Nine years of iron superconductors, what have we learnt

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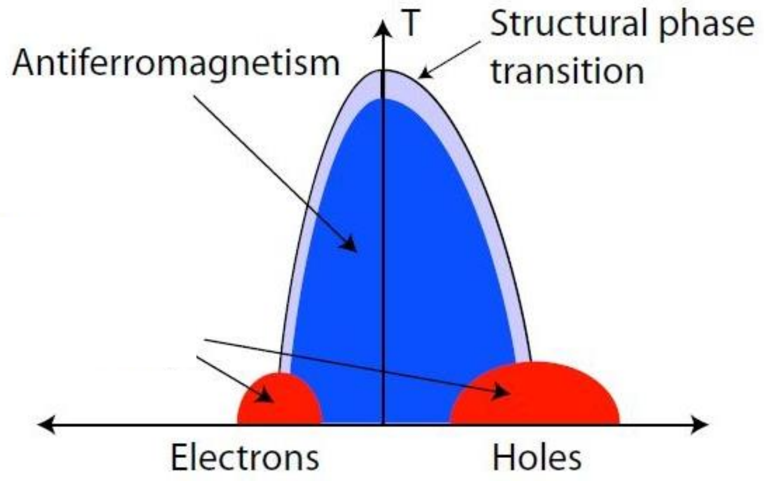


Outline

- Conventional vs non-conventional superconductors.

- Iron superconductors, basic properties & models
  - The materials
  - Non-universal phase diagrams
  - Band structure & multi-orbital character. Basic models

- Electronic correlations in iron superconductors. Hund metal physics

- Ordered phases

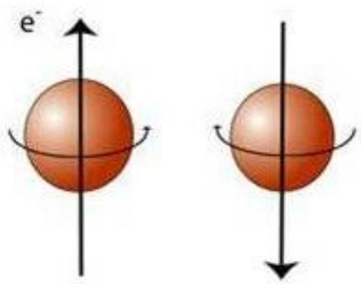
  - The magnetic state
  - Superconductivity: mechanism & order parameter
  - The nematic state: spin & orbital interplay

- Other issues

- Summary and future prospects.

Introduction to superconductivity

- 1911. Discovery. Resistivity vanishes below a critical temperature Tc
- 1933. Meissner effect. Superconductors expel the magnetic fields
- 1957. BCS Theory for superconductivity. Phase transition. Cooper pairs which condense & electron-phonon mechanism



$$\Psi = \prod_{\mathbf{k}=\mathbf{k}_1,\cdots,\mathbf{k}_{N/2}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} a^{\dagger}_{\mathbf{k}\uparrow} a^{\dagger}_{-\mathbf{k}\downarrow} \right) |0\rangle$$

$$E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2} \longrightarrow \text{Gap at the Fermi surface}$$

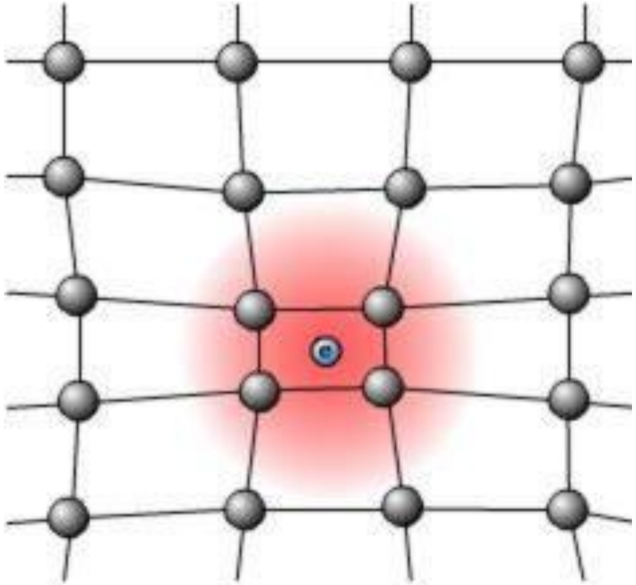
Electrons have equal charge & repel each other,
where is the attractive interaction coming from?

↓

Which is the mechanism of superconductivity?

Conventional vs non-conventional superconductors

- 1957. BCS Theory for superconductivity. Cooper pairs which condense & electron-phonon mechanism



In BCS theory the attraction between the electrons is mediated by the interaction with the vibrations of the atomic lattice (electron-phonon mechanism)

This mechanism works in many materials: The conventional superconductors

Non-conventional superconductors

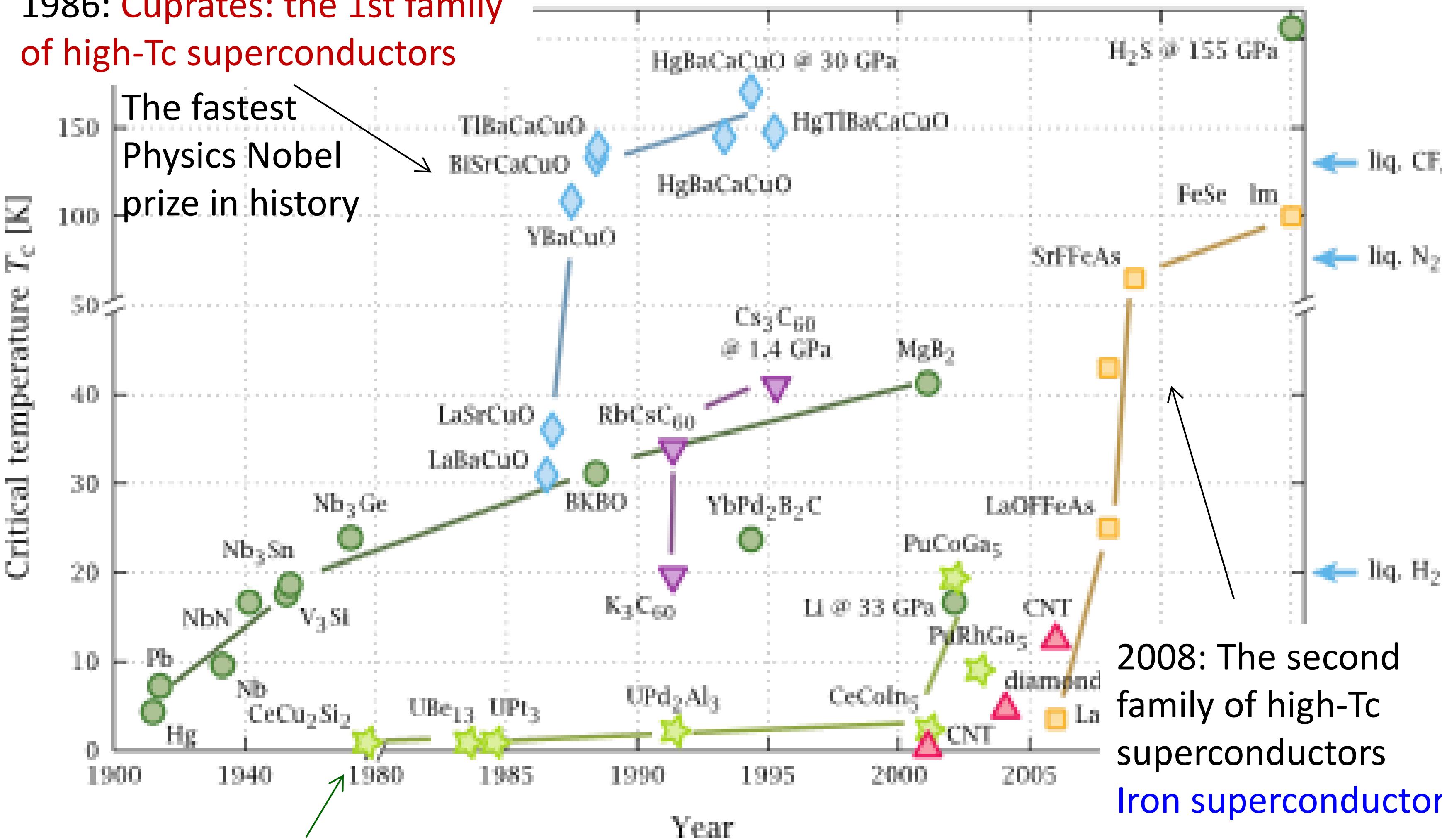
- Other possible sources of pairing were soon proposed: spin fluctuations, plasmons, …:

Note that 3He is a superfluid mediated by ferromagnetic spin fluctuations

Superconducting materials

1986: Cuprates: the 1st family of high-Tc superconductors

The fastest Physics Nobel prize in history

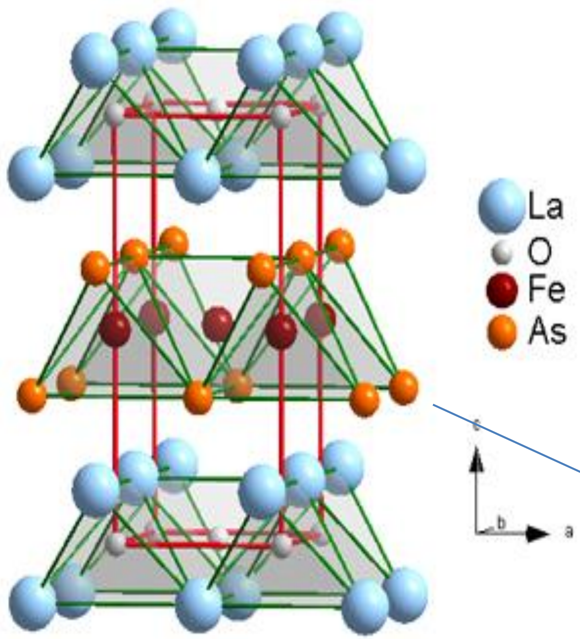


2008: The second family of high-Tc superconductors

Iron superconductors.

Superconductivity in heavy fermion compounds

In 2008 it starts the iron age



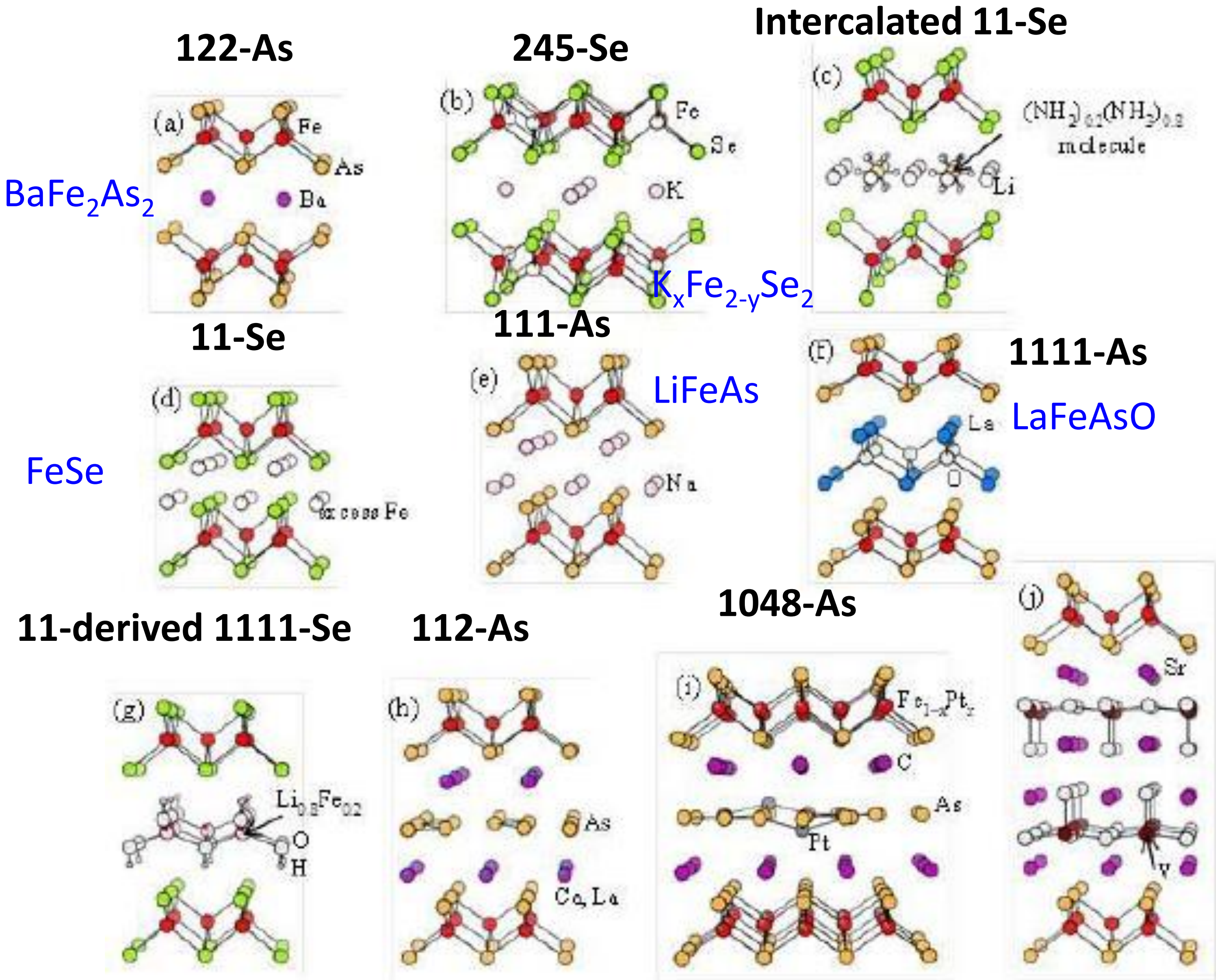
FeAs layer

The iron age

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

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

Iron superconductors: the materials, FeAs & FeSe layers



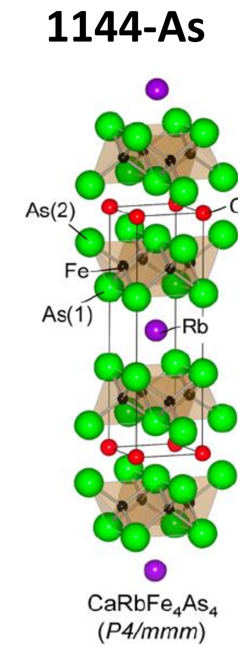
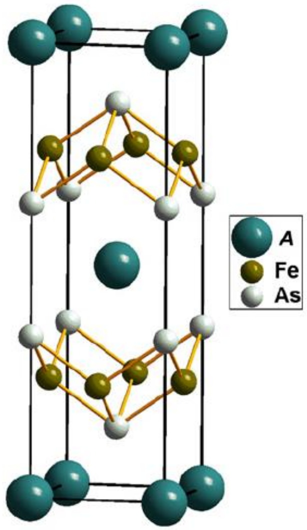


Fig: Iyo et al, JACS 138, 3410 (2016)

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

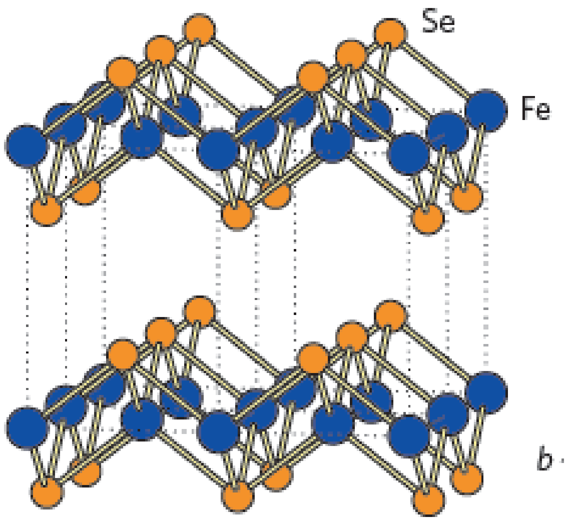
Iron superconductors: the materials, FeAs & FeSe layers



122-family ($BaFe_2As_2$, Sr_2As_2, …)

Most studied compounds due to availability of single crystals

FeSe (11 family)

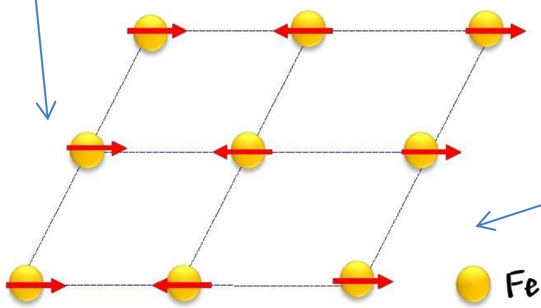


- In bulk and ambient pressure Tc=8 K
- Synthesized in monolayer form with higher Tc (65 K or above 100 K?)
- Phase diagram (nematic phase)
- Tiny Fermi surfaces. BEC-BCS crossover

Fig: Baek et al, Nat. Mat. 14, 210 (2015)

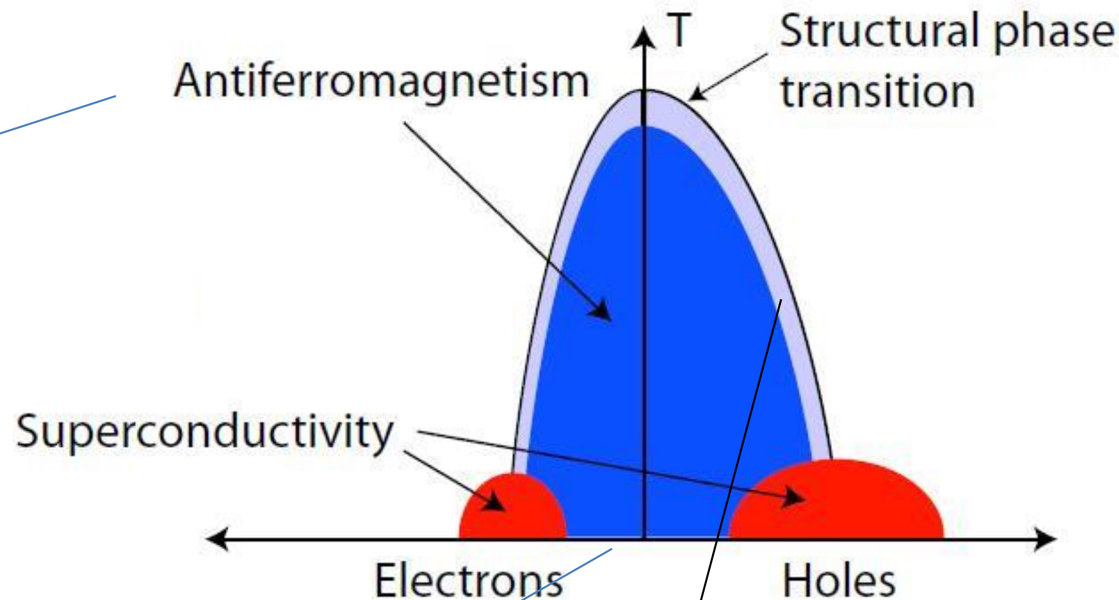
The phase diagram of early discovered iron superconductors

Ferromagnetic in Y direction



Antiferromagnetic in X direction

Pnictides (FeAs systems)



Undoped system
(6 electrons per Fe)

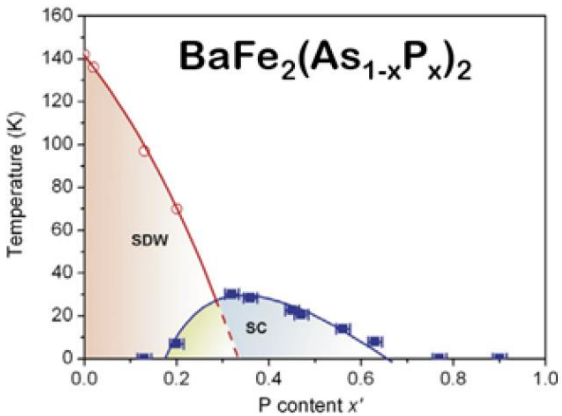
Nematic state
(anisotropic in plane)

Fig: Lanzara's webpage

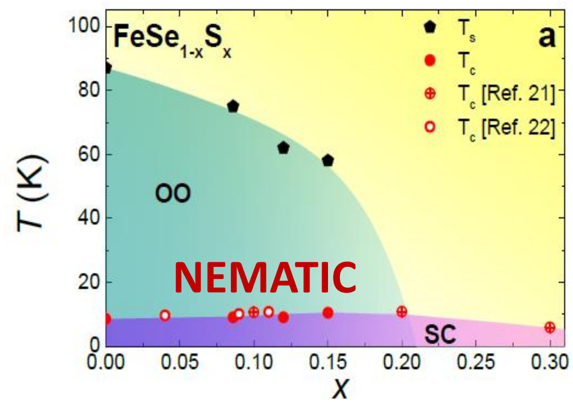
De la Cruz et al, Nature 453, 899 (2008), Zhao et al, Nature Materials 7, 953 (2008)

High-Tc superconductivity in iron based materials: The phase diagram

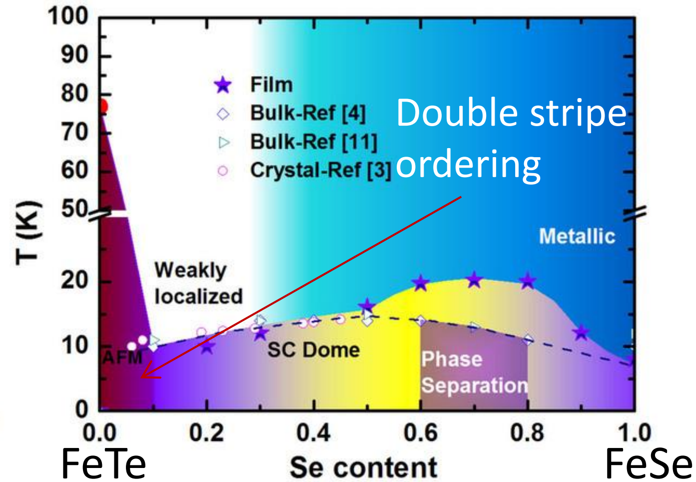
Isovalent substitution



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

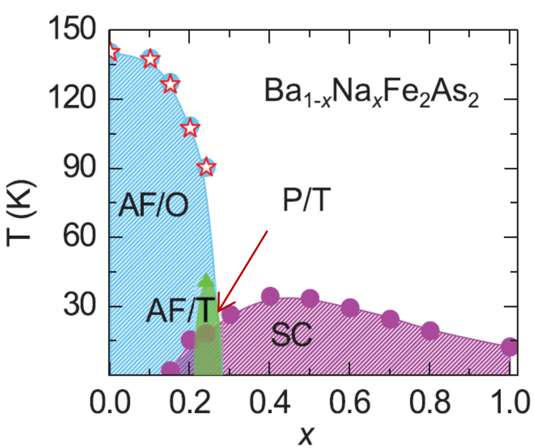


Watson et al, PRB 92, 121108 (2015)

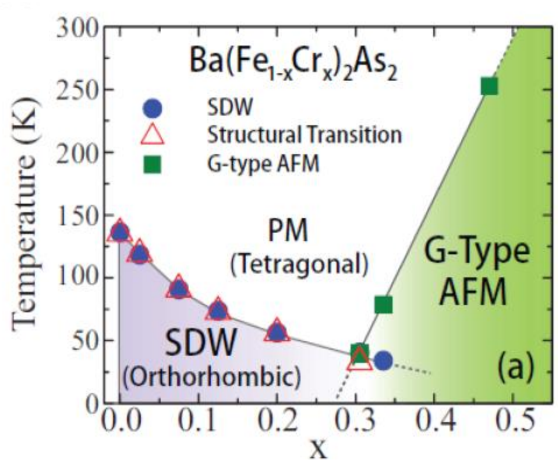


Zhuang et al, Sci. Rep. 4 7273 (2014)

Hole doping

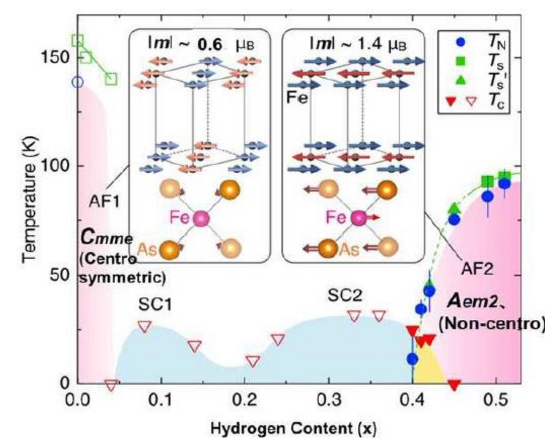


Avci et al,
Phys. Rev. B 88, 094510 (2013)



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

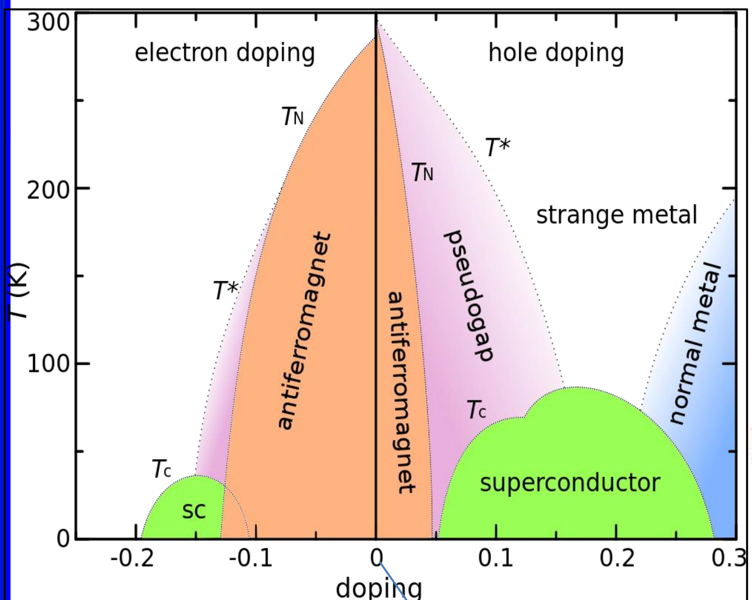
Electron doping



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

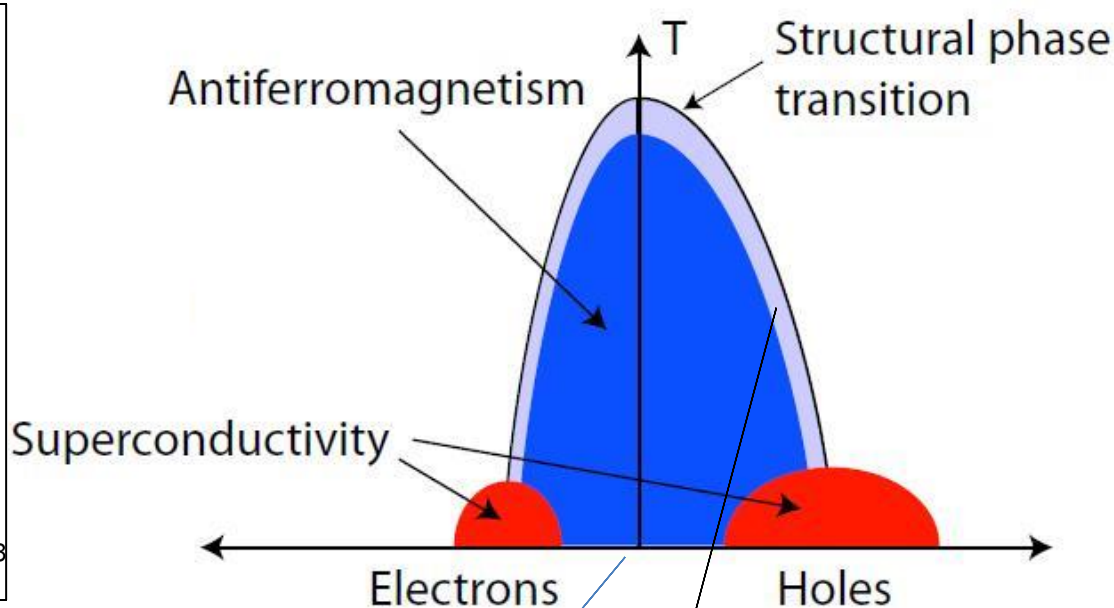
The phase diagram of early discovered iron superconductors

Cuprates



Mott Insulator

Pnictides (FeAs systems)



Metallic

Nematic state
(anisotropic in plane)

Fig: Lanzara's webpage

The phase diagram of early discovered iron 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 that of cuprates related?
- Which is the origin of the nematic phase?

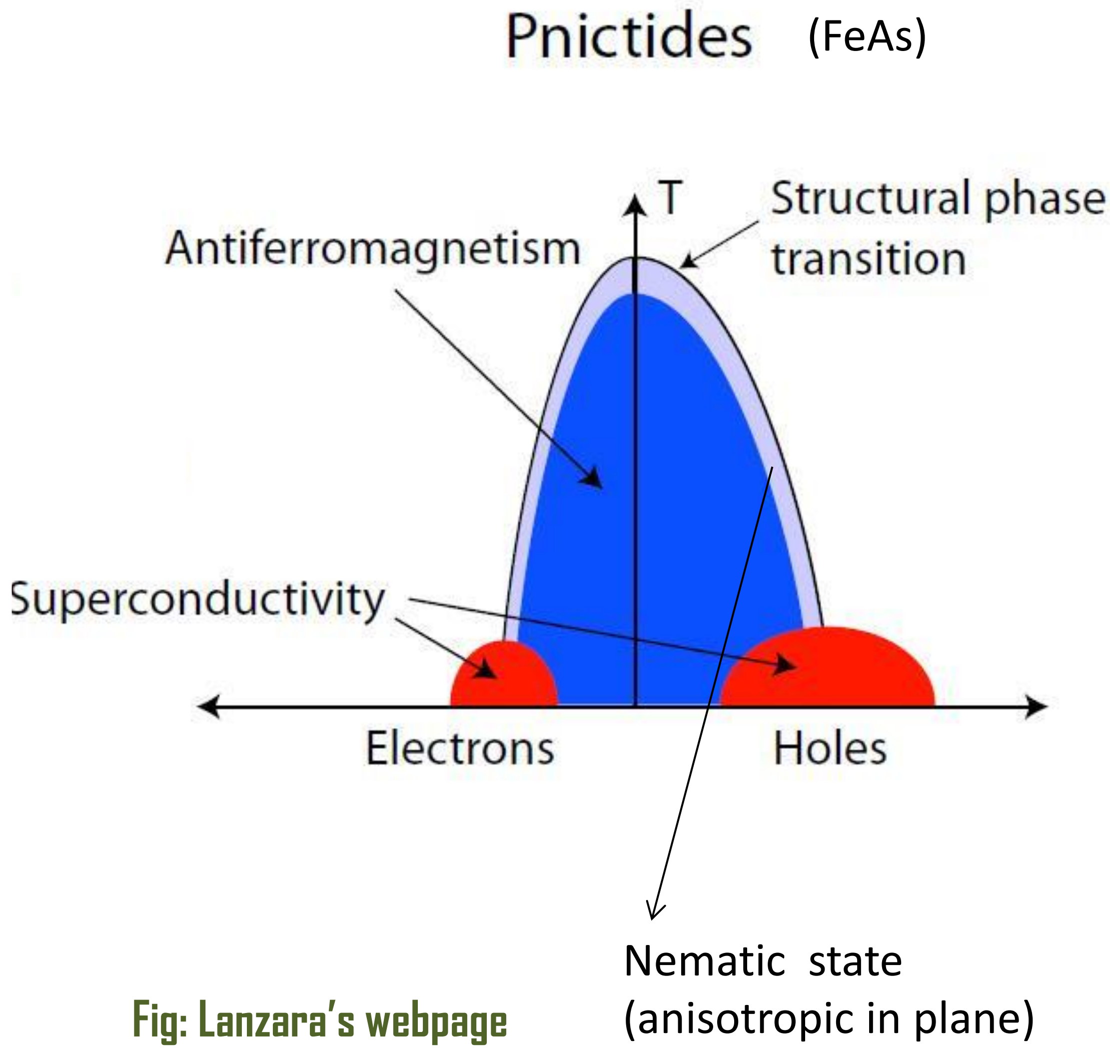


Fig: Lanzara's webpage

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

To study the iron superconductors:

Systems under study

- Different families & compounds
- Role of hole & electron doping with different dopants
- Role of pressure
- Role of temperature
- Isovalent doping
- Role of disorder …

Many techniques

- ARPES
- Resistivity
- Neutrons
- STM
- NMR
- Raman
- Optical conductivity
- Quantum oscillations
- X-ray
- Magnetic torque …

Theory

- Ab-initio
- Microscopic models
- Effective models (different assumptions)
- Approximations: RPA, Hartree-Fock, Renormalization Group, Slave-spin
  DMFT
  Landau-Ginzburg ….
  Spectroscopic properties

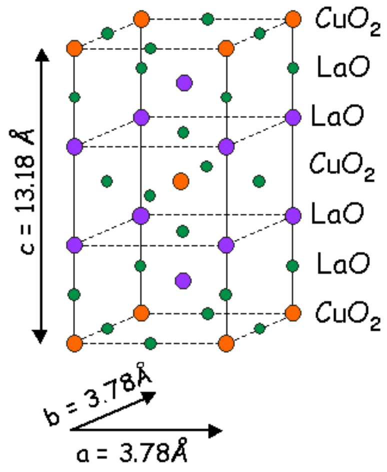
The phase diagram of early discovered iron superconductors

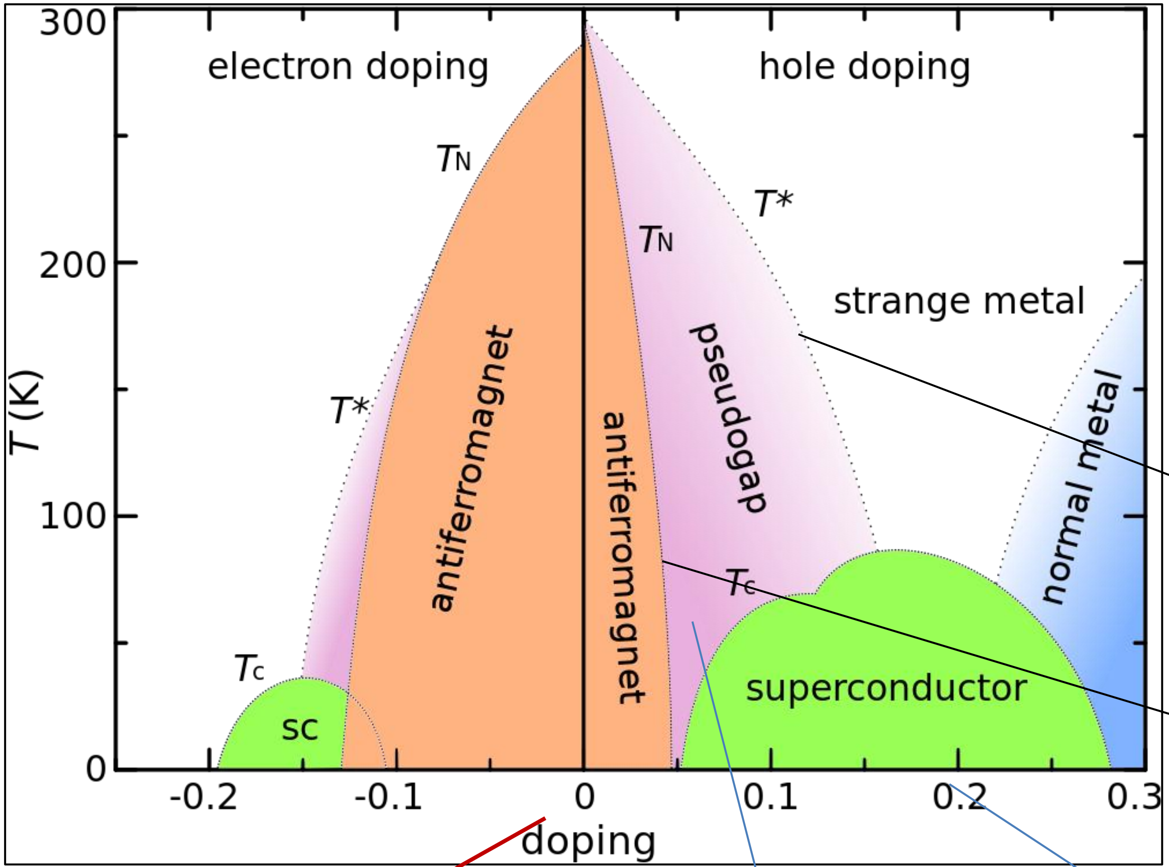
- ❑ Which is the origin of the high-Tc superconductivity?
- ❑ Can we find new materials with higher Tc?
- ❑ Are the physics of iron superconductors and that of cuprates related?
- ❑ Which is the origin of the nematic phase?

Key issues:

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

The physics of high-Tc superconducting cuprates





Pseudogap region: very strange properties

D-wave Superconductivity Appears when antiferromagnetism is suppressed

Tendency towards anisotropic states (stripes)

Quantum critical point?

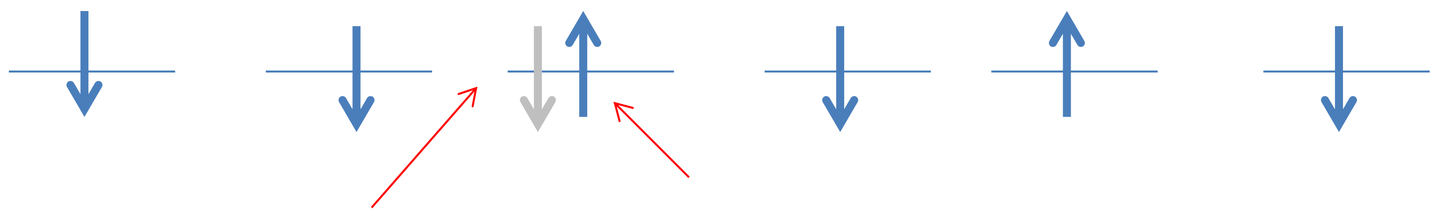
The parent compound (zero doping) is a Mott insulator

Mott insulators

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

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

Repulsion in undoped cuprates is so strong that it can drive the system into an insulating state

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

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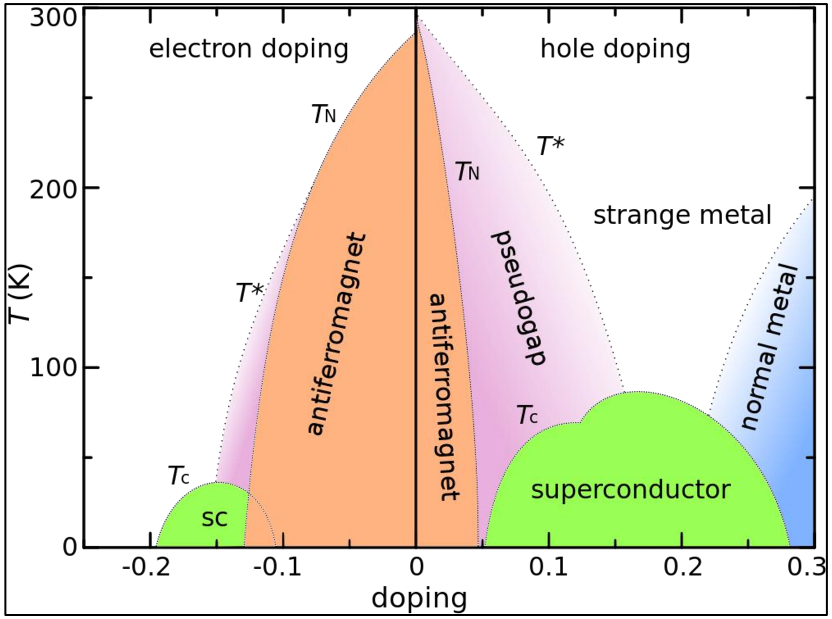
The physics of high-Tc superconducting cuprates



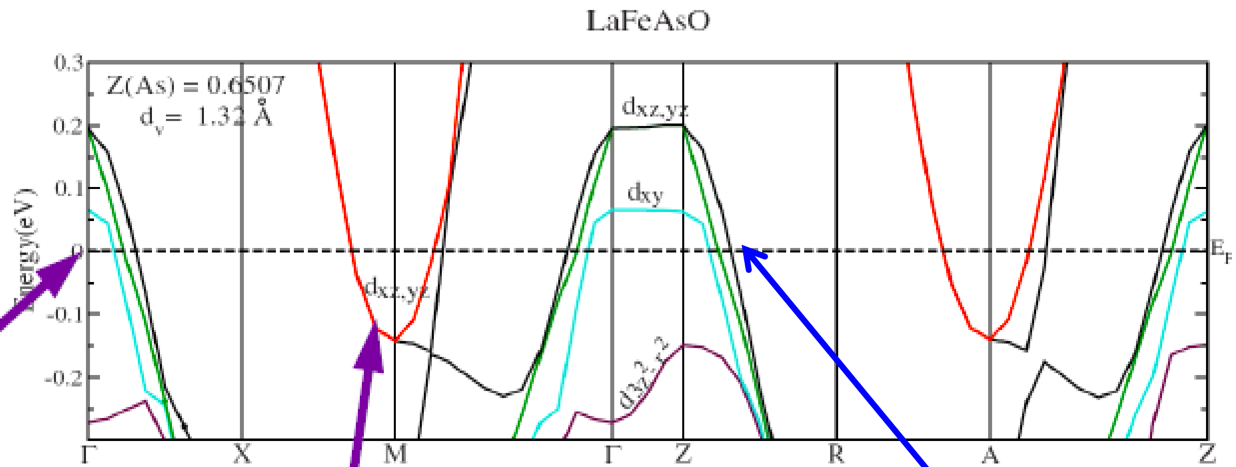
- Proximity to antiferromagnetism
- Possible role of quantum criticality
- Possible role of anisotropic states

Cuprates: doping a Mott insulator in 2D

Are the strong (Mott) correlations a requisite for the high-Tc superconductivity?

Band structure & multi-orbital character.

DFT calculations



Hole pockets

Electron pockets

Vildosola et al, PRB 78, 064518 (2008)

Several Fe bands cross the Fermi level

Basic models to describe iron superconductors

Tight-binding + interaction Hamiltonians treated in different approximations

Allow to study the strength of correlations & include the orbital degree of freedom

Basic models to describe iron superconductors

Tight-binding + interaction Hamiltonians treated in different approximations

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

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

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

Hund's coupling

In general only local interactions are included but some models include 1st nearest neighbors to discuss the nematic state of FeSe

Basic models to describe iron superconductors

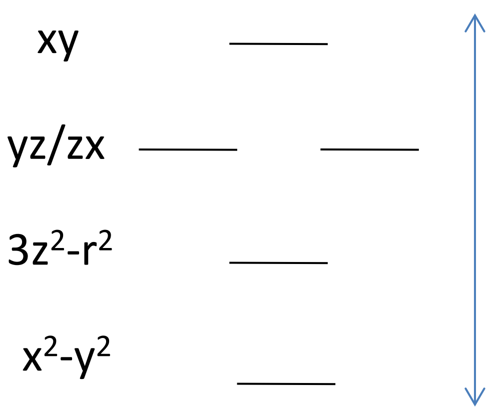
$$H = \sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^{\dagger} c_{j,\beta,\sigma} + h.c. + U \sum_{j,\gamma} n_{j,\gamma,\uparrow} n_{j,\gamma,\downarrow}$$

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

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

Hund's coupling

Small crystal field differences



At least the 5 Fe d-orbitals are necessary to describe the electronic properties (maybe even more):

Undoped system 6 electrons in 5 orbitals

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Mott insulators vs weakly correlated metals

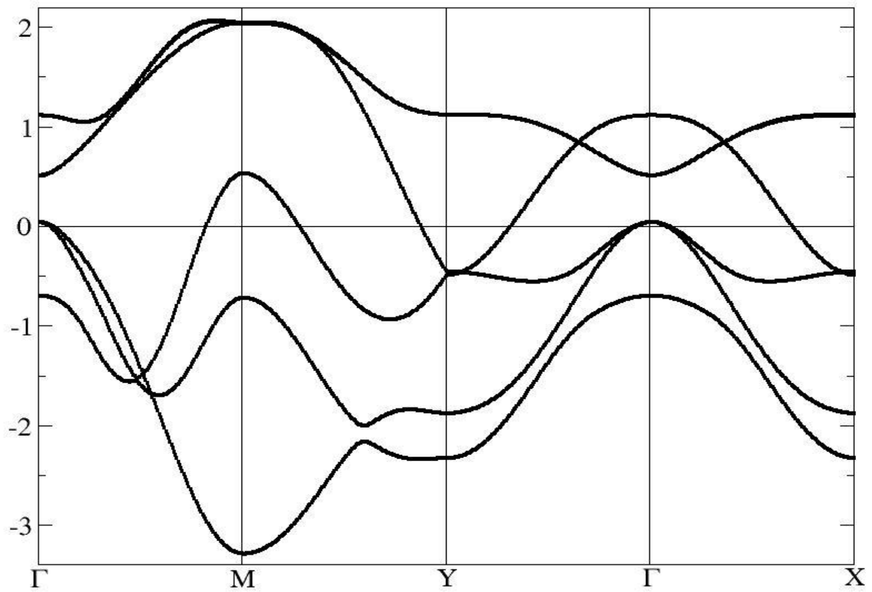
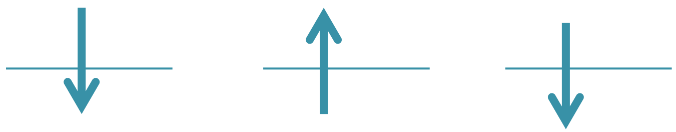


Fig: Calderón et al, PRB, 80, 094531 (2009)

Weakly interacting Metal:
Electrons delocalized in real space, localized in k-space.
Description in terms of electronic bands
Ordered phases: Fermi surface instabilities



Mott Insulator:
Electrons localized in real space, delocalized in k-space.
Spin models. Description as localized spins is meaningful
Ordered phases: interactions between spins

Basic models to describe iron superconductors

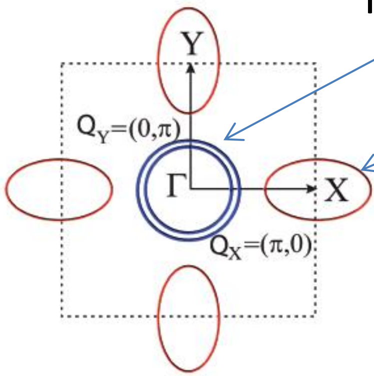
Tight-binding + interaction Hamiltonians treated in different approximations

Models with focus on electronic states close to the Fermi surface (k-space models), Itinerant description.

Spin models which assume that the electrons are localized,
real space description

Basic models

- **Weakly correlated models**. Focus on the Fermi surface bands close to the Fermi level (k-space description, assumes weakly correlated metal)



Hole pockets

Electron pockets

Necessary to include the orbital content

- **Localized Electrons**. Focus on spin models (real space description, assumes localized electrons)

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

Heisenberg Hamiltonian to 1st and 2nd nearest neighbors (a J_3 term to 3rd nearest neighbors included to explain the Magnetic order of FeTe)

$$K_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j \right)^2$$

Iron superconductors: Basic properties and models

- High-Tc superconductivity in materials with FeAs or FeSe layers. Many compounds belonging to at least 11 families. Tc up to 65 K or even aborve 100 K (monolayer FeSe)?

- The phase diagram is not unique. The most common phases are stripe antiferromagnetic, nematic phase, superconducting phase. Other magnetic orders (like double stripe in FeTe or C4 phase in hole-doped systems) have been observed. Some compounds show two superconducting domes.

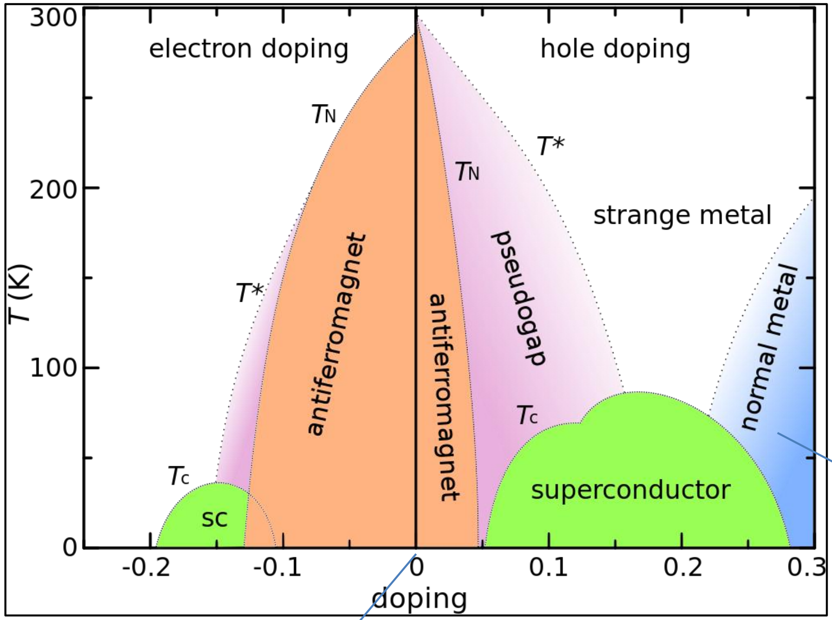
- Phase diagram with common features to that of cuprates (but also important differences)

- Iron superconductors are multi-orbital systems.

- Different approaches to study these materials:

    - Multi-orbital interacting models
    - Low energy models (Fermi surface physics)
    - Spin models (localized electrons)

The physics of high-Tc superconducting cuprates



- Proximity to antiferromagnetism
- Possible role of quantum criticality
- Possible role of anisotropic states

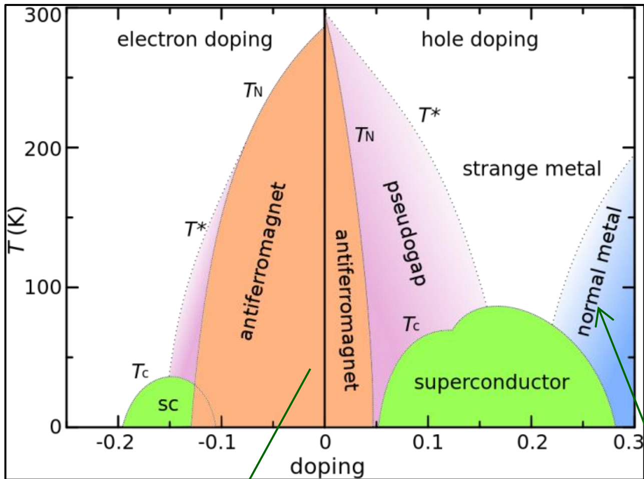
Normal metal:
Itinerant system
description in k-space
Fermi surface instabilities

Mott insulator
Localized system
Spin models in
Real space

Cuprates: doping a Mott insulator in 2D

Are the strong (Mott) correlations a requisite for the high-Tc superconductivity?

Correlations in iron superconductors



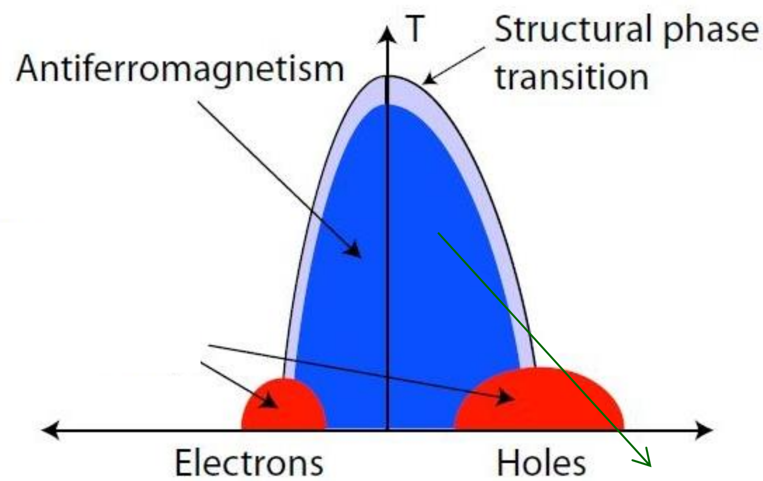
Cuprates phase diagram

Itinerant electrons

Mott insulator

Localized electron
(very strong correlations)

FeAs based superconductors



Metallic state

Does this mean that the electrons are not correlated in iron superconductors?

Strong correlations: enhanced mass

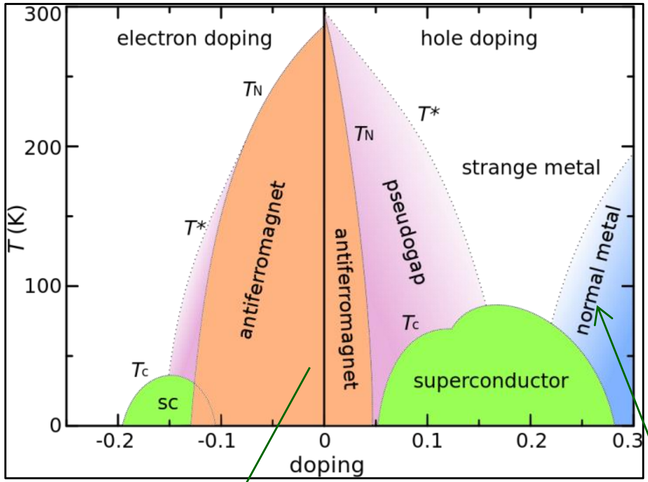
- Many body states, important deviations from DFT predictions which is based on an independent particle description (band theory)

- In some cases, the single-particle band description fails completely. Mott insulators: expected to be metals by band theory but insulators due to correlations

- Fermi liquid: in most cases at low energies and temperatures it is still possible to describe the system in terms of single particle bands and excitations (quasiparticles) with renormalized properties (mass m*, specific heat, spin susceptibility, Drude weight …)

Enhanced electronic mass m* as a measure of correlations

Correlations in iron superconductors



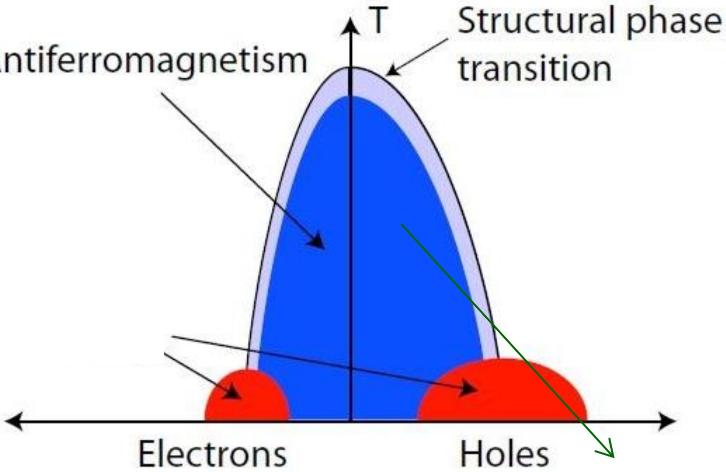
Cuprates phase diagram

Itinerant electrons

Mott insulator

Localized electron
(very strong correlations)

FeAs based superconductors



Metallic state

Does this mean that the electrons are not correlated in iron superconductors?

Mass enhancements in FeAs systems m* ~2-3
(in chalcogenides even larger)

Not clear which should be the best starting point to describe iron superconductors

Correlations in iron superconductors: Hund's physics

So far dichotomy:

Fermi surface physics

Weak correlations
Itinerant electrons
No local moments

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)

Mott physics

Strong correlations
Localized electrons
Local Moments

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

Correlations in iron superconductors: Hund's physics

So far dichotomy:

Fermi surface physics

Weak correlations
Itinerant electrons
No local moments

Mott physics

Strong correlations
Localized electrons
Local Moments

Hund physics

Strong correlations
Local moments
Itinerant electrons

↓

Hund metal
(new concept)

Important role, not only in iron superconductors but also in multi-orbital oxides and other systems

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,PRB 92, 075136 (2015)

Correlations in iron superconductors: Hund's physics

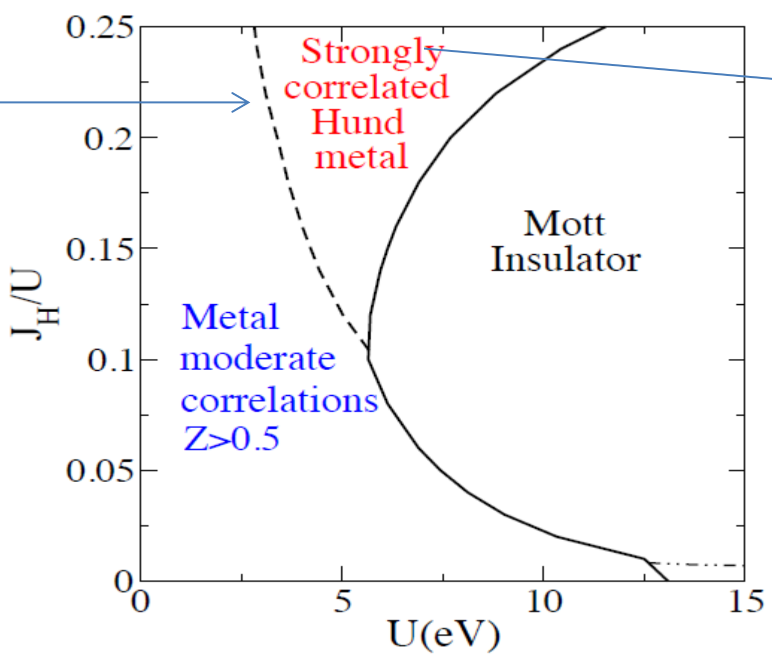
$$H = \sum_{i,j,\gamma,\beta,\sigma} t_{i,j}^{\gamma,\beta} c_{i,\gamma,\sigma}^{\dagger} c_{j,\beta,\sigma} + h.c. + U \sum_{j,\gamma} n_{j,\gamma,\uparrow} n_{j,\gamma,\downarrow}$$
$$+ (U' - \frac{J_H}{2}) \sum_{j,\gamma>\beta,\sigma,\tilde{\sigma}} n_{j,\gamma,\sigma} n_{j,\beta,\tilde{\sigma}} - 2J_H \sum_{j,\gamma>\beta} \vec{S}_{j,\gamma} \vec{S}_{j,\beta}$$
$$+ J' \sum_{j,\gamma\neq\beta} c_{j,\gamma,\uparrow}^{\dagger} c_{j,\gamma,\downarrow}^{\dagger} c_{j,\beta,\downarrow} c_{j,\beta,\uparrow} + \sum_{j,\gamma,\sigma} \epsilon_{\gamma} n_{j,\gamma,\sigma}$$

Hund's coupling

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

6 electrons (undoped)

Crossover



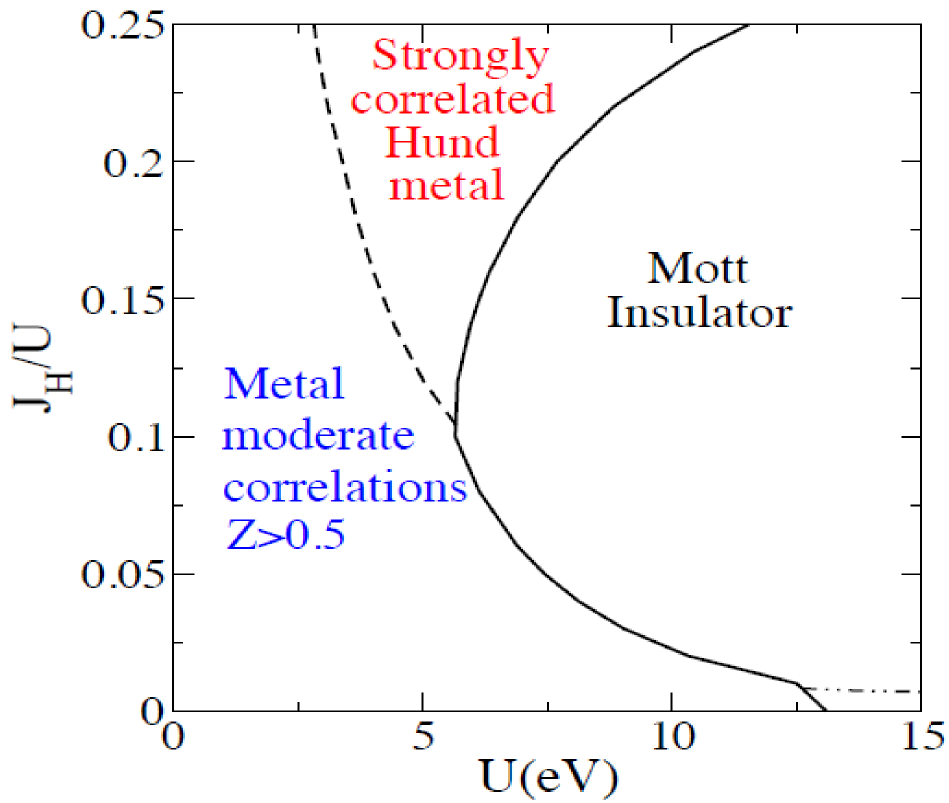
Strong correlations between electrons (large mass enhancement) due to Hund's rule coupling. Large local spin moments.

But electrons can hop between neighboring atoms.

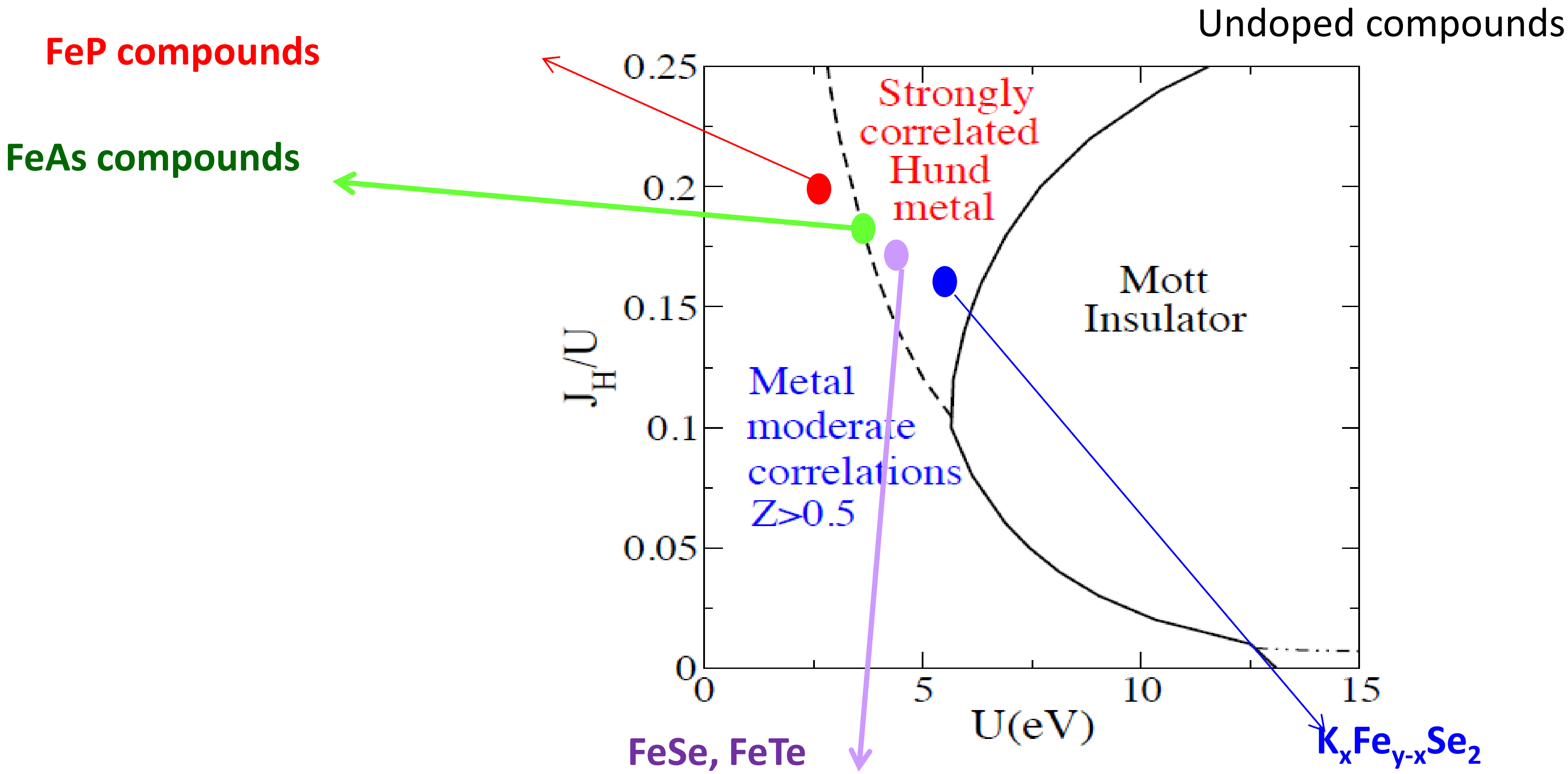
Orbital decoupling: Different orbitals present different strength.

Yu & Si, PRB 86, 085104 (2012)

Correlations in iron superconductors: Hund's physics



Correlations in iron superconductors: Hund's physics

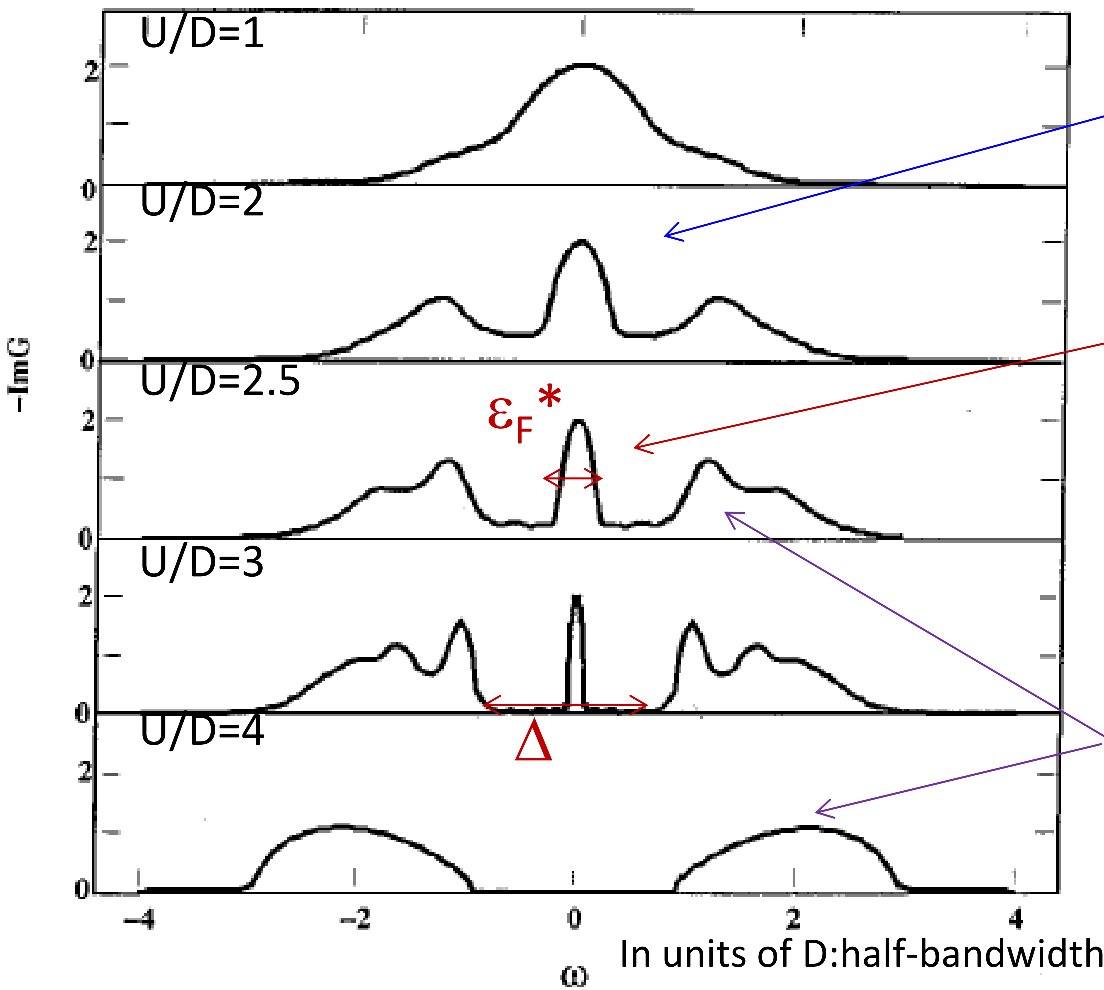


From analysis of: ARPES,
Neutron & Xray experiments,
Quantum oscillations,
Comparison with theory …

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

Mott transition. Paramagnetic state. DMFT picture. 1band

Increasing interaction



Three peak structure

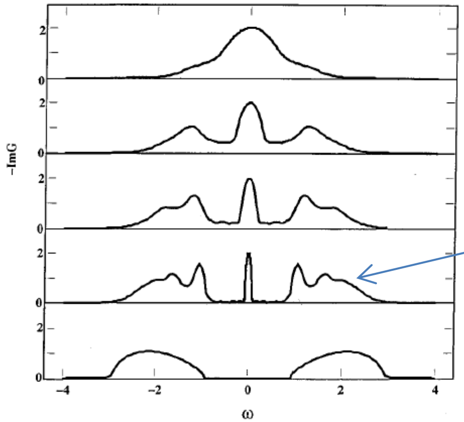
Heavy quasiparticles
Single-particle part
of the excitation
(coherent:bands)

Hubbard bands-
many body states
(incoherent or continuum)

Infinite dimensions

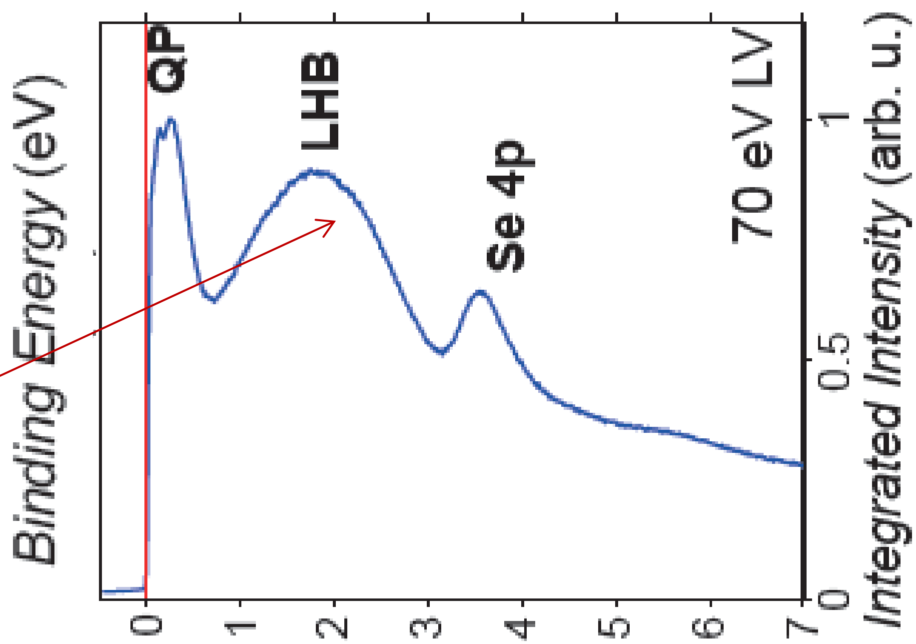
Georges et al , RMP 68, 13 (1996)

Correlations in iron superconductors



Hubbard bands very wide and spread in Hund metals:
It is difficult to identify them

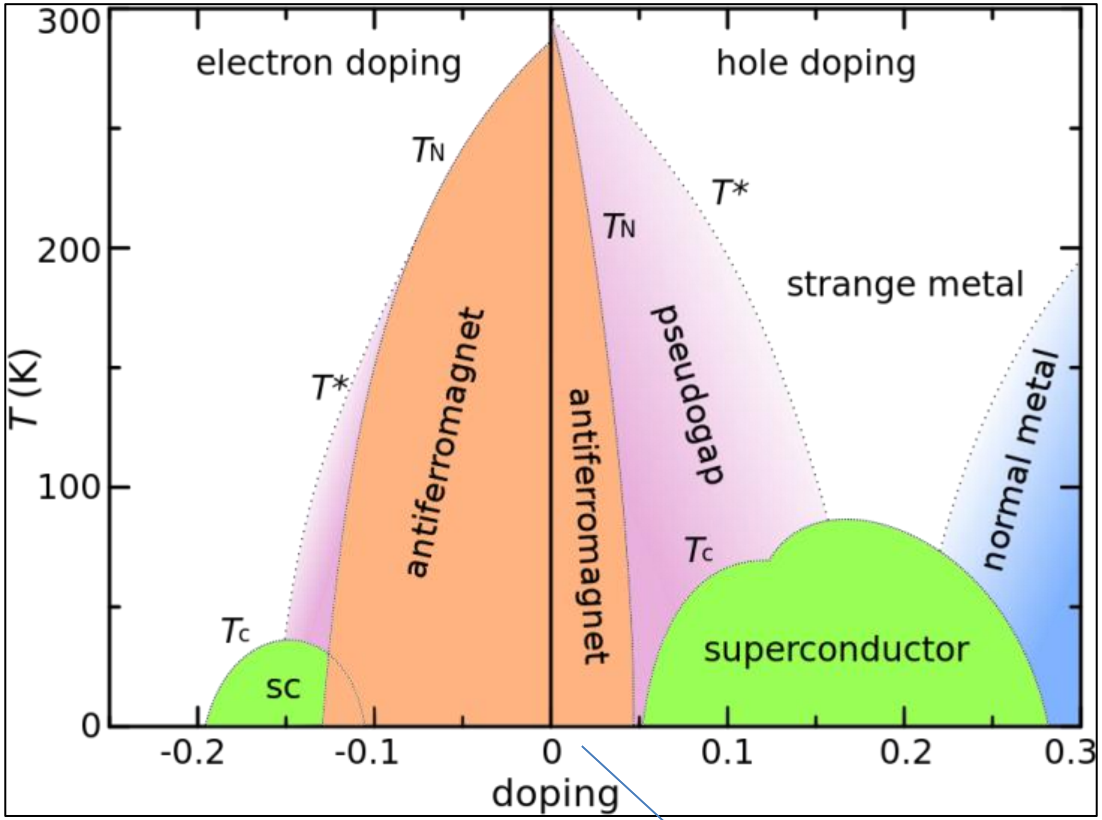
Observation of Lower Hubbard Band in FeSe (ARPES)



Clear evidence of
strong correlations
in iron superconductors

Watson et al, arXiv:1612.02676; Evtushinsky et al, arXiv:1612.02313

Correlations and doping



Mott insulator (half-filling)

Correlations increase when the filling approaches half-filling (Mott insulator)

Correlations in iron superconductors as a function of doping

Theory

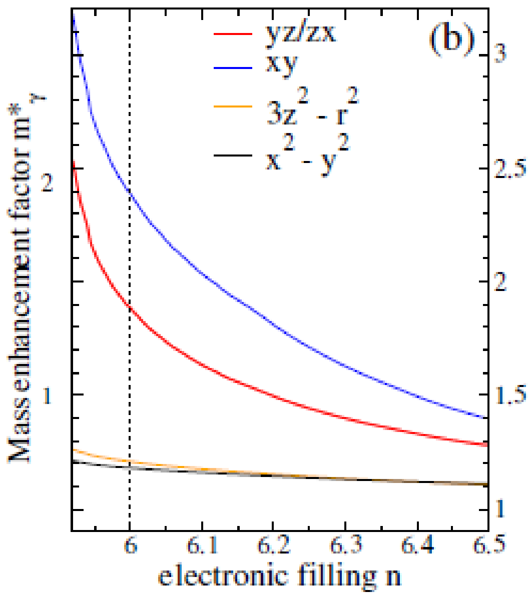


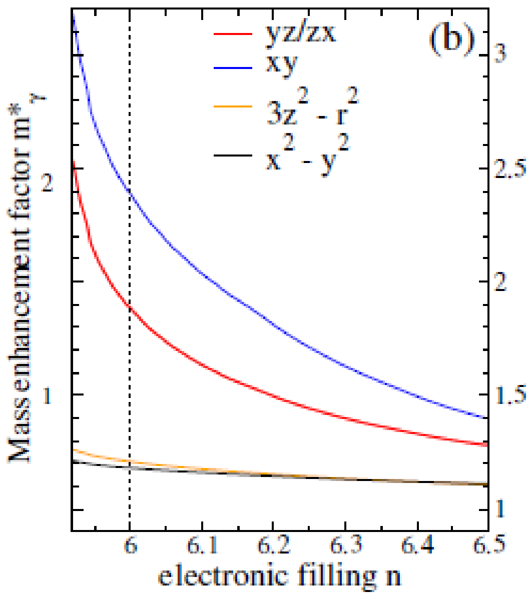
Fig: Pizarro, Calderón, Liu, Muñoz, Bascones, PRB in press (2017)

Correlations increase towards the half-filled Mott insulator (n=5)

Ishida& Liebsch, PRB 82, 1551006 (2010) Werner et al, Nature Phys. 8, 331 (2012) Calderon et al, PRB 90, 115128 (2014) de Medici et al, PRL 112, 177001 (2014)

Correlations in iron superconductors as a function of doping

Theory



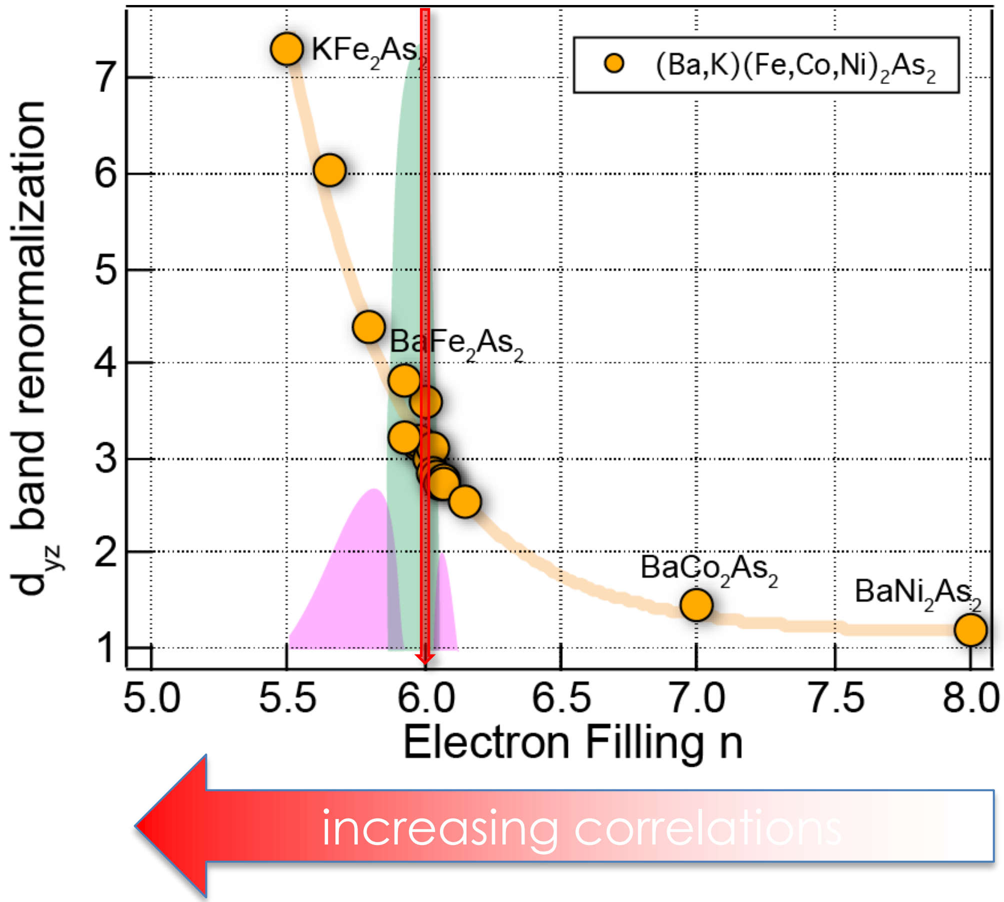
Correlations increase towards the half-filled Mott insulator (n=5)

$BaMn_2As_2$

half-filling

Experiment

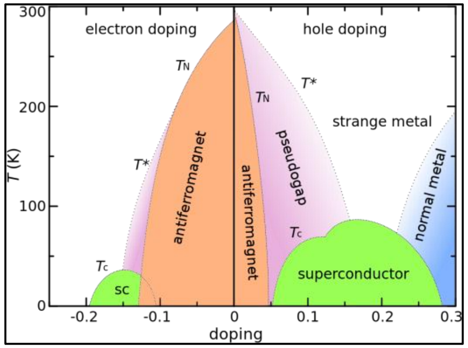
undoped



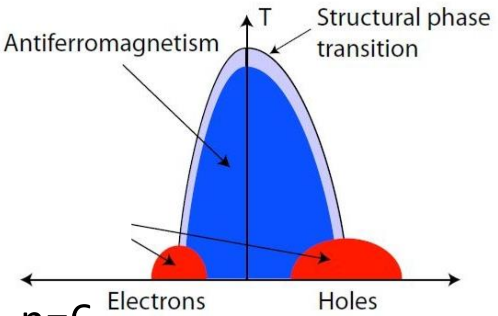
Courtesy, Ming Yi, UC Berkeley (ARPES)

A new way to look at the phase diagram of iron superconductors

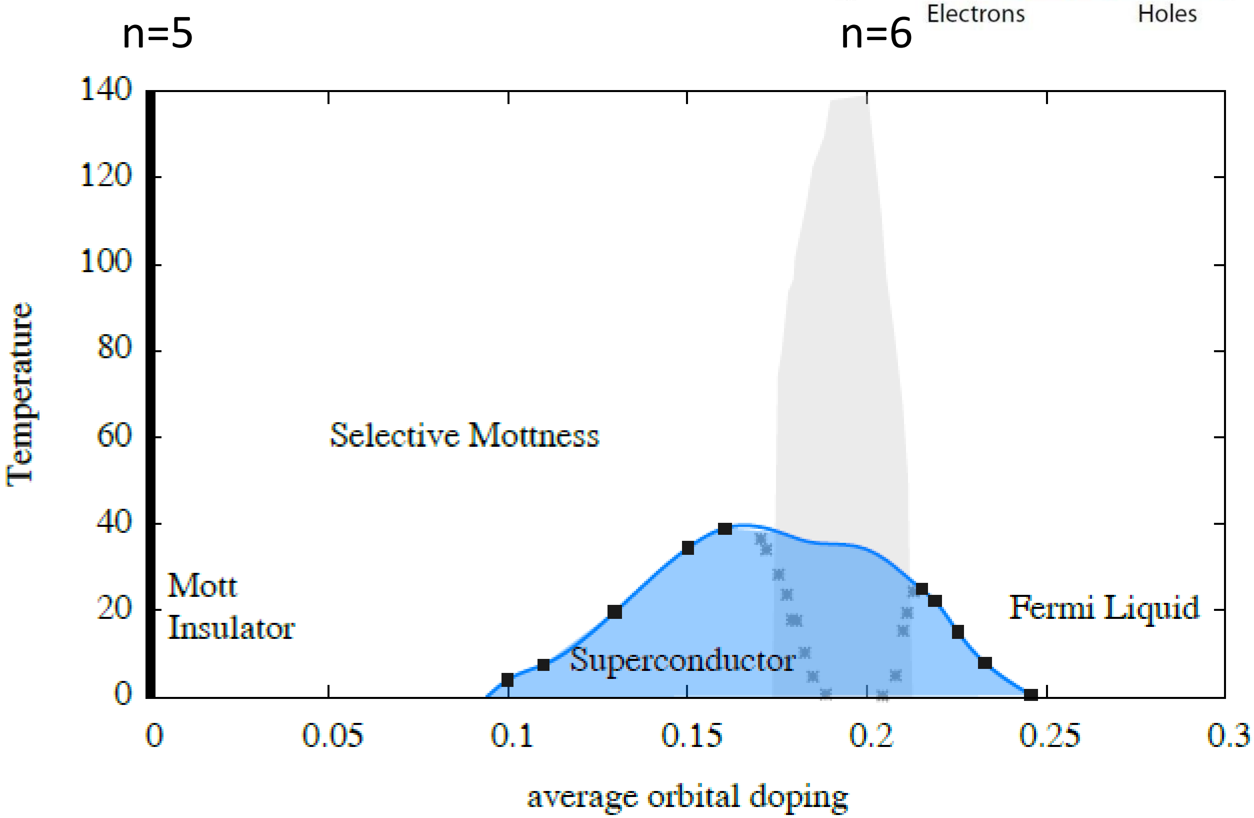
Cuprates



Iron superconductos (FeAs)



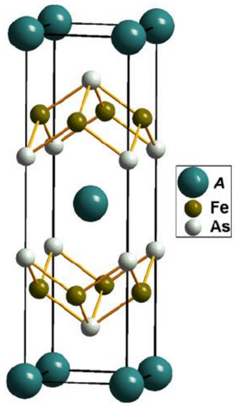
Iron superconductors as electron doped Mott insulators

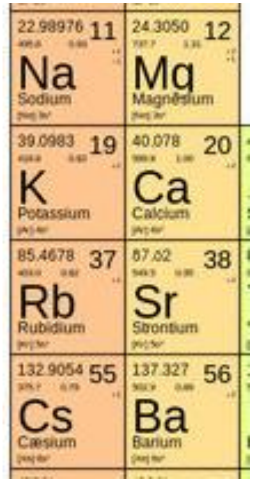


Ishida& Liebsch, PRB 82, 1551006 (2010)

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

The lattice is also important to understand the correlations



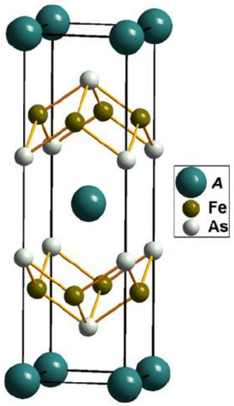


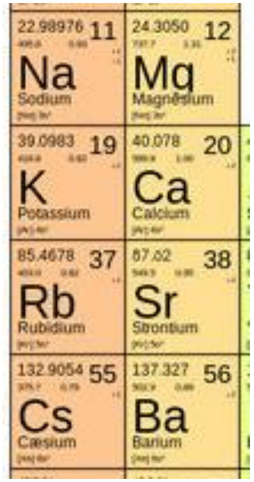
Isostructural & Isovalent compounds

KFe_2As_2 → $RbFe_2As_2$ → $CsFe_2As_2$

Increasing correlations (experimental & theoretical evidence)

The lattice is also important to understand the correlations



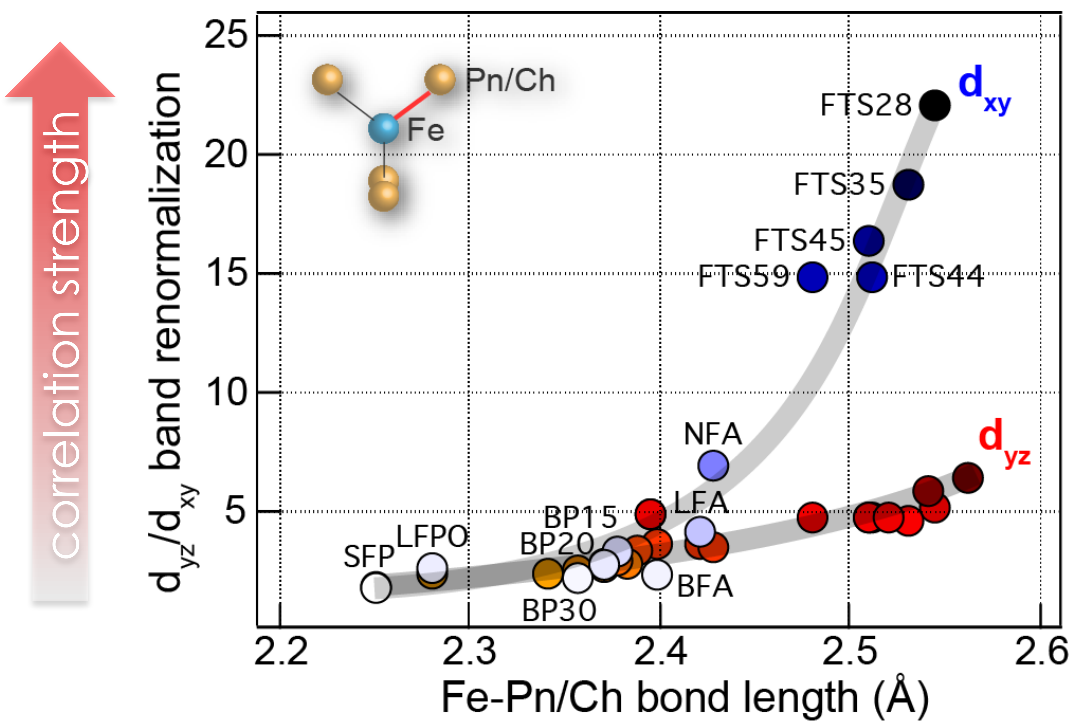


Isostructural & Isovalent compounds

KFe_2As_2 → $RbFe_2As_2$ → $CsFe_2As_2$

Increasing correlations (experimental & theoretical evidence)

**Undoped compounds only*



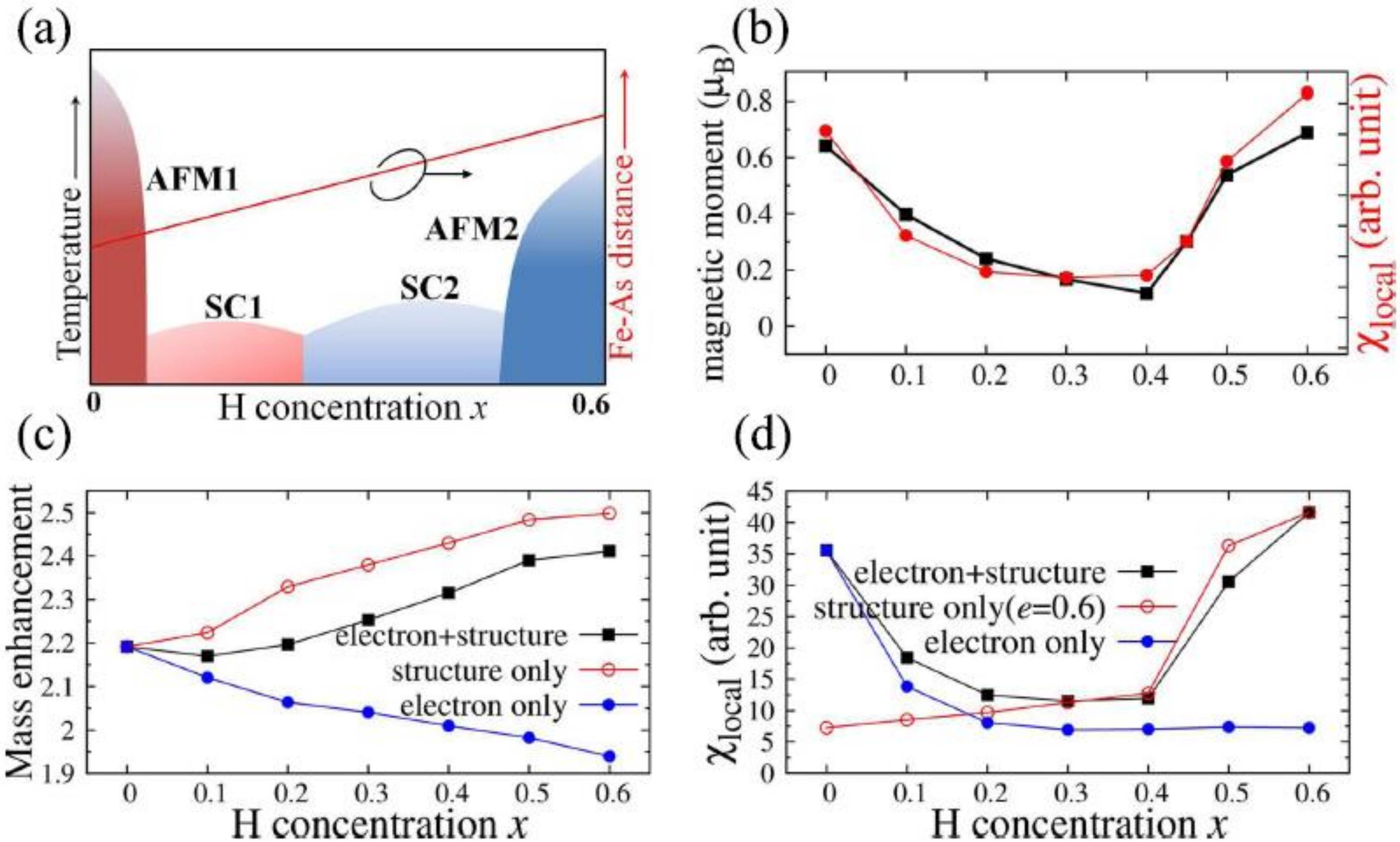
longer bond length
➔electrons more localized

Courtesy, Ming Yi, UC Berkeley (ARPES)

The lattice is also important to understand the correlations

Two superconducting domes in $LaFeAsO_{1-x}H_x$

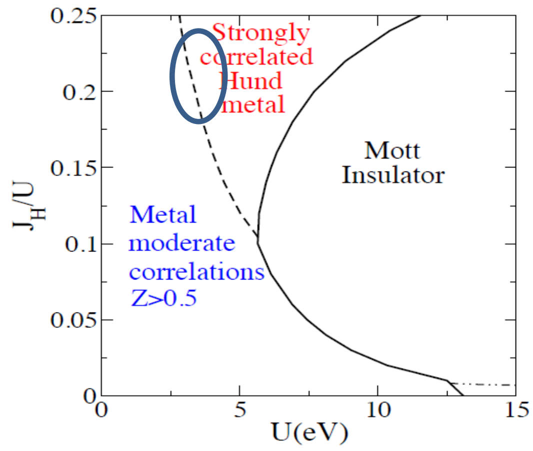
Substitution of oxygen by hidrogen dopes the FeAs layer with electrons



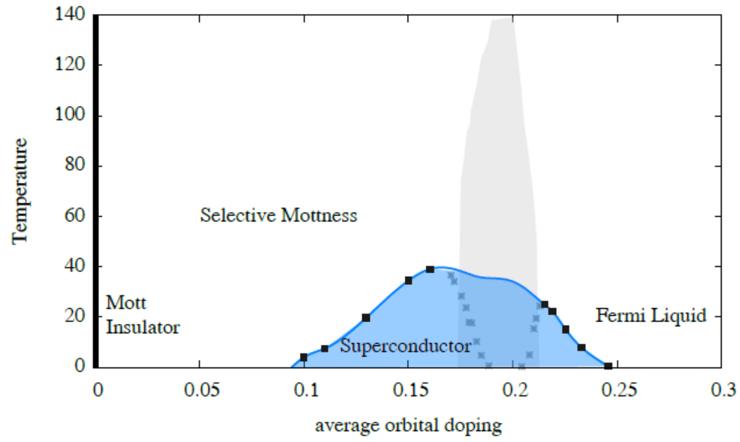
Moon et al, arXiv:1612.05520

The lattice is also important to understand the correlations

- ❑ Hund metal: Correlations induced by Hund's rule & U. Local moments but itinerant electrons. Orbital decoupling

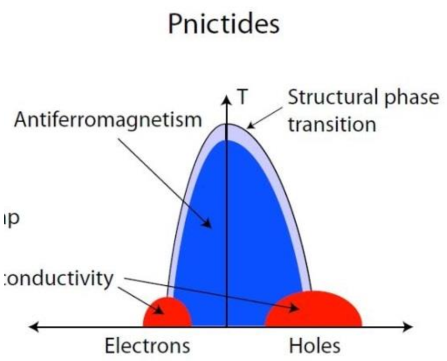


- ❑ Correlations increase with hole-doping towards the half-filled Mott insulator.
The phase diagram revisited. Connection with cuprates



- ❑ The electronic filling determines the correlation but the lattice is also important

Ordered phases: spin and orbital interplay



Origin of instabilities

Primary role of spin degrees of freedom

- Nematicity is a consequence of Magnetism
- Superconductivity induced by magnetic fluctuations

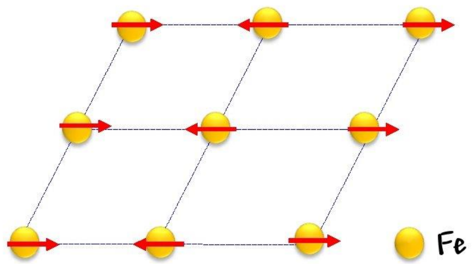
Primary role of orbital degrees of freedom

- Magnetism is a consequence of Nematicity
- Superconductivity induced by orbital fluctuations

Orbital and spin degrees of freedom are coupled
difficult to disentangle who comes first

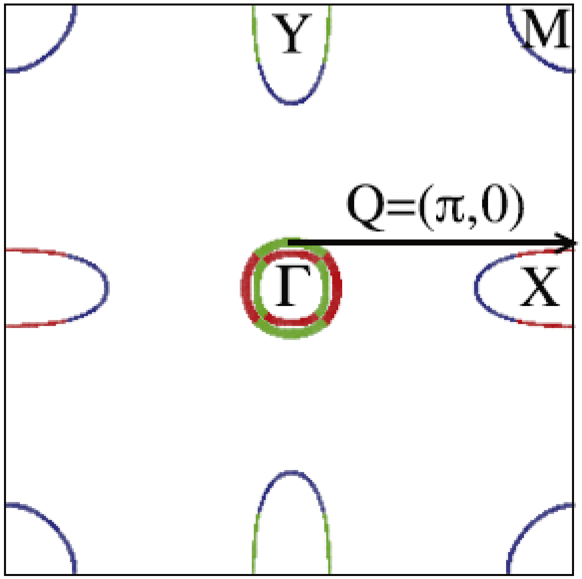
Magnetism in iron superconductors

Stripe magnetism Q=(π,0)



Magnetism in iron superconductors

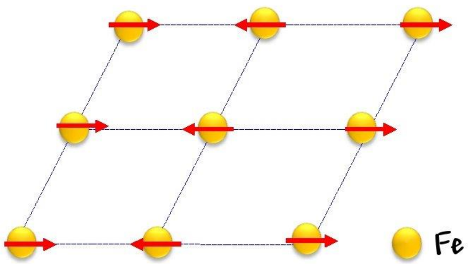
Fermi surface physics



Local moments (Heisenberg like)

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

$J_2/2>J_1$ Stripe order



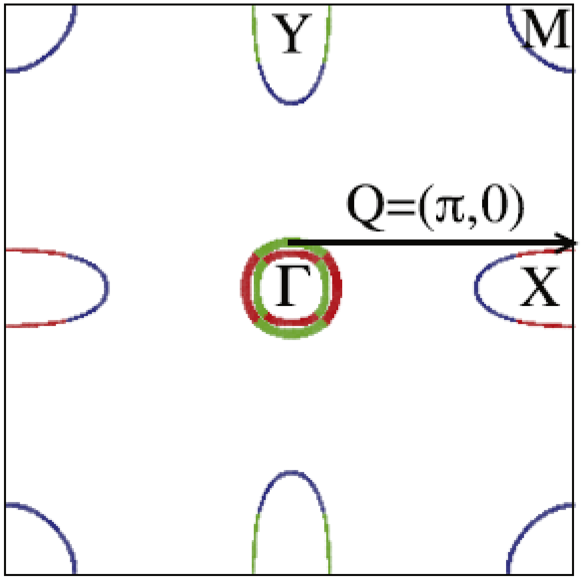
Stripe magnetism Q=(π,0)

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)

Magnetism in iron superconductors

Fermi surface physics



Against this model

- Double stripe in FeTe
- Magnetic ordering in $LaFeAsO_{1-x}H_x$
- Energy scale of spin waves

Local moments (Heisenberg like)

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

$J_2/2>J_1$ Stripe order

To explain neutrons it is necessary to include

$$K_{ij}\left(\mathbf{S}_i\cdot\mathbf{S}_j\right)^2$$

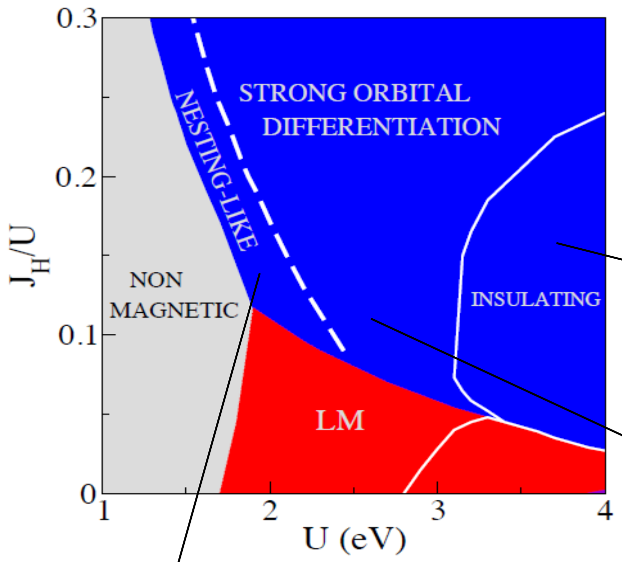
Against this model

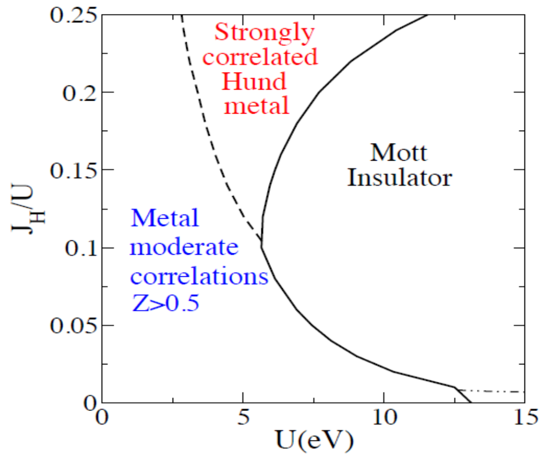
- C4 phase in hole-doped 122 family
- Experimental magnetic moment too low
- Signatures of itinerancy in spin waves

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

Magnetism in iron superconductors

Hartree-Fock magnetic phase diagram





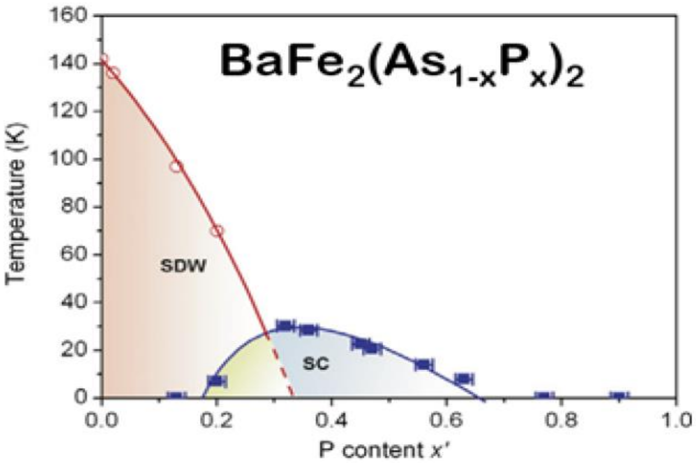
Heisenberg like magnetism (localized electrons/spins)

Double exchange like physics with some itinerant and some Localized orbitals

Nesting like magnetism (Fermi Surface physics)

E. Bascones leni@icmm.csic.es

Superconductivity in iron superconductors



Superconductivity appears when
an antiferromagnetic phase is suppressed
This happens in many non-conventional
superconductors

Origin of superconductivity?

~~Conventional (electron-pnonon)~~

Non-conventional

Spin fluctuations

Orbital fluctuations
(enhanced by phonons)

Fluctuations from
Localized spins

Spin fluctuations ,
Fermi surface
instability

Superconductivity in iron superconductors: the gap function

Origin of superconductivity?: Non conventional

Spin fluctuations

Fluctuations from Localized spins

s±, d-wave gap depending on parameters

Little predictive power (no clear value of the parameters or orbital dependence)

Si et al

Spin fluctuations , Fermi surface instability

s± in FeAs undoped systems
d-wave in strongly doped systems

Hirschfeld, Scalapino, et al

Orbital fluctuations (enhanced by phonons)

s++ in FeAs undoped systems

The superconducting order parameter **does not change sign** in the Brillouin zone

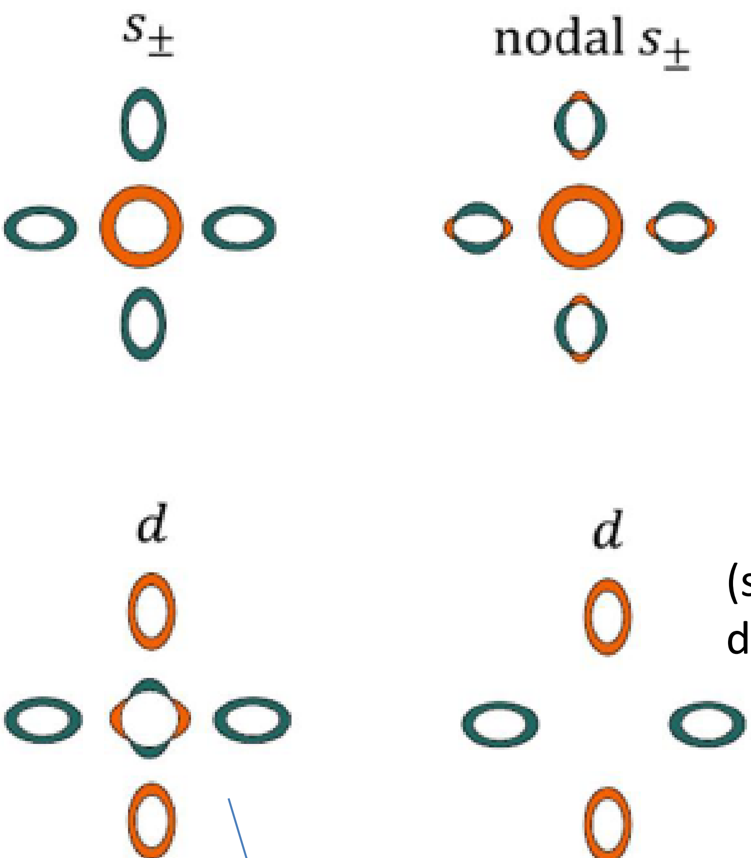
Kontani et al

The superconducting order parameter **changes sign** in the Brillouin zone

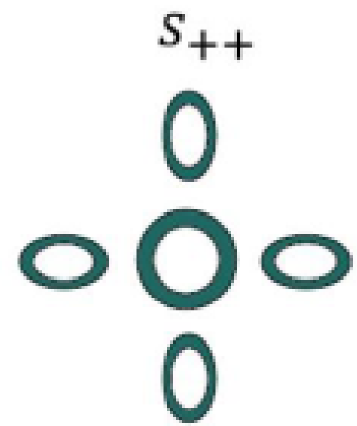
Superconductivity in iron superconductors: the gap function

Origin of superconductivity?: Non conventional

Sign changing order parameters



(strongly electron doped system)



In systems with electron and hole pockets the absence of nodes points excludes d-wave

E. Bascones leni@icmm.csic.es

Superconductivity in iron superconductors: the gap function

Nodes in the gap function

(specific heat, penetration length, ARPES,STM)

Table 1. Gap structures in Fe-based materials deduced from thermodynamic and transport measurements. OD=overdoped, OP=optimally doped, UD=underdoped. Symbol * indicates possible evidence for "*c*-axis nodes".

Family	Full gap	Highly anisotropic	Strong nodal
1111	$PrFeAsO_{1-y}$[52K] [293] SmFeAs(O,F)[55K] [295]	LaFeAs(O,F)[26K] [214] NdFeAs(O,F) [214]	LaFePO[6K] [203, 204, 294]
122	(Ba,K)Fe_2As_2[40K] [146, 236, 296, 242] Ba(Fe,Co)$_2As_2$ [OP,23K] [238, 208]	Ba(Fe,Co)$_2As_2$ [OD] [238, 241]* Ba(Fe,Ni)$_2As_2$ [297]* Ba(Fe,Co)$_2As_2$ [UD] [241]*	KFe_2As_2 [4K] [211, 309] $BaFe_2$(As,P)$_2$[OP,31K] [205, 149] (Ba,K)Fe_2As_2 [UD] [242]
111	LiFeAs [18K] [298, 258]		LiFeP [6K] [299]
11		Fe(Se,Te) [27K] [231, 246]	

Excludes d-wave in these systems

Differences among materials:

The order parameter in some materials presents nodes but in other materials it is nodeless

Hirschfeld, Korshunov, Mazin, Rep. Prog. Phys 74, 124508 (2011)

Superconductivity in iron superconductors: the gap function

Sign change of the order parameter vs Absence of sign change

- Many experiments measure the magnitude of the order parameter but not the sign
- No definitive experiment contrary to what happened in cuprates with d-wave

s±

Supported by many experiments (neutron resonance, Josephson junctions, QPI from STM, **localized states around non-magnetic impurities** in STM)

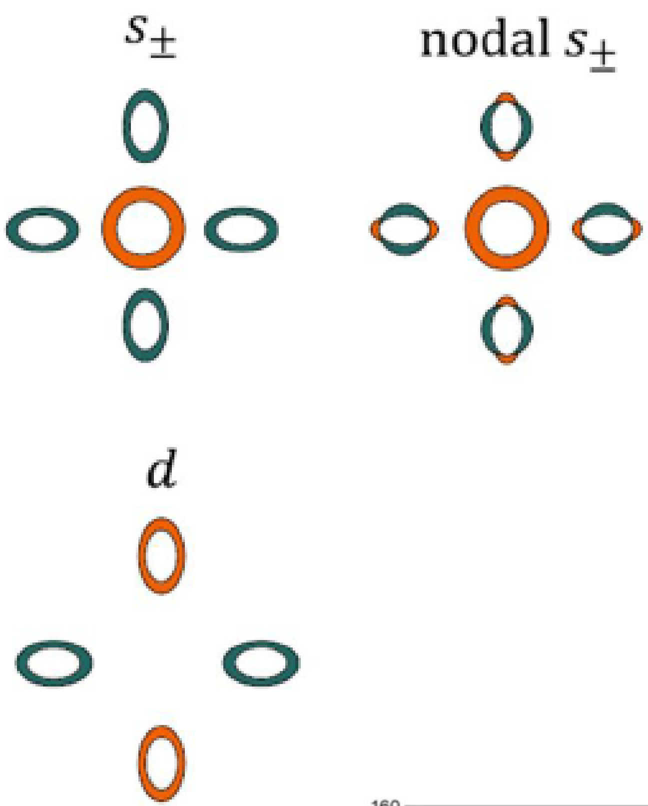
s++

Early supported by the effect of disorder on the gap.

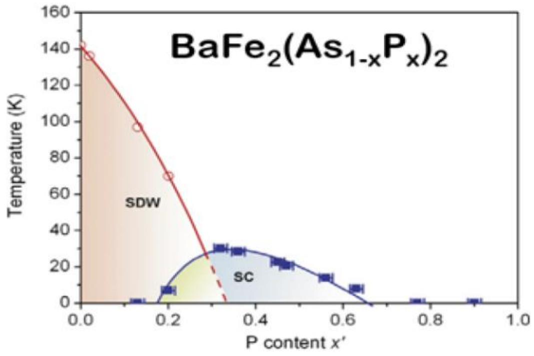
Role of disorder revisited

Hirschfeld, Comptes Rendus Physique 17, 197 (2016)

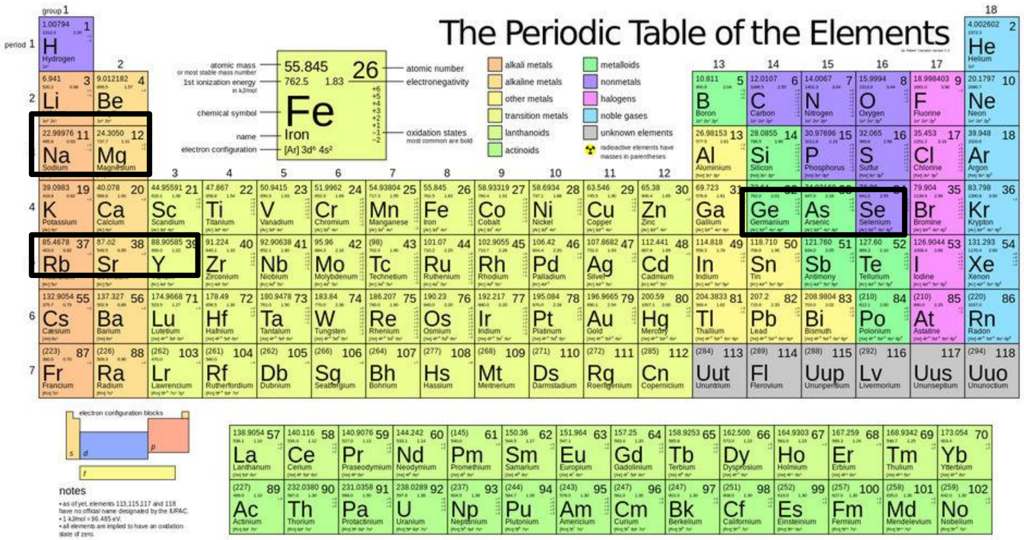
Superconductivity in iron superconductors: the gap function



- The symmetry of the order parameter seems consistent with predictions from spin fluctuations theory of superconductivity
- Most probably s± in undoped FeAs systems, it can be d-wave in some electron doped chalcogenides and in (strongly hole-doped) KFe_2As_2
- Not clear whether the spin fluctuations come from itinerant or localized spins.
- Generic agreement, but still some inconsistencies between theory (itinerant) and experiment with the k-dependent amplitude of the order parameter.

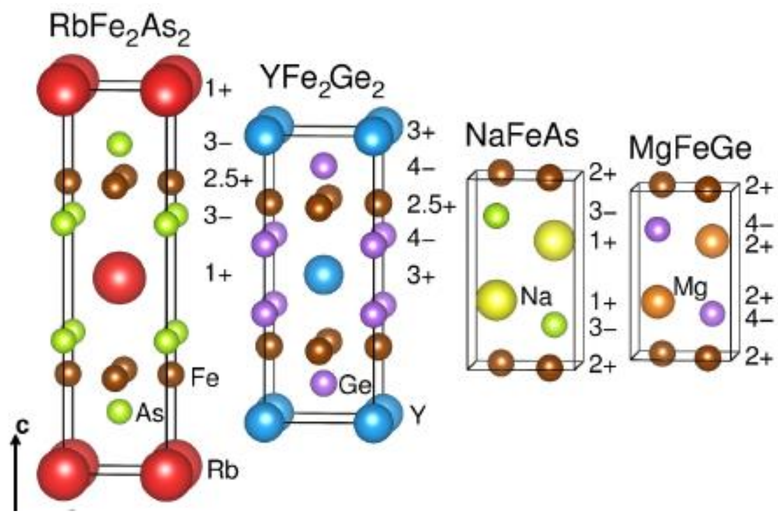


Absence of superconductivity in the germanides



Iron superconductors: FeAs, FeSe layers

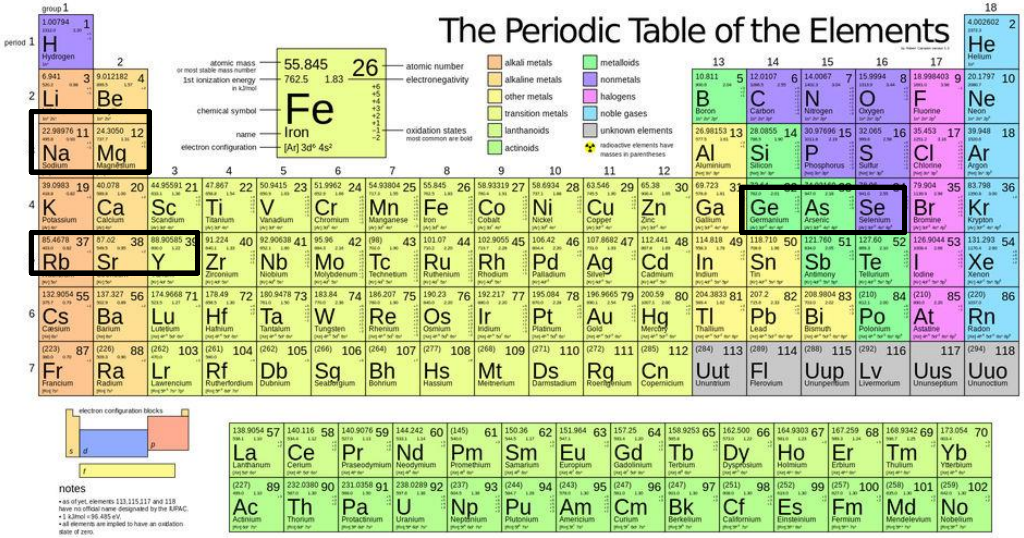
What about systems with **FeGe** layers?



Isostructural and isovalent FeGe compounds not superconducting or maybe with very low Tc

E. Bascones leni@icmm.csic.es

Absence of superconductivity in the germanides



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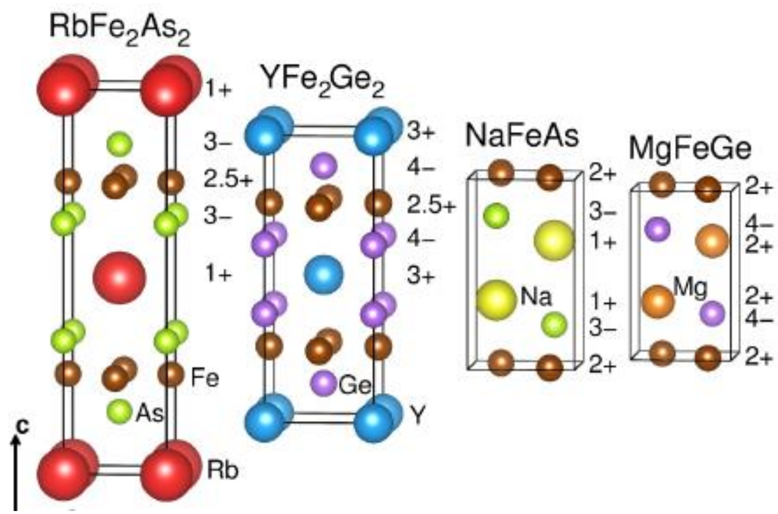
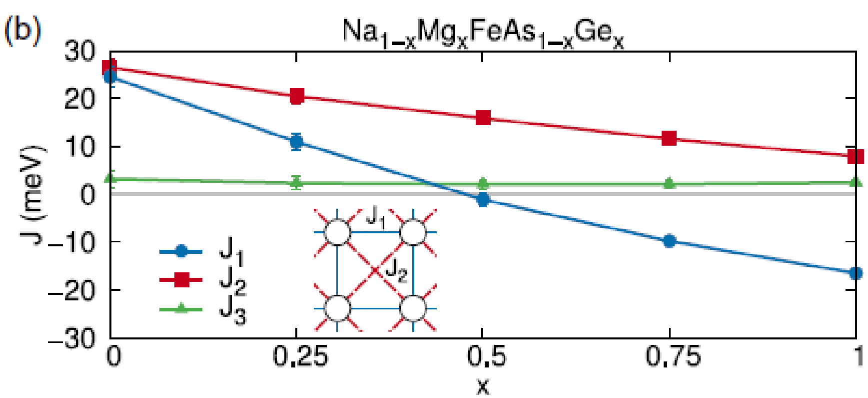


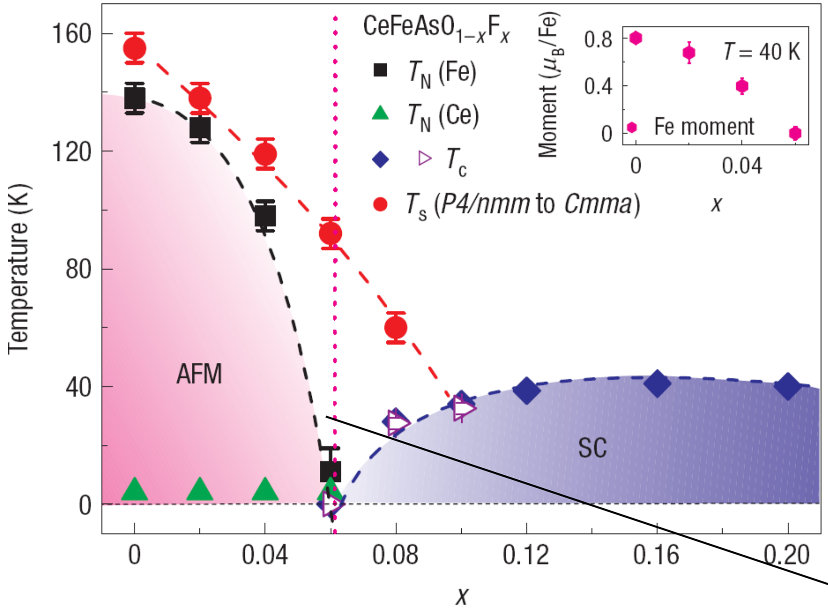


Isostructural and isovalent FeGe compounds not superconducting or maybe with very low Tc

Ferromagnetic tendencies in FeGe!
Non trivial role of cation states

Guterding, Jeschke, Mazin, Glasbenner, Bascones, Valenti, PRL 118, 017204 (2017)

Nematicity in iron superconductors



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

A structural transition precedes the antiferromagnetic phase in many compounds a≠b

Tetragonal symmetry broken

Very strong anisotropic electronic properties on spite of a very small lattice change (resistivity, optical conductivity, neutrons, ARPES, …)

Nematicity in iron superconductors

Nature & origin of the structural transition & nematic state

Elastic transition
(ionic lattice)

Electronic origin of the transition

Nematicity in iron superconductors

Nature & origin of the structural transition & nematic state

Elastic transition
(ionic lattice)

Electronic origin of the transition

Lattice & electrons are coupled

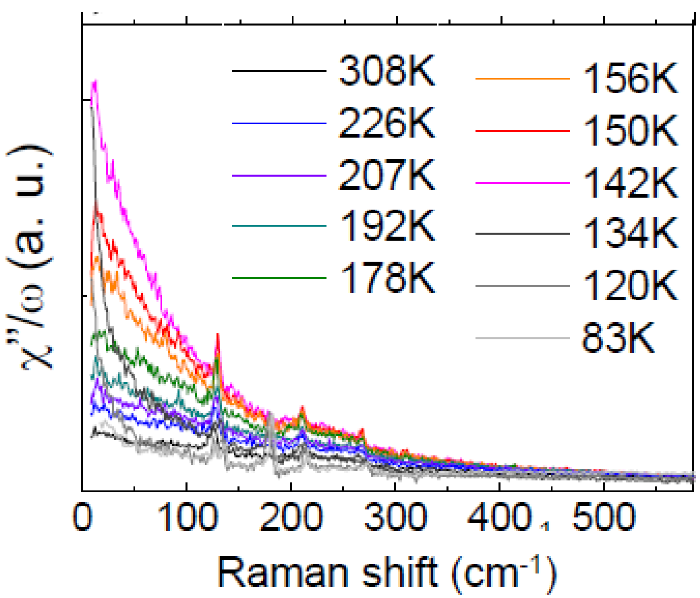
Nematicity in iron superconductors

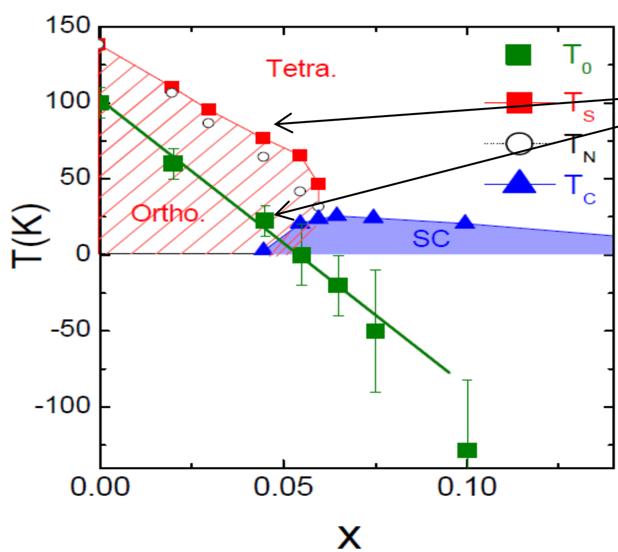
Nature & origin of the structural transition & nematic state

Elastic transition
(ionic lattice)

Electronic origin of the transition

Raman experiments (in B_{1g} symmetry) measure the bare electronic susceptibility





The coupling to the lattice increases the transition temperature

Gallais & Paul, Comptes Rendus Physique 17, 113 (2016)

Nematicity in iron superconductors

Nature & origin of the structural transition & nematic state

Electronic origin of the transition

Ising **spin**-nematic state
Selects magnetic moment
Q=(π,0) or **Q=(0,π)**
(Precursor of stripe AF)

Most **popular** model
for **FeAs systems**
(elastic constants same
temperature dependence
as spin fluctuations)

Orbital order
yz and zx orbitals inequivant

Onsite Ferro-orbital
(different occupation)

$\varepsilon(n_{zx}-n_{yz})$

Phonons?

No evidence of this
state in realistic
theoretical models

Nematicity in iron superconductors

Nature & origin of the structural transition & nematic state

Elastic transition
(ionic lattice)

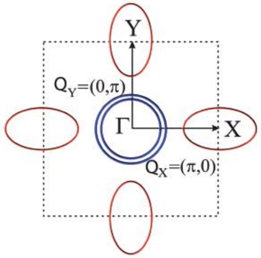
Electronic origin of the transition

Ising **spin**-nematic state
Selects magnetic moment
Q=(π,0) or **Q=(0,π)**
(Precursor of stripe AF)

Early predicted
with localized
spin models

$$\boxed{K_{ij}\left(\mathbf{S}_i \cdot \mathbf{S}_j\right)^2}$$

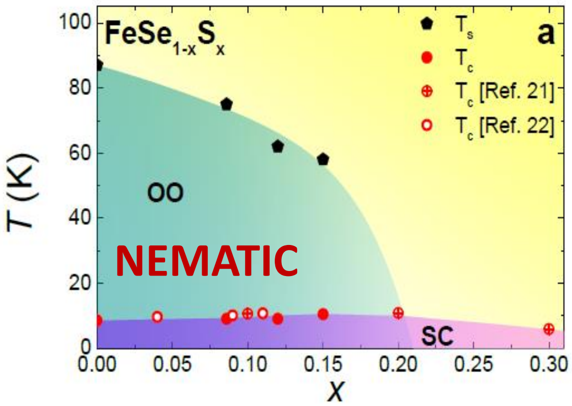
Itinerant
band version



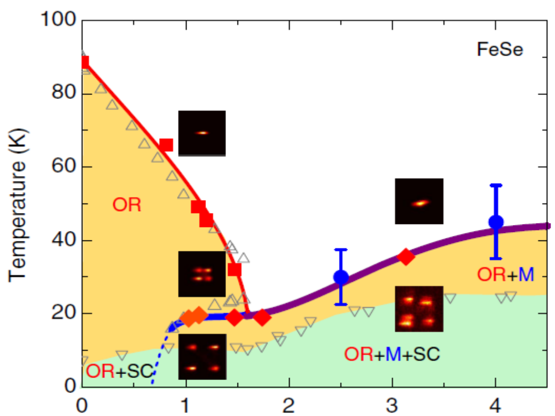
The itinerant version is more popular but no clear difference in the nematic state between the two models experimentally

Nematicity in iron superconductors. FeSe

Nature & origin of the structural transition & nematic state



Watson et al,
PRB 92, 121108 (2015)



Kothapalli et al,
Nat. Comm 7, 12728 (2015)

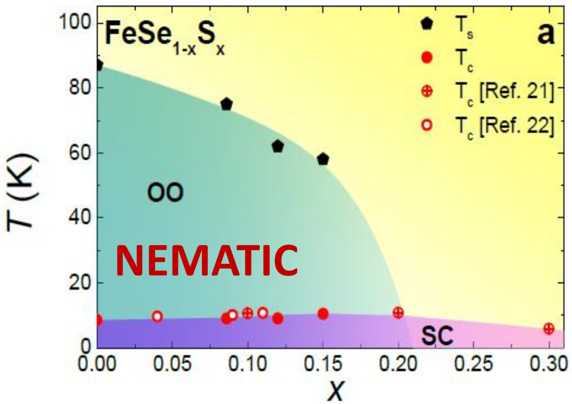
Electronic origin of the transition

Orbital order

yz and zx orbitals inequivant

Nematicity in iron superconductors. FeSe

Nature & origin of the structural transition & nematic state



Watson et al,
PRB 92, 121108 (2015)

Electronic origin of the transition

Orbital order

yz and zx orbitals inequivant

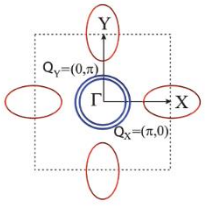
Onsite Ferro-orbital (different occupation)

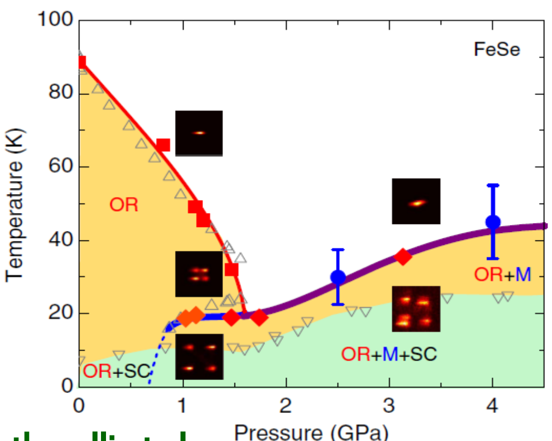
$$\varepsilon(n_{zx}-n_{yz})$$

Phonons?

D-**bond** order (Intersite interactions)

Sign-changing Orbital order (spin fluctuations)





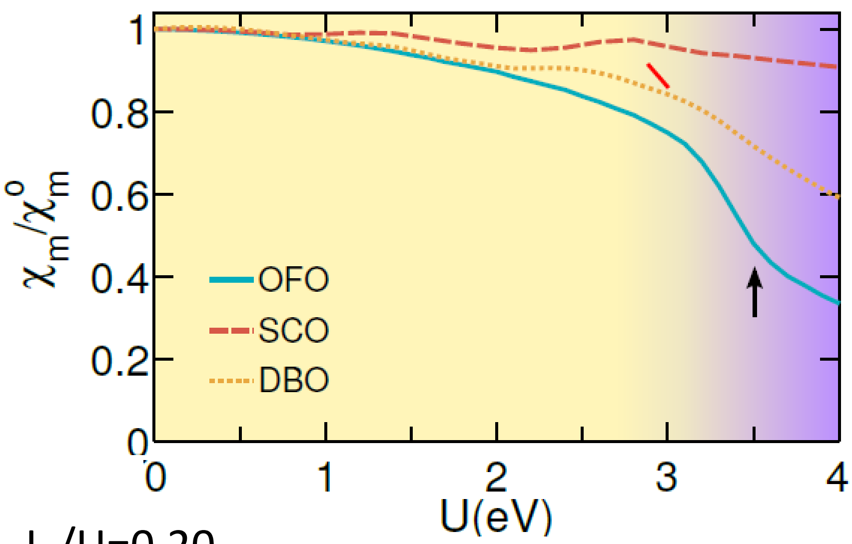
Kothapalli et al,
Nat. Comm 7, 12728 (2015)

(controversial) ARPES experiments which suggest unconventional order

Nematicity in iron superconductors. FeSe

Nature & origin of the structural transition & nematic state

Electronic origin of the transition



$J_H/U=0.20$

Orbital order :FeSe

yz and zx orbitals inequivant

OFO

Onsite Ferro-orbital (different occupation)

$\varepsilon(n_{zx}-n_{yz})$

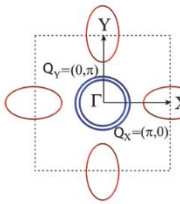
Phonons?

DBO

D-**bond** order (Intersite interactions)

SCO

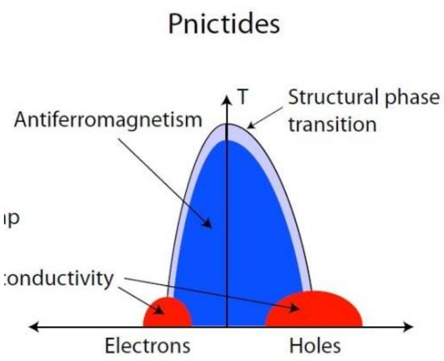
Sign-changing Orbital order (spin fluctuations)



Hund's physics strongly suppresses Onsite OFO order and it has the weakest effect on sign changing order (SCO) which is the most plausible orbital order in FeSe

Fanfarillo, Giovannetti, Capone, Bascones, arXiv: 1609.06672

Ordered phases: spin and orbital interplay



Origin of instabilities

Primary role of spin degrees of freedom

- Nematicity is a consequence of Magnetism
- Superconductivity induced by magnetic fluctuations

Primary role of orbital degrees of freedom

- Magnetism is a consequence of Nematicity
- Superconductivity induced by orbital fluctuations

Other issues

- Quantum criticality. Evidence of AF criticality in $BaFe2(As_{1-x}P_x)_2$ at optimal doping. Lack of effect in Tc of critical nematicity in $FeSe_{1-x}S_x$

- Monolayer or few layer FeSe on STO or other substrates. Tc enhancement and non-trivial role of doping.

- Disorder: non-universal suppression of Tc, effect on the gap, localized bound states, QPI, nucleation of magnetic clusters, effect on nematicity …

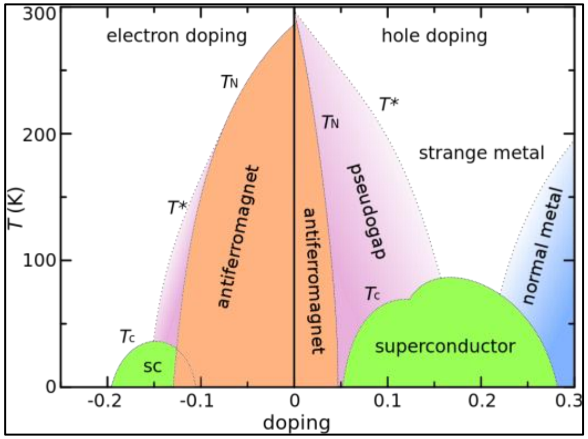
- The experimental Fermi surface: spin fluctuations, non-local effect of interactions.

- BCS vs BEC crossover in FeSe

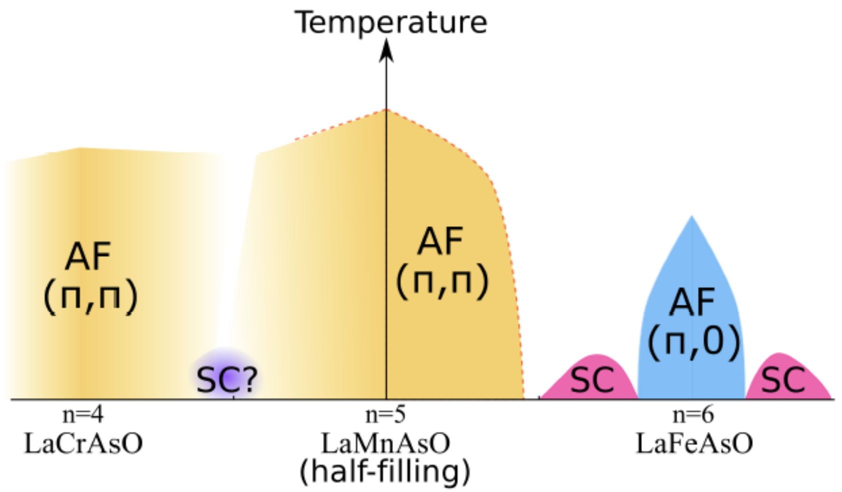
- Three-dimensionality and the folded Brillouin zone (possible UC pairing states)

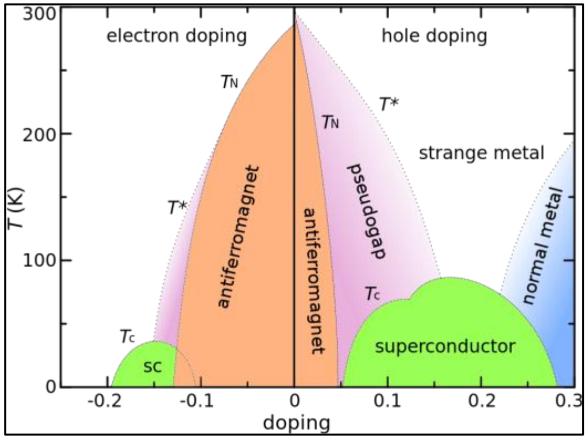
- Spin-orbit coupling

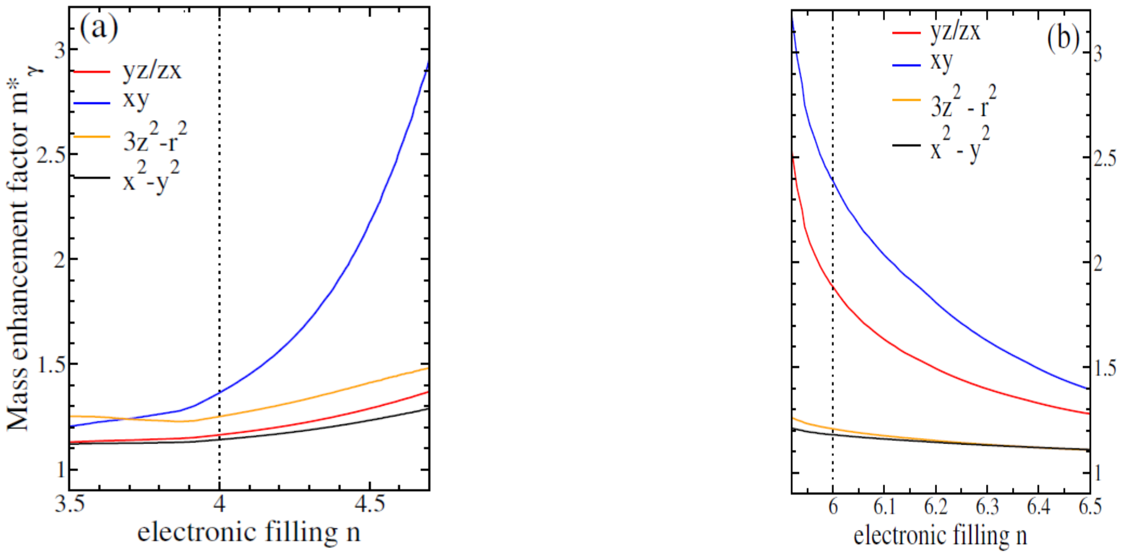
Future prospects: Search for high-Tc in Chromium materials



Future prospects: Search for high-Tc in Chromium materials







Superconductivity, if present, most probably d-wave

Pizarro, Calderón, Liu, Muñoz, Bascones, PRB in press (2017)

9 years of iron superconductors: what we have learnt

- 11 families of FeAs or FeSe based superconductors. FeSe in monolayer form. High-Tc superconductivity seems absent in FeGe systems

- Superconductivity, magnetism and nematicity present in the phase diagram, which is non-universal (nematicity w/wout AF, two domes, different magnetic orders …)

- Key developments in understanding multi-orbital & multi-band systems. Hund's coupling.

- Correlations. Hund metal physics: high-spin, itinerancy, orbital decoupling. Increase of correlations approaching the half-filled Mott insulator (n=5)-connection with cuprates physics. Role of the lattice. Not clear yet the best starting point for effective models.

- Not clear the nature of magnetism (itinerancy, but some states not explained by nesting). Double exchange physics?

- Superconductivity most probably mediated by antiferro-magnetic fluctuations. Order parameter most probably $s\pm$ FeAs systems with electron & hole pockets (both nodal & nodeless examples) and d-wave in systems with only electron or only hole-pockets.

- Structural transition is electronic, most probably Ising-spin nematic in FeAs systems, but could be of orbital nature in FeSe. Hund's physics opposes onsite ferro-orbital ordering. Spin fluctuations could lead to sign changing orbital order.

Thanks

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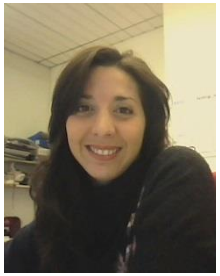

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