ORBITAL SELECTIVITY IN IRON-BASED SC:
STRONG AND WEAK-CORRELATED PERSPECTIVES

Intertwined Order and Fluctuations in Quantum Material

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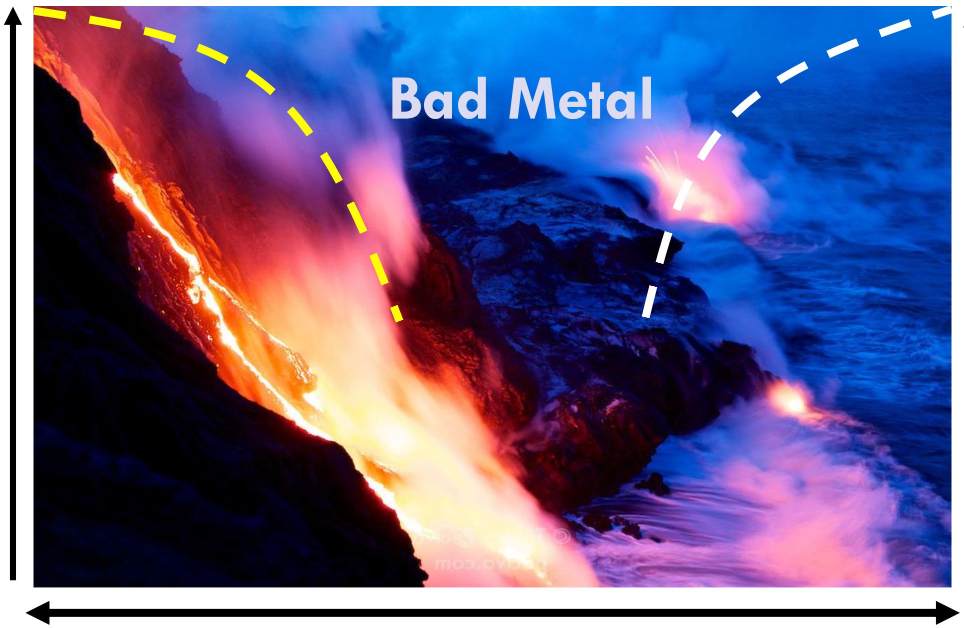
UNCONVENTIONAL SC & CORRELATIONS

High Temperature

Strong Correlation

Local electronic spin/charge interactions, localization phenomena, no FS



Tuning parameter

Low Temperature

Fermi Liquid

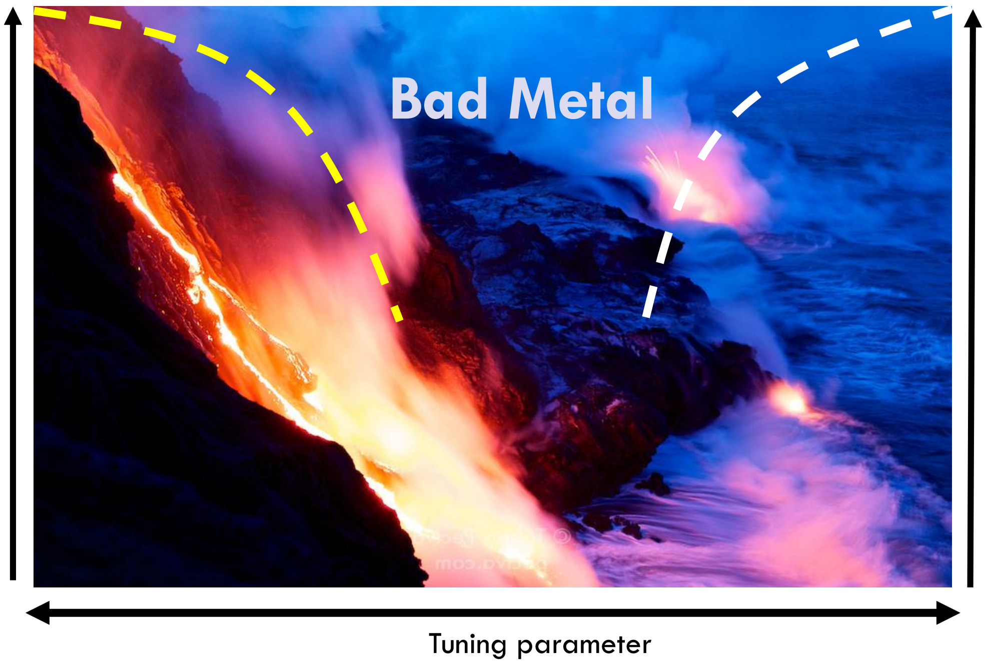
Coherent qp, collective modes weakly coupled to itinerant electrons, well defined FS

Unconventional SC emerges at low temperature from a state that is far from an ideal metal

UNCONVENTIONAL SC & CORRELATIONS

Strong Correlation

Local electronic spin/charge interactions, localization phenomena, no FS



Fermi Liquid

Coherent qp, collective modes weakly coupled to itinerant electrons, well defined FS

