The role of Hund's coupling in the nematicity of iron superconductors:

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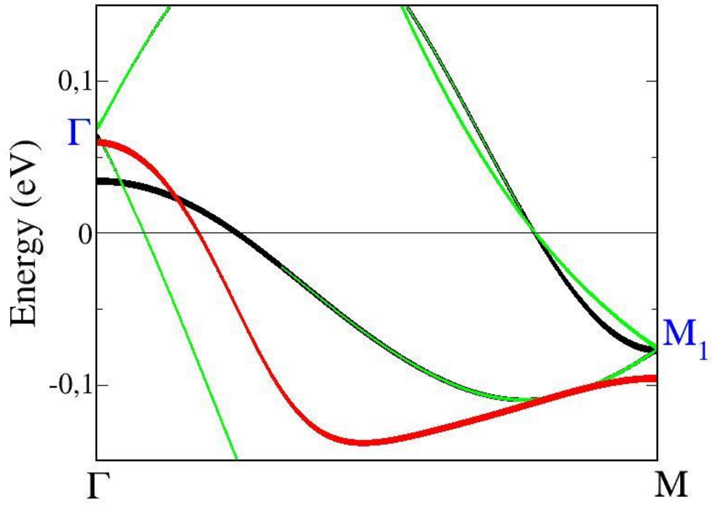
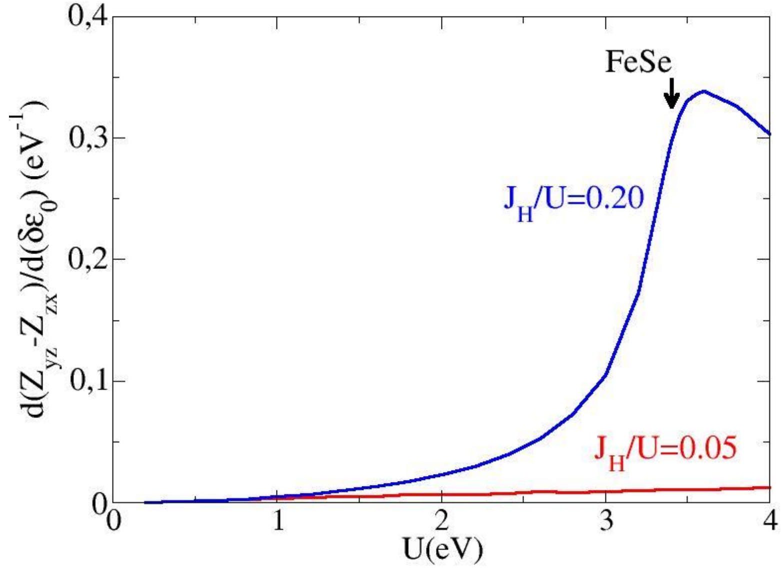
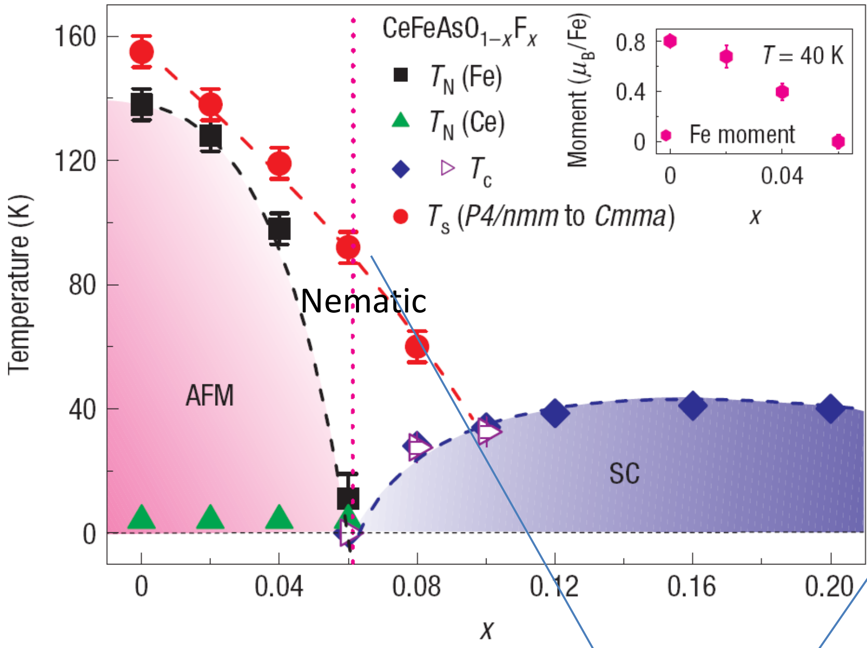




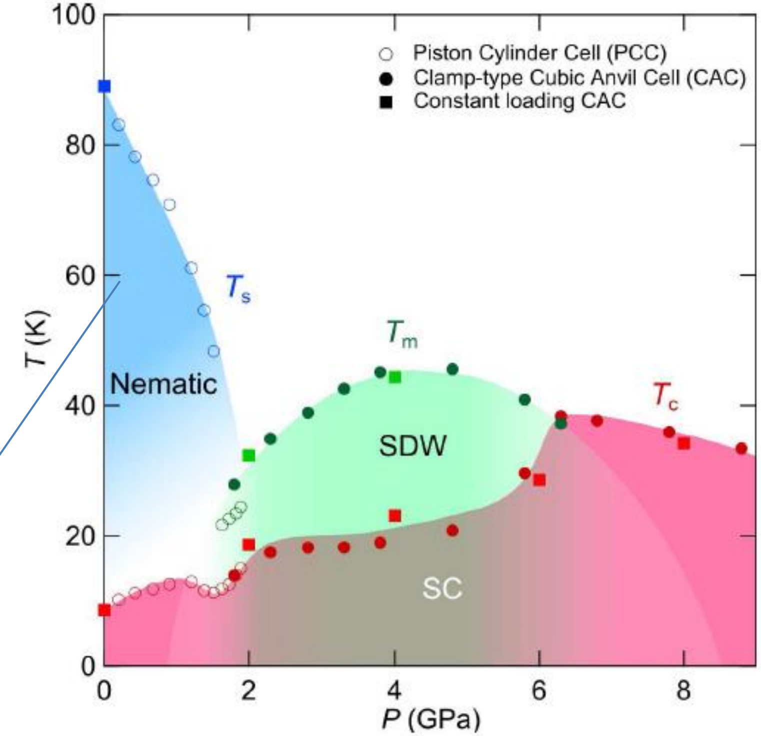
Nematicity in FeSe

$CeFeAsO_{1-x}F_x$



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

FeSe

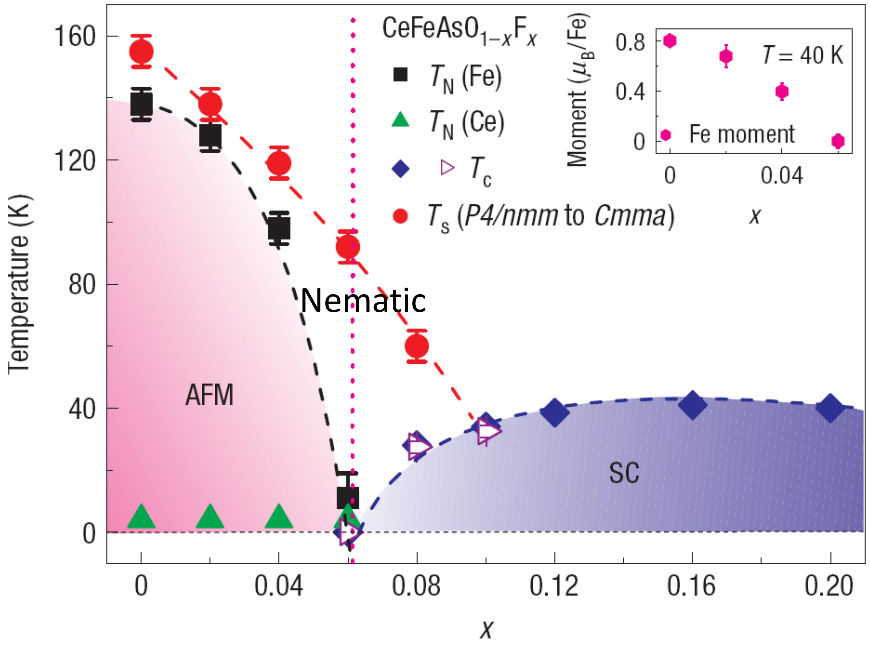


Sun et al, arXiv 1512.06951

Tetragonal symmetry is broken.
Orthorhombic distortion
Electronic properties strongly anisotropic

Nematicity in FeSe

$CeFeAsO_{1-x}F_x$



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

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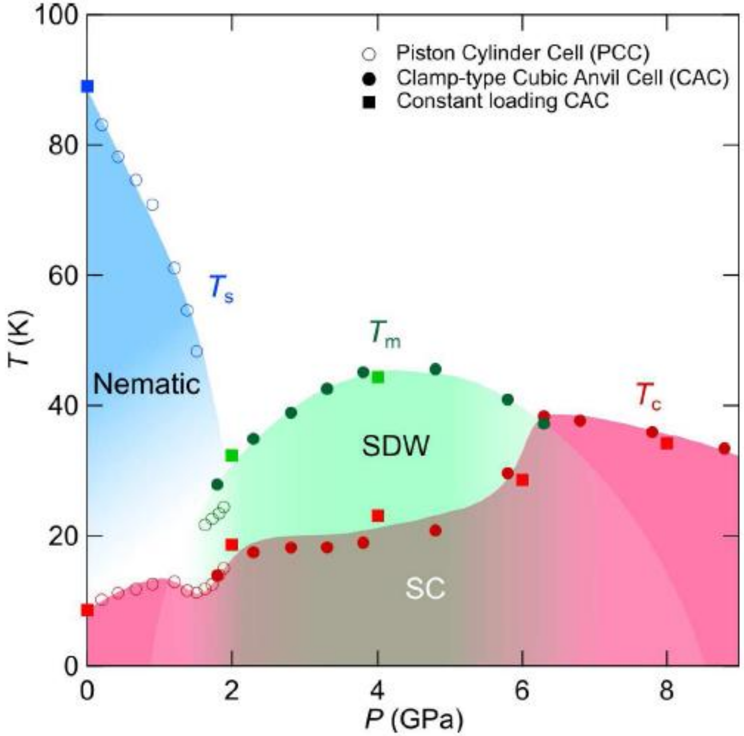


Sun et al, arXiv 1512.06951

Spin degree of freedom

Ising-spin nematic?
Quadrupolar orders?

