# Modelling correlated superconductors

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UNIVERSITÄT
FRANKFURT AM MAIN

*Topology Matters / SPICE*
*Mainz  July 26, 2017*

# Collaborators

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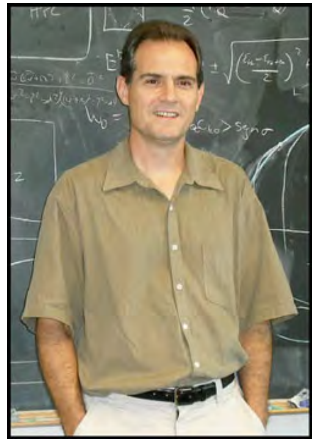

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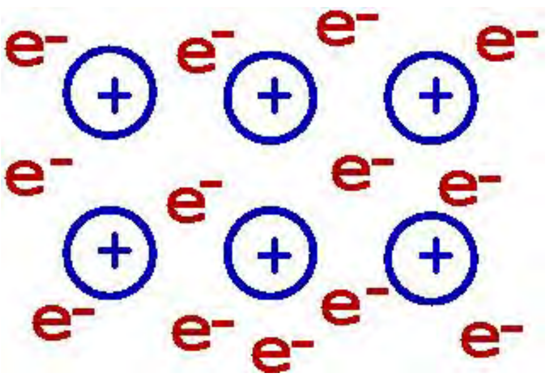
**Alexander von Humboldt** Foundation

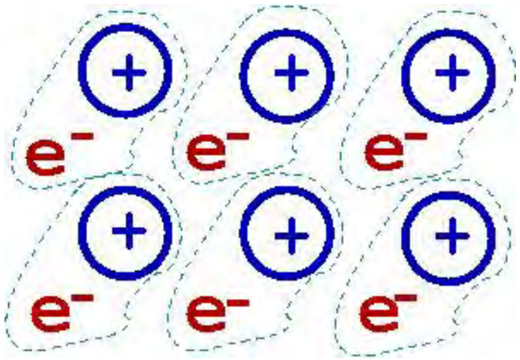
- Systems with strongly interacting electrons:

**very large entanglement of the many-body electron wavefunction**

- Metal:




- Insulator:

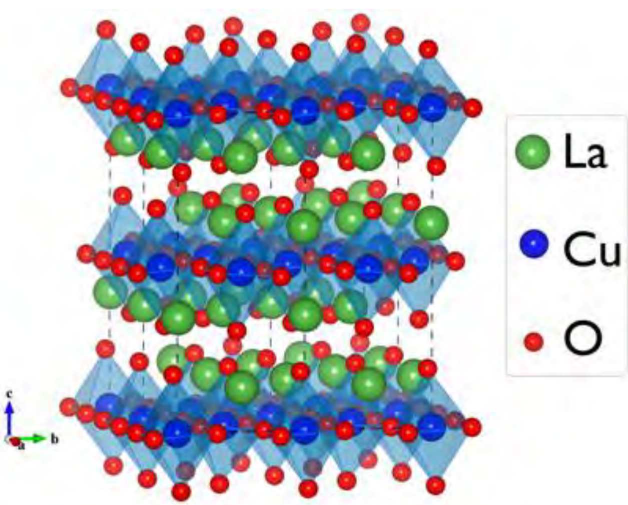


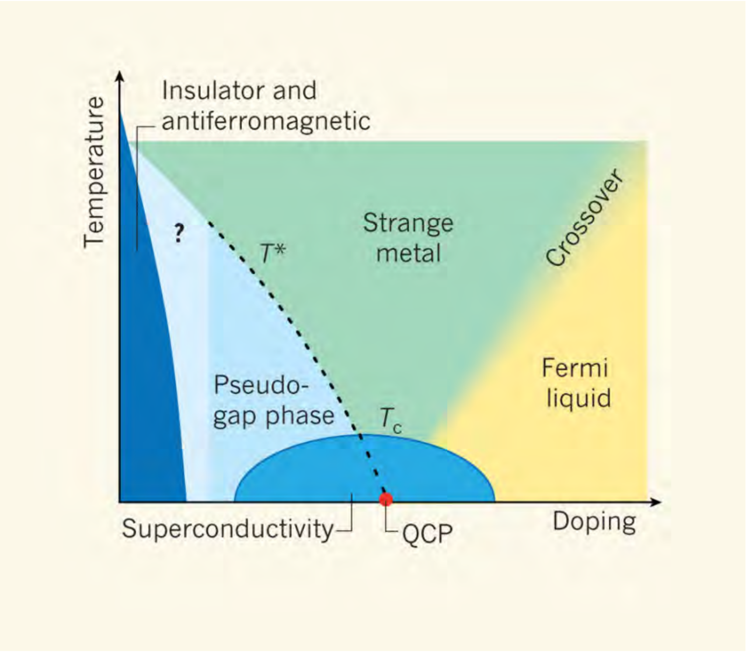

***Mott insulators***

# high-Tc Cu-based superconductors

- Complex phase diagrams: **High-Tc superconductors**

**$La_{2-x}Sr_xCuO_4$**




*C. Varma Nature 468, 184 (2010)*

***Competing ordered phases***

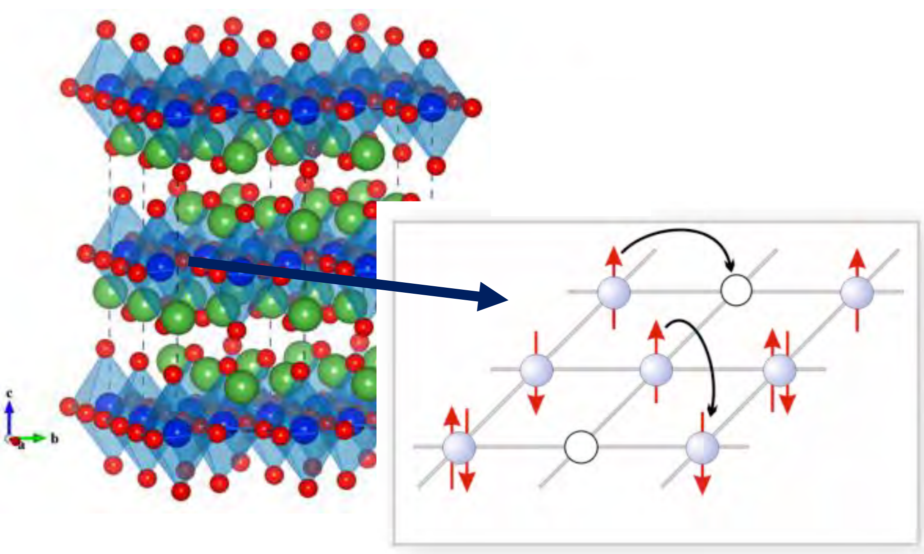
**Correlation:**

- Mott transition: metal - insulator

# high-Tc Cu-based superconductors

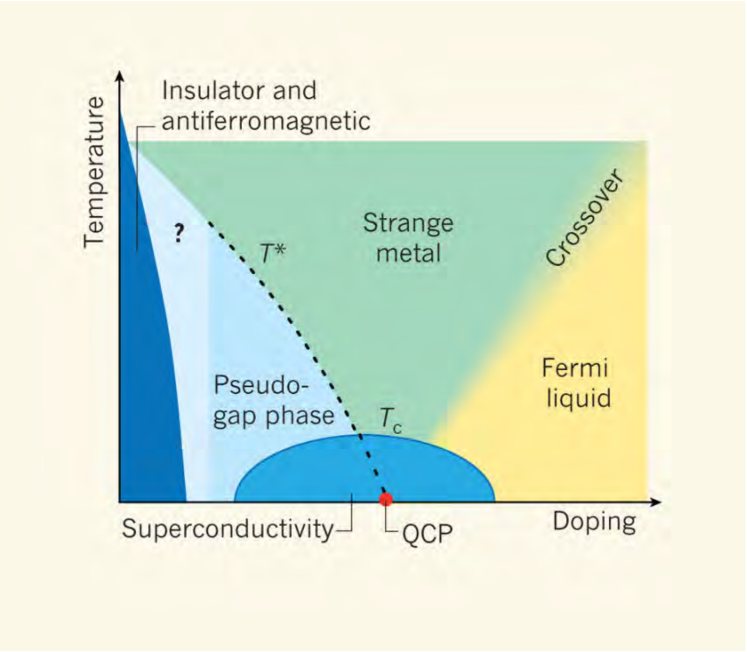
- Complex phase diagrams: **High-Tc superconductors**

**$La_{2-x}Sr_xCuO_4$**



Hubbard model

$$H_{\text{Hubbard}} = t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



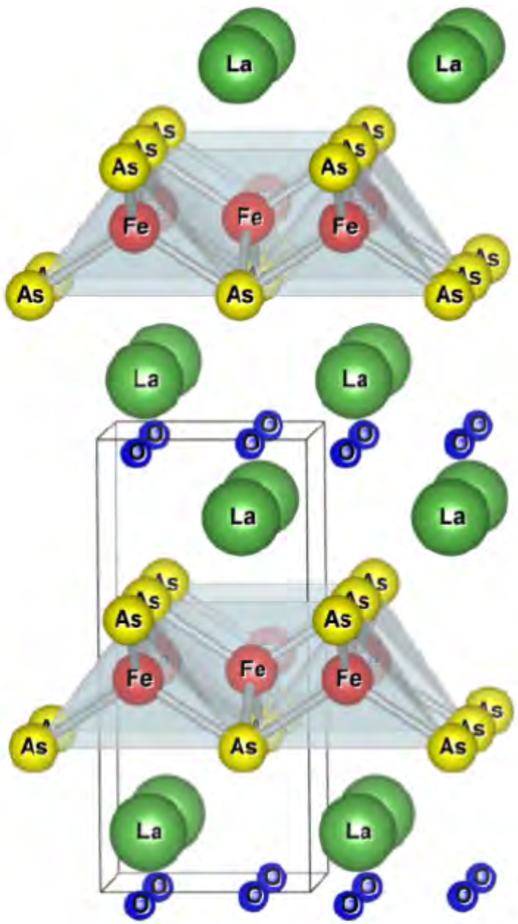

*C. Varma Nature 468, 184 (2010)*

***Competing ordered phases***

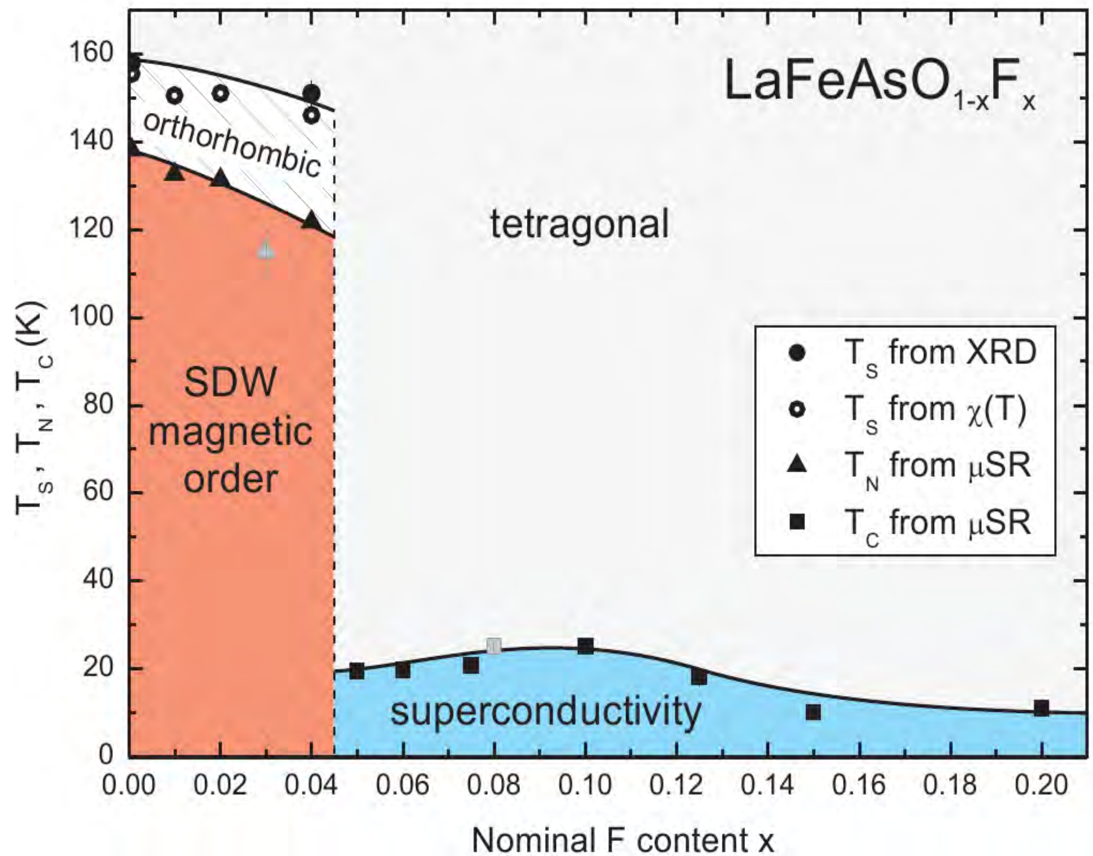
**Correlation:**

- Mott transition: metal - insulator

# 2008: a new iron age




- $T_c$= 26K

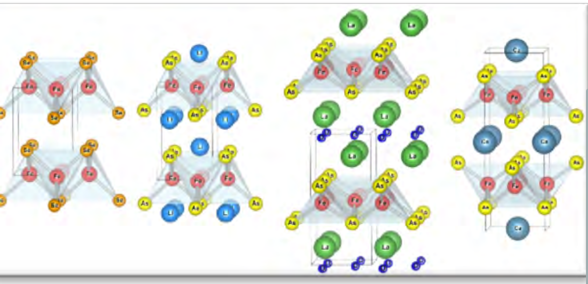



**1111**

*Kamihara et al. JACS 130, 3296 (2008)*

*Luetkens et al. Nat. Mat. Lett. (2008)*

# Fe-based superconductors



- Families:

**pnictides**

**1111** *RE*O(F)FeAs ( $T_{cmax}$=55K SmOFeAs)

**122** *AE*$Fe_2As_2$ ($T_{cmax}$=38K $BaFe_2As_2$ upon doping)

**111** *AM*FeAs ($T_{cmax}$= 18K LiFeAs)

**chalcogenides**

**11** FeSe ($T_{cmax}$= 8K )

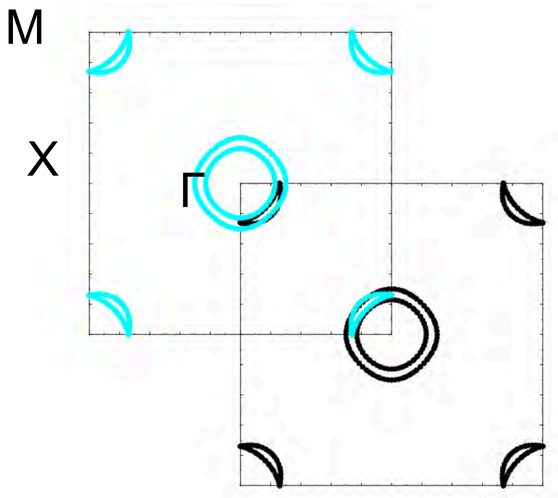
$A_xFe_{2-z}Se_2$ (A=K, Cs,Rb) $T_{cmax}$=30K → Under P Tc ↑

- FeSe under pressure ($T_{cmax}$ =37K)
- FeSe with molecular intercalation ($T_{cmax}$=44K)
- FeSe monolayer on $SrTiO_3$ ($T_{cmax}$ ~ 100K?)

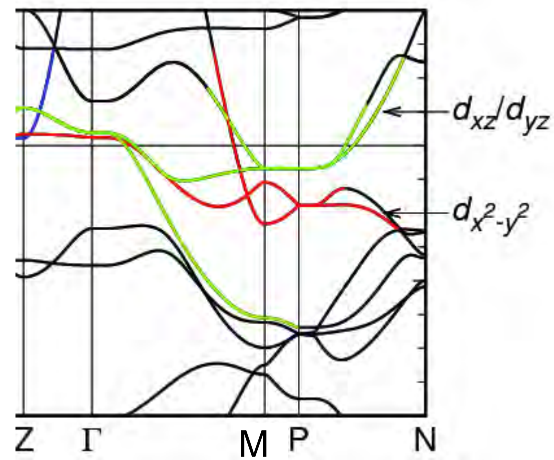
$CaKFe_4As_4$

# Fe-based superconductors

- nesting-driven magnetism:

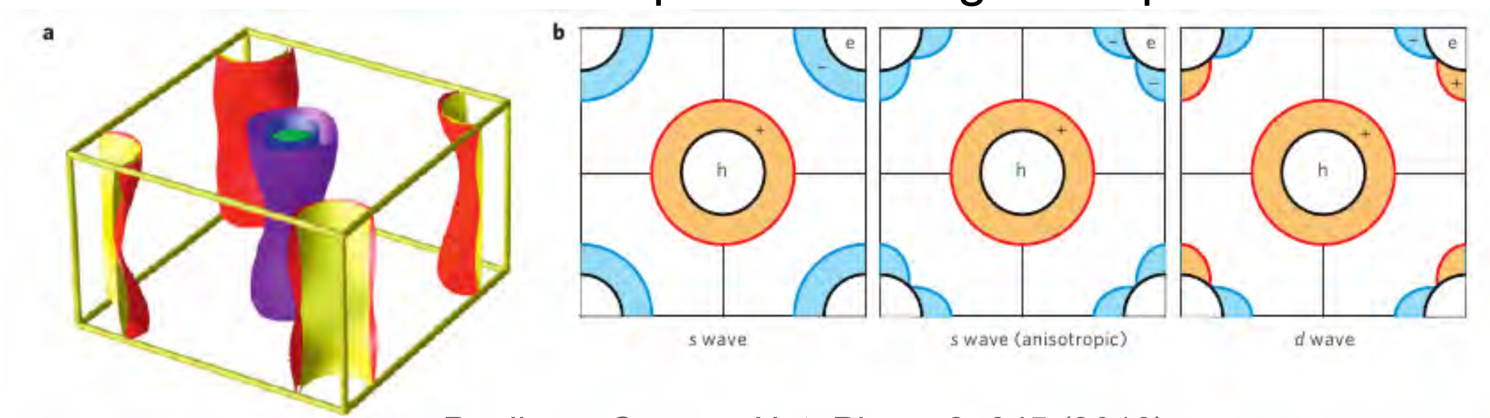



- multiorbital systems:

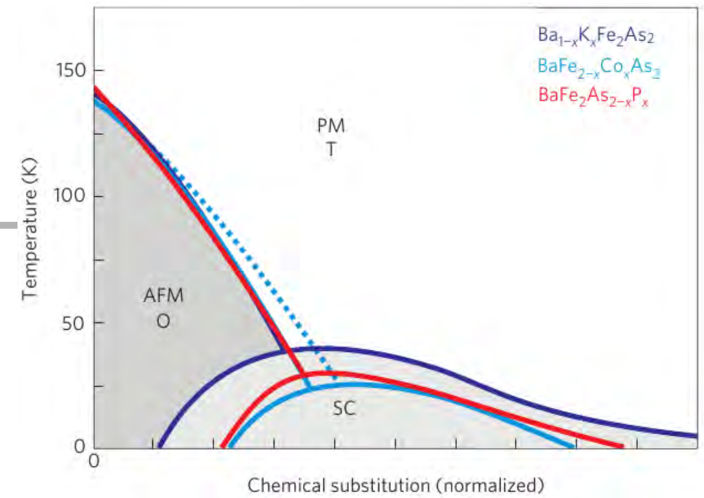



*Fink et al. PRB (2009) ARPES*
*Ruillier-Alberque et al. PRL (2012) Transport*

- superconducting order parameter:




*Paglione, Greene Nat. Phys.* ***6****, 645 (2010)*
*Hirschfeld, Korshunov, Mazin Rep. Prog. Phys.* ***74****, 124508 (2011)*




- **correlation effects**

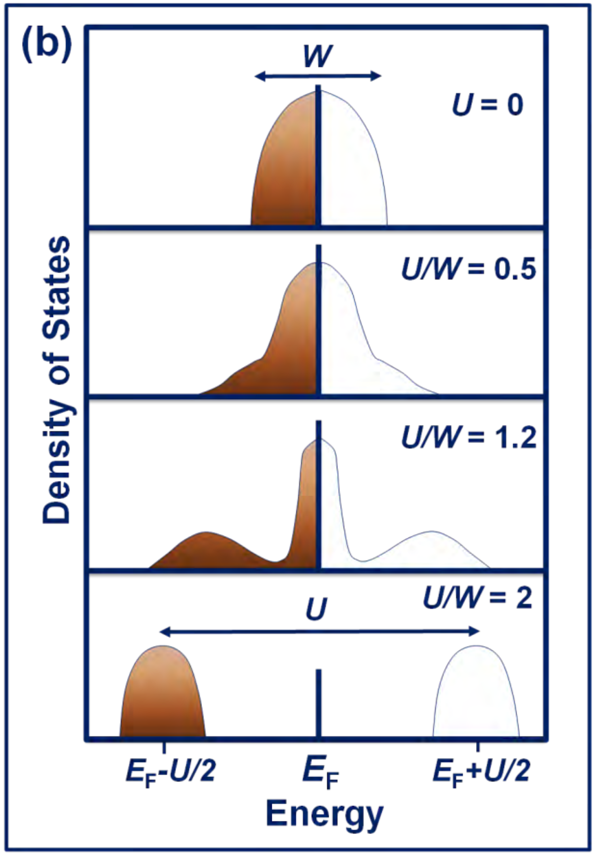
- **nature of magnetism**
  (role of spin-orbit coupling and symmetry)

***ab initio*** **density functional theory**
**+ many-body methods**

→ superconductivity

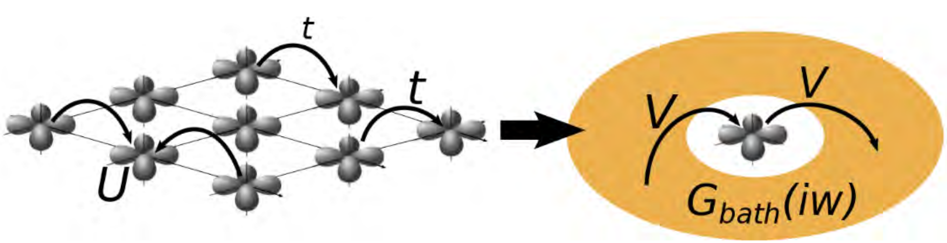
# correlation effects

$$\hat{H} = -\sum_{<ij>,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

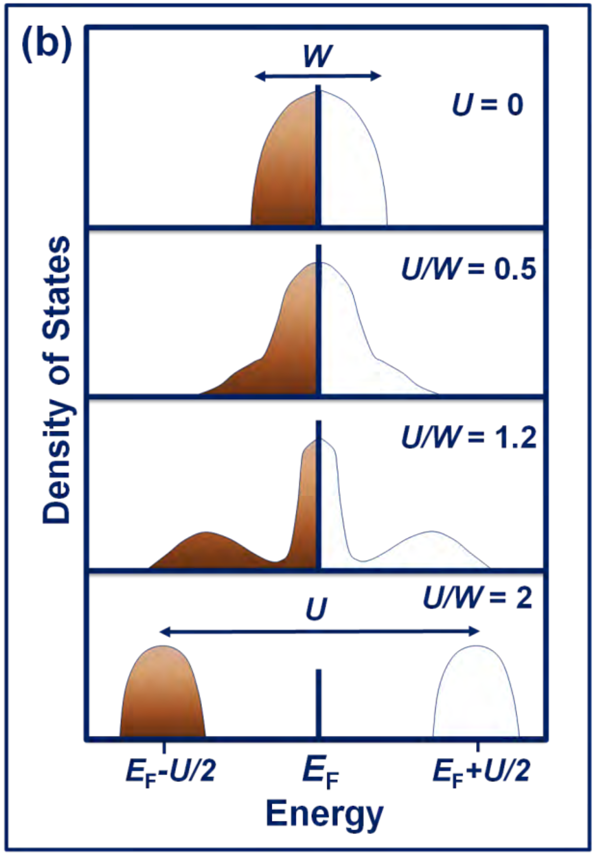


# correlation effects

$$\hat{H} = -\sum_{<ij>,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$




G. Kotliar, D. Vollhardt Phys. Today 57, 53 (2004)
A. Georges, G. Kotliar PRB 45, 6479 (1992)
T. Maier, M. Jarrell, T. Pruschke, M. Hettler RMP 77, 1027 (2005)




Density Functional theory +
**Dynamical Mean Field Theory (DMFT)**

Multiorbital systems:
role of Hund‘s coupling $J_H$ ?
Hund‘s metals

*Yin, Haule, Kotliar Nat Mat. **10**, 932 (2011)*
*Ferber ,Jeschke, Valenti PRL **109**, 236403 (2012)*

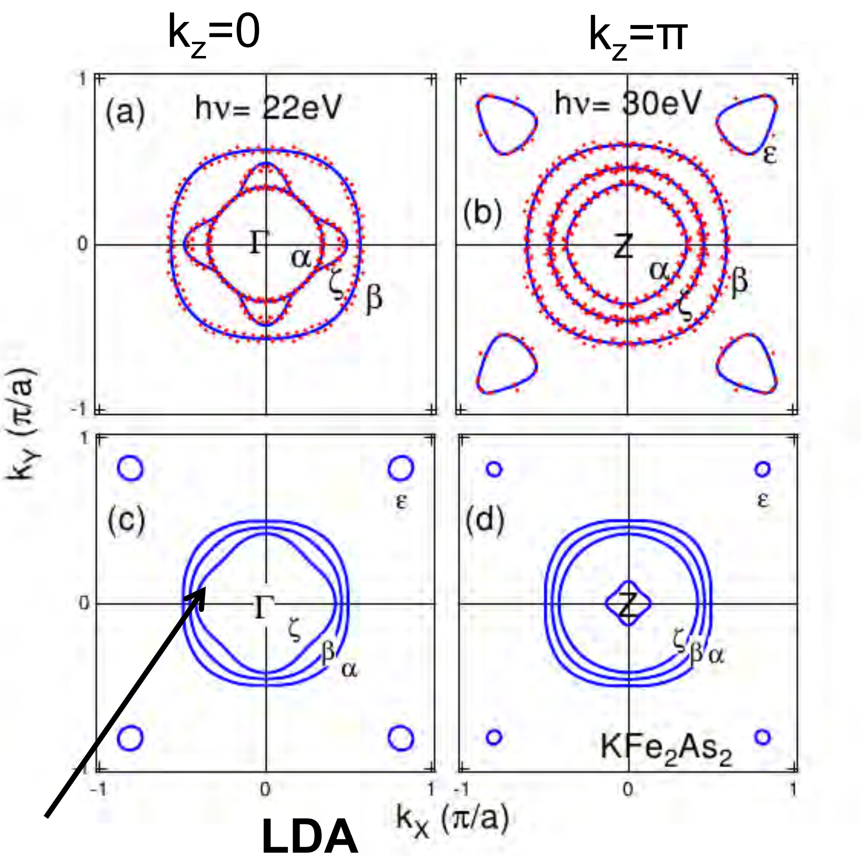
# correlation effects: how important?

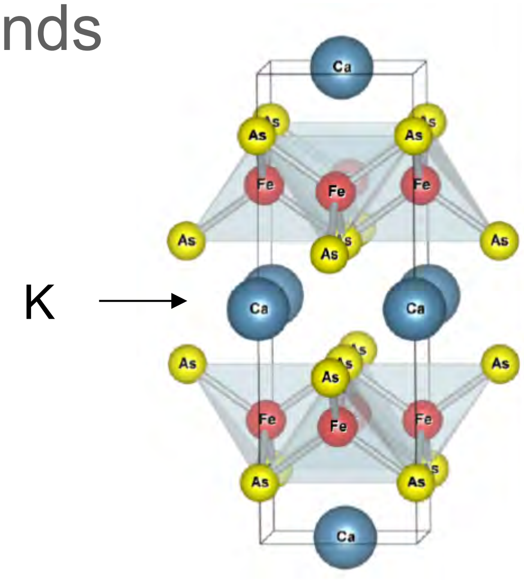
## Traces in experiment:

- ARPES: renormalization of bands

$KFe_2As_2$ at ambient pressure

$T_c$= 3.4K




*ARPES: Yoshida et al. arXiv:1205.6911*
*Okazaki et al. Science **337**, 1304 (2012)*
*dHvA: Terashima et al. PRB **87**, 224512 (2013)*

**ARPES, de Haas van Alphen, optical conductivity, resistivity, thermodynamics…**

# correlation effects: how important?

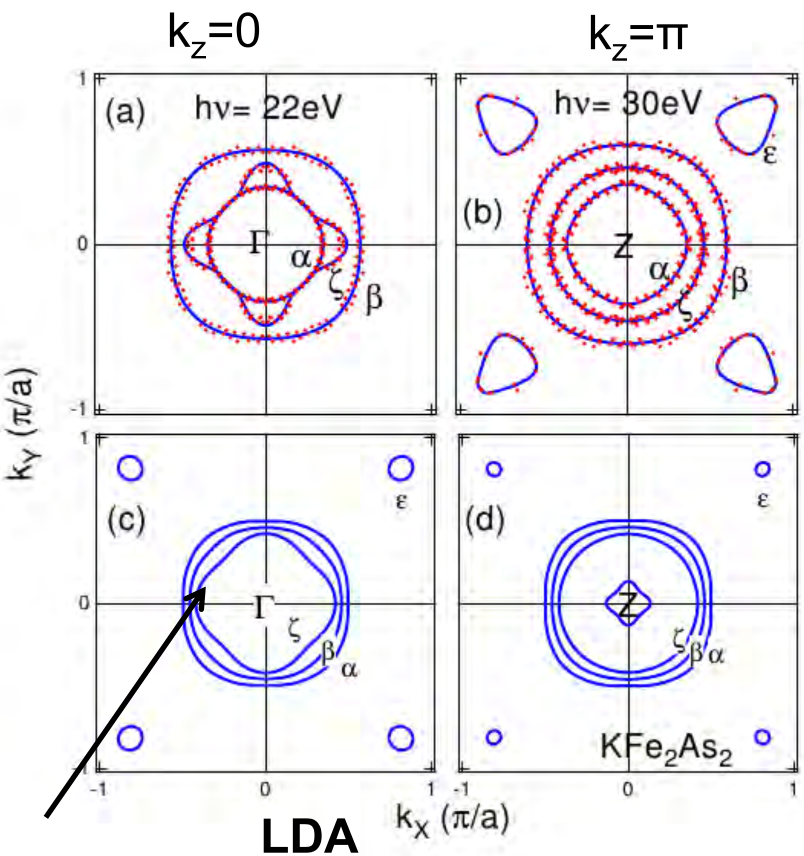
## Traces in experiment:

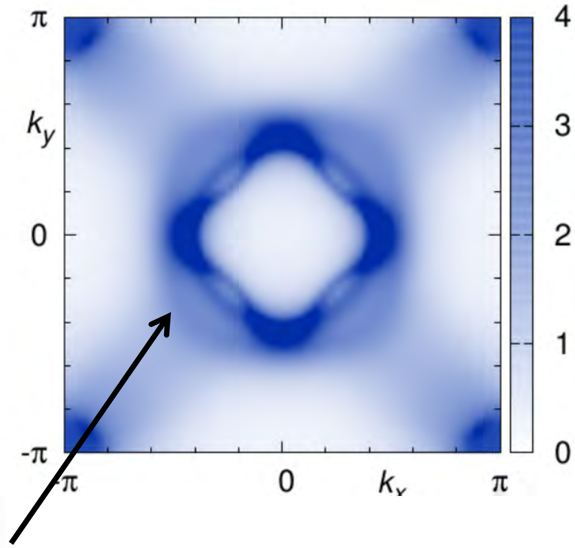
$KFe_2As_2$ at ambient pressure

- ARPES: renormalization of bands

LDA+DMFT

$T_c$= 3.4K




U= 4 eV
$J_H$= 0.8 eV

(change of topology)

*Backes, Guterding, Jeschke, Valenti NJP **16**, 083025 (2014)*

*Guterding, Backes, Jeschke, Valenti PRB **91**, 140503(R) (2015)*

## correlation effects: how important?

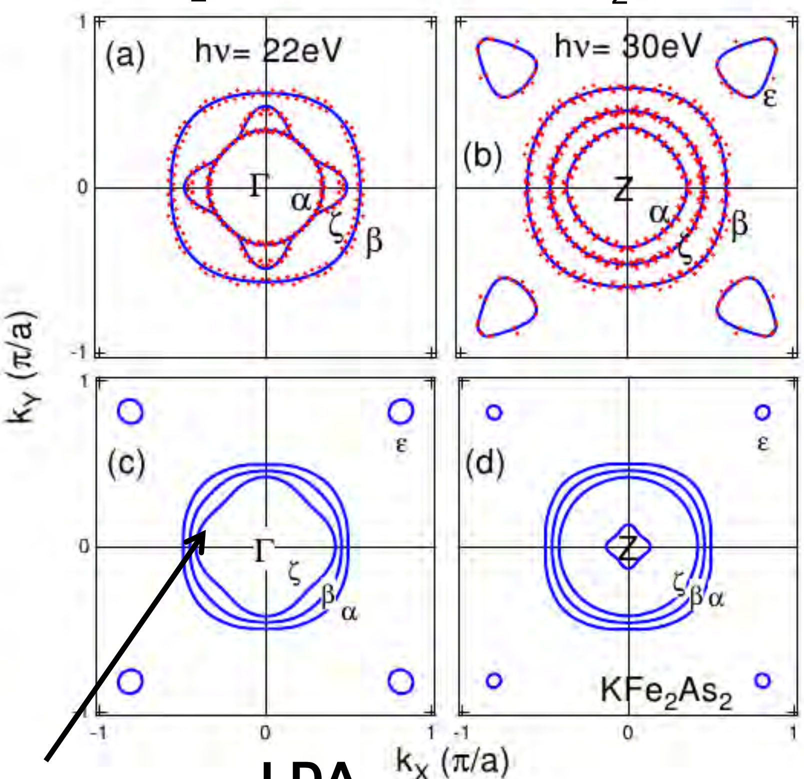
# Traces in experiment:

$KFe_2As_2$ at ambient pressure

$T_c$= 3.4K

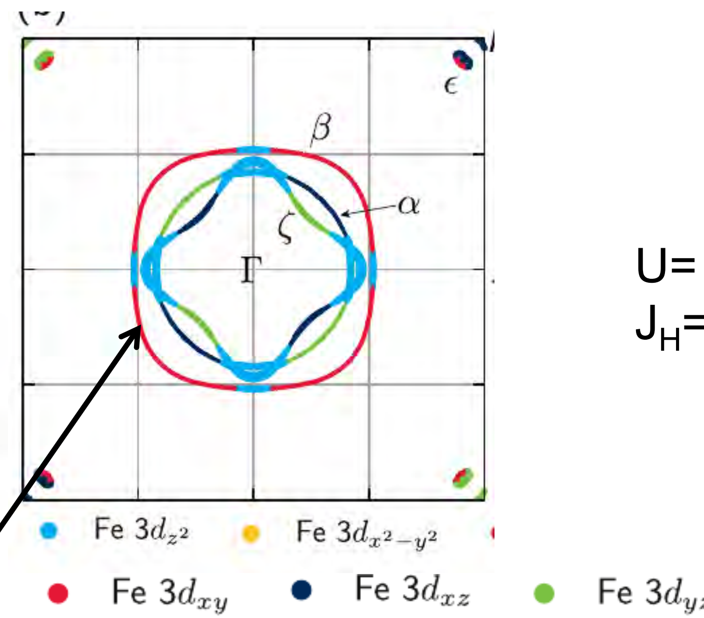
- ARPES: renormalization of bands

k$_z$=0 k$_z$=π




LDA

LDA+DMFT




U= 4 eV
$J_H$= 0.8 eV

| Orbital | $d_{xy}$ | $d_z^2$ | $d_{x^2-y^2}$ | $d_{xz/yz}$ |
|---|---|---|---|---|
| $\frac{m^*}{m_{LDA}}$ | 2.72 | 1.89 | 1.56 | 2.02 |

orbital-selective correlations

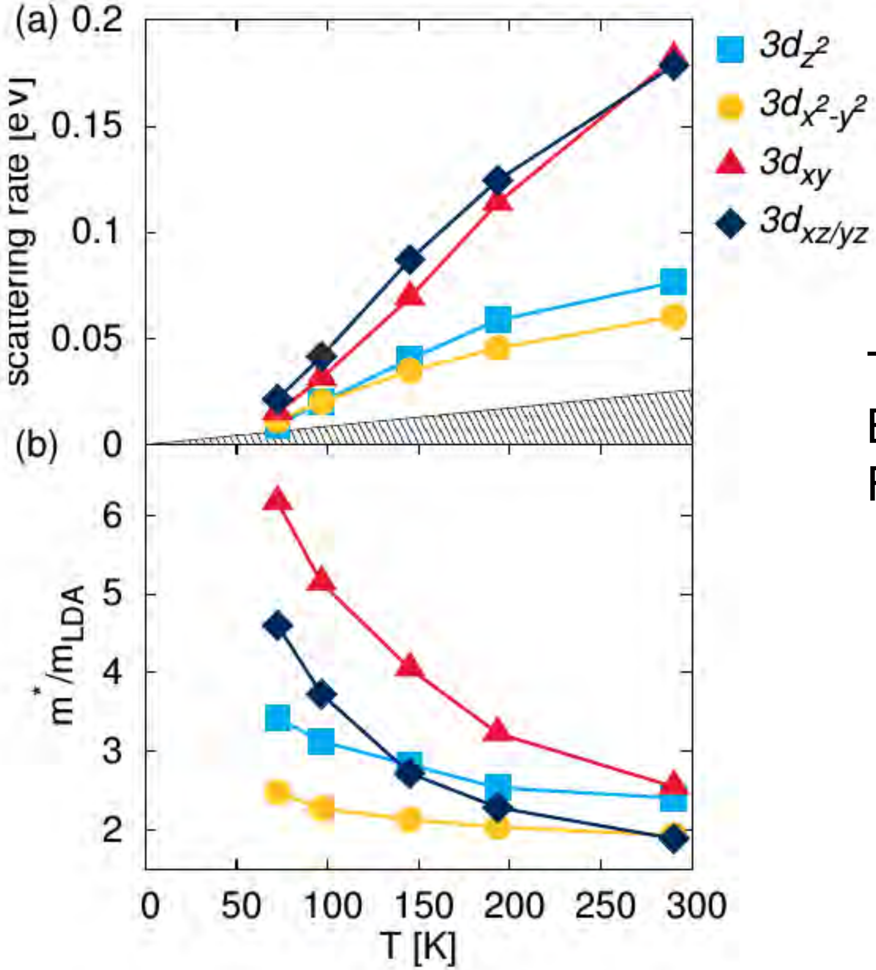
*Backes, Guterding, Jeschke, Valenti NJP **16**, 083025 (2014)*
*Guterding, Backes, Jeschke, Valenti PRB **91**, 140503(R) (2015)*

# Coherence-incoherence crossover

U= 4 eV  $J_H$= 0.8 eV   LDA+DMFT

**$KFe_2As_2$**

Temperature dependence




orbital-selective correlations

(inverse of the quasiparticle lifetime)

$T^*_{theo}$~50K

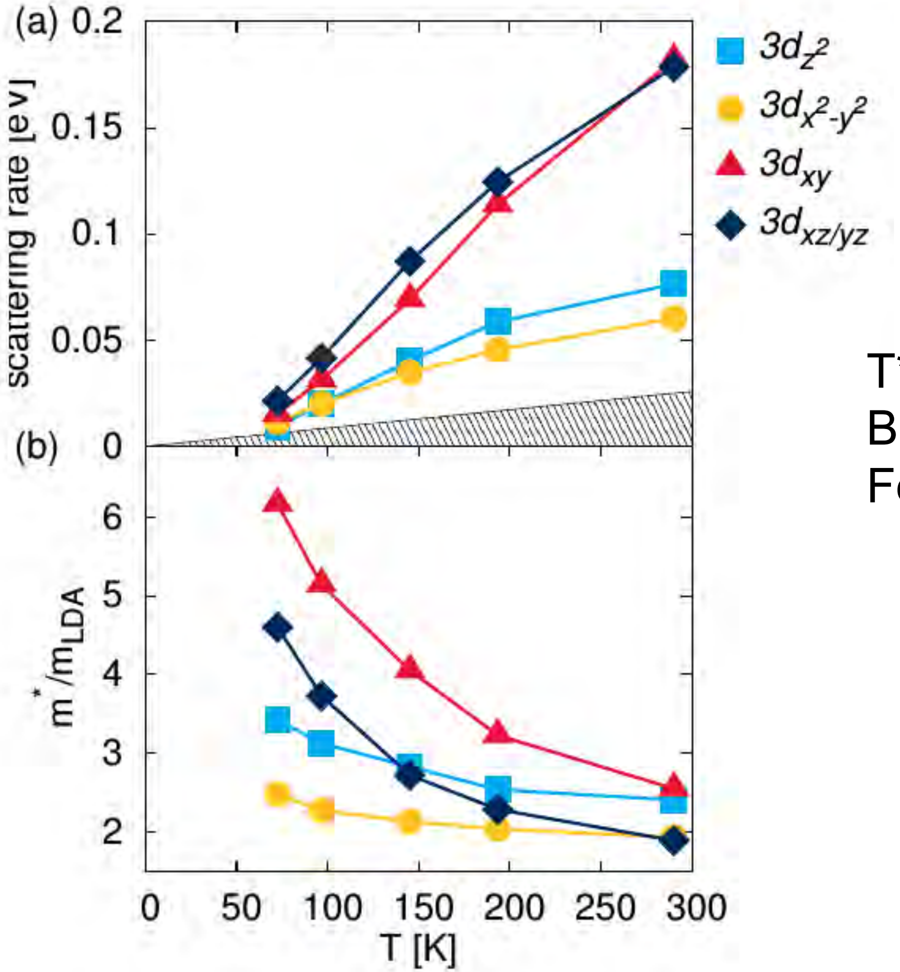
T*:
Bad metal –
Fermi liquid

# Coherence-incoherence crossover

U= 4 eV  $J_H$= 0.8 eV    LDA+DMFT

**$KFe_2As_2$**

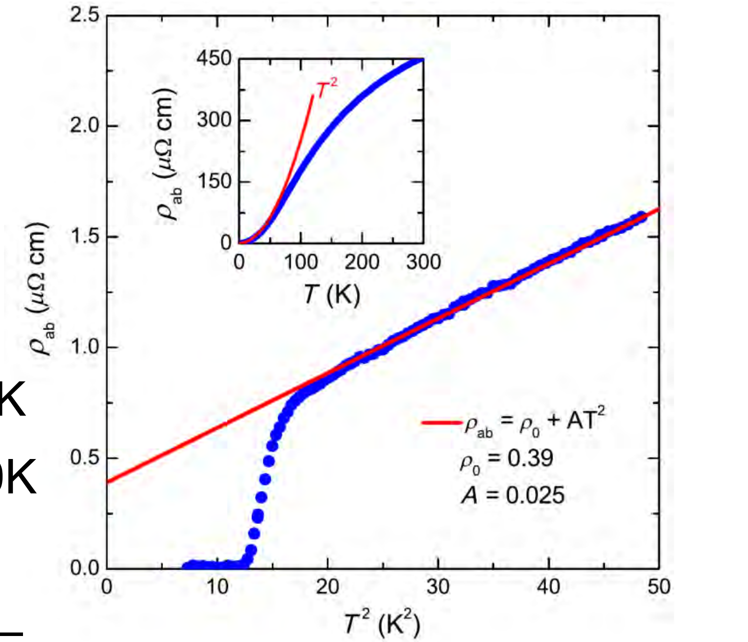
Temperature dependence

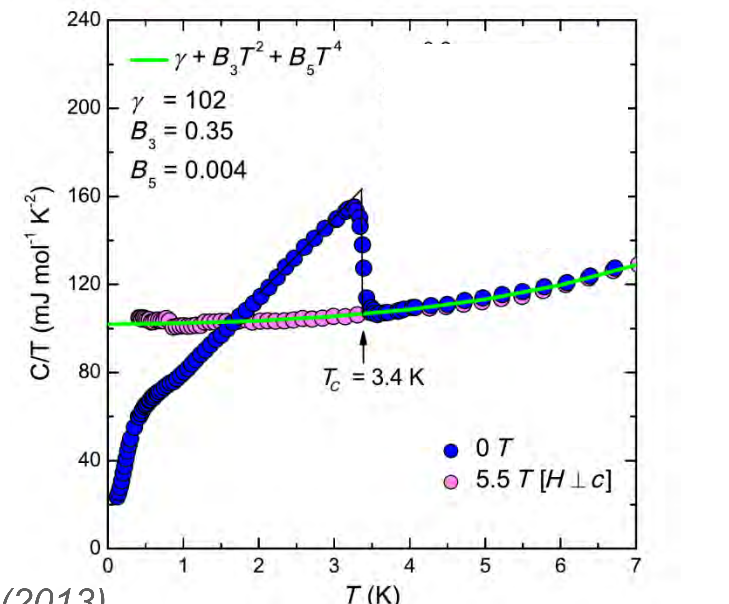



$T^*_{exp}$~70K

$T^*_{theo}$~50K

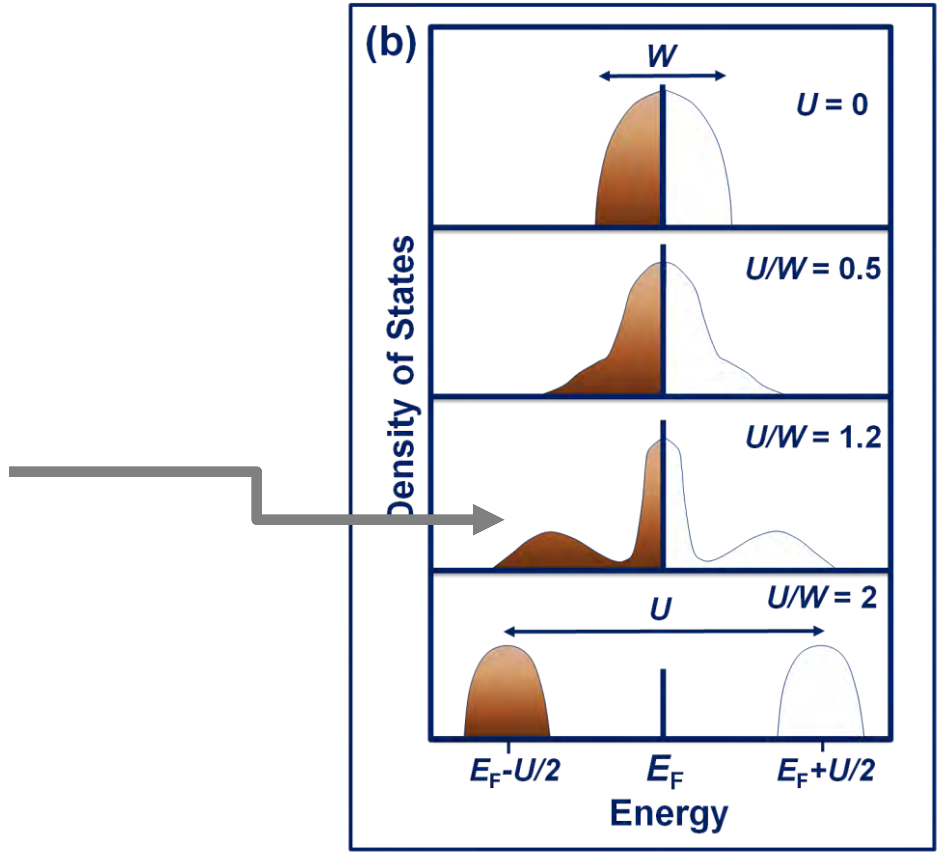
T*:
Bad metal – Fermi liquid



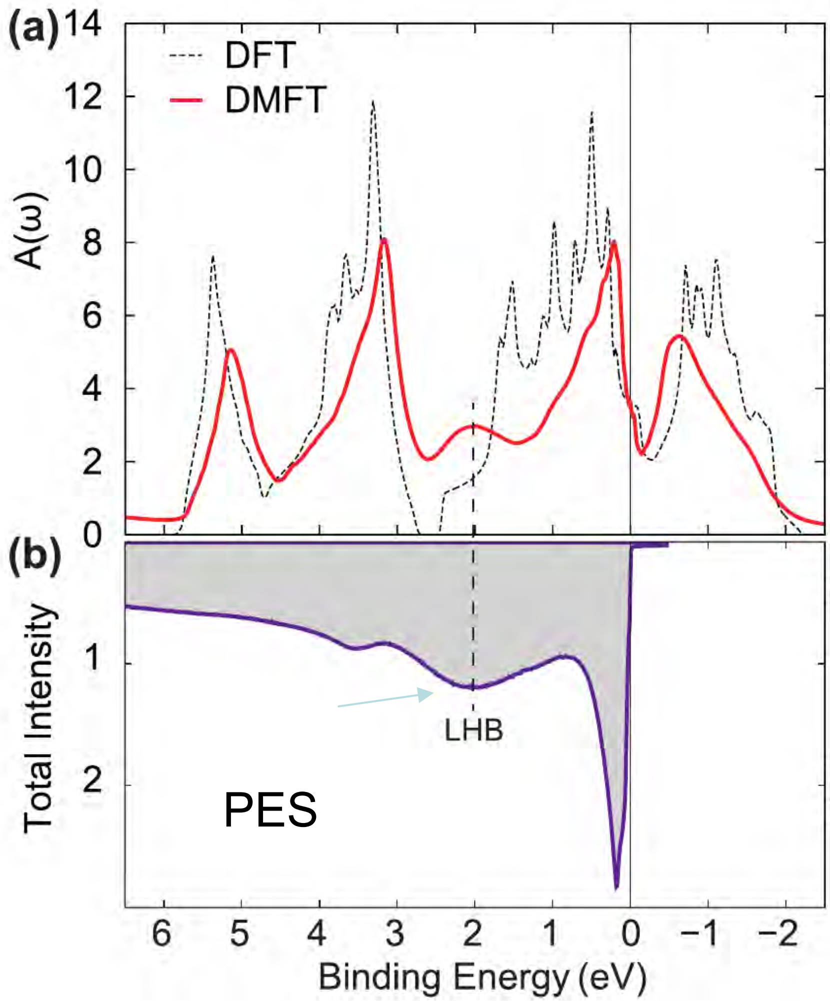

*Backes, Jeschke, Valenti  PRB **92**, 195128 (2015)*

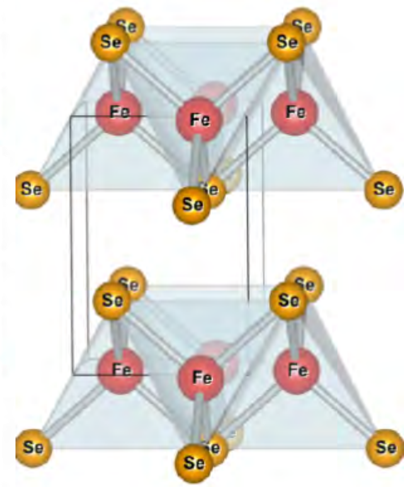
*Hardy et al. PRL **111**, 027002 (2013)*


(b)
W
U = 0
U/W = 0.5
U/W = 1.2
U/W = 2
U
Density of States
E_F-U/2
E_F
E_F+U/2
Energy

# FeSe: correlation effects

Formation of Hubbard-like bands as a fingerprint of strong correlations



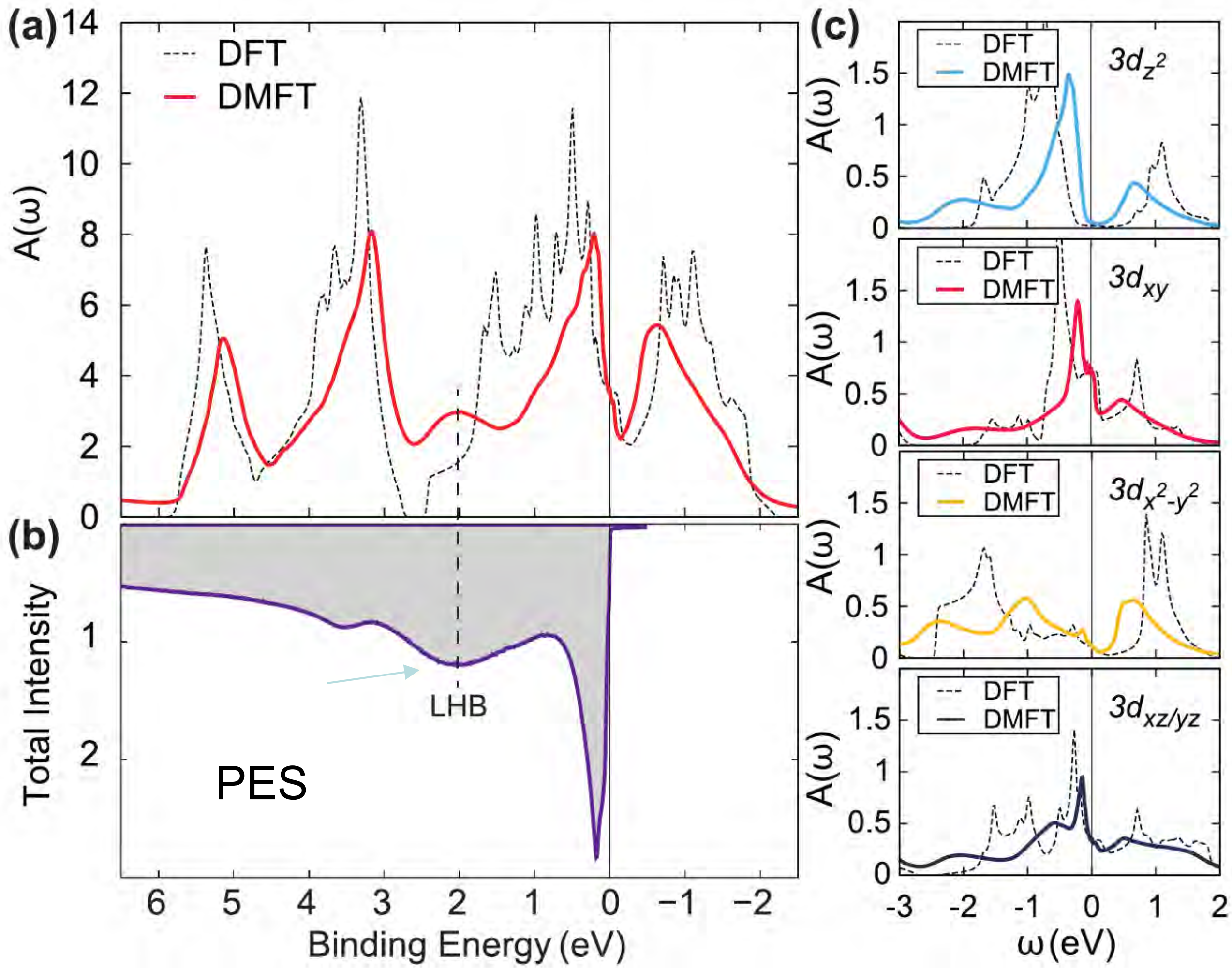



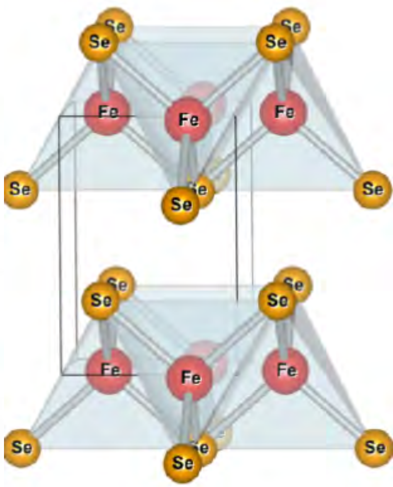

*Watson,Backes,Haghighirad,Hoesch,Kim,Coldea,Valenti PRB 95,081106(R) (2017)*

*Evtushunsky, Büchner,Borisenko et al. arXiv:1612.02313*
*Skornyakov,Anisimov,Vollhardt,Leonov arXiv:1703.03236*

# FeSe: correlation effects

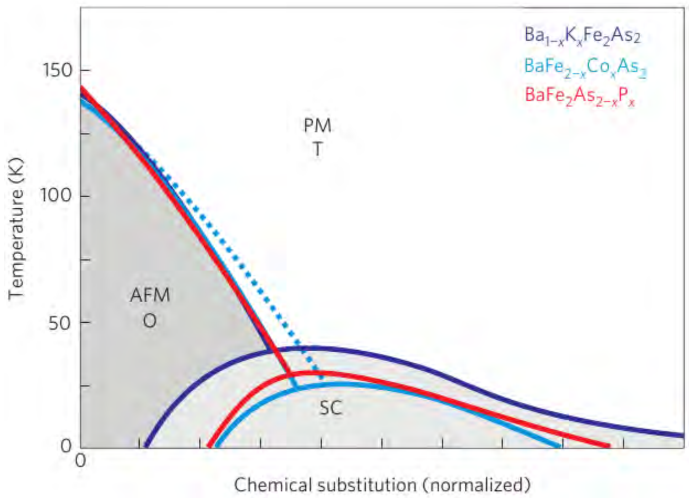
Formation of Hubbard-like bands as a fingerprint of strong correlations

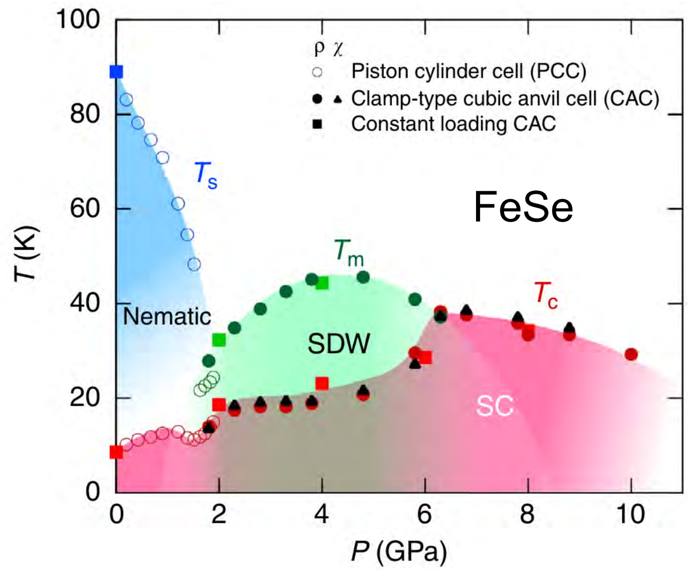



*Watson, Backes, Haghighirad, Hoesch, Kim, Coldea, Valenti PRB 95, 081106(R) (2017)*

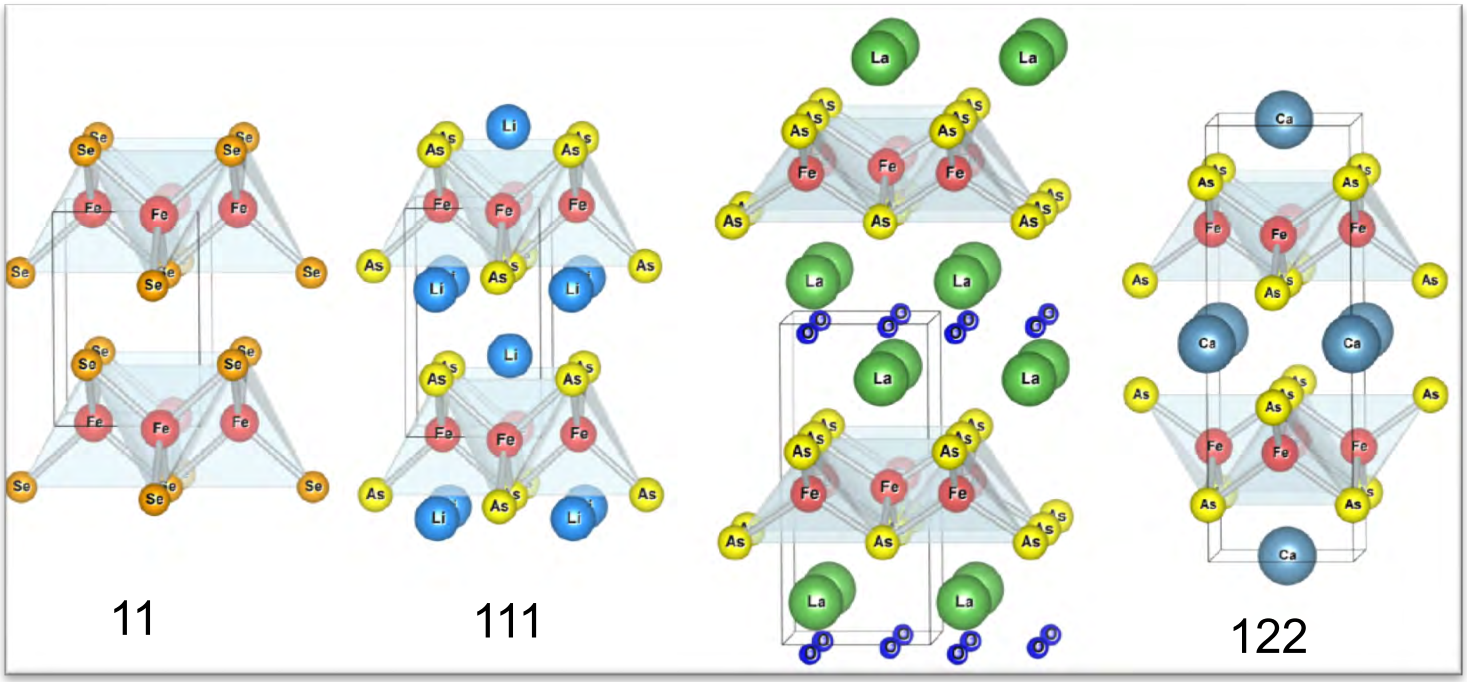
*Discovery of orbital-selective Cooper pairing in FeSe (quasiparticle interference imaging)*
*Sprau et al. Science 357, 75 (2017)*




# nature of magnetism?

magnetism as key ingredient for unconventional superconductivity




1111

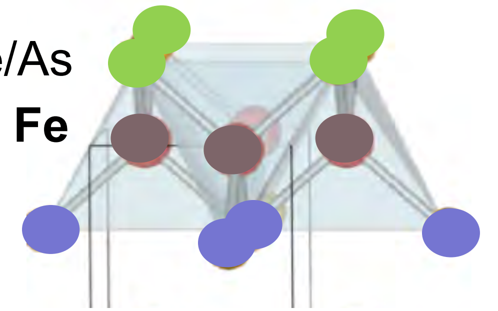
**Symmetry:** **tetragonal**

| | |
|---|---|
| 11, 111, 1111 | P4/nmm (129) |
| 122 | I4/mmm (139) |

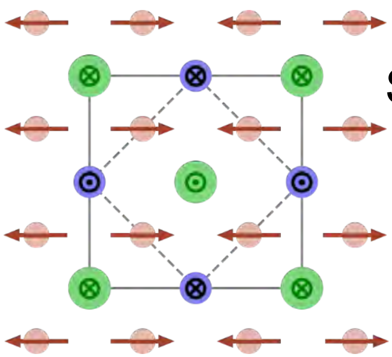
→ C4
→ glide symmetry across the Fe-As planes

# $Q_1=(\pi,0)$ $Q_2=(0,\pi)$ Magnetic Orders

**Breaks:**
- rotational symmetry
  C4→ C2
- time-reversal symmetry

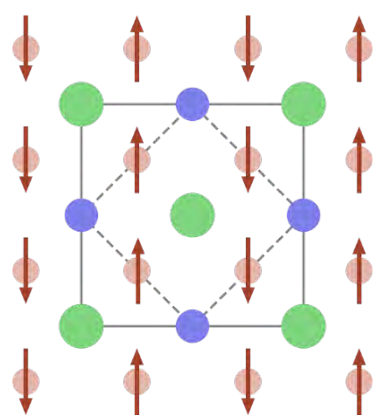



Stripe **M||Q** $\mathbf{M_1}$ or $\mathbf{M_2}$=0




$$\boldsymbol{m}(\boldsymbol{R}) = \boldsymbol{M}_1 \cos(\boldsymbol{Q}_1 \cdot \boldsymbol{R}) + \boldsymbol{M}_2 \cos(\boldsymbol{Q}_2 \cdot \boldsymbol{R}).$$

Stripe **M⊥Q**



*Dai RMP 87, 855 (2015)*

# $Q_1=(\pi,0)$ $Q_2=(0,\pi)$ Magnetic Orders

**Breaks:**
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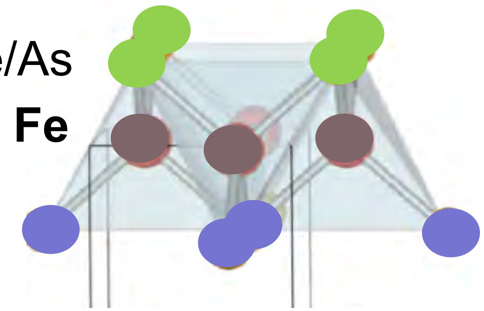
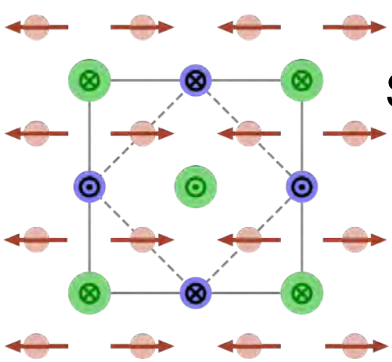
- time-reversal symmetry




Stripe **M||Q** **$M_1$** or **$M_2$**=0

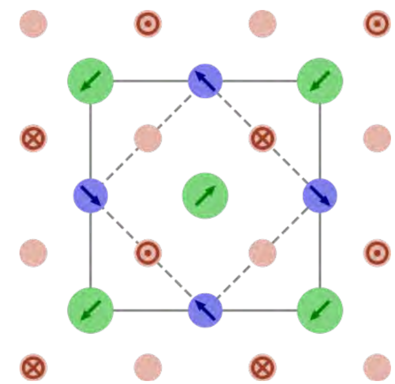



$$m(R) = M_1 \cos(Q_1 \cdot R) + M_2 \cos(Q_2 \cdot R).$$

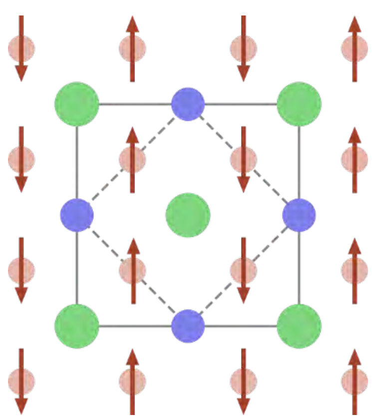
C4 preserved

**$M_1=\pm M_2$**

Spin Charge Density Wave



Stripe **M⊥Q**



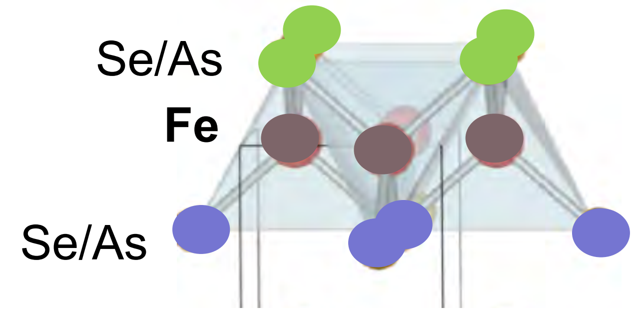
*O'Halloran et al. PRB 95, 075104 (2017)*

*Meier,…,Borisov,Valenti,…,Canfield Arxiv:1706.01067*

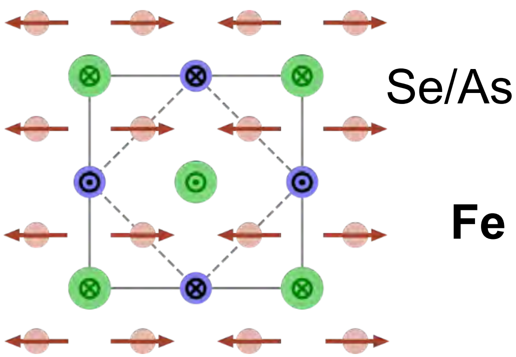
# $Q_1=(\pi,0)$ $Q_2=(0,\pi)$ Magnetic Orders

**Breaks:**
- rotational symmetry
  C4→ C2
- time-reversal symmetry

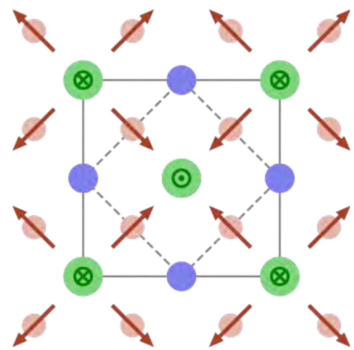
**Breaks:**
- Glide symmetry
- time-reversal symmetry




Stripe **M||Q**




Hedgehog (non-collinear $\mathbf{M}_i$)
Spin Vortex Crystal ($\mathbf{M}_i||\mathbf{Q}_i$)



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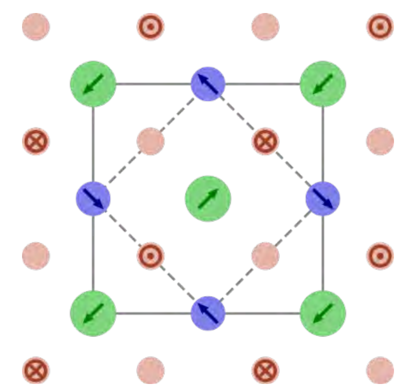
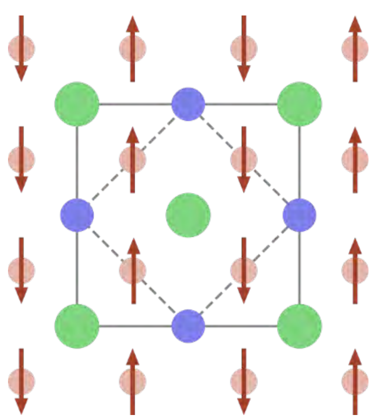
C4 preserved

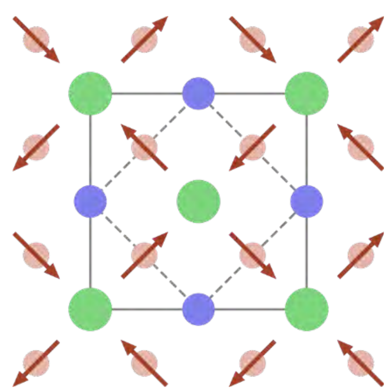
Spin Charge Density Wave



Stripe **M⊥Q**



Loops
Spin Vortex Crystal ($\mathbf{M}_i \perp \mathbf{Q}_i$)



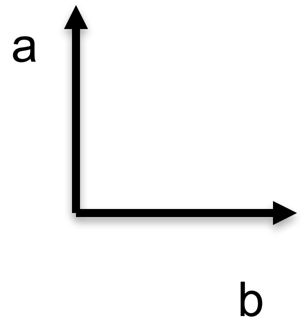
*O'Halloran et al. PRB 95, 075104 (2017)*

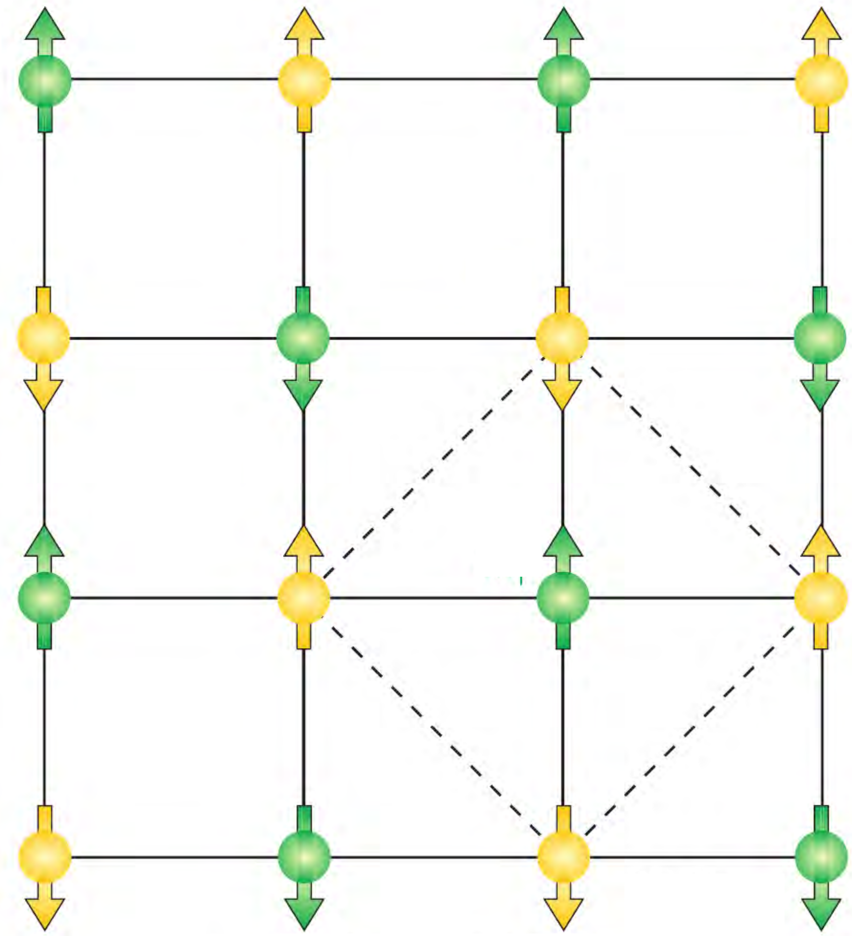
*Meier,…,Borisov,Valenti,…,Canfield Arxiv:1706.01067*

## Fe-plane

tetragonal → orthorhombic

**Breaks:**
- rotational symmetry
  C4→ C2
- time-reversal symmetry

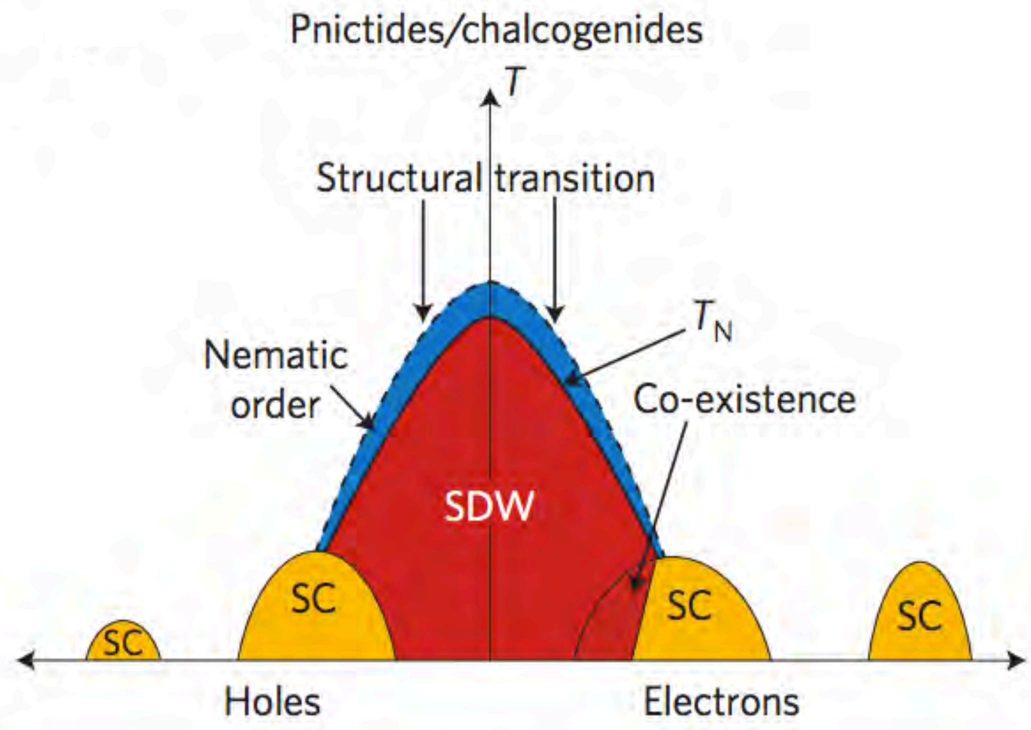


$Q_2 = (0,\pi)$

# A third phase: Nematic phase

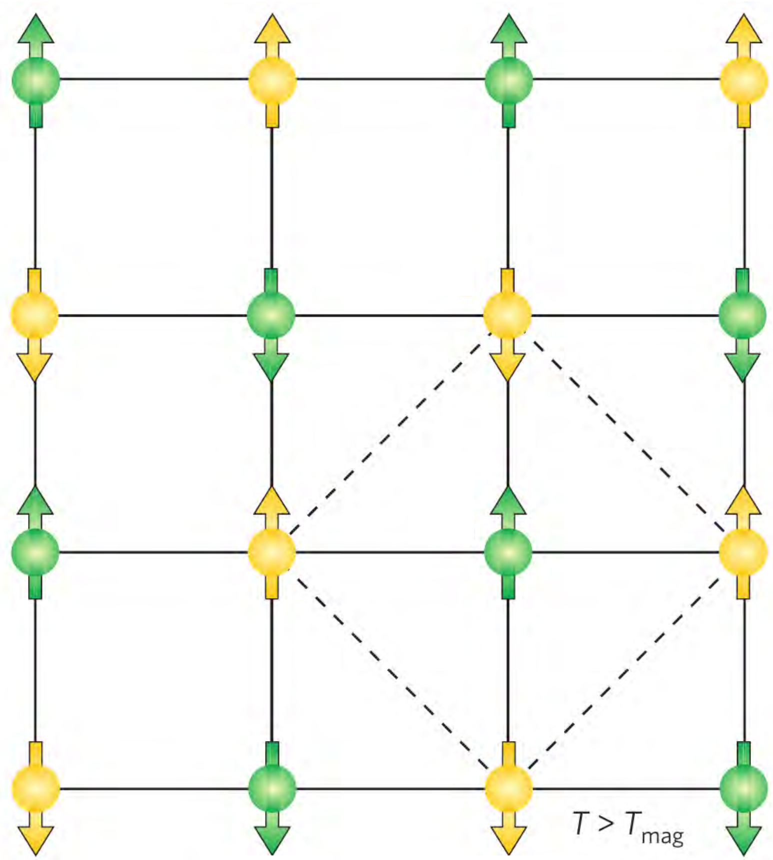
($Ba_{1-x}K_xFe_2As_2$ $BaFe_{2-x}Co_xAs_2$ )



# A third phase: Nematic phase

## Superconducting phase / Ordered magnetic phase / **Nematic Phase**

($Ba_{1-x}K_xFe_2As_2$ $BaFe_{2-x}Co_xAs_2$ )




- Breaks rotational symmetry: C4 → C2

- Preserves time-reversal symmetry

**Origin?**
- **structural distortions**
- **charge/orbital**
- **spin**

electronic nematic order

*Fernandes et al. Nature Physics (2014)*

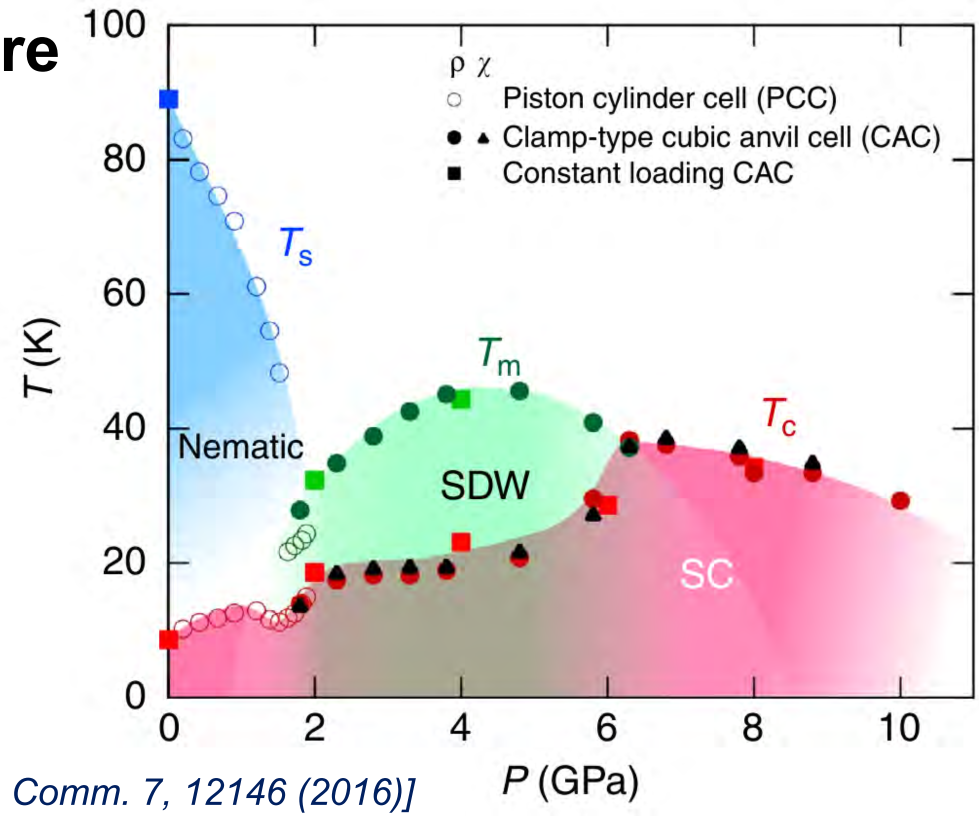
# FeSe: 8K superconductor

## FeSe under pressure

C4→C2

**1) Nematic phase**

**no magnetic ordering**

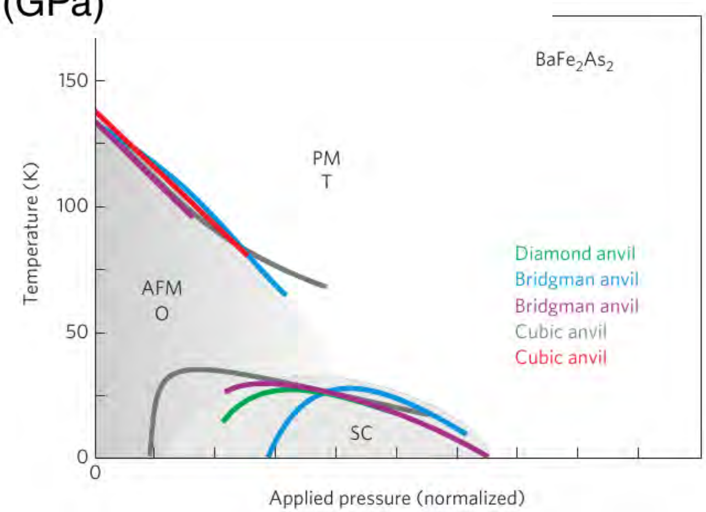



*[Sun et al. Nature Comm. 7, 12146 (2016)]*

**2) Superconducting $T_c$ goes up**

→ 37K under pressure

Compare f.i. to Ba122




*Rotter et al. Ang. Chem. 47, 7949 (2008)*
*Kimber et al. Nat. Mat. 8, 471 (2009)*
*Paglione , Greene Nat. Phys. 6, 645 (2010)*

.

# Summary of some experimental observations

## - Fermi surface: extremely small hole and electron pockets (ARPES, dHvA)

*Terashima et al. PRB 90, 144517 (2014)*

*Audouard et al. arXiv 1409.6003*

*Watson et al. PRL 115, 027006 (2015)*

*Fedorov et al. Sci. Rep. 6, 36834 (2016)*

*Kushnirenko et al. arXiv:1702.02088 (anomalous T-dependence)*

## - absence of spin fluctuations in NMR but (π,0) magnetic fluctuations in INS

*Baek et al. Nature Mat. 14, 2010 (2015)*

*Boehmer et al. PRL 114, 10052 (2015)*

*Rahn et al. PRB. 91, 180501(R) (2015)*

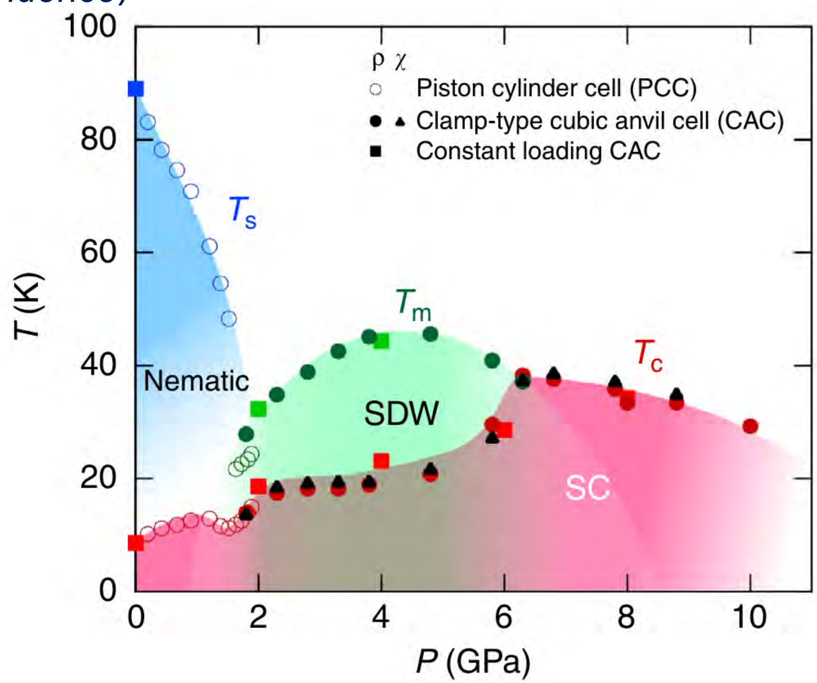
*Wang et al., Nat. Mat. 15, 159 (2016)*

## - Pressure-induced AFM transition (AC magnetization, μSR, resistance Mössbauer, X-ray)

*Bendele et al. PRL 104, 087003 (2010)*

*Terashima et al. J. Phys. Soc. Jpn 84, 063701 (2015)*

*Kothapali et al. arXiv 1603.04135*




*[Sun et al. Nature Comm. 7, 12146 (2016)]*

## - dxz/dyz splitting and orbital order in the nematic phase

*Maletz et al. PRB 89, 220506(R) (2014)*

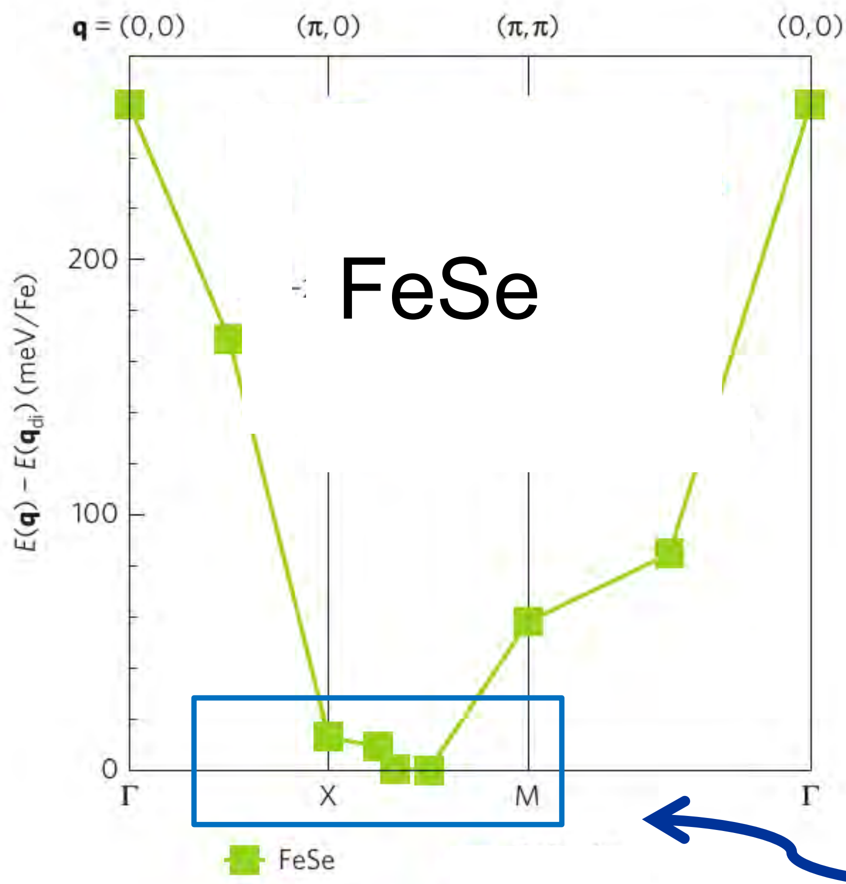
*Watson et al. PRB 91, 155106 (2015)*

(list not complete)

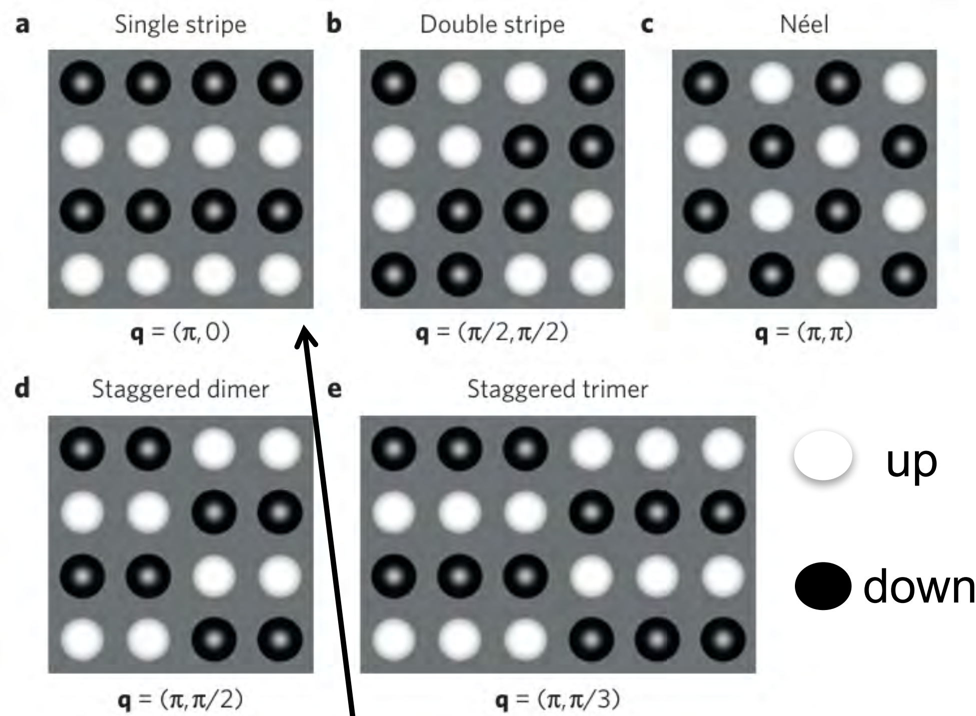
# What can we learn from ab initio calculations?

# FeSe: magnetism?

**magnetic GGA total energy calculations (ELK, WIEN2k, FPLO)**




tetragonal experimental structure




Competing magnetic states:
**q**= (π,Q) $0 < Q < \pi/2$

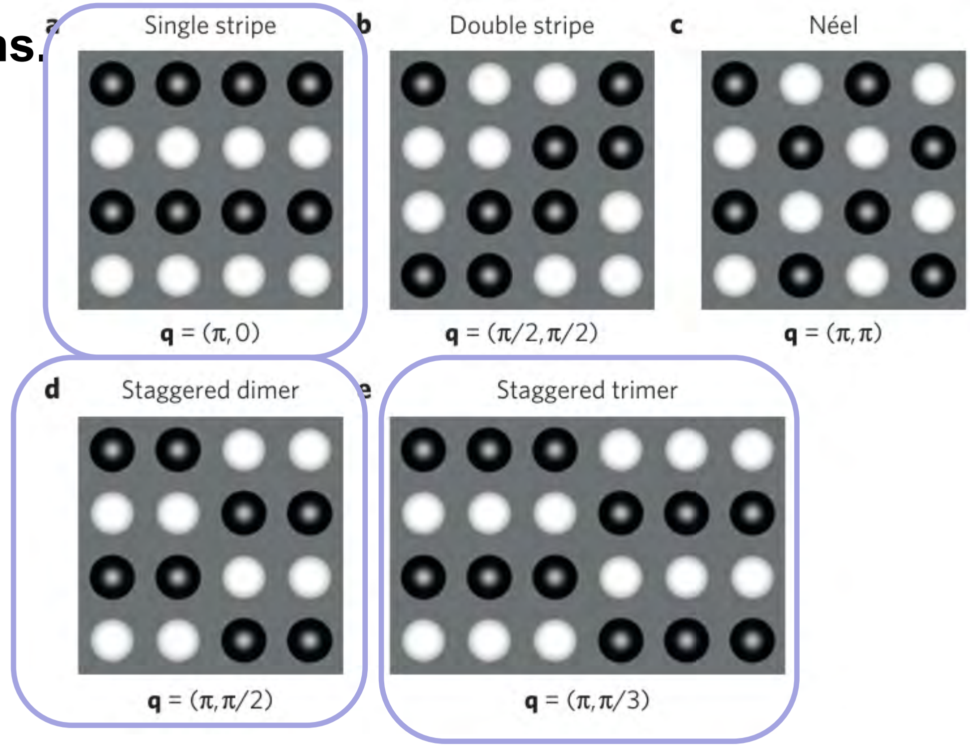
**magnetic frustration!**

Soft magnetic fluctuations along the transverse direction

*Glasbrenner,Mazin,Jeschke,Hirschfeld,Fernandes,Valenti Nat.Phys. 11, 953 (2015)*

# FeSe: magnetism?

**magnetic GGA total energy calculations.**
**(ELK, WIEN2k, FPLO)**




Competing magnetic states:

**q**= (π,Q) $0 \leq Q \leq \pi/2$

→ magnetic long-range order is destroyed by spin fluctuations

→ BUT all low-lying states break the x ←→ y symmetry in the same way and don't compete in terms of **nematicity**

C4→C2

→ **nematic order** is promoted!

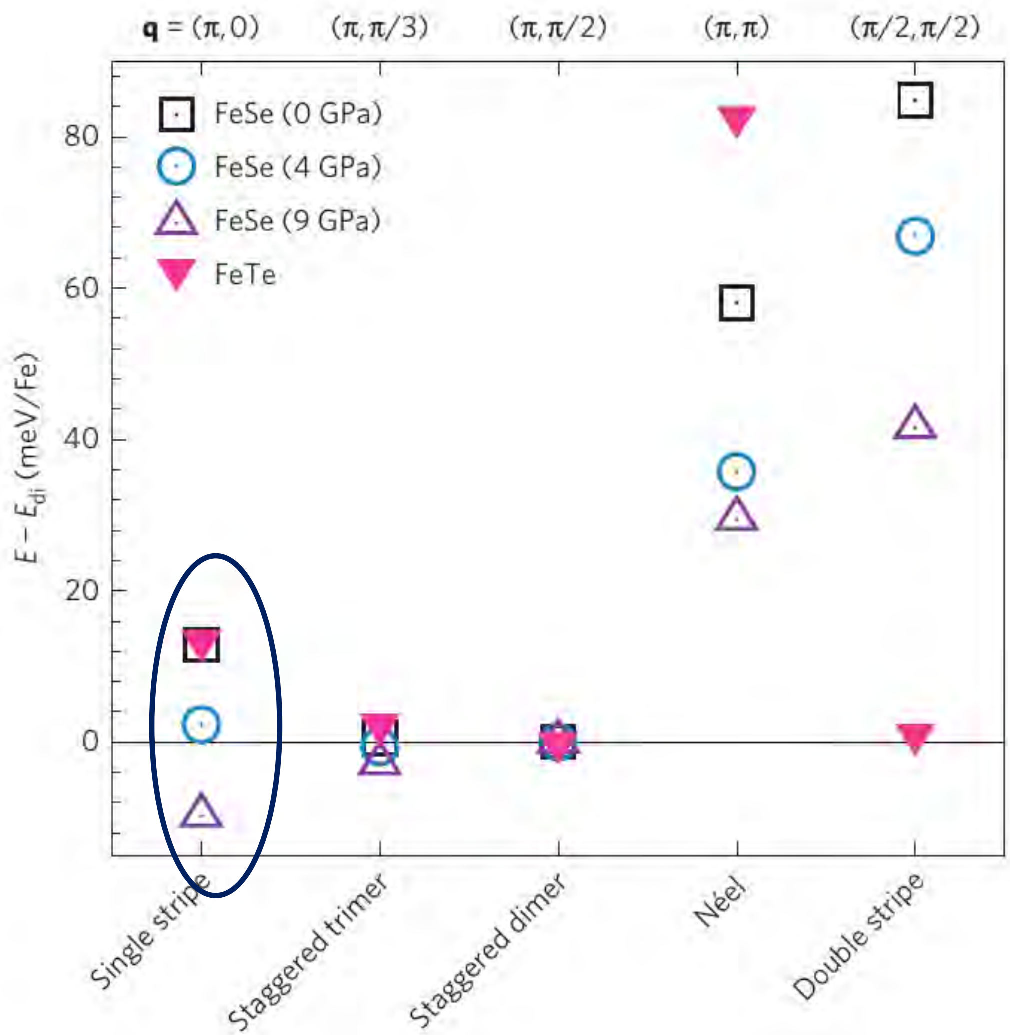
*Glasbrenner, Mazin, Jeschke, Hirschfeld, Fernandes, Valenti Nat.Phys. 11, 953 (2015)*

# FeSe under pressure

**GGA total energy calculations.**
**(ELK, WIEN2k, FPLO)**

-Under pressure fluctuations with q=(π,0) dominate

Consequences?



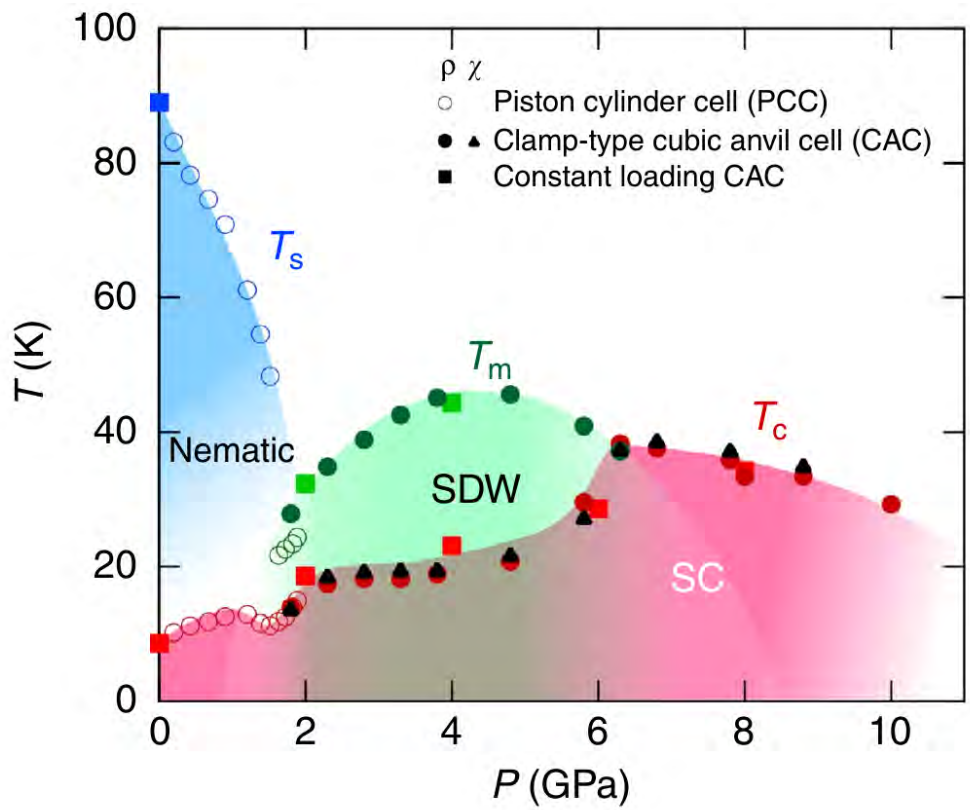
# FeSe under pressure

## Superconductivity?

**q**= (π,Q)   0 < Q < π/2  :

pair-breaking spin fluctuations

-Under pressure fluctuations with **q**=(π,0) dominate




*[Sun et al. Nature Comm. 7, 12146 (2016)]*

Fluctuation with  **q**=(π,0)

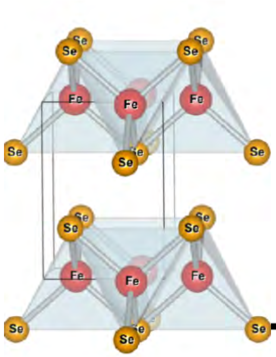
promote  s+- superconductivity  → **rise of $T_c$ with pressure**

P>9 Gpa

(a) Magnetism is generally suppressed, fluctuations diminish

(b) Tc goes down

# Why is bulk FeSe so special?




| Material | Fe-As/Se Distance (Å) |
|---|---|
| LaFeAsO | 1.32 |
| $BaFe_2As_2$ | 1.36 |
| NaFeAs | 1.43 |
| FeSe (0 GPa) | 1.48 |
| FeSe (4 GPa) | 1.42 |
| FeSe (9 GPa) | 1.42 |
| FeTe | 1.77 |

stripe order

magnetic degeneracy

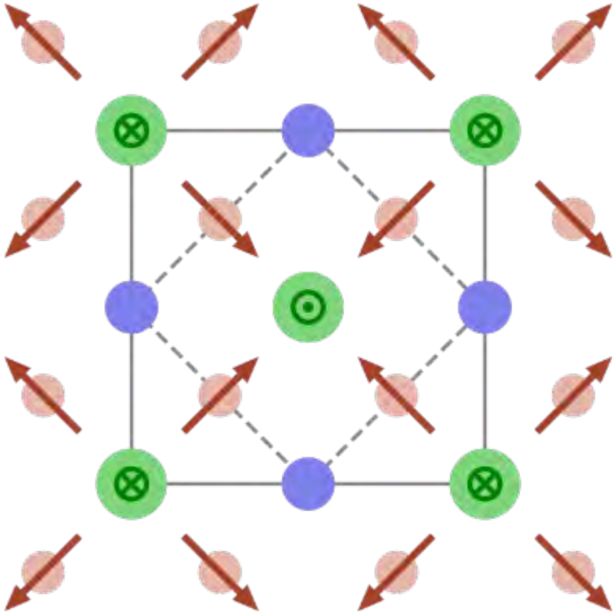
double stripe order

critical Fe-Se distance?

**Magnetic order breaks:**
- Glide symmetry
- time-reversal symmetry

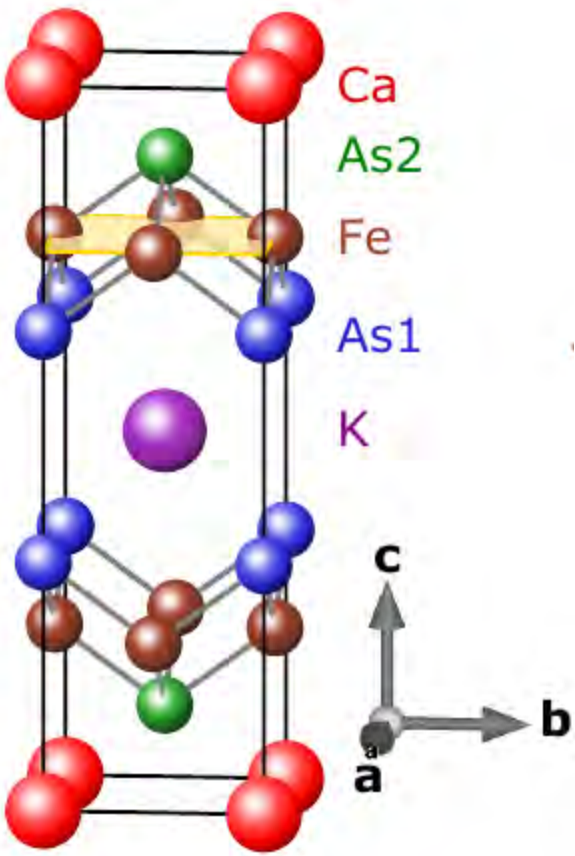
?

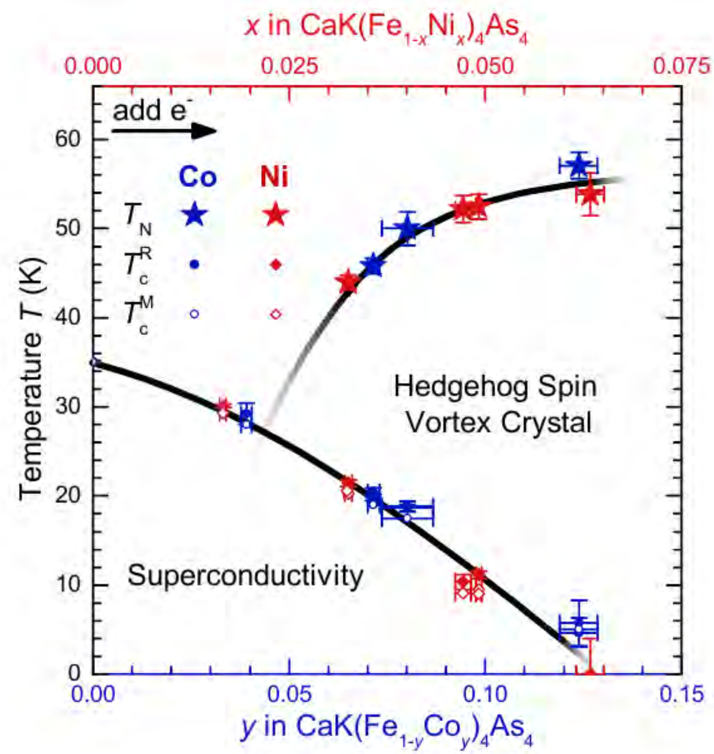
Hedgehog
Spin Vortex Crystal (**$\mathbf{M_i} || \mathbf{Q_i}$**)

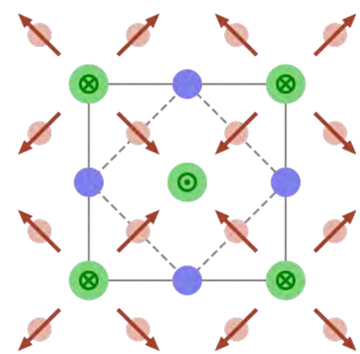


**Magnetic order breaks:**
- Glide symmetry
- time-reversal symmetry

$CaKFe_4As_4$



*Meier,…,Borisov,Valenti,…,Canfield*
*Arxiv:1706.01067*

outlook

## Correlation effects

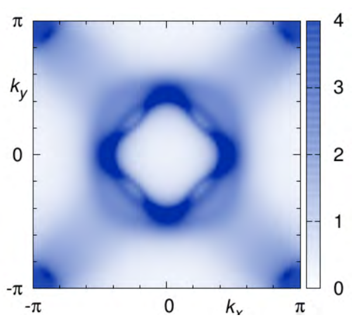
**DFT+DMFT**

- Strong band renormalization
- **Orbital-selective correlations**

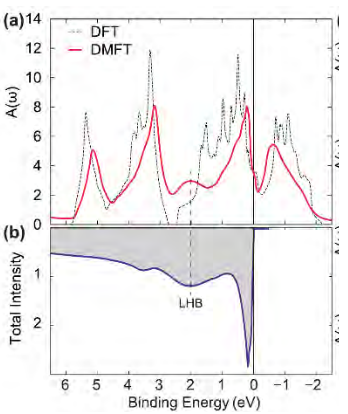
→ *change of Fermi-surface topology*
→ *orbital-selective Cooper pairing*

- Hubbard-like lower bands

$KFe_2As_2$




FeSe



# Correlated superconductors: Fe pnictides/chalcogenides

outlook

## Correlation effects

**DFT+DMFT**

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FeSe

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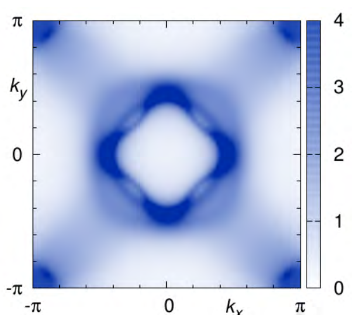
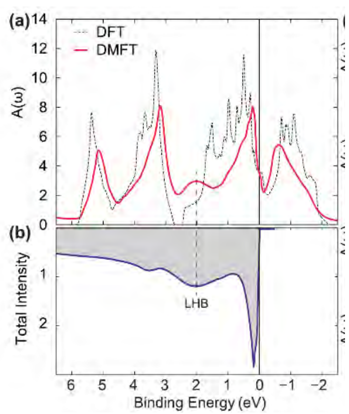
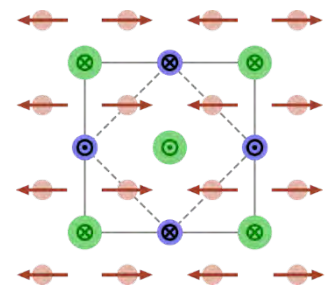


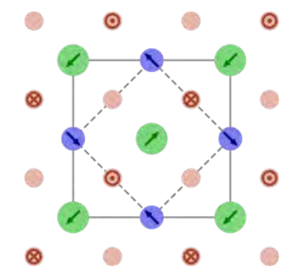

## Magnetism

$$m(R) = M_1 \cos(Q_1 \cdot R) + M_2 \cos(Q_2 \cdot R)$$

stripe order



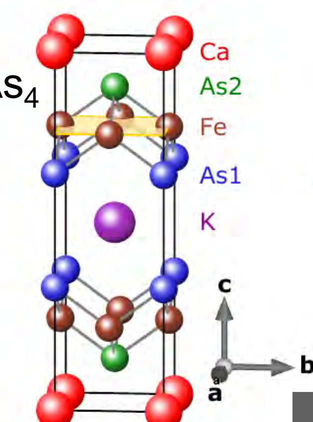
SCDW order

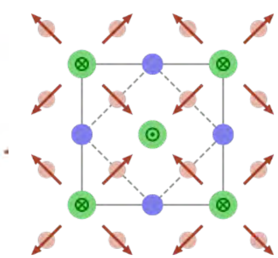


(nematic phases FeSe)
(magnetic frustration)

Hedgehog order (Skyrmion)

$CaKFe_4As_4$



superconductivity

# Correlated superconductors: Fe pnictides/chalcogenides

outlook

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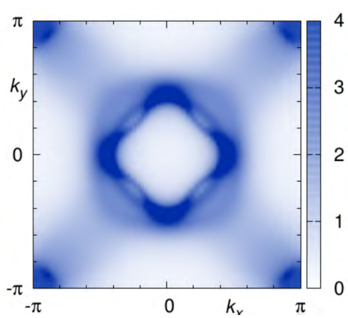
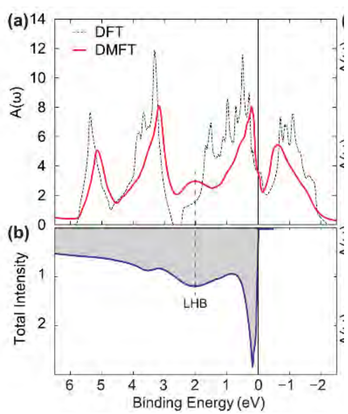



FeSe

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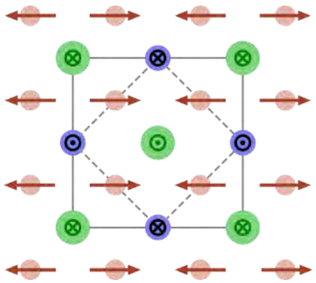
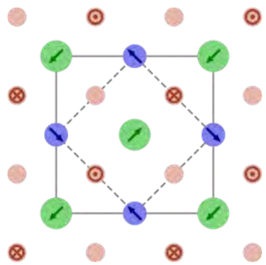


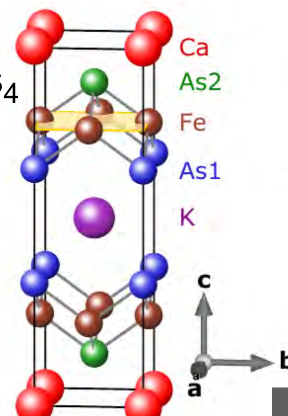
SCDW order



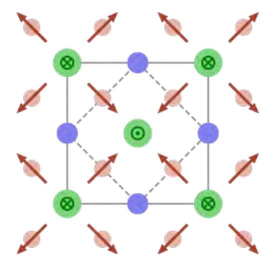
(nematic phases FeSe)

(magnetic frustration)

$CaKFe_4As_4$




Hedgehog order (Skyrmion)



**THANK YOU!**

superconductivity