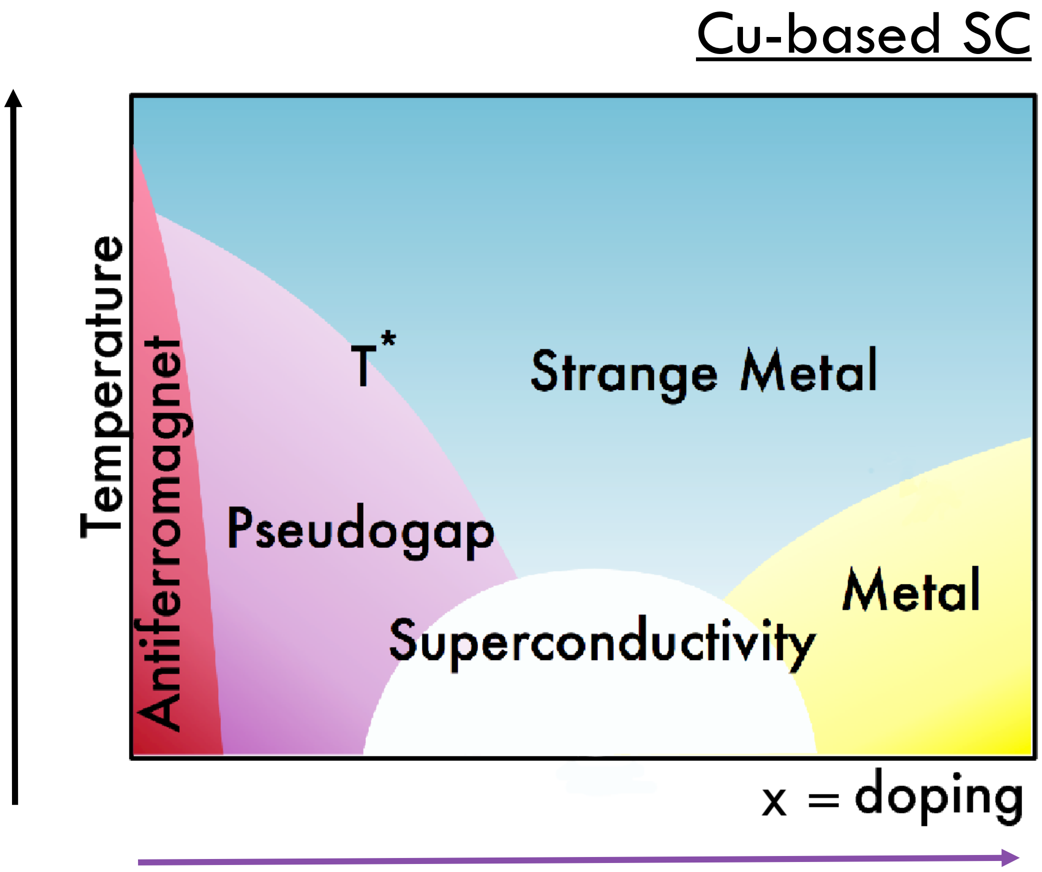
Hubbard Model
Slave Technique, DMFT …

Perturbative approach,
Effective Action, GL theory …

High - Energy Physics

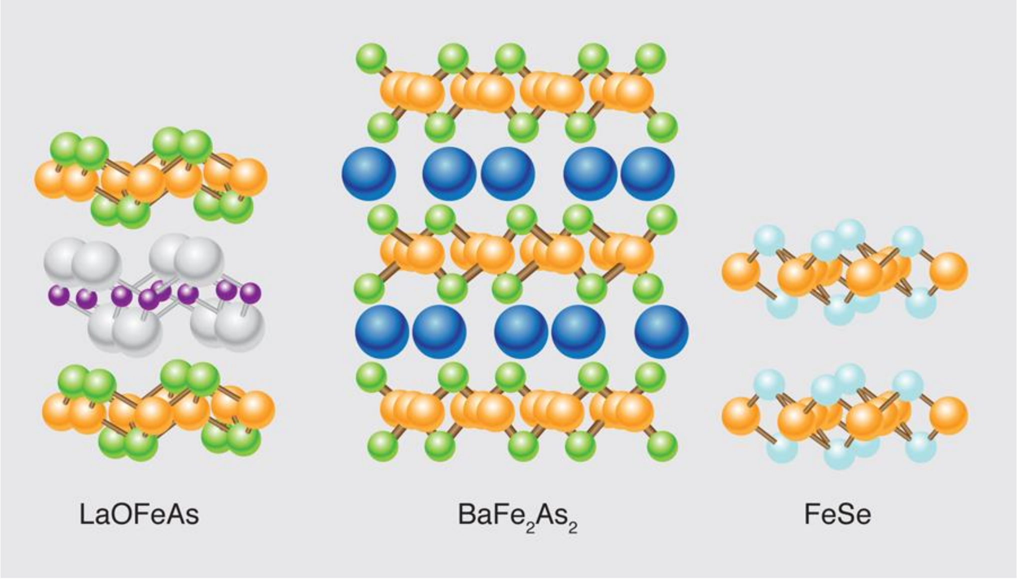
Low- Energy Physics

UNCONVENTIONAL SC & CORRELATIONS:
CUPRATES AS PROTOTYPICAL EXAMPLE

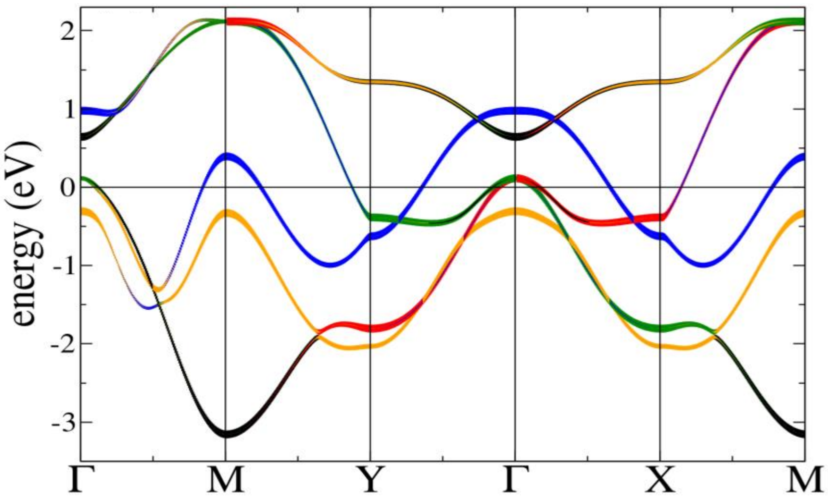


MULTIORBITAL PHYSICS IN CORRELATED SYSTEMS

Cuprates are the exception! Many unconventional superconductors are multiorbital systems: A_3C_{60}, Sr_2RuO_4 ...



