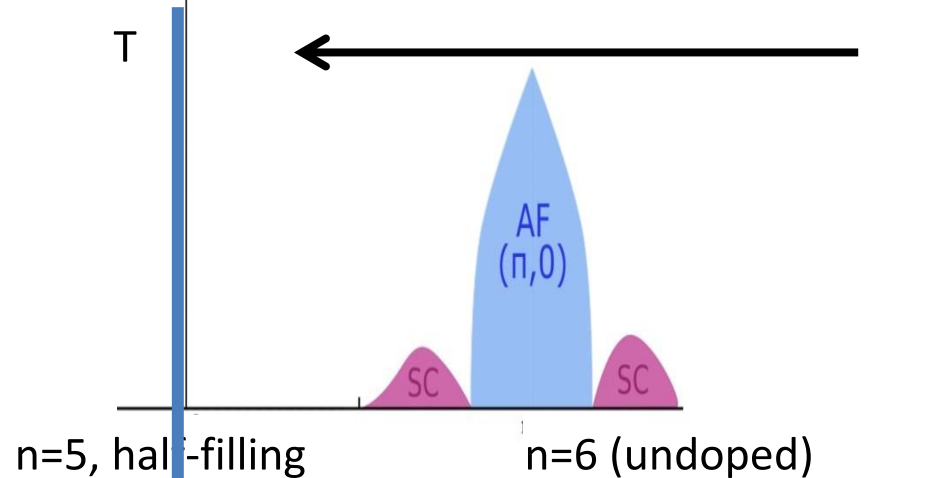
The connection between cuprates & iron superconductors

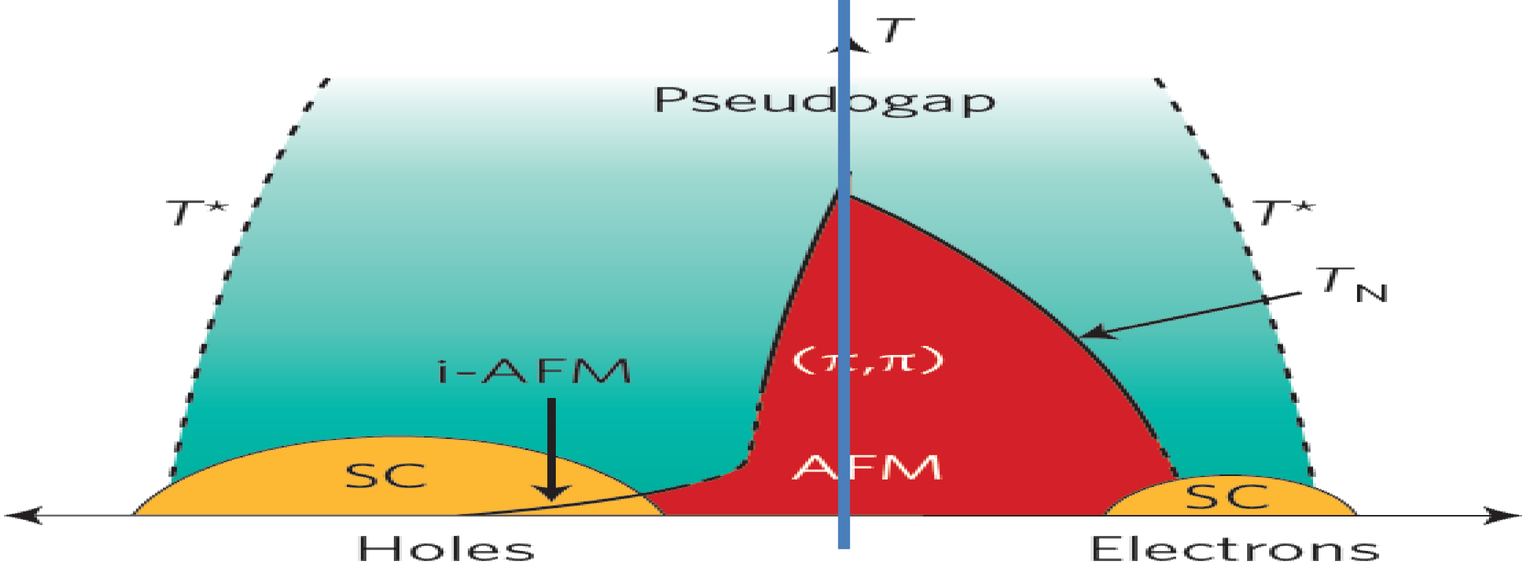
Ishida & Liebsch, PRB 81, 054513 (2010)

Mott insulator at Half-filling as the parent compound of iron superconductors

Increasing correlations towards half-filling



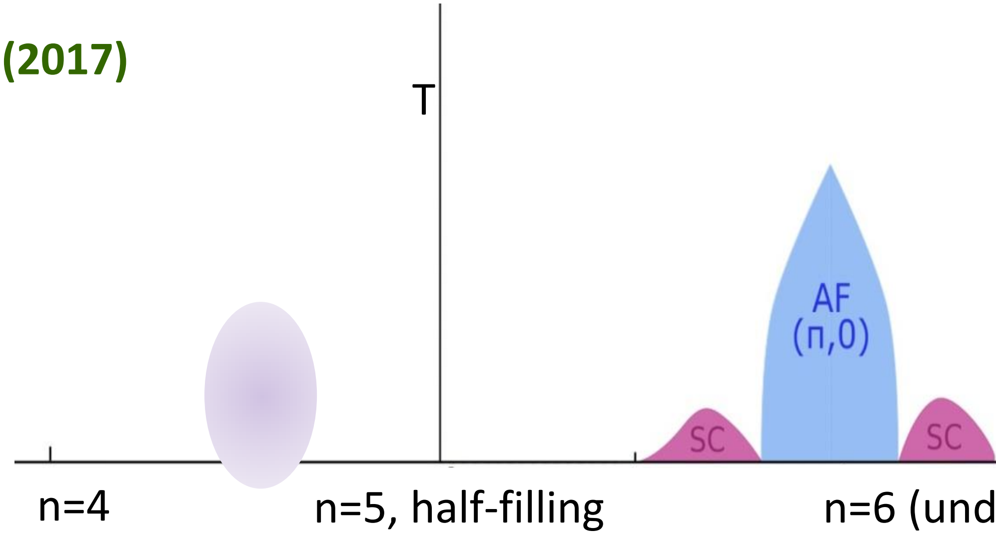
"Undoped" iron superconductors x=1.2 compared with electron doped cuprates



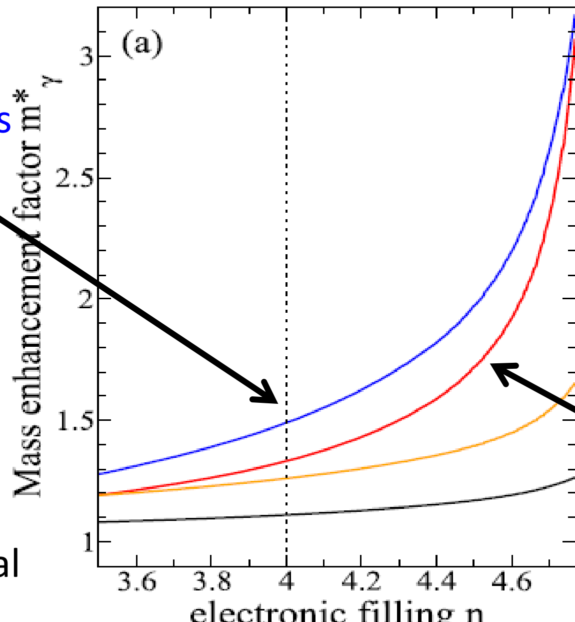
Search for superconductivity at the other side of half-filling

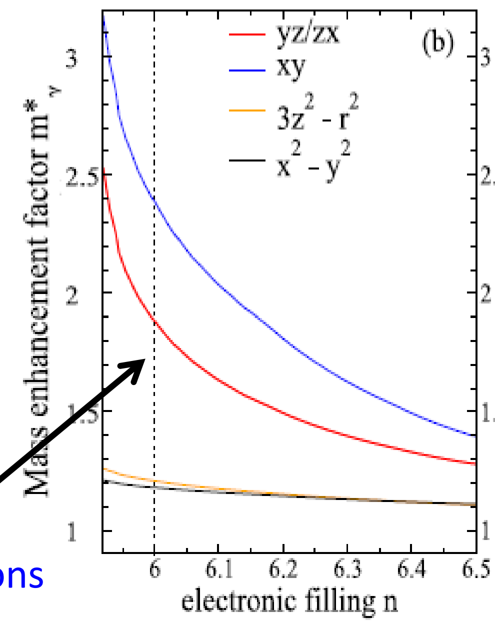
Pizarro et al, PRB 95, 075115 (2017)

Search for doping levels at which the strength of correlations is similar to that found in the pnictides



n=4 compounds are less correlated than undoped Fe-compounds





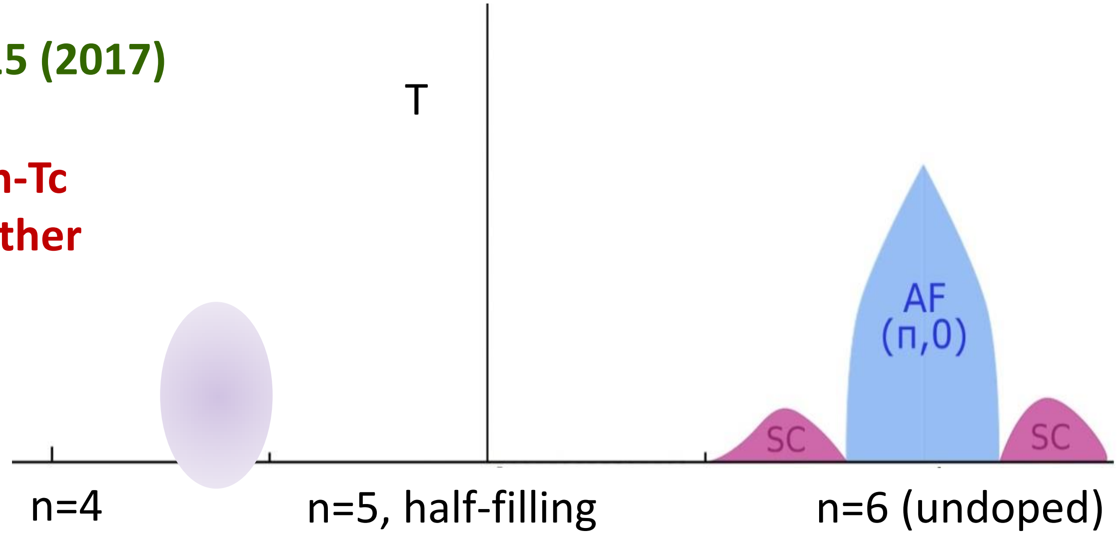
Similar correlations at n=4.5 and n=6

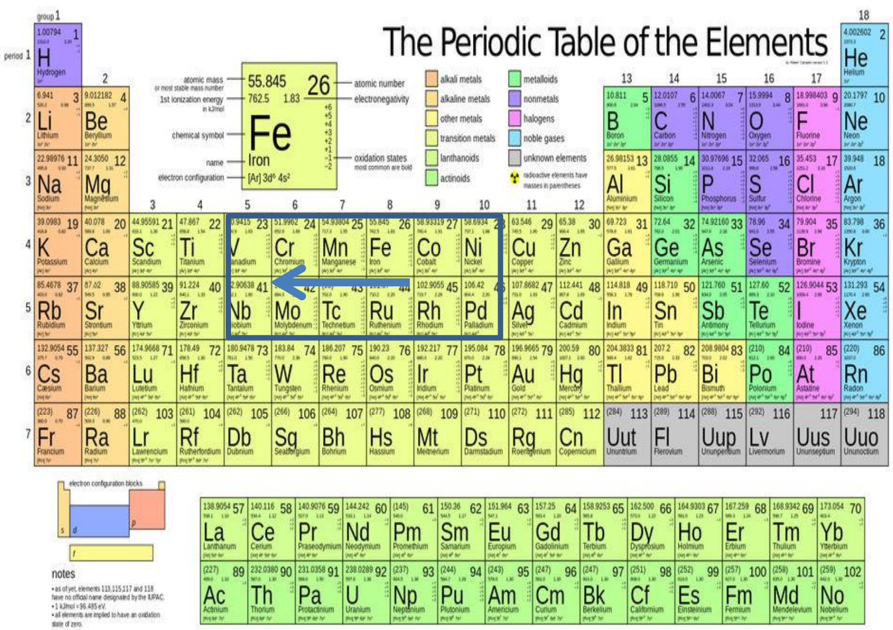
See also, Edelmann et al Phys. Rev. B 95, 205118 (2017)

Search for superconductivity at the other side of half-filling

Pizarro et al, PRB 95, 075115 (2017)

Our proposal: look for high-Tc superconductivity at the other side of half-filling n<5





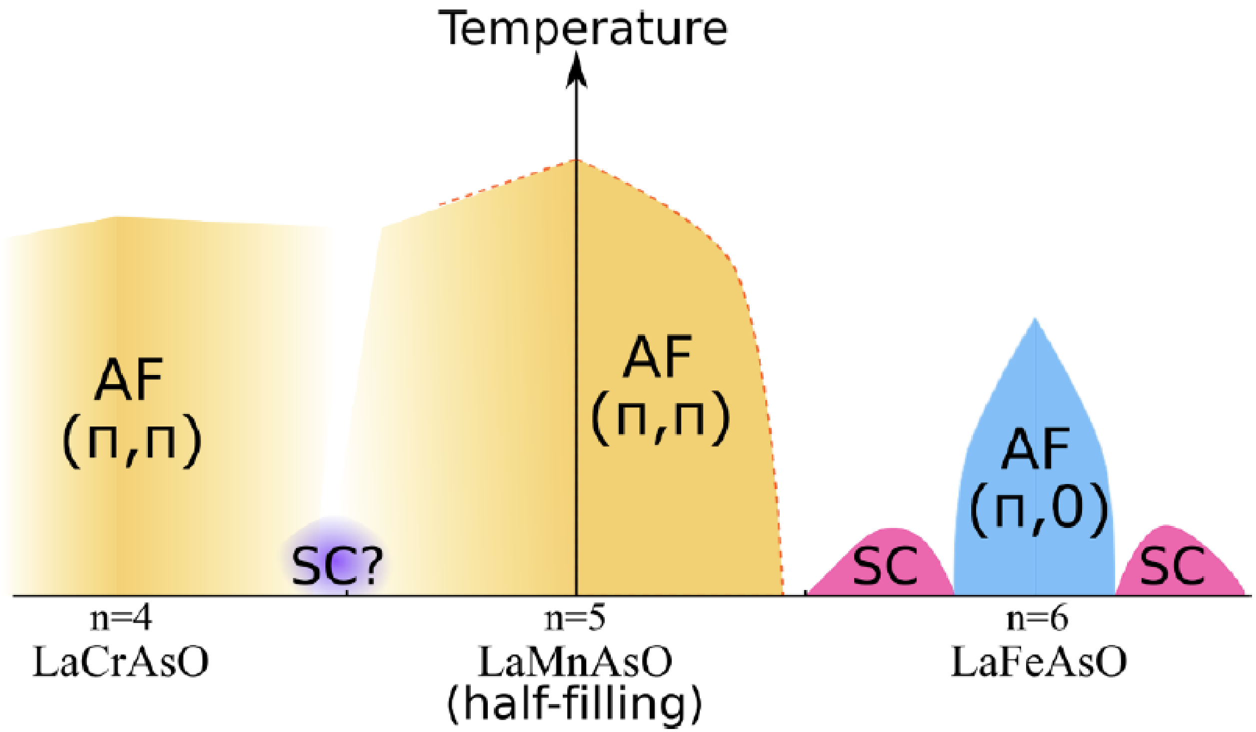
Fe^{2+} :n=6

Mn^{2+} :n=5

Cr^{2+} :n=4

Search for superconductivity & strong correlations in electron doped Cr-pnictides & chalcogenides with the same lattice structures as in iron superconductors.

Search for superconductivity at the other side of half-filling

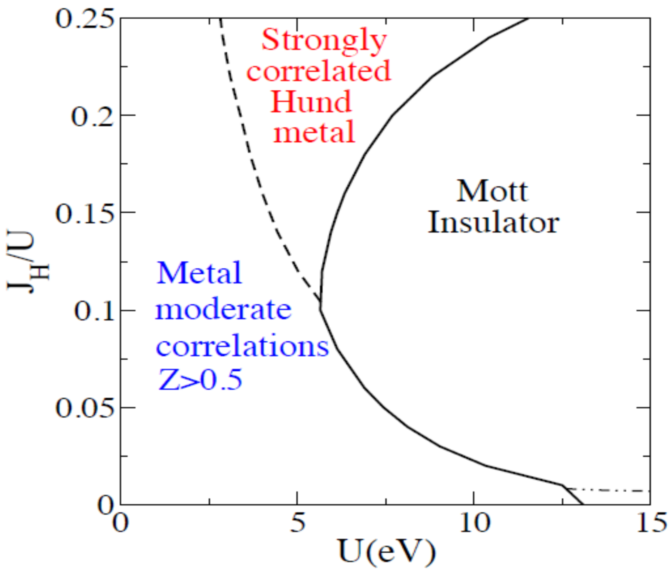


If they are found to be antiferromagnetic → Apply pressure to suppress magnetism and search for superconductivity

J.M. Pizarro et al, PRB 95, 075115 (2017)

Summary: Electronic correlations in iron superconductors

Status



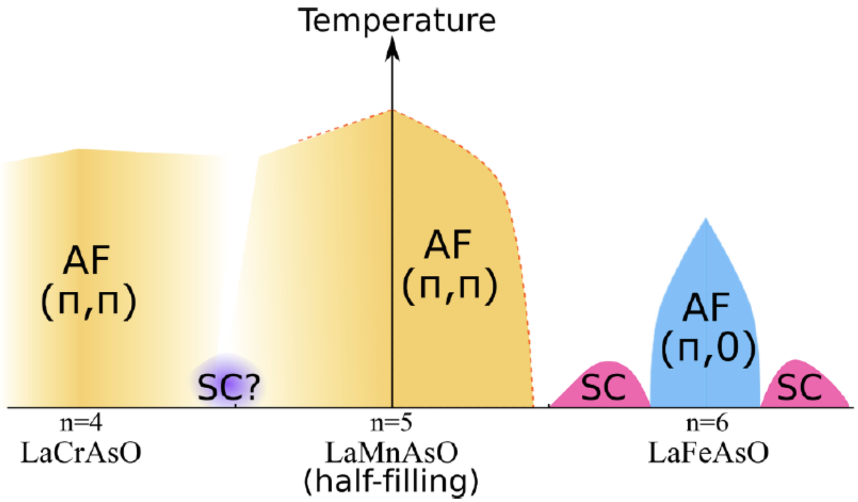
Review: E.B. et al, Comptes Rendus Physique 17, 36 (2016)

Interesting effect of Pressure in $BaFe_2S_3$

J.M. Pizarro & E:B: arXiv:1803.00282

Opportunities

Search for high-Tc superconductivity in chromium pnictides & chalcogenides



If they are found to be AF
apply pressure to suppress AF

J.M. Pizarro et al, PRB 95, 075115 (2017)

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Collaborators & Acknowledgments

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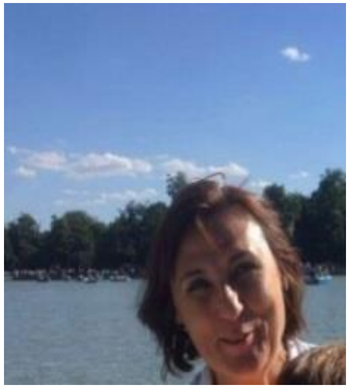

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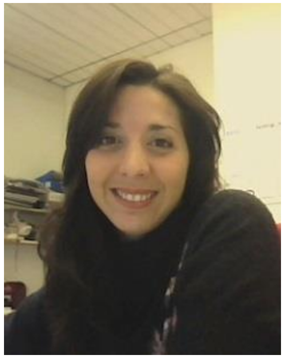

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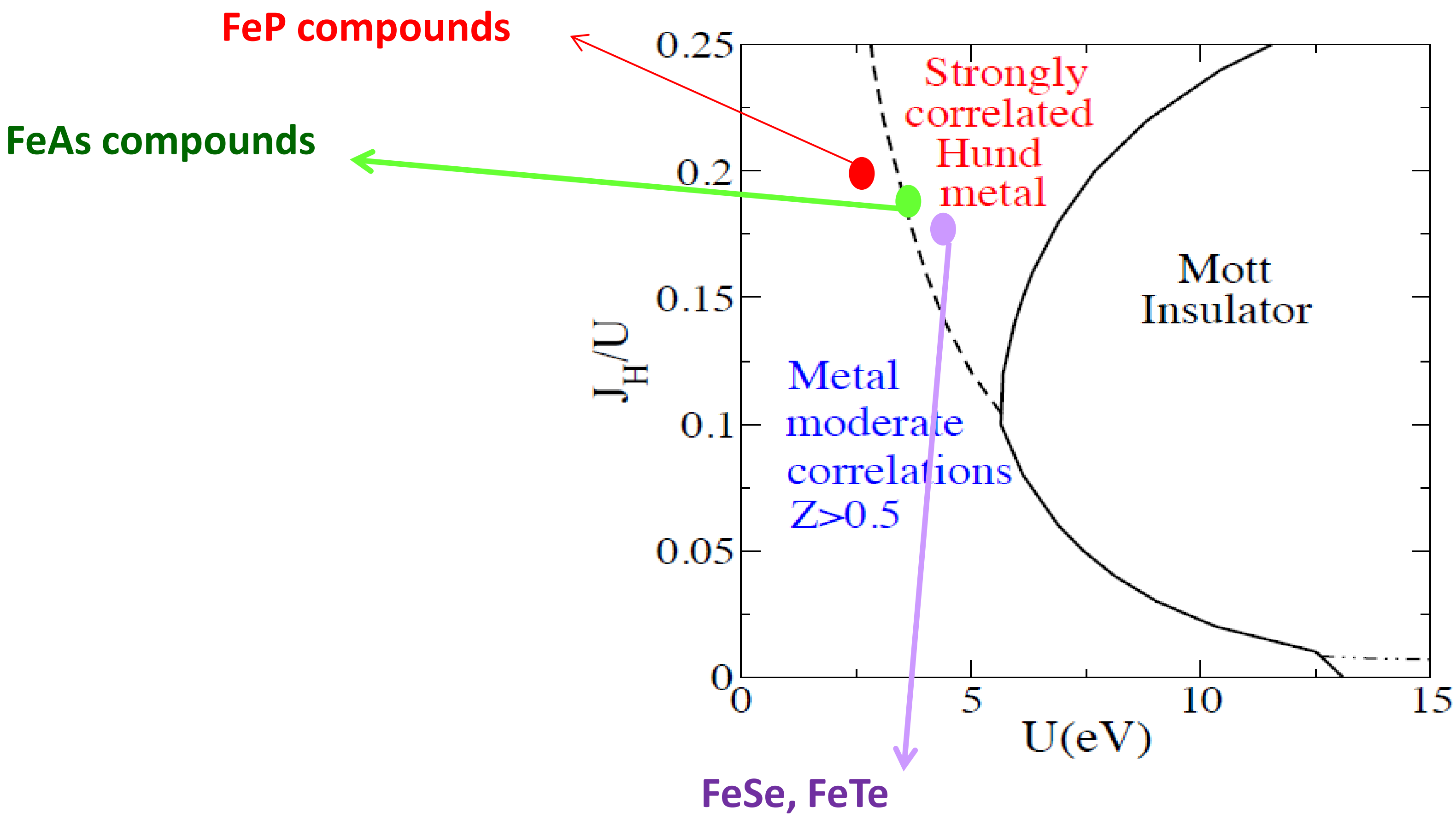
GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

FUNDACION RAMON ARECES

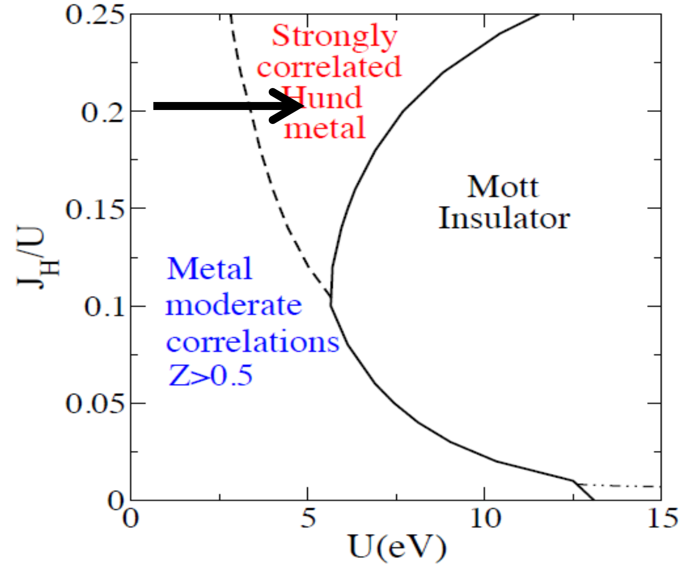
Strength of correlations in quasi-1d $BaFe_2S_3$

Undoped compounds



Strength of correlations in quasi-1d $BaFe_2S_3$

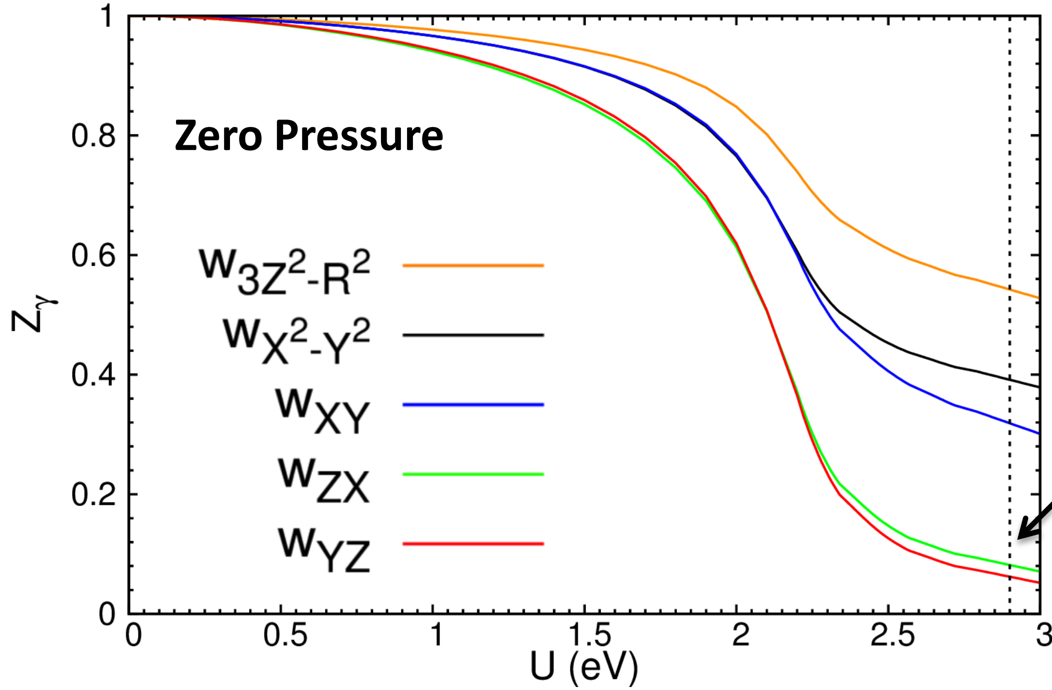
Quasiparticle weight (inverse mass enhancement): measurement of correlations



$1 \geq Z \geq 0$

Independent particle.
Non correlated

Mott insulator



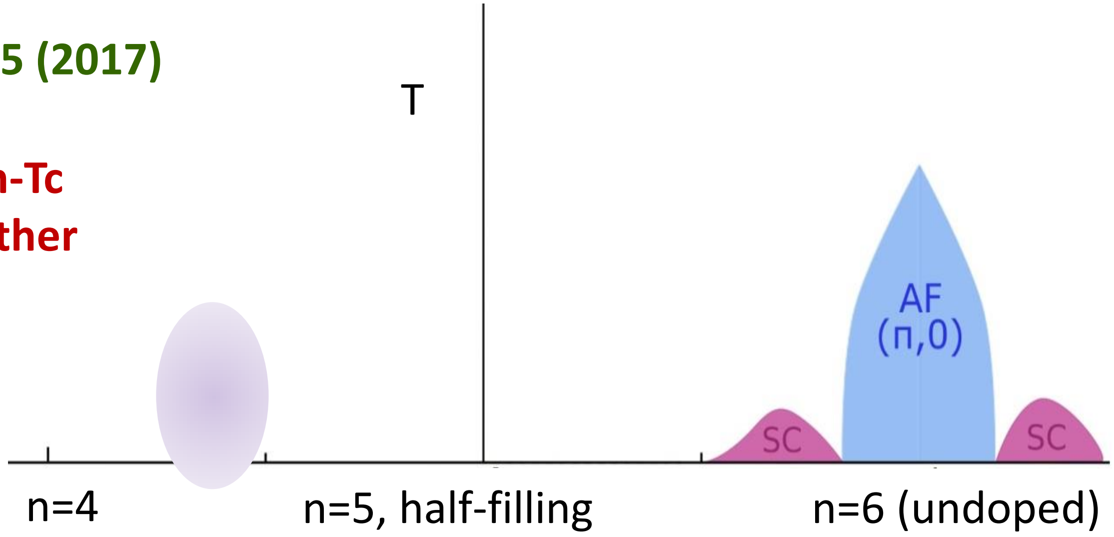
Two very strongly correlated orbitals
m*~12-15
but not a Mott insulator at T=0

J.M. Pizarro & E:B: arXiv:1803.00282

Chromium pnictides and chalcogenides

Pizarro et al, PRB 95, 075115 (2017)

Our proposal: look for high-Tc superconductivity at the other side of half-filling n<5

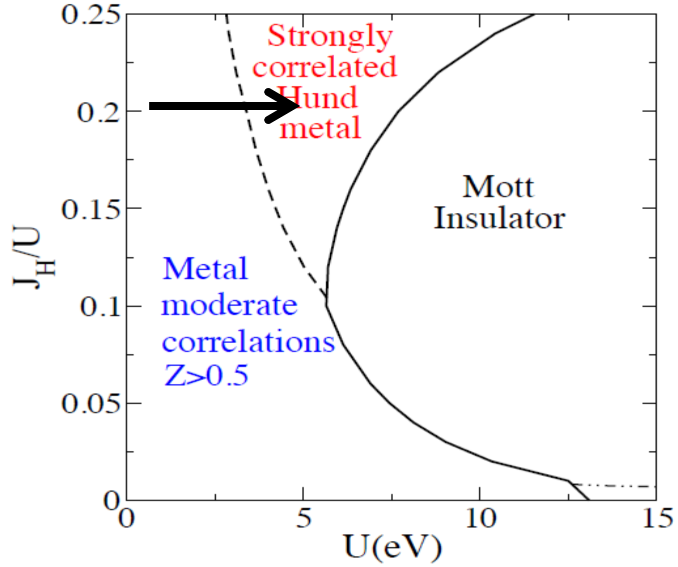


n=4 Undoped materials
(already synthesized)
LaCrAsO
$BaCr_2As_2$
$SrCr_2As_2$ → Dope them with Fe, Co at the Cr site, with La, Y at the cation site (Ba, Sr, Eu) or with F, H at the O site
$EuCr_2As_2$
$Ba_2Ti_2Cr_2As_4O$
Many other compounds or families (like 111) could be synthesized

Search for superconductivity & strong correlations in electron doped Cr-pnictides & chalcogenides with the same lattice structures as in iron superconductors.

Strength of correlations in quasi-1d $BaFe_2S_3$

Quasiparticle weight (inverse mass enhancement): measurement of correlations



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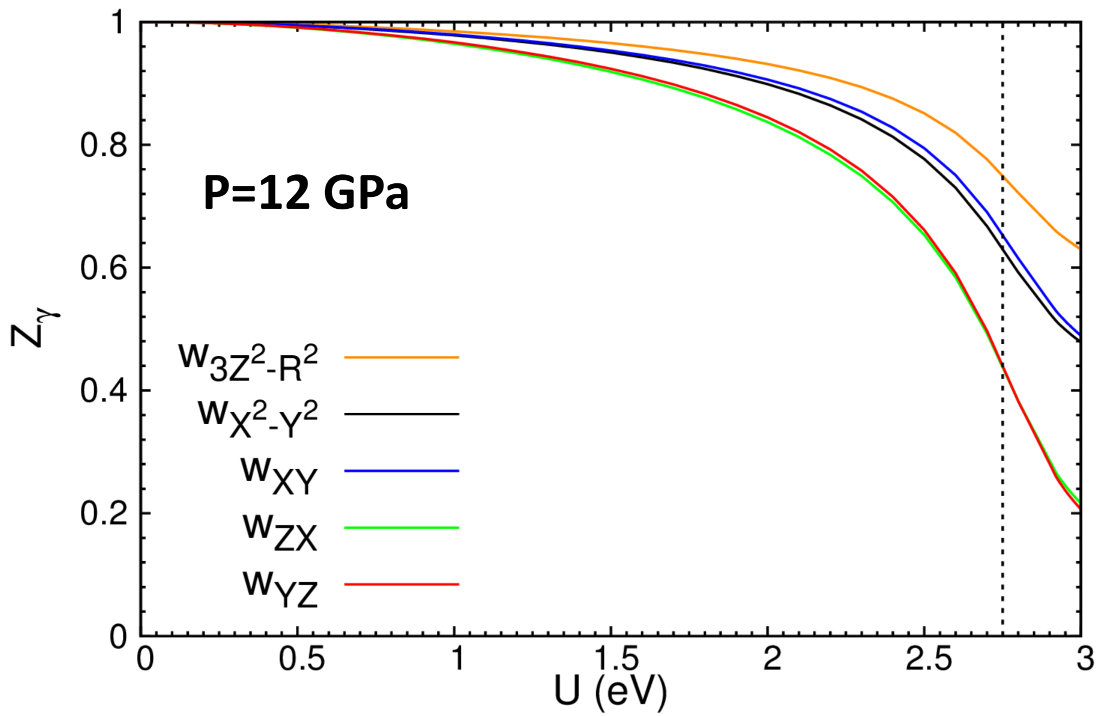
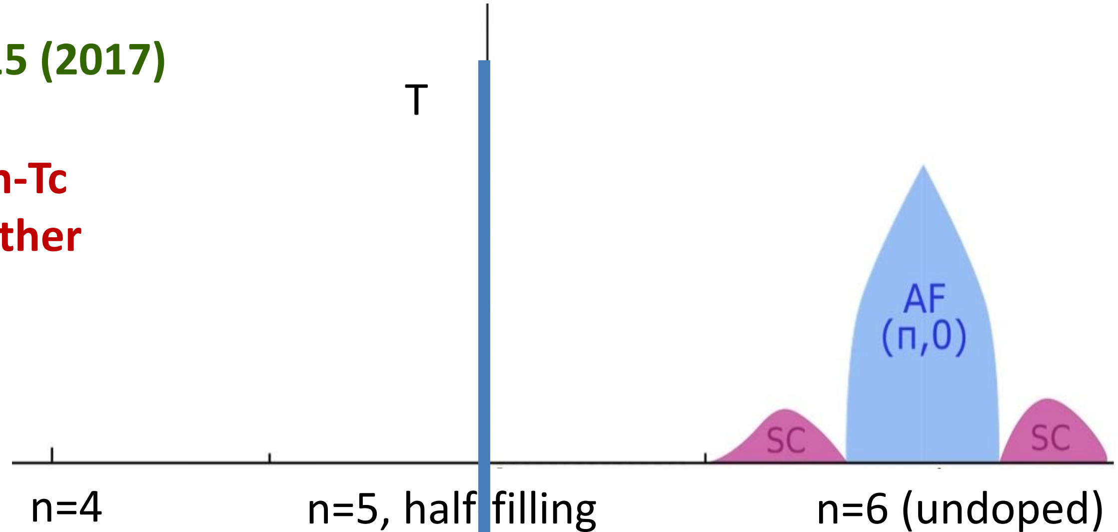


J.M. Pizarro & E:B: arXiv:1803.00282

Search for superconductivity at the other side of half-filling

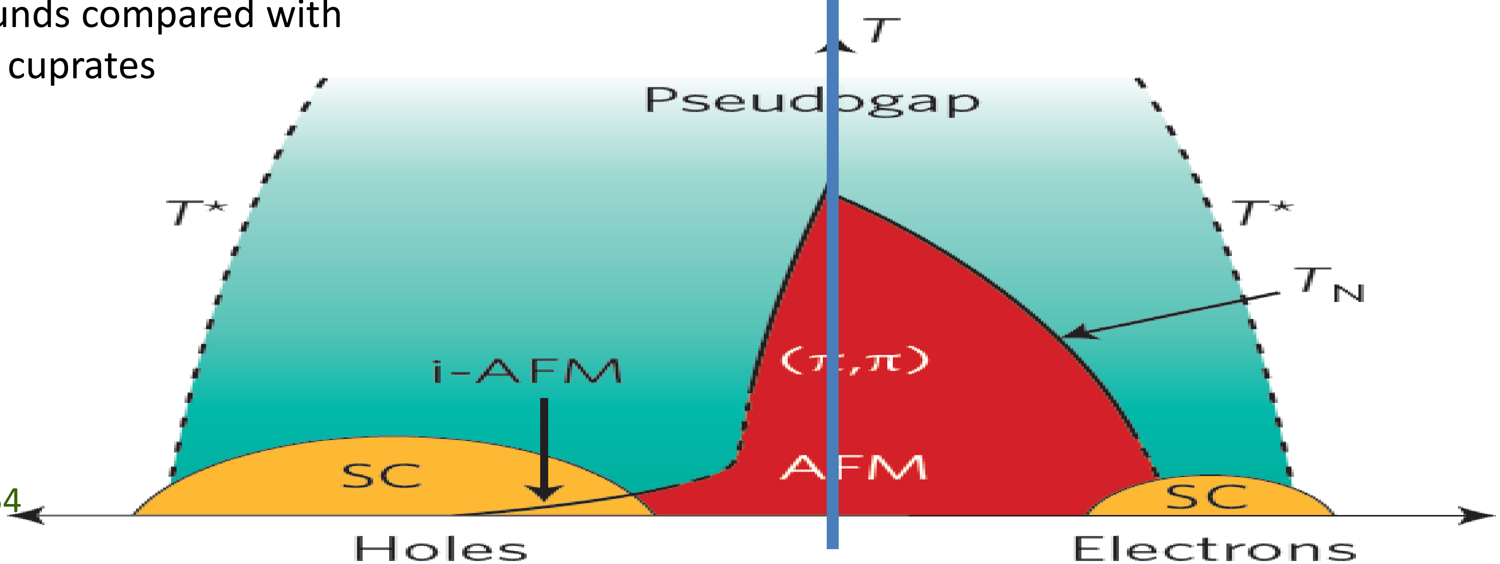
Pizarro et al, PRB 95, 075115 (2017)

Our proposal: look for high-Tc superconductivity at the other side of half-filling n<5



"Undoped" iron superconductors x=1.2
Compared with electron doped cuprates

n<5 compounds compared with
Hole-doped cuprates

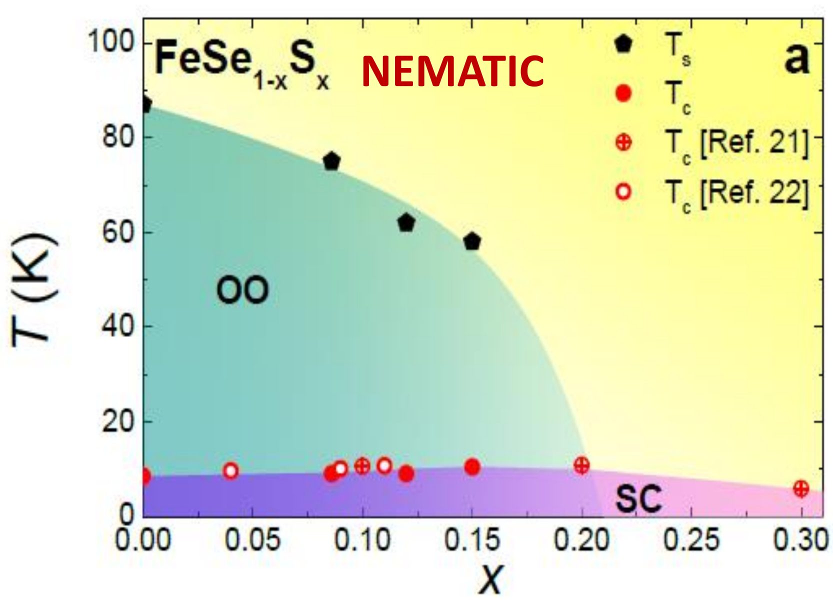


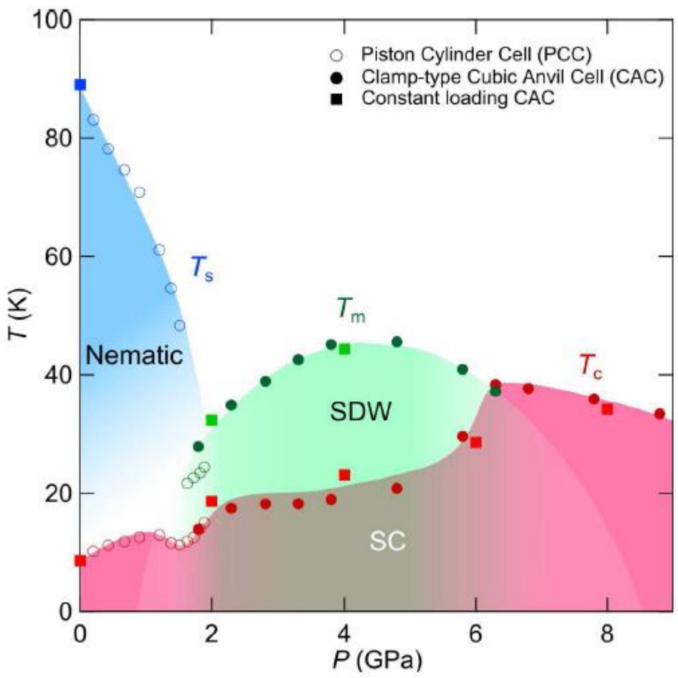
See also:
Edelmann et al,
arXiv:1610.10054

Iron superconductors: High-Tc superconductivity, magnetism and nematicity

Different materials present different phase diagrams

FeSe





Watson et al,
PRB 92, 121108 (2015)

Sun et al, Nat Commun. 7, 12146 (2016)