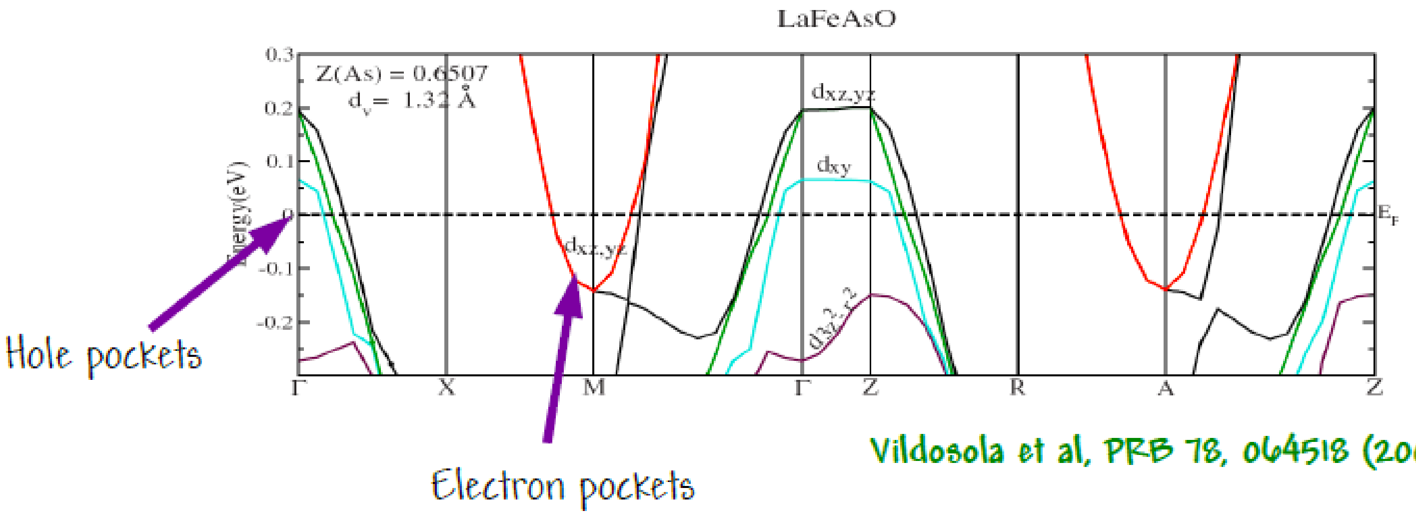
Orbital degree of freedom

Ferro-orbital onsite ordering Δ (n_{zx}-n_{yz})?
d-wave nematic bond order $\Delta\Sigma_k$(coskx-cosky)(n_{zx}(k)+n_{yz}(k)) ?

Correlations in iron superconductors: The role of multi-orbital physics

Experimentally electronic bands similar to those predicted by LDA but strongly renormalized (narrower bands with enhanced mass) are observed

Local correlations are important



Vildosola et al, PRB 78, 064518 (2008)

LDA: Fe bands at the Fermi level.
Several orbitals involved

Minimum model : **5 orbitals**
(6 electrons when undoped)

Multi-orbital character may play an important role in the correlations and instabilities

Hund's coupling: key role in the correlations

The role of Hund's coupling in the nematicity of iron superconductors

- Hamiltonian: 5 orbital Hubbard-Kanamori Hamiltonian (only local interactions included). Tight binding model from LDA for FeSe

- Interactions treated at single-site mean-field slave-spin.
  - Included: local correlations (quasiparticle weight-mass enhancement)
  - Not included: finite-range spin fluctuations

- Study of the response of the system to a nematic perturbation
  - Onsite order: Ferro-orbital ordering $\Delta\,(n_{zx}-n_{yz})$?
  - Bond order: d-wave nematic $\Delta\Sigma_k(\cos kx-\cos ky)(n_{zx}(k)+n_{yz}(k))$?
  - Anisotropy in the hopping to 1st nn

The role of Hund's coupling in the nematicity of iron superconductors

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Outline

- ❑ Correlations in iron superconductors: the role of Hund's coupling. Hund metals

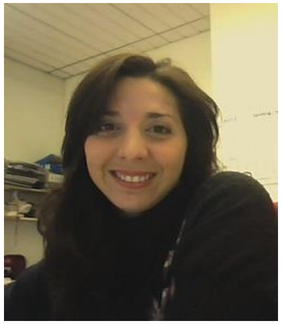
- ❑ Nematicity:

  - Response of the system to an anisotropic perturbation: ferro-orbital ordering and correlations

  - Consequences in the band structure (ARPES)

- ❑ Summary

Thanks to my Collaborators



Nematicity and Correlations

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Nematicity

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Correlations in iron superconductors: The role of multi-orbital physics

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

Tight-binding (hopping) — Intra-orbital repulsion

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

Inter-orbital repulsion — Hund's coupling

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

Pair hopping — Crystal field

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

Two interaction parameters: U, J_H

Local Interactions

Correlations in iron superconductors: The role of multi-orbital physics

Local density-density interactions only

two electrons in the same orbital

two electrons in different orbitals with the same spin

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

$$+ U' \sum n_{a\uparrow} n_{b\downarrow}$$

two electrons in different orbitals with different spin

Ising approximation:
Spin-flip part of Hund's term
& pair-hopping neglected

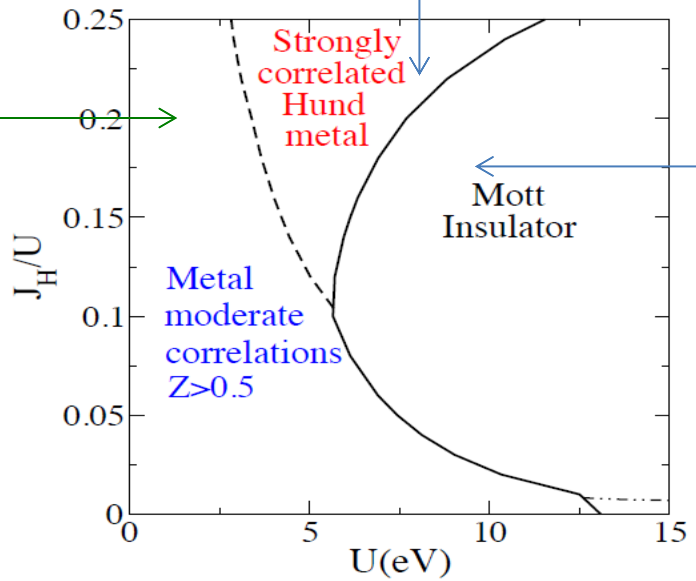
$U' = U - 2J_H$ ⟶ Two interaction parameters: U, J_H

Correlations in iron superconductors: The role of multi-orbital physics

Correlations diagram corresponding to a 5 orbital Tight-binding model suitable for iron superconductors with n=6 electrons (undoped)

Correlated **high-spin state** but still itinerant (double exchange)

Fermi surface Physics (nesting …)



Local moment physics (Heisenberg, exchange …)

Technique:
Single site Slave-spin,
Local correlations

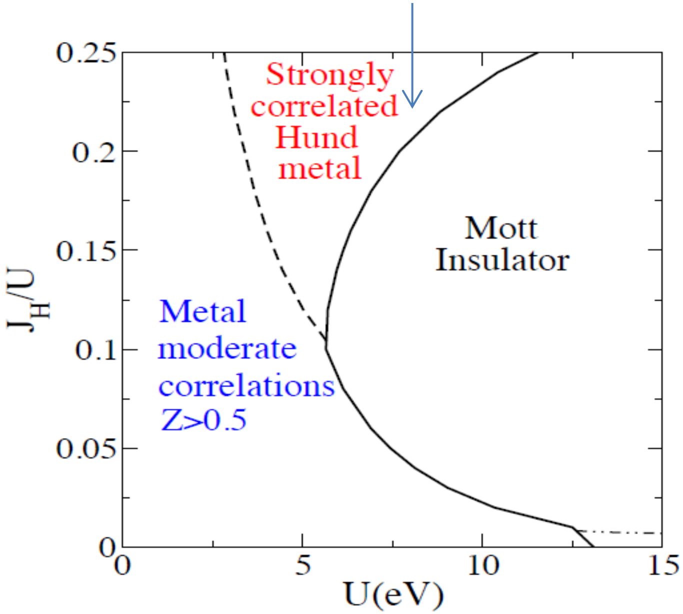
Review: EB et al, Comptes Rendus Physique 17,36 (2016)

Yu & Si, PRB 86, 085104 (2012)
Similar diagram in (π,0) Hartree-Fock: **EB et al, PRB 87, 174508 (2012)**

See also: Werner et al, PRL 101 (2008), Haule & Kotliar NJP 11(2008), Ishida & Liebsch PRB 81 (2010) Liebsch & Ishida, PRB 82 (2010), de Medici et al PRL 107 (2011) & PRB 83(2011), Werner et al, Nat. Phys 8 (2011), Lanata et al PRB (2013), de Medici et al PRL 112, (2014), Calderon et al ,PRB 90 (2014) Fanfarillo & EB, PRB 92 (2015)

Correlations in iron superconductors: The role of multi-orbital physics

high-spin state but still itinerant (double exchange)



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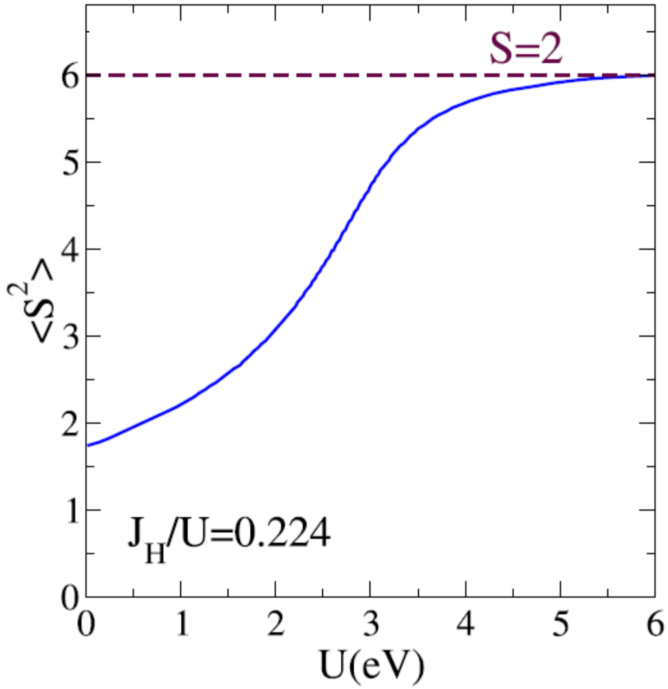
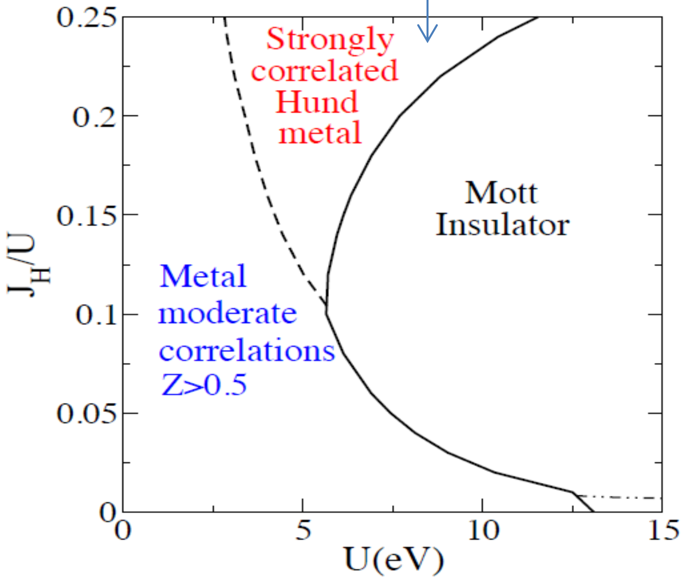


Lanata et al, PRB 87, 045122 (2013)
Fanfarillo & EB, PRB 92, 075136 (2015)

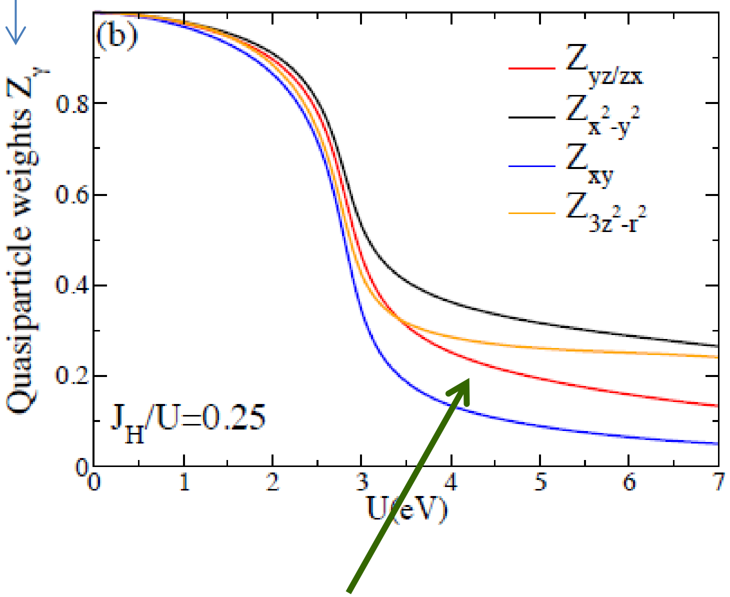
Review: Bascones et al, Comptes Rendus Physique 17,36 (2016)

Correlations in iron superconductors: The role of multi-orbital physics

high-spin state



Inverse of electronic mass renormalization



Technique: Single site Slave-spin, Local correlations

Correlation strength in different orbitals is different. **Orbital dependent mass enhancement**

Yu & Si, PRB 86, 085104 (2012)

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

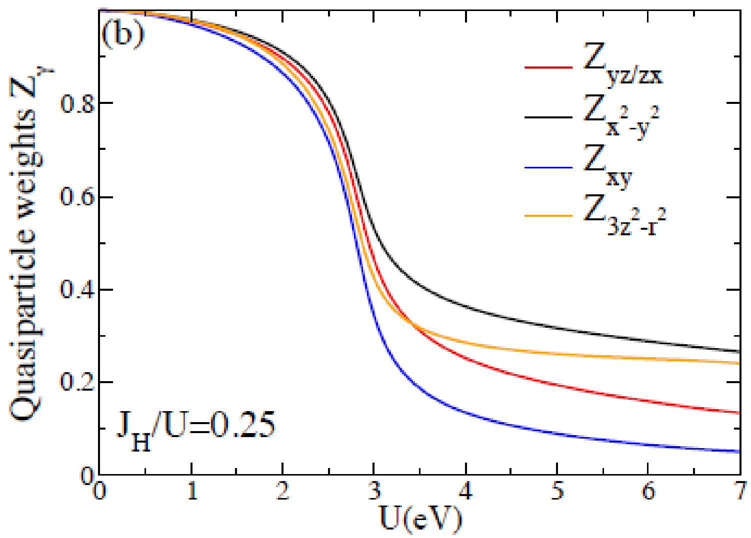
Hund metals: decoupling

two electrons in the same orbital

two electrons in different orbitals with the same spin

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

two electrons in different orbitals with different spin

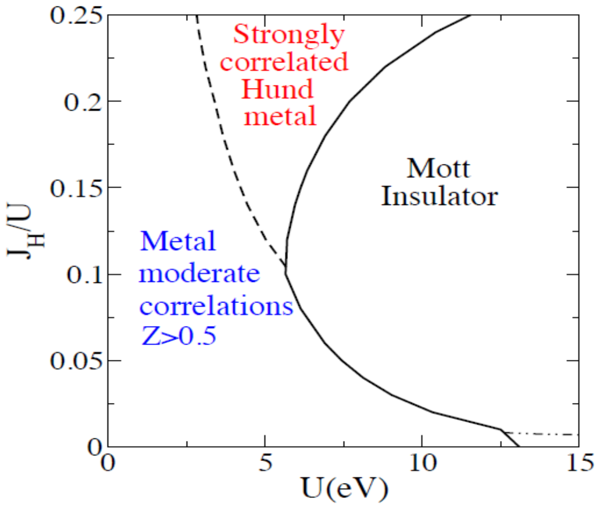


As the atoms becomes spin polarized the effective interaction between the electrons in different orbitals decreases. It vanishes at $J_H=U/3$

Fanfarillo & EB, PRB 92, 075136 (2015)

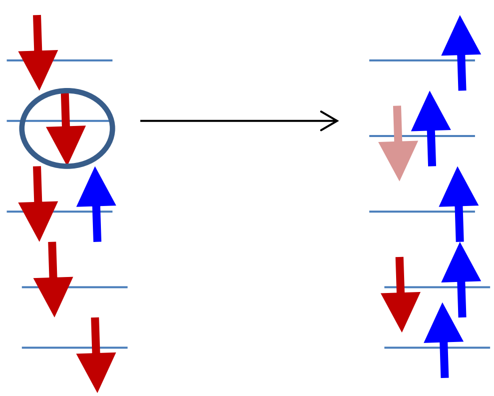
$U' = U - 2J_H$

Correlations in iron superconductors: The role of multi-orbital physics



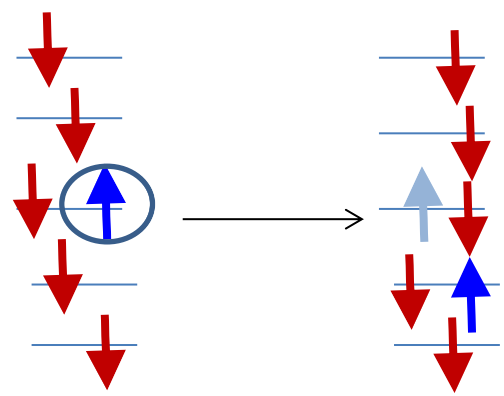
Strong correlations but still itinerancy

Strong correlations: Forbidden process
(increases # of **double occupied orbitals** & decreases spin polarization)



U+ 3 J_H

Metallicity: Allowed process
(no increase in # of **double occupied orbitals** & increases spin polarization)

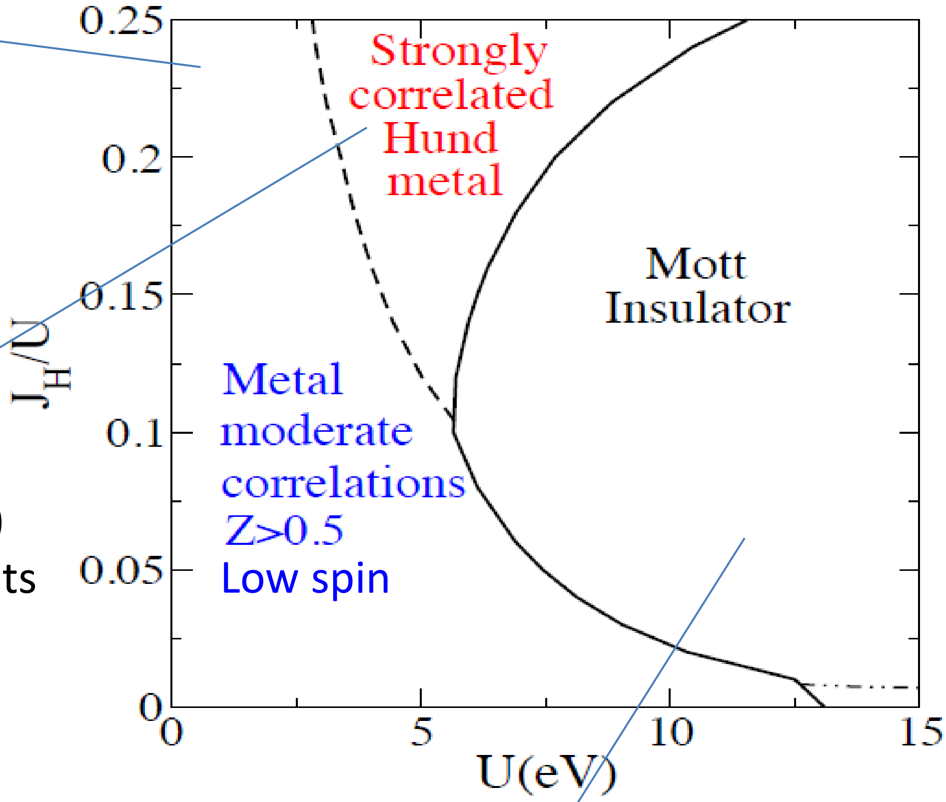


U- 3 J_H

Fanfarillo & EB, PRB 92, 075136 (2015)

Iron superconductors in the correlations diagram

Weakly correlated
Fermi surface physics



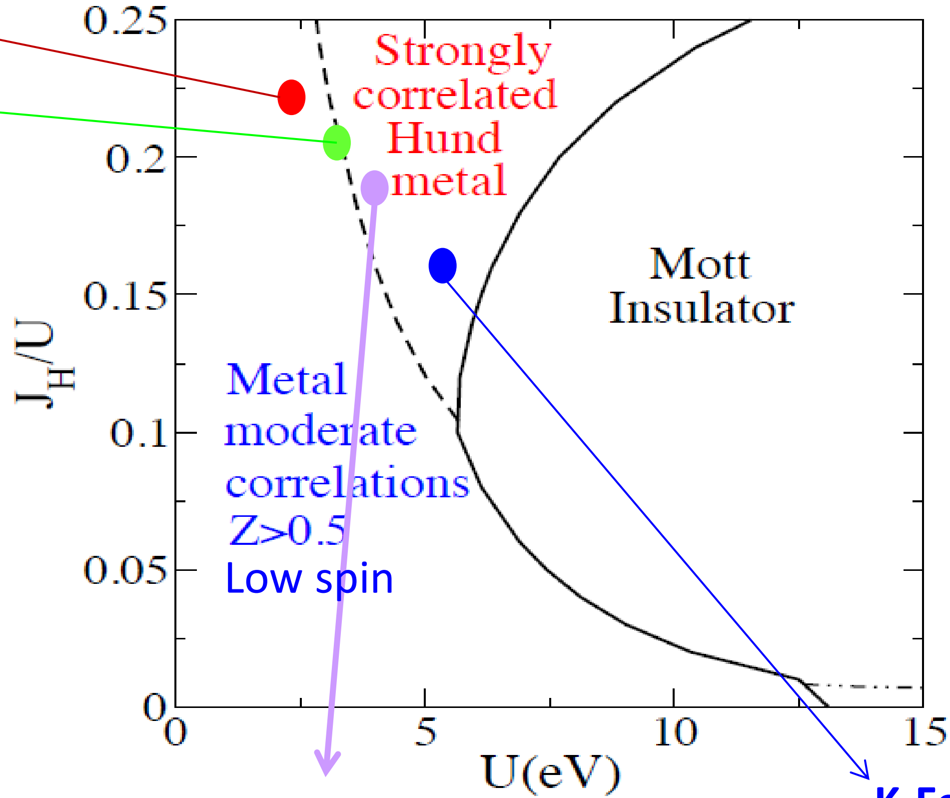
High-spin (double exchange like physics)
Strong correlations: mass enhancements
Orbital differentiation
Metal (partial itinerancy)

Localized spin moments
(Heisenberg models …)

Iron superconductors in the correlations diagram

FeP compounds

Undoped FeAs compounds
(more correlated when hole-doped)



$K_xFe_{y-x}Se_2$

FeSe, FeTe

From comparison with: ARPES, Quantum oscillations, specific heat, doping dependence, X-ray, neutron spectroscopy, optical Conductivity, spin susceptibility, Orbital selectivity, and **predictions** from DMFT+constrainted LDA, …

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

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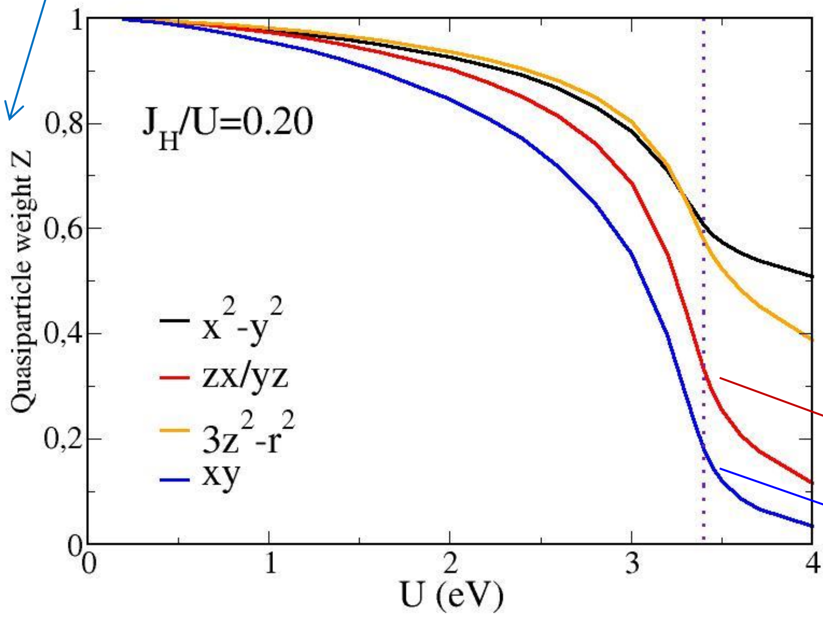
Iron superconductors in the correlations diagram

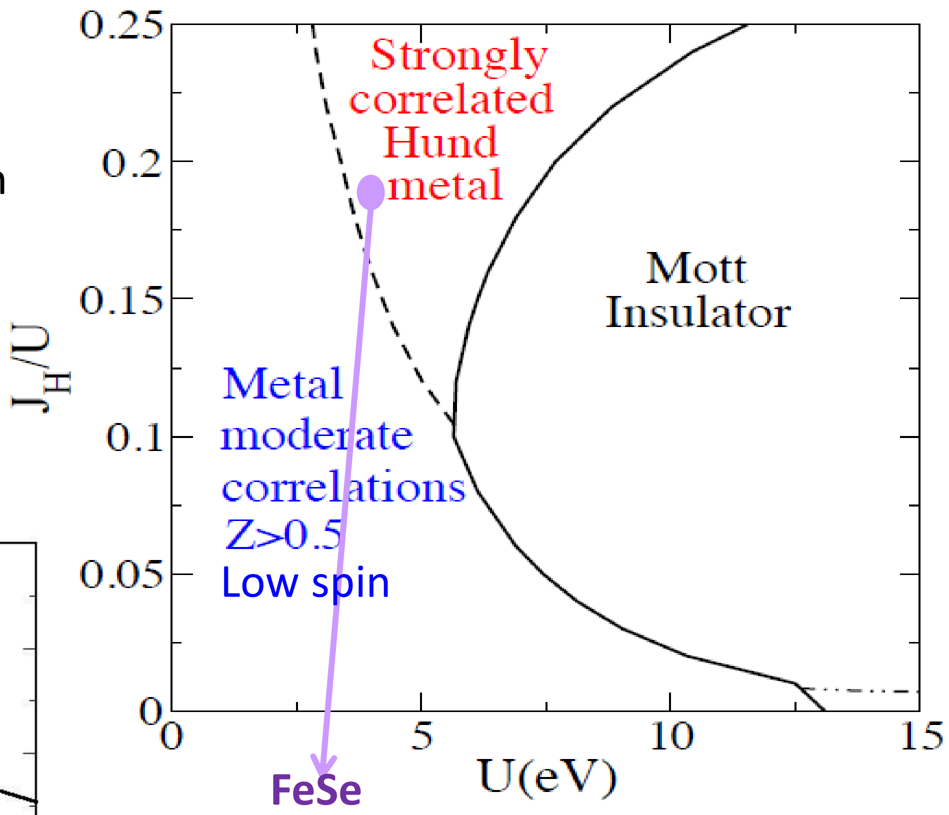
FeSe

ARPES and Quantum oscillations experiments in FeSe are consistent with orbital dependent renormalization mass . Close to the Fermi surface

$m^*_{zx/yz}$~3 m^*_{xy}~5

Inverse renormalization of the mass



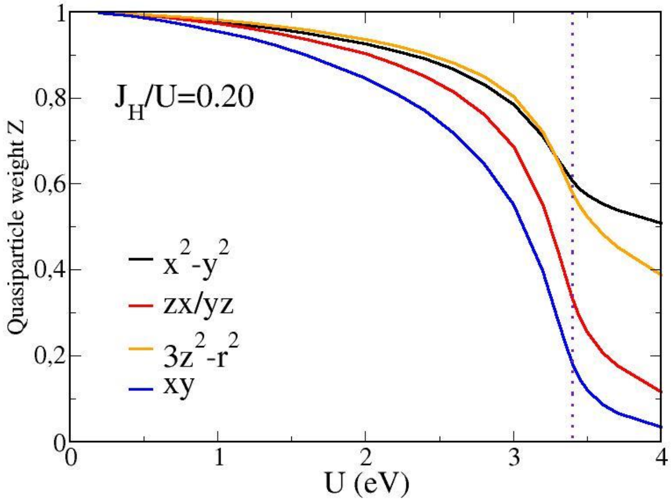


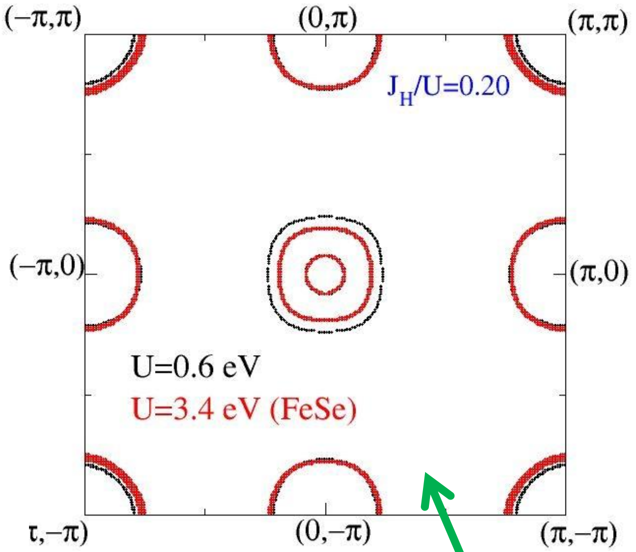
$m^*_{zx/yz}$~3

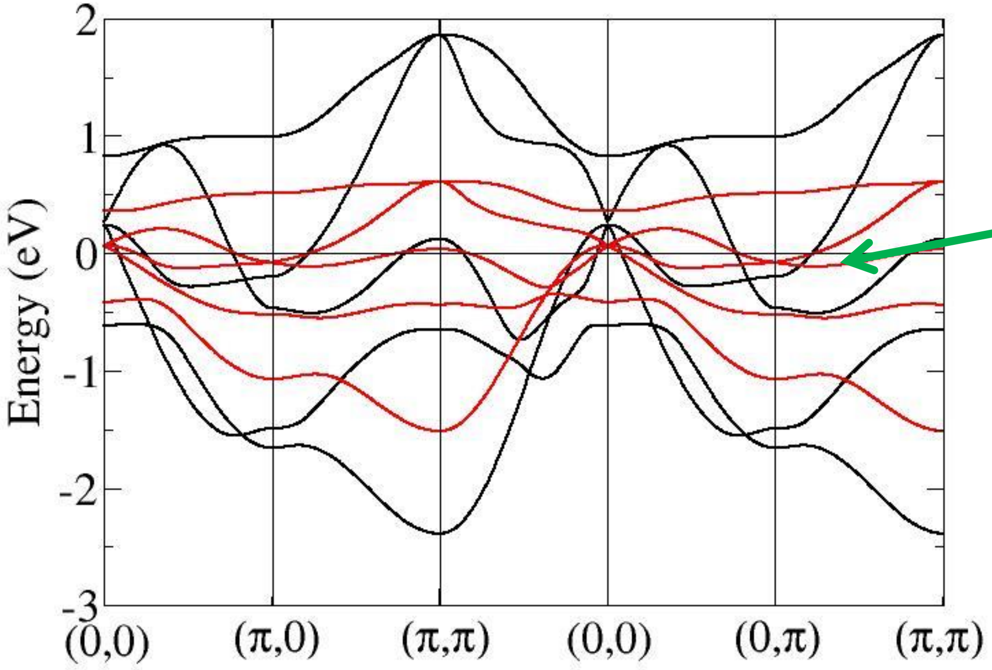
m^*_{xy}~5

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

Correlations in FeSe







Shrinking of the Fermi surface not due to local correlations

1-Fe unit cell

Hund's coupling and ferro-orbital ordering

Response of the system to an onsite level splitting

ε_{zx}

ε_{yz}

$\updownarrow \delta\varepsilon_0$

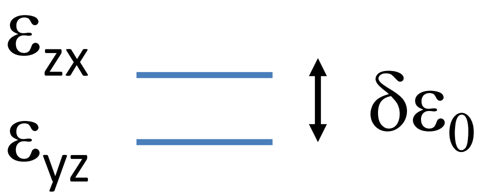
$$n_{yz}-n_{zx}=\frac{d(n_{yz}-n_{zx})}{d(\delta\varepsilon_0)}\,\delta\varepsilon_0$$

$$\delta\varepsilon_0=\varepsilon_{zx}-\varepsilon_{yz}$$

How does the response of
the system depend on interactions?

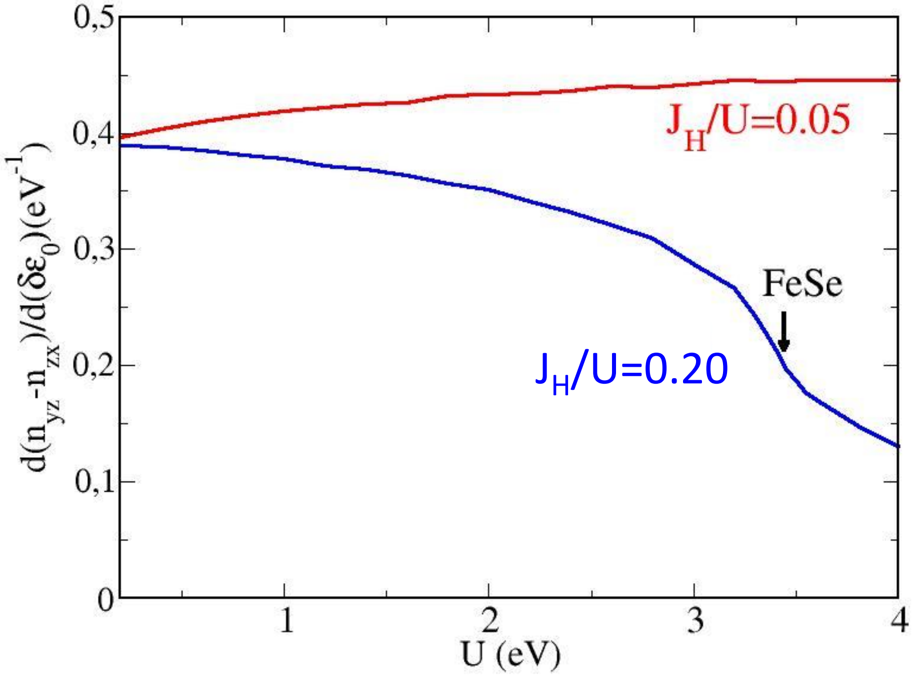
Hund's coupling and ferro-orbital ordering

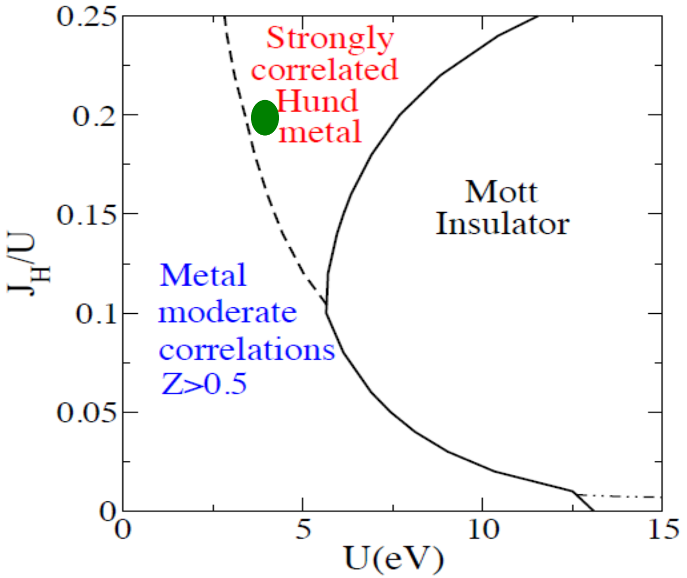
Response of the system to an onsite level splitting



$$n_{yz}-n_{zx}=\frac{d(n_{yz}-n_{zx})}{d(\delta\varepsilon_0)}\,\delta\varepsilon_0$$

$$\delta\varepsilon_0=\varepsilon_{zx}-\varepsilon_{yz}$$





Anisotropic Quasiparticle weight

Response of the system to an onsite level splitting

ε_{zx}

ε_{yz}

$\updownarrow \; \delta\varepsilon_0$

$$Z_{yz}-Z_{zx}=\frac{d(Z_{yz}-Z_{zx})}{d(\delta\varepsilon_0)}\,\delta\varepsilon_0$$

$$\delta\varepsilon_0=\varepsilon_{zx}-\varepsilon_{yz}$$

Anisotropy in the correlation strength

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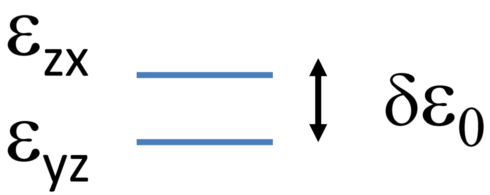
Anisotropic Quasiparticle weight

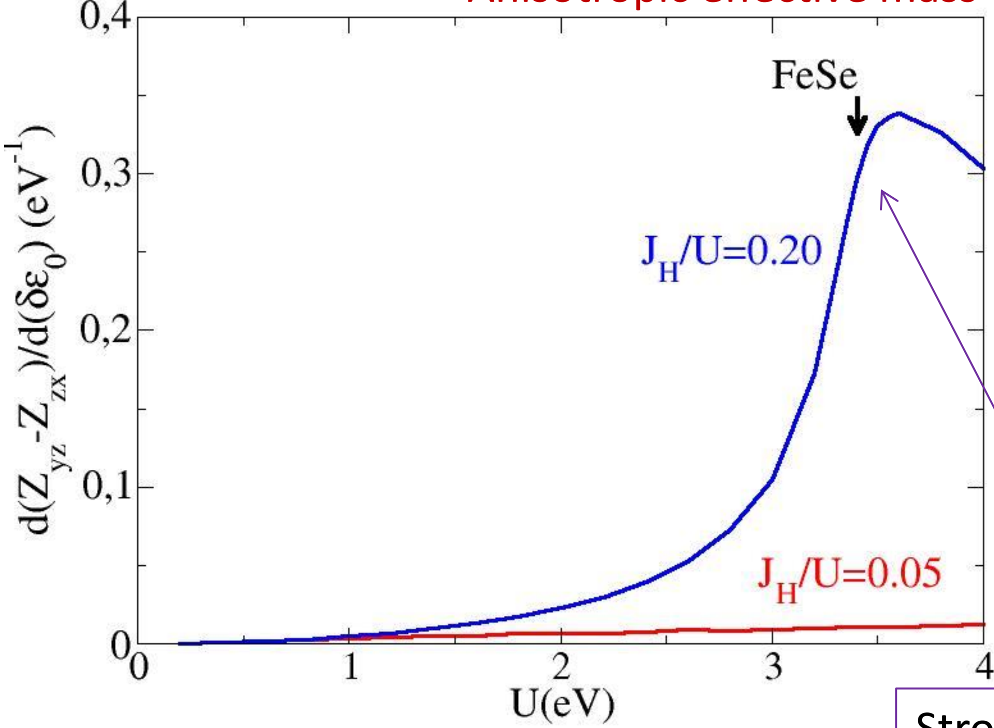
Response of the system to an onsite level splitting

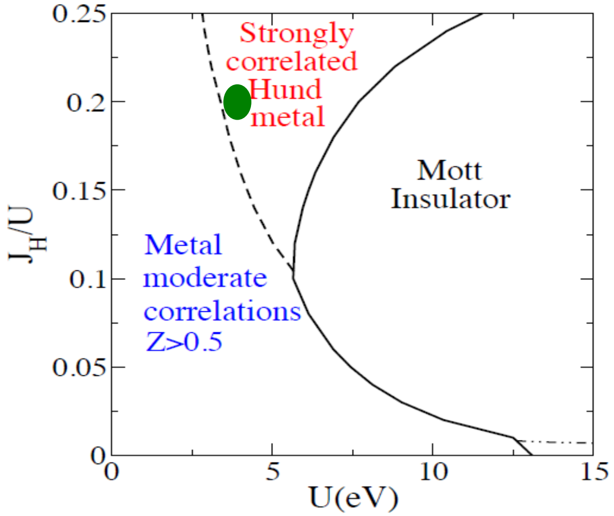


$$Z_{yz}-Z_{zx}=\frac{d(Z_{yz}-Z_{zx})}{d(\delta\varepsilon_0)}\,\delta\varepsilon_0$$

$$\delta\varepsilon_0=\varepsilon_{zx}-\varepsilon_{yz}$$

Anisotropic effective mass





Strongly enhanced response, but finite peak

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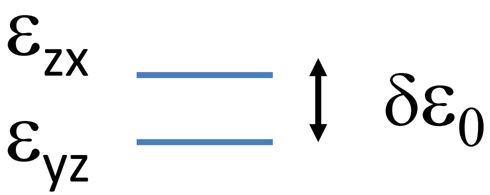
Anisotropic Quasiparticle weight

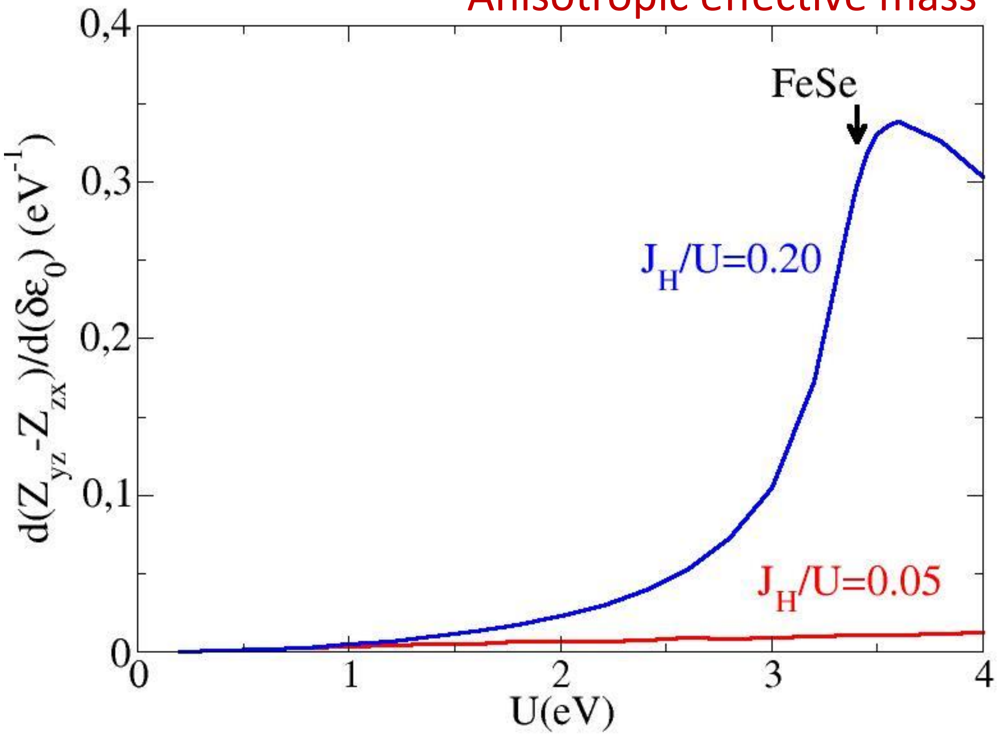
Response of the system to an onsite level splitting

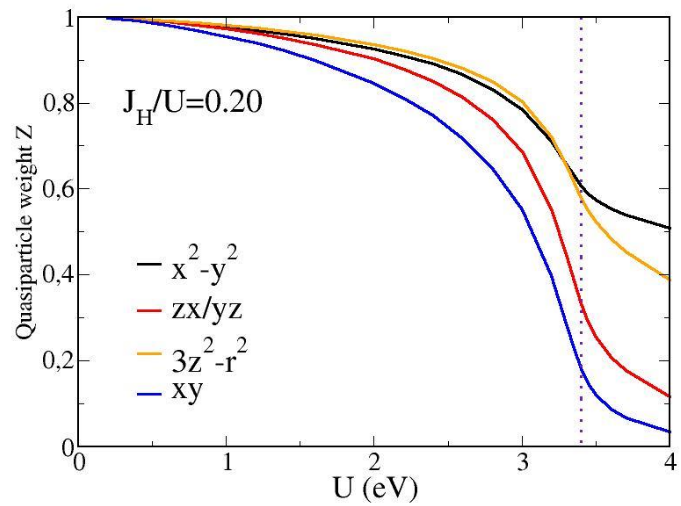


$$Z_{yz}-Z_{zx}=\frac{d(Z_{yz}-Z_{zx})}{d(\delta\varepsilon_0)}\,\delta\varepsilon_0$$

$$\delta\varepsilon_0=\varepsilon_{zx}-\varepsilon_{yz}$$

Anisotropic effective mass





$\delta\varepsilon_0$~75 meV

$Z_{yz}-Z_{zx}$~0.025

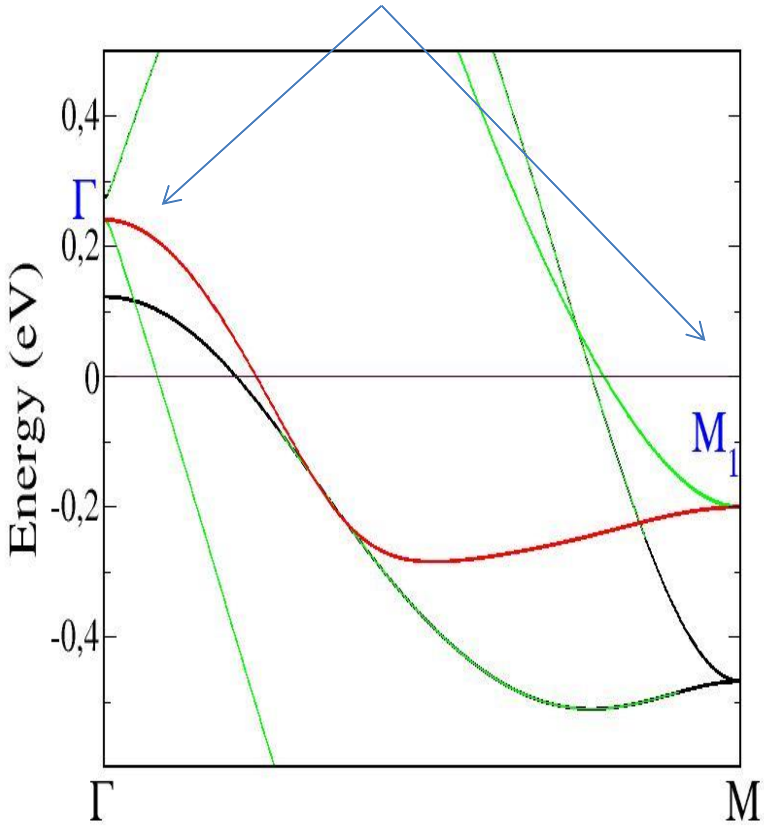
Similar effects for a d-wave nematic bond order

Effect of the nematicity on the band structure

2-Fe unit cell

zx: green **yz:red**

In the tetragonal state (no nematicity):
Degeneracy of zx and yz bands at symmetry points



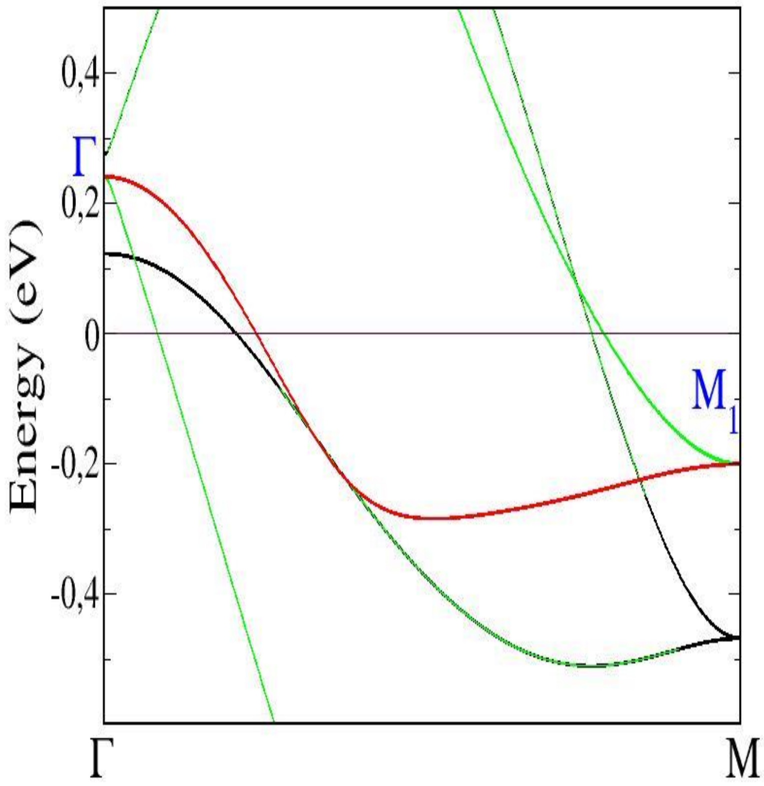
Effect of the nematicity on the band structure

2-Fe unit cell

zx: green   yz:red

In the nematic state finite splitting appears between zx and yz bands at the symmetry points.
The splitting gives information on the kind of nematic order

Naive splitting used to interpret ARPES experiments



Onsite order: $\delta\varepsilon_0(n_{zx}-n_{yz})$

Splitting at $M_1 \sim \delta\varepsilon_0$
Splitting at $\Gamma \sim \delta\varepsilon_0$

Bond d-wave order:

$\Delta\Sigma_k(\cos kx-\cos ky)(n_{zx}+n_{yz})$

Splitting at $M_1 \sim 4\Delta$
Splitting at $\Gamma \sim 0$

Effect of the nematicity on the band structure

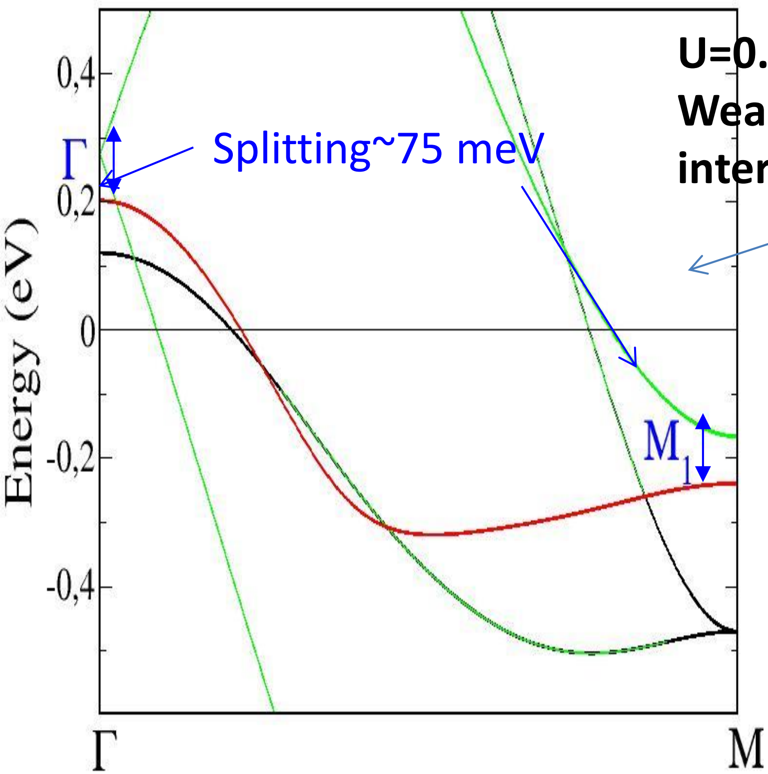
2-Fe unit cell

zx: green yz:red

In the nematic state finite splitting appears between zx and yz bands at the symmetry points. The splitting gives information on the kind of nematic order

$\delta\varepsilon_0=\varepsilon_{zx}-\varepsilon_{yz}$=75 meV

Naive splitting used to interpret ARPES experiments



U=0.2 eV
Weak interactions

Onsite order: $\delta\varepsilon_0(n_{zx}-n_{yz})$

Splitting at M_1~$\delta\varepsilon_0$
Splitting at Γ~$\delta\varepsilon_0$

Bond d-wave order:

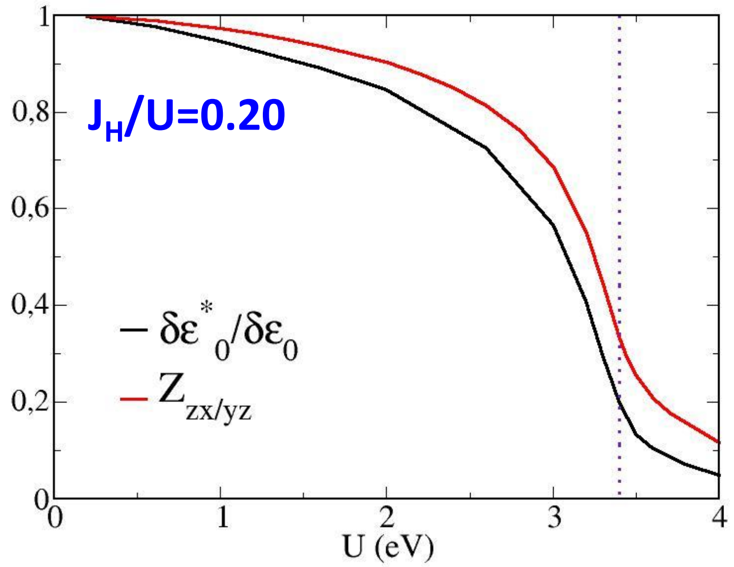
$\Delta\Sigma_k$(coskx-cosky)$(n_{zx}+n_{yz})$

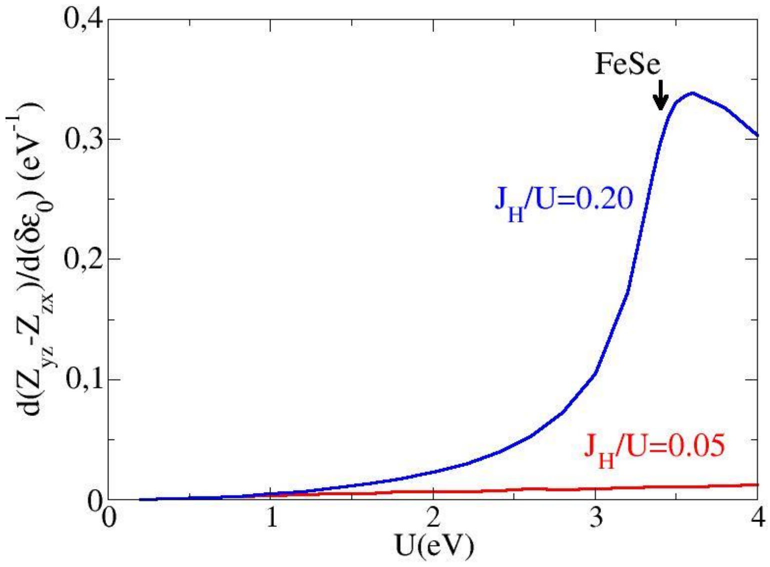
Splitting at M_1~4Δ
Splitting at Γ~0

Experiment still controversial

Effect of Onsite orbital ordering on the band structure

$\delta\varepsilon_0(n_{zx}-n_{yz})$





Shift at the symmetry points

$$\delta\varepsilon_{zx}(k) \sim \delta\varepsilon^*_{0,zx}+\delta Z_{zx}(2t^{y}_{zx,zx}\cos k_y +4t'_{zx,zx}\cos k_x \cos k_y)$$

$$\delta\varepsilon_{yz}(k) \sim \delta\varepsilon^*_{0,yz}+\delta Z_{yz}(2t^{x}_{yz,yz}\cos k_x +4t'_{yz,yz}\cos k_x \cos k_y)$$

$t^{y}_{zx,zx}=t^{x}_{yz,yz} \sim -0.32$ eV

$t'_{zx,zx}=t'_{yz,yz} \sim 0.23$ eV

Tight binding parameters

K dependence in 1-Fe unit cell

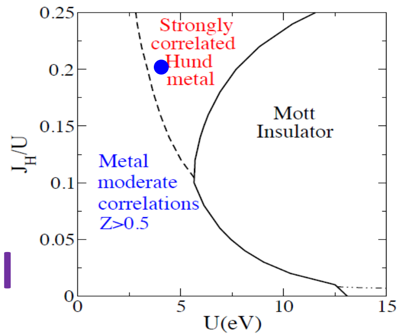
Effect of Ferro-orbital ordering on the band structure

Splitting at $M_1 \sim \delta\varepsilon^*_0 + \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx})$

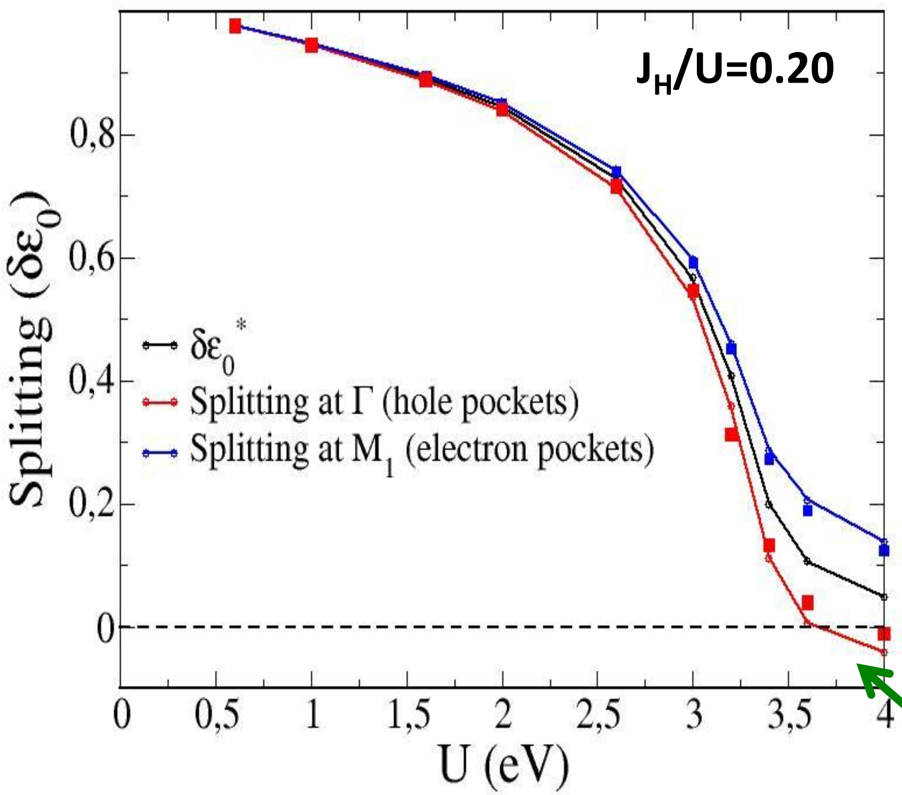
Splitting at $\Gamma \sim \delta\varepsilon^*_0 - \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx})$

0.29 eV

FeSe



2-Fe unit cell



Splittings at symmetry points between zx/yz orbitals are modified with respect to naive expectations

Accidental sign reversal

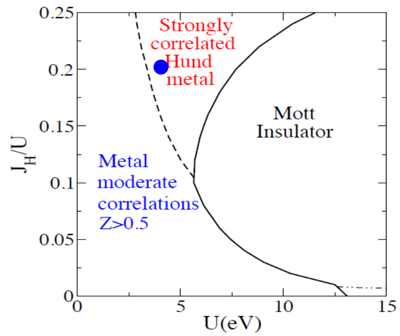
Effect of Ferro-orbital ordering on the band structure

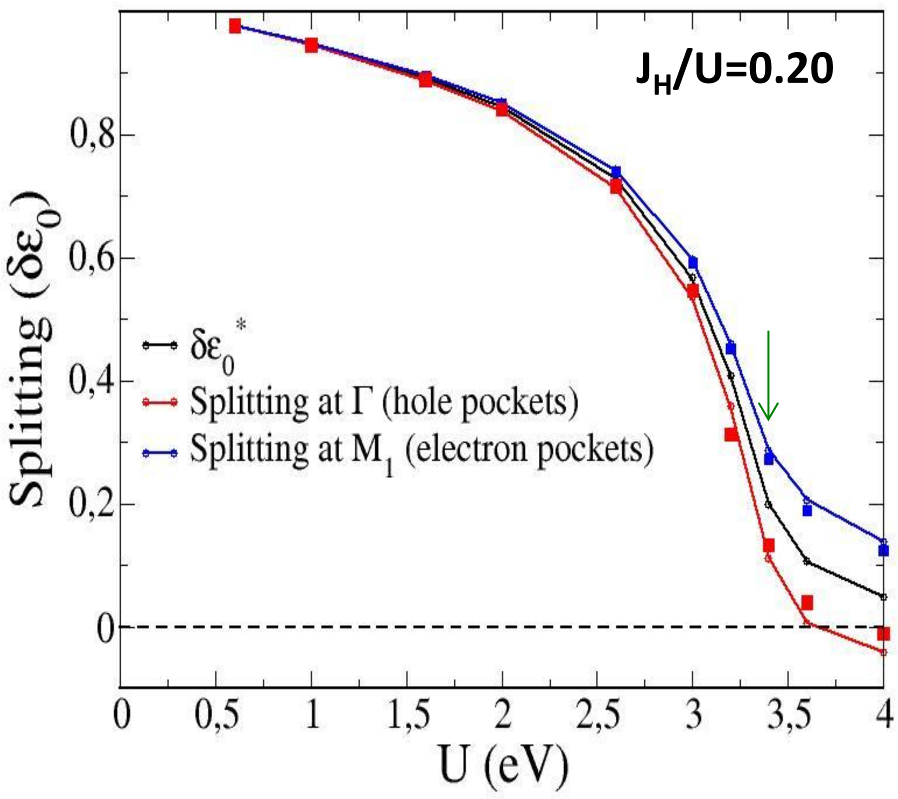
Splitting at $M_1 \sim \delta\varepsilon^*_0 + \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx})$

Splitting at $\Gamma \sim \delta\varepsilon^*_0 - \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx})$

0.29 eV

FeSe

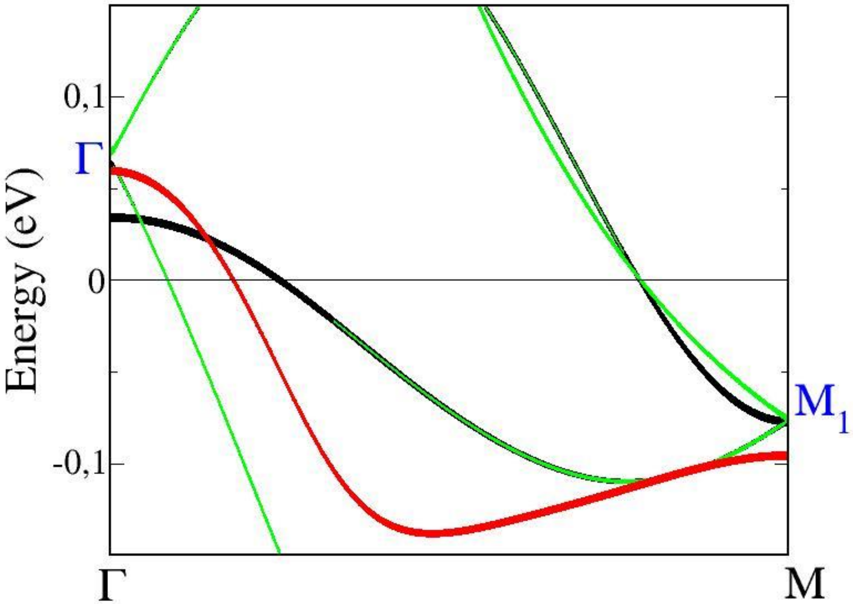




2-Fe unit cell

zx: green yz:red

U=3.4 eV $J_H/U=0.20$ $\delta\varepsilon_0$=75 meV



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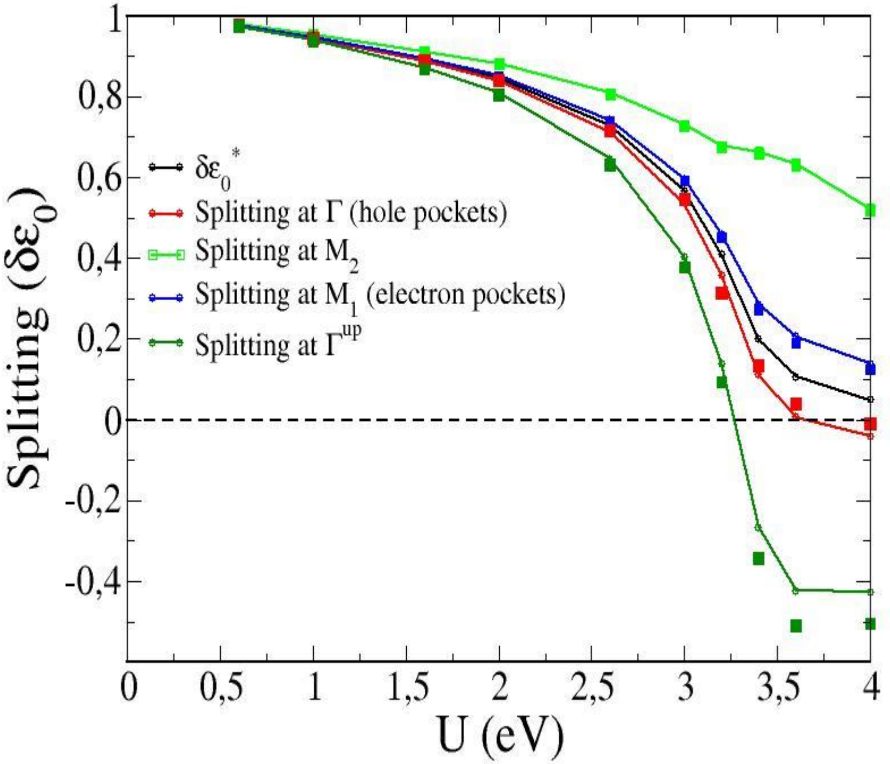
Different splittings at Γ, Γ^{up}, M_1, M_2

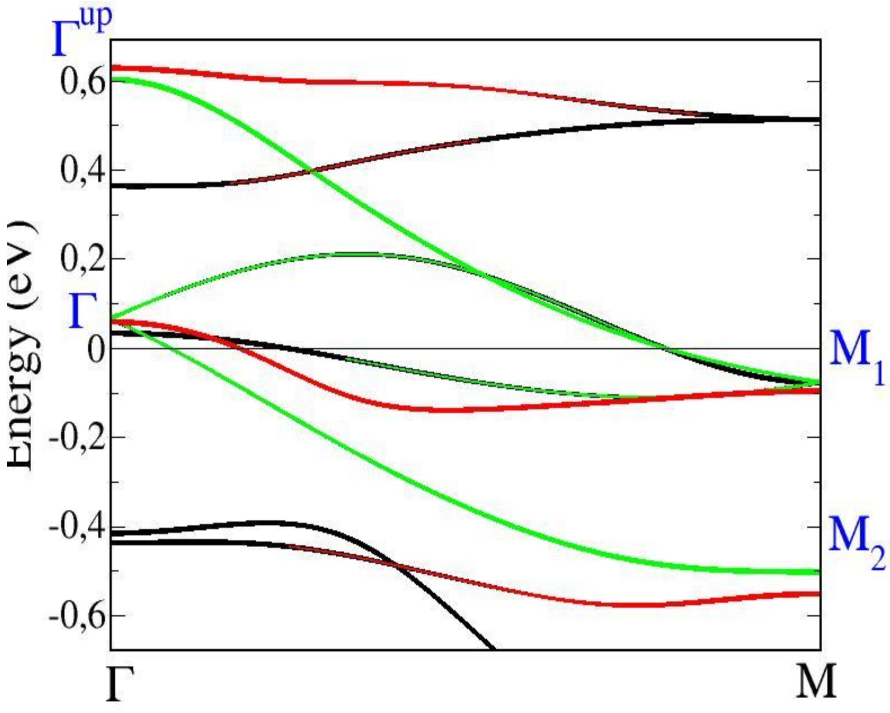
$$M_1 \sim \delta\varepsilon^*_0 + \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx})$$

$$\Gamma \sim \delta\varepsilon^*_0 - \delta Z(\underbrace{2t^y_{zx,zx} + 4t'_{zx,zx}}_{\sim 0.29\ \text{eV}})$$

$$M_2 \sim \delta\varepsilon^*_0 + \delta Z(-2t^y_{zx,zx} + 4t'_{zx,zx})$$

$$\Gamma^{up} \sim \delta\varepsilon^*_0 - \delta Z(\underbrace{-2t^y_{zx,zx} + 4t'_{zx,zx}}_{\sim 1.56\ \text{eV}})$$





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Different splittings at Γ, Γ^{up}, M_1, M_2

$$M_1 \sim \delta\varepsilon^*_0 + \delta Z(2t^y_{zx,zx} + 4t'_{zx,zx})$$

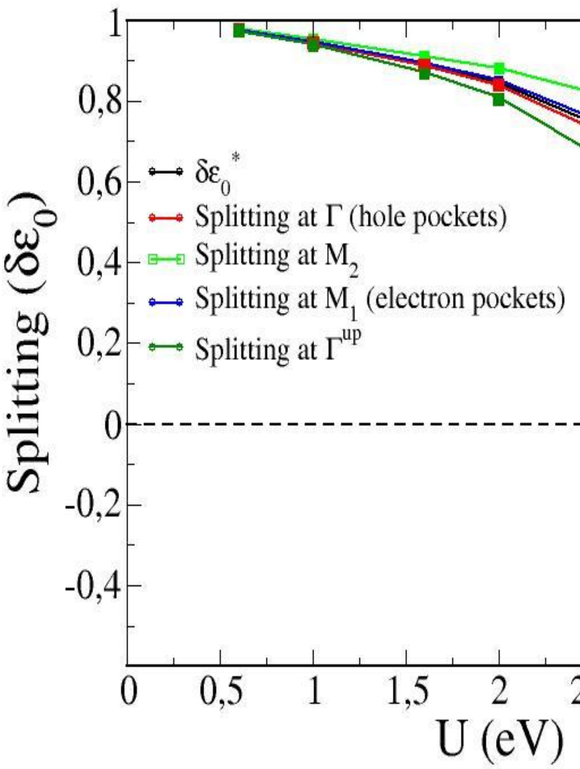
$$\Gamma \sim \delta\varepsilon^*_0 - \delta Z(\underbrace{2t^y_{zx,zx} + 4t'_{zx,zx}}_{\sim 0.29\ \text{eV}})$$

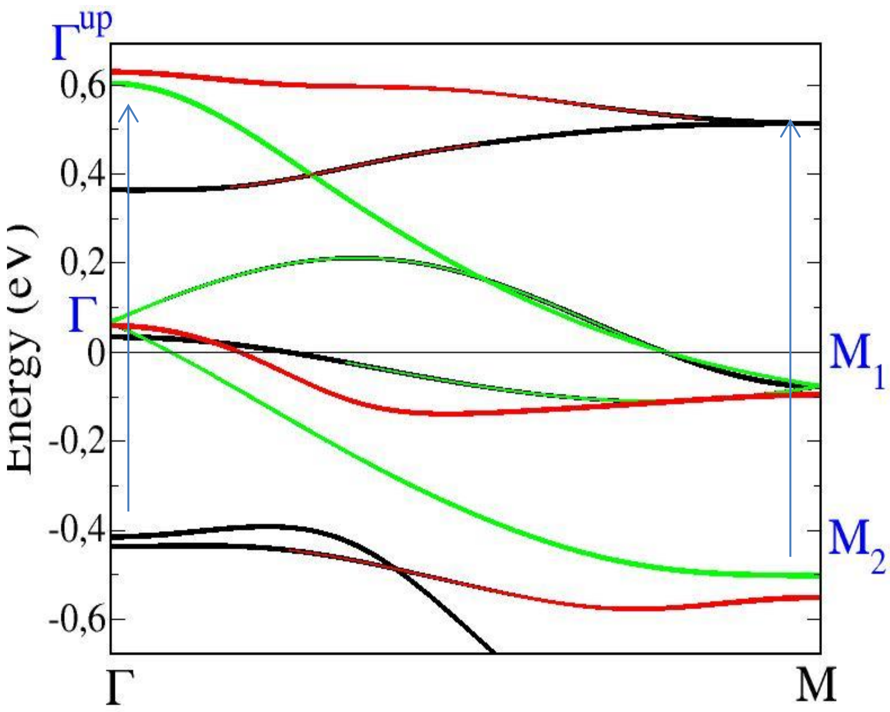
~0.29 eV

$$M_2 \sim \delta\varepsilon^*_0 + \delta Z(-2t^y_{zx,zx} + 4t'_{zx,zx})$$

$$\Gamma^{up} \sim \delta\varepsilon^*_0 - \delta Z(\underbrace{-2t^y_{zx,zx} + 4t'_{zx,zx}}_{\sim 1.56\ \text{eV}})$$

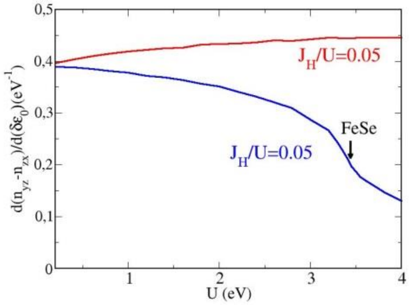
~1.56 eV





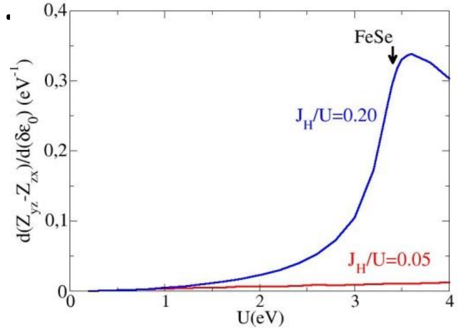
Role of Hund's coupling in the nematicity of iron superconductors

- ❑ Strong suppression of ferro-orbital ordering due to Hund's coupling, operative for interactions suitable for FeSe

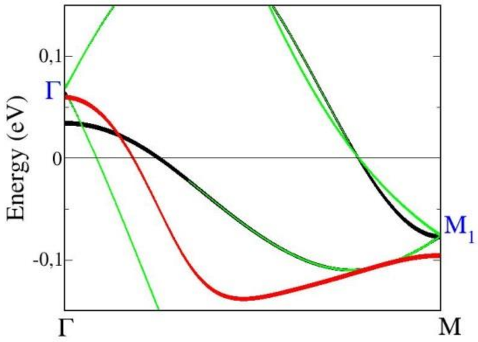


- ❑ Anisotropic quasiparticle weight in presence of other sources of anisotropy (ferro-orbital ordering, hopping anisotropy, d-wave nematic, strain ….).

  Enhanced response at the crossover to the Hund metal (FeSe)



- ❑ Impact on the band structure: Splittings between zx/yz at symmetry points different from naive expectations. Important for the interpretation of ARPES experiments



- ❑ Further information from the splittings at M_2 and Γ^{up} (optical conductivity)

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