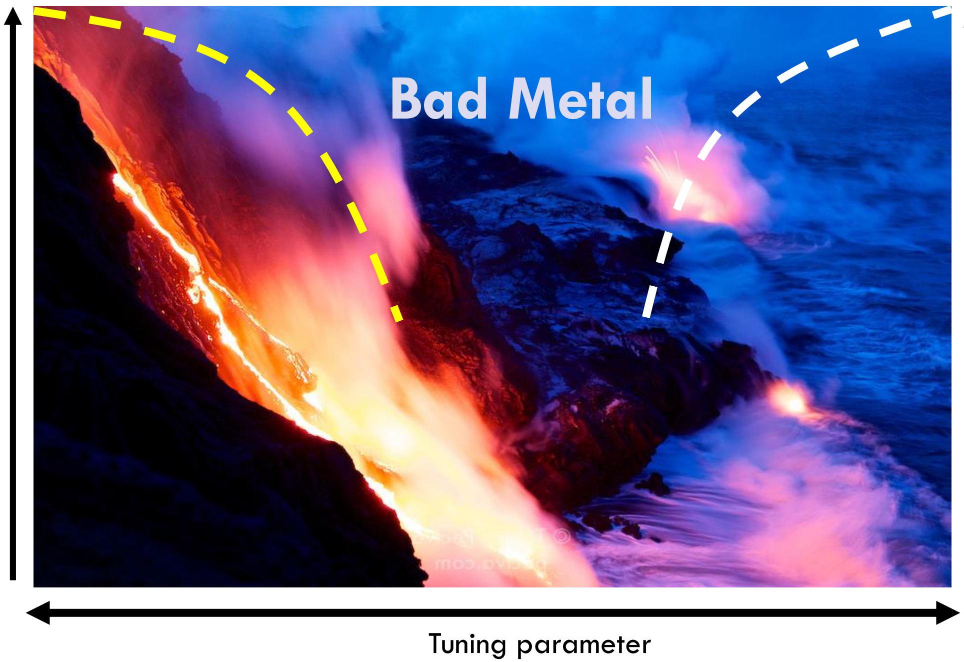
… and Iron-based SC



UNCONVENTIONAL SC & CORRELATIONS FOR MULTIORBITAL SYSTEMS

H-E Physics + Orbital dof

Hubbard Model
Slave Technique,
DMFT …



L-E Physics + Orbital dof

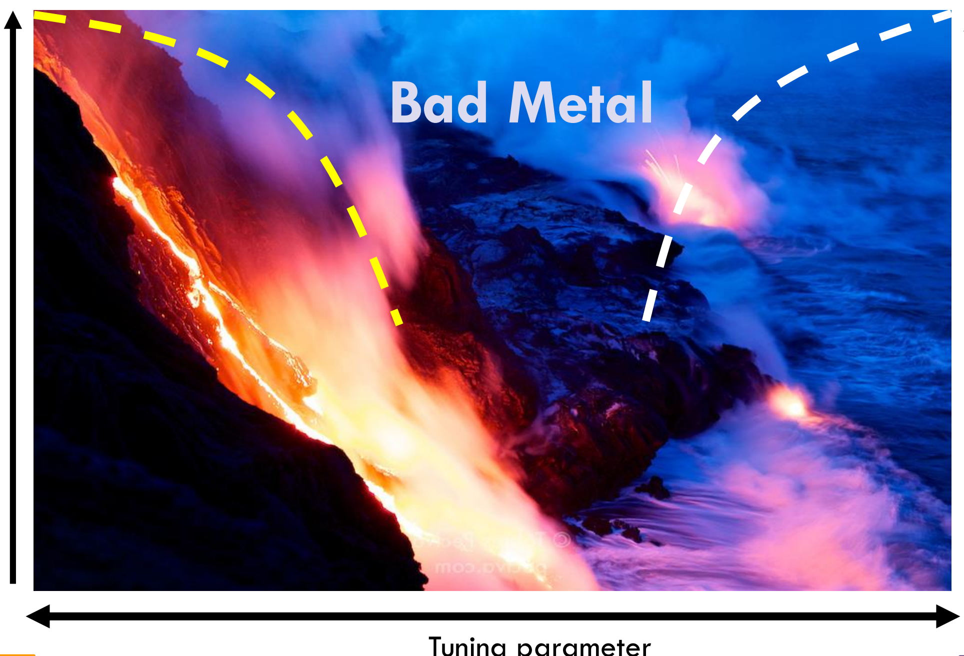
Perturbative approach,
Effective Action,
GL theory …

Is this picture relevant for multiorbital system e.g. IBS?

UNCONVENTIONAL SC & CORRELATIONS FOR MULTIORBITAL SYSTEMS

H-E Physics + Orbital dof

Hubbard Model
Slave Technique,
DMFT …



L-E Physics + Orbital dof

Perturbative approach,
Effective Action,
GL theory …

Hund's Metal Physics

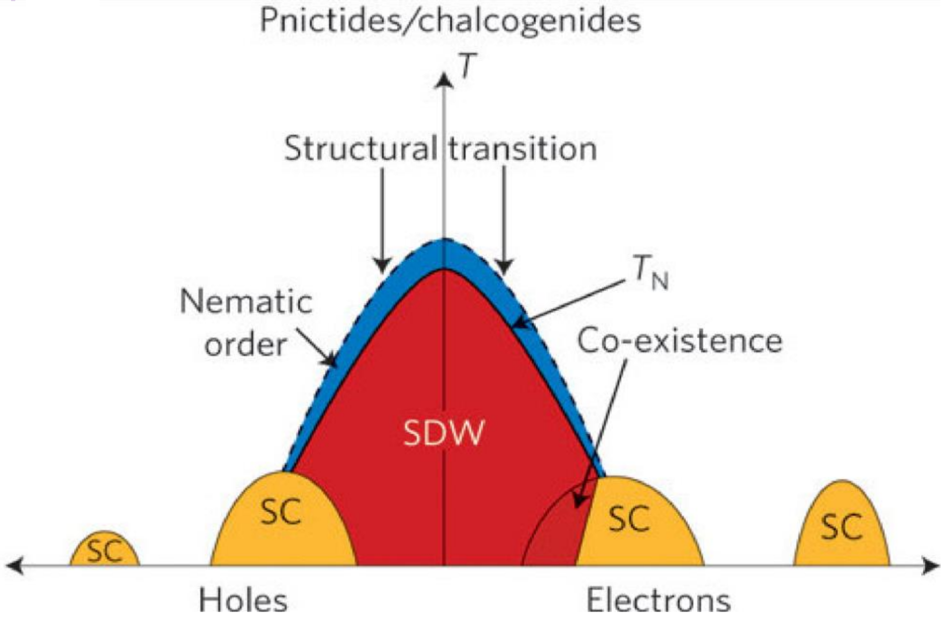
Orbital Selective Mott Physics

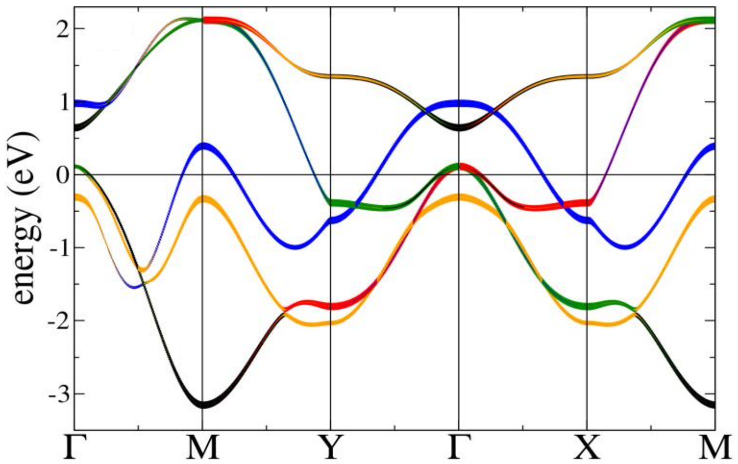
Orbital Selectivity is emerging from both High & Low energy approaches as a key feature of IBS physics

Orbital Nesting Instability

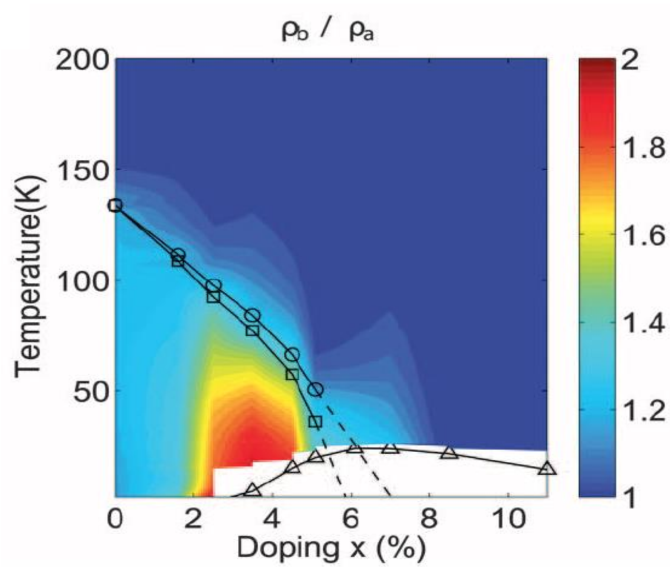
Orbital Selective Spin-Fluctuations

IRON-BASED SC:
OVERVIEW





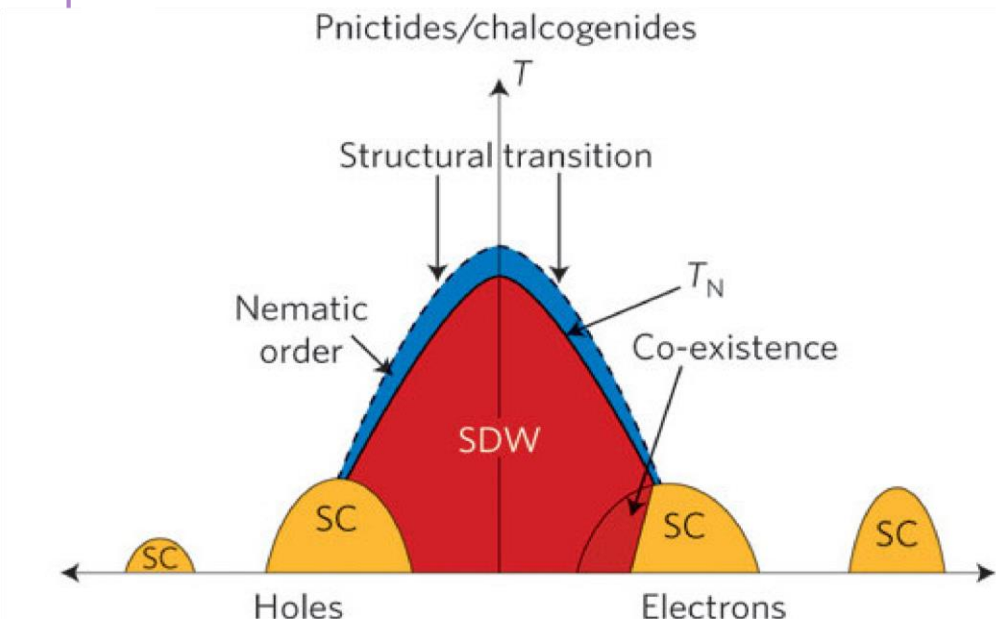
5 d-Fe orbitals contribute to the multiband electronic bands. FSs of h/e-pockets

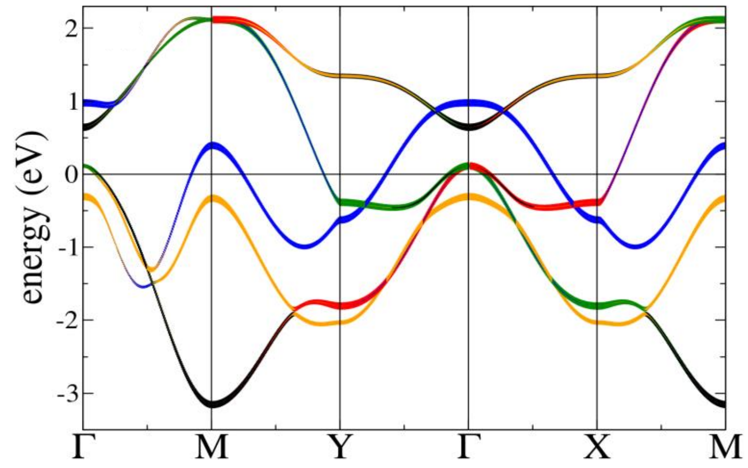


Chu et al. Science 13 (2010)

- Structural Transition
- Nematic Phase
- Spin Density Wave
- Superconductivity

IRON-BASED SC:
WEAK CORRELATED VIEW

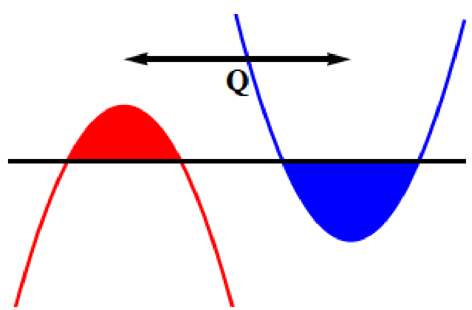




Spin-Mediated Low-Energy Model

Hole+Electron **bands** + **interband** interaction mediated by collective spin mode with characteristic energy and coupling (NO orbital information)

✓Metallicity of the parent compound
✓Hole+Electron pockets nested at the spin mode Q-vector

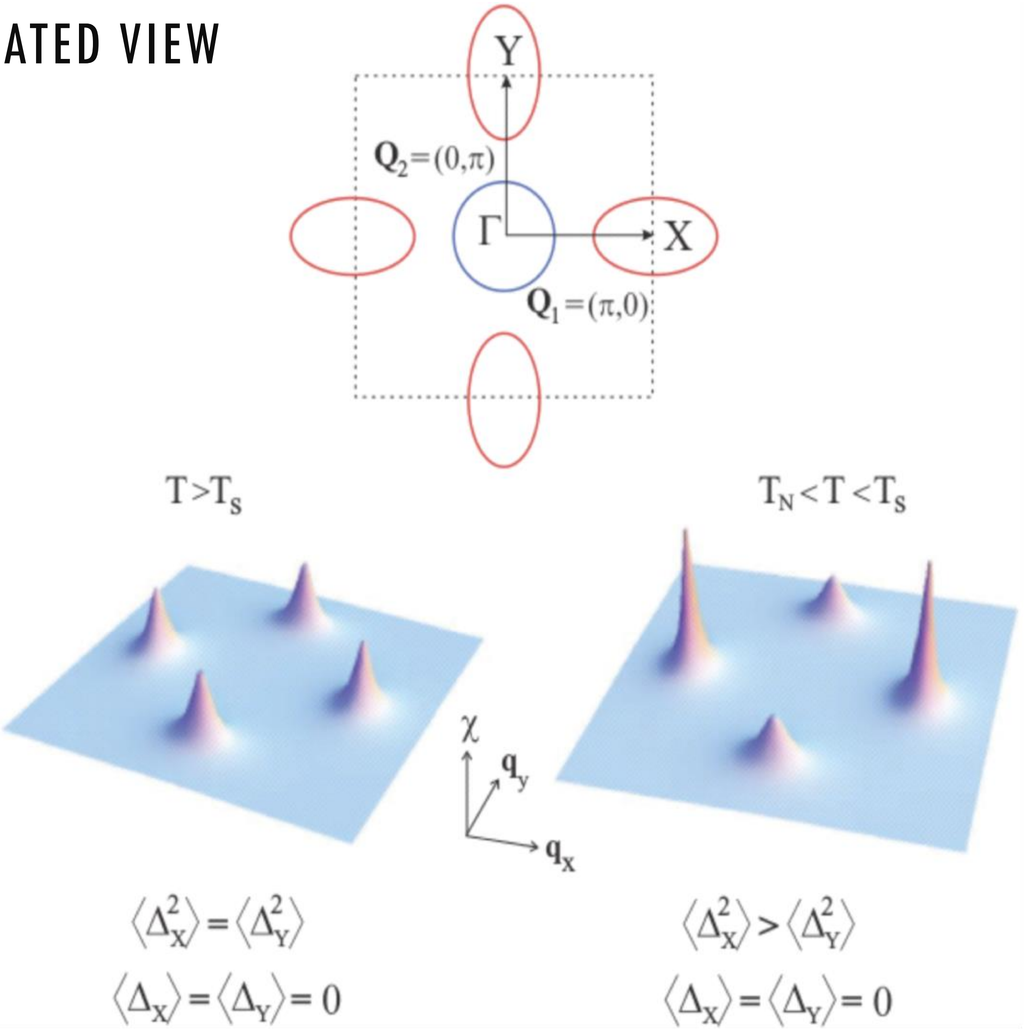


Mazin et al. PRL 101 (2008), Chubukov et al. PRB 78 (2008), Stanev et al. PRB 78 (2008) …

IRON-BASED SC:
WEAK CORRELATED VIEW

Spin-Mediated Low-Energy Model

- SDW at perfect nesting
- $s\pm$ SC out of perfect nesting
- Nematicity from anisotropic spin fluctuations:
  Z_2 broken while O(3) preserved



Fernandes et al. NatPhys 10 (2014)

ARE WE MISSING SOMETHING?

- Contrasting evidences of strong correlation:

✓ LDA vs ARPES overall in good agreement if the mass is strongly renormalized (~3/9 orbital and material dependent)

✓ Correlation degree sensitive to e/h-doping (effective mass asymmetry for e/h-doping)

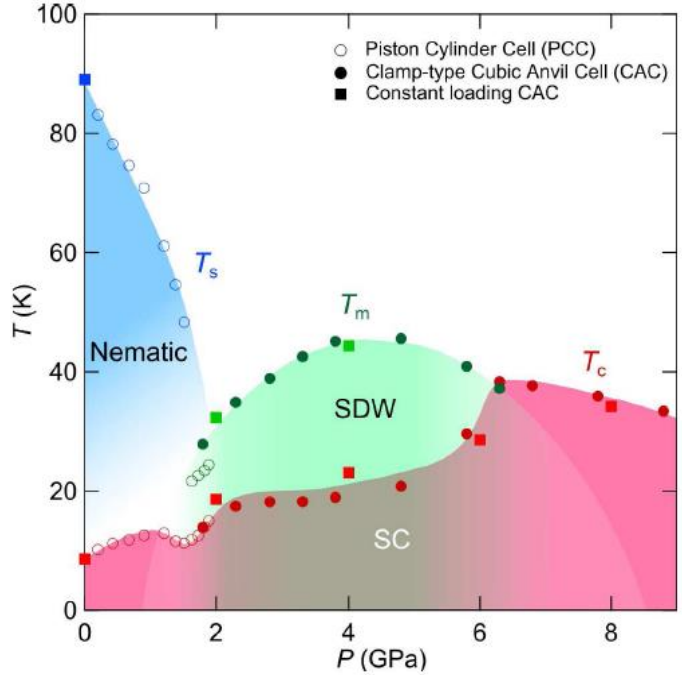
- The Case of FeSE:

Similar nesting condition of 122, different behavior

✓ HUGE NEMATIC phase WITHOUT magnetism (although sizeble spin-fluctuations from experiments e.g. Wang et al NatMat 2015)

✓ Sign-change ORBITAL ORDER in the nematic phase: orbital splitting with opposite sign at the Γ and M points.

✓ UNDER PRESSION nematicity decays abruptly and magnetism emerges.

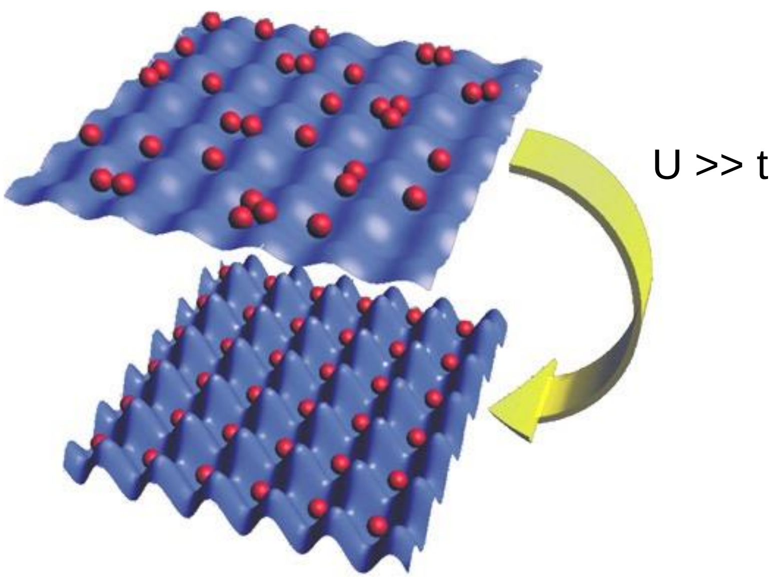


Sun et al. NatComm (2016)

MOTT-HUBBARD INSULATOR: SINGLE ORBITAL CASE HALF FILLING

The conduction band is half-filled BUT the system is insulating because of the strong Coulomb repulsion (t vs U)

At half-filling ($n = 1$) :



Increasing U

Quasiparticle Spectral Weight Suppressed $Z \sim 1/m^*$ increasing of correlation

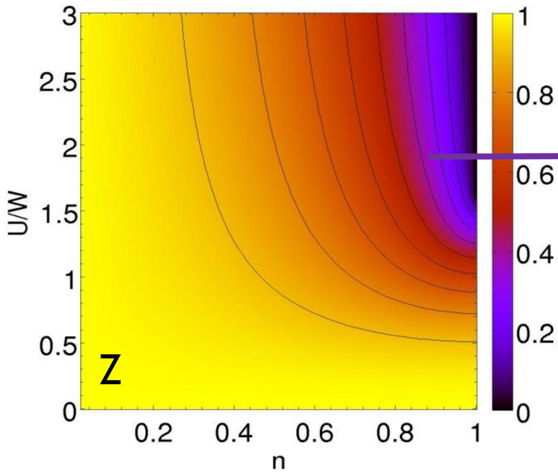
From Z=1 FL – Metal to
Z=0 Correlated electrons - Insulator

Charge Fluctuations Suppressed: localization of the electrons

Spin Fluctuations Enhanced
atoms are locally spin polarized

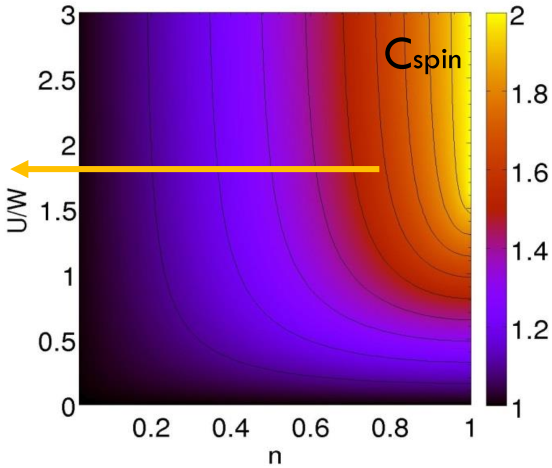
MOTT-HUBBARD INSULATOR: SINGLE ORBITAL CASE IN DOPING

Far from half-filling
($n \neq 1$) :

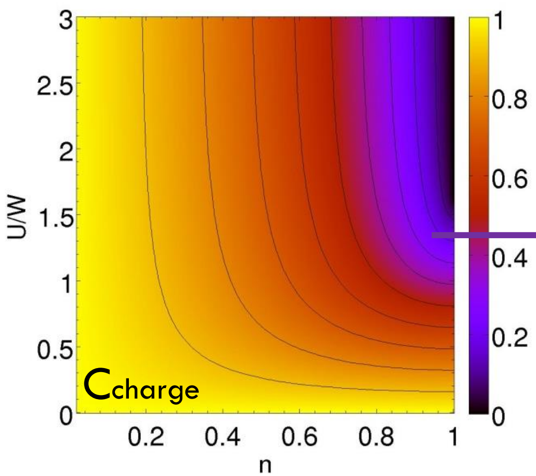


Small but finite Z:

Correlated bad metal
close to the Mott insulator



High Spin
Correlation



C_{charge} suppressed:

Quasi - Localized Electrons

MULTIORBITAL MODEL: U, JH

Density-Density Multiorbital Interacting Hamiltonian:

tb (hopping term) Intra-orbital repulsion

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

Inter-orbital repulsion Hund's coupling

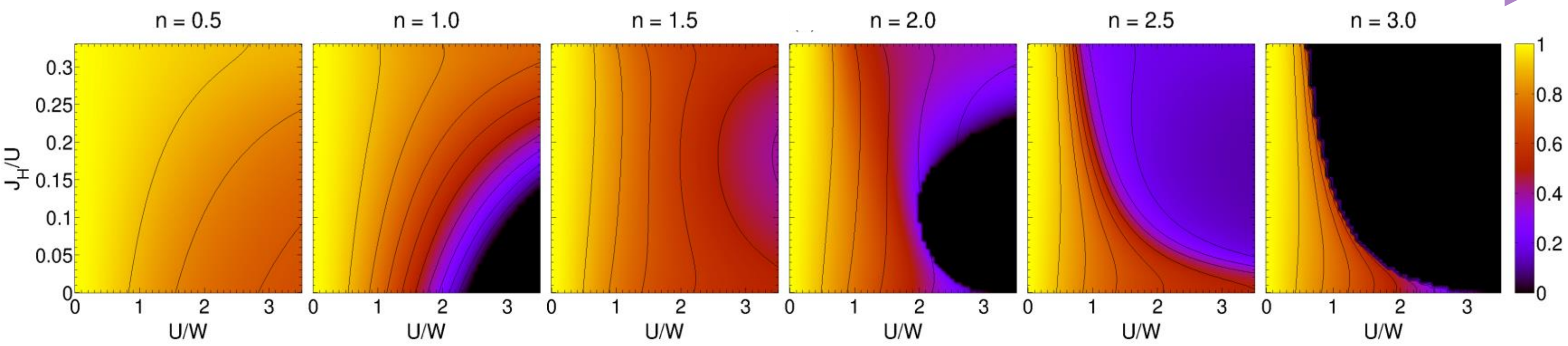
$$+ \left(U' - \frac{J_H}{2}\right) \sum_{j,\gamma>\beta,\sigma,\tilde{\sigma}} n_{j,\gamma,\sigma} n_{j,\beta,\tilde{\sigma}} - 2J_H \sum_{j,\gamma>\beta} \vec{S}_{j,\gamma} \vec{S}_{j,\beta}$$

Interactions are local and satisfy rotational invariance: $U' = U - 2J_H$

t, U, and J_H energy scales of the model

MORE IS DIFFERENT: 3 ORBITALS

Quasiparticle Spectral Weight $Z(U, J_H)$ from $n = 0.5$ to hf

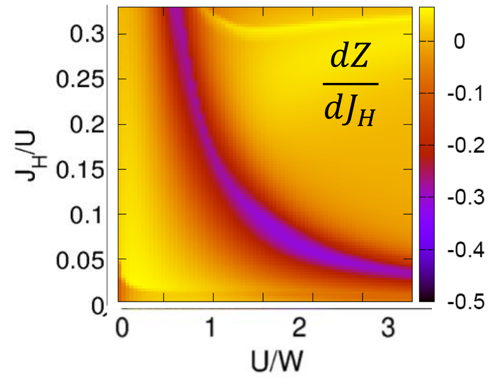


- Bad metals close to HF Mott Insulator

- Hund's metal boundary follows the MI transition line

- 2(4) el/3orb:
Hund induces correlated metal state

$n = 2.5$

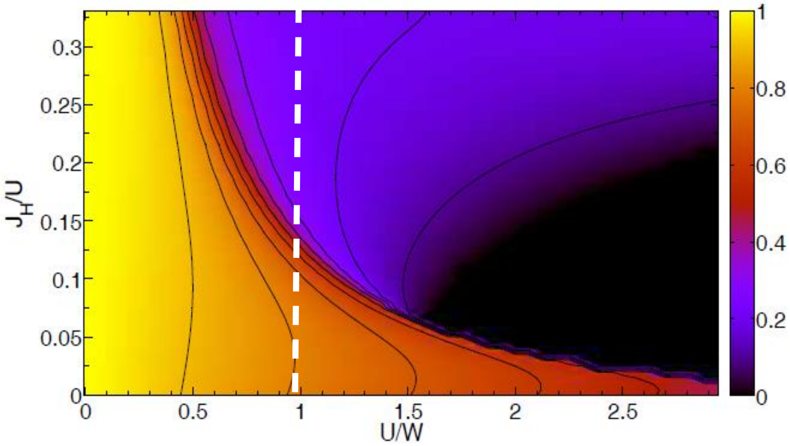


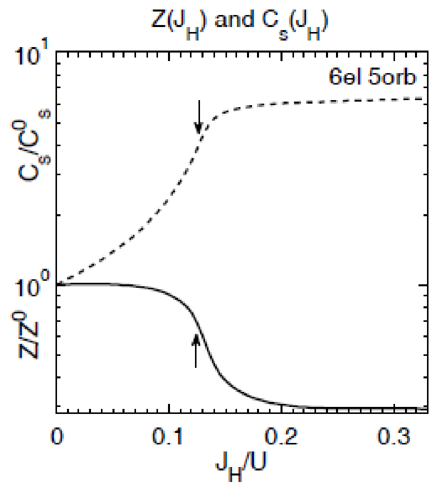
Fanfarillo & Bascones, PRB 92(2015)

THE IBS CASE: 6 ELECTRONS IN 5 ORBITALS

Fanfarillo & Bascones, PRB 92(2015)

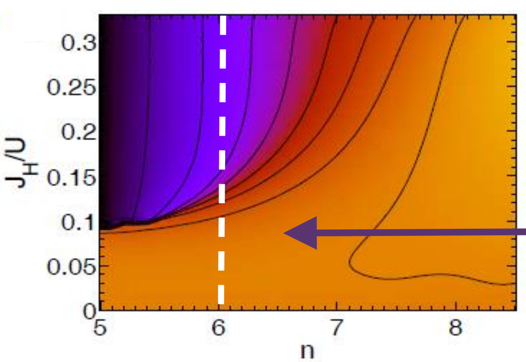
$Z(U, J_H)\ n = 6$



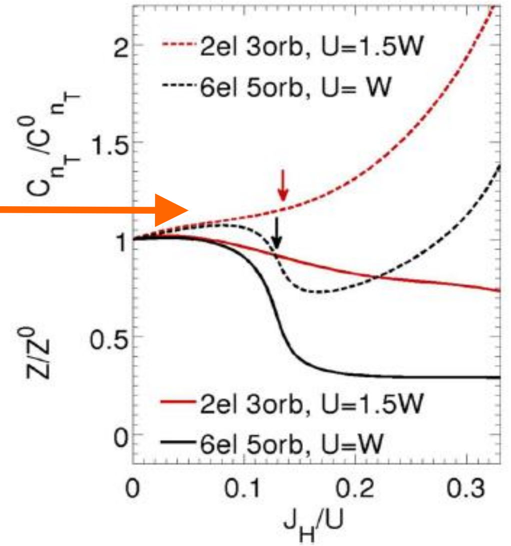


Hund's coupling induced high spin configuration

$Z(J_H, n)\quad U = W$



Z and charge fluctuations:
Correlation vs Localization



Hund'metal linked to the hf n=5 Mott insulator
doping asymmetry around n=6

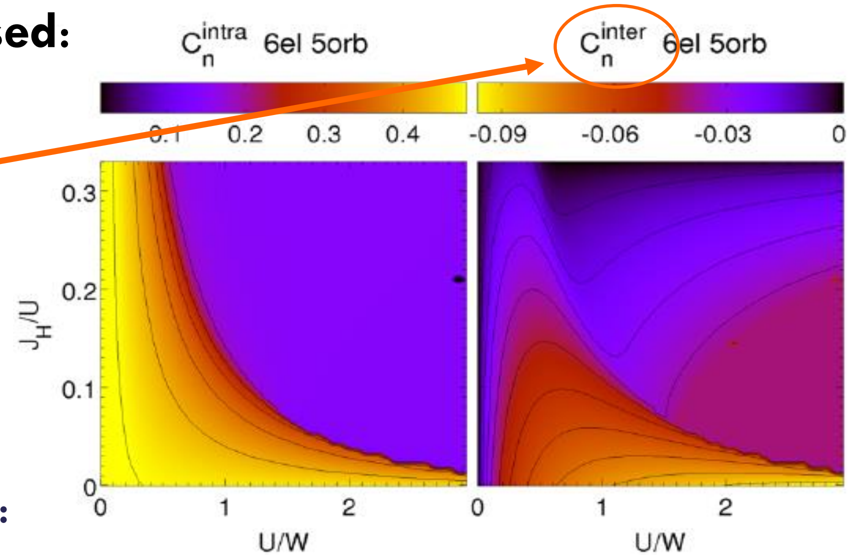
HUND'S METAL: ORBITAL DECOUPLING

As the **double occupancies are suppressed:**

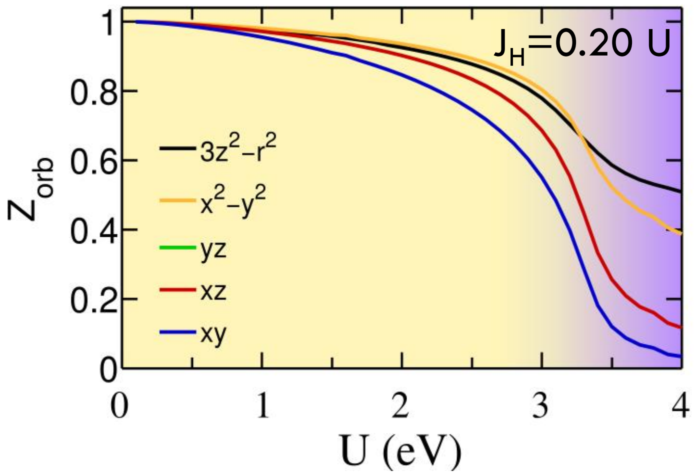
- atoms becomes *spin polarized*

- *orbitals decoupled*

Effective interorbital interaction decreases inside the polarized phase



Small Crystal Field Splitting + Hund's coupling:



-*Orbital Selective Physics*

Each orbital has a different $Z_a \sim 1/m_a^*$ proportional to the orbital filling

Each orbital behaves as a doped Mott insulator

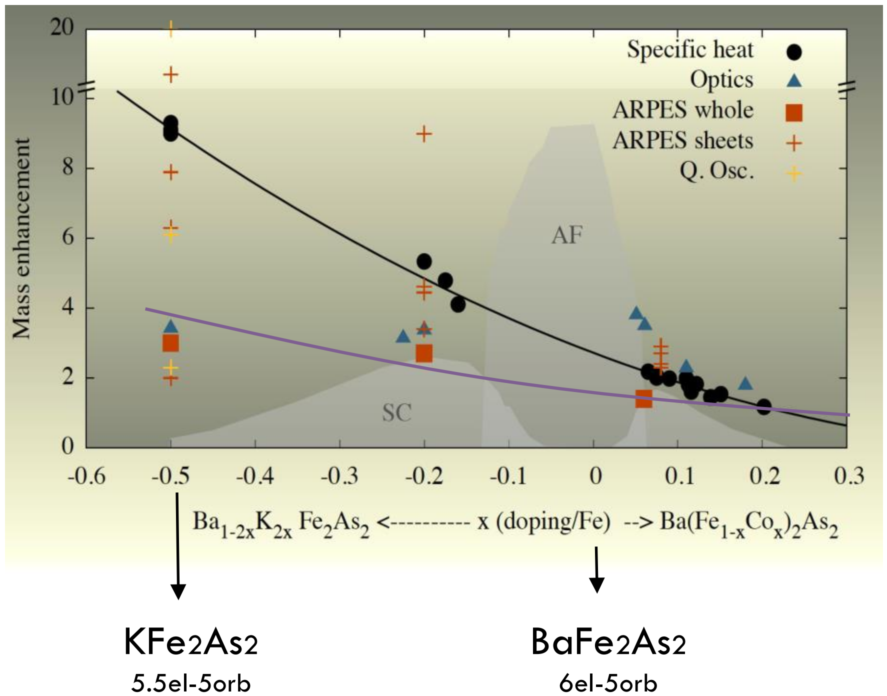
Fanfarillo & Bascones, PRB 92 (2015)

HUND'S PHYSICS IN IBS

De Medici *et al* PRL 112 (2014)

Increasing Experimental Evidence of IBS as Hund's Metals:

- Doping dependence of 122 m*
- Sommerfeld coefficient evolution through the AFe_2As_2 series A= K, Rb, Cs
- Hubbard Band in FeSe
- …



m* strongly orbital selective
Hund's metal and Selective Mottness

•m*increases reducing the # of electrons (from n=6 to n=5)

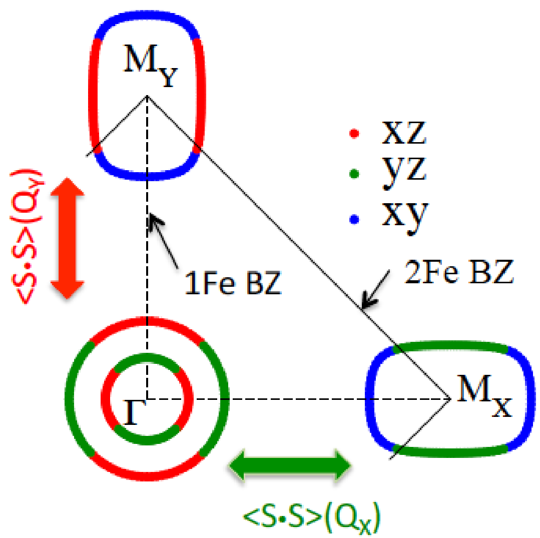
ORBITAL NESTING PICTURE:

MULTIORBITAL PHYSICS AT LOW-ENERGY

From the Orbital to the FS:

Rotation of the fermion from the orbital to the band basis lead to a tensorial effective action for the spin interaction

Fanfarillo et al. PRB 91(2015), Christensen et al. PRB 93 (2016)



However:

- only 3 orbital manly contribute to the FS

Low-energy description from symmetry adapted Hamiltonian by Cvetovic & Vafek PRB 88 (2013)

- Dominant INTRAORBITAL spin-fluctuation

Spin Fluctuations select different orbital along X or Y

$$\langle \mathbf{S} \cdot \mathbf{S} \rangle (\mathbf{Q}_X) \Rightarrow \langle \mathbf{S}^{yz}_{\mathbf{Q}_X} \cdot \mathbf{S}^{yz}_{\mathbf{Q}_X} \rangle$$
$$\langle \mathbf{S} \cdot \mathbf{S} \rangle (\mathbf{Q}_Y) \Rightarrow \langle \mathbf{S}^{xz}_{\mathbf{Q}_Y} \cdot \mathbf{S}^{xz}_{\mathbf{Q}_Y} \rangle$$

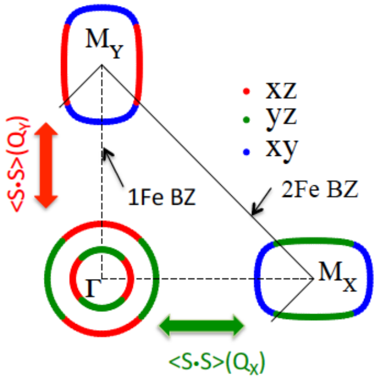
Fanfarillo et al PRB 94 (2016)
Fanfarillo arXiv 1706.08953

FS T-EVOLUTION in FeSe: explaining the tiny pockets!

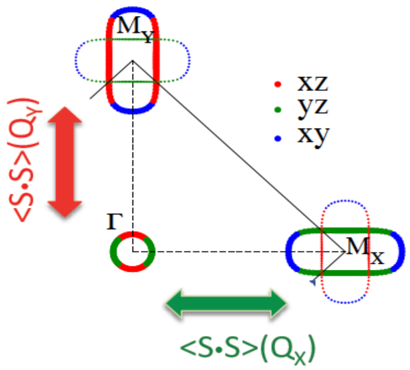
✓ Electrons coupled to orbital selective spin-fluctuation: ORBITAL SELECTIVE self-energy corrections

✓ Real part of the self-energy: mass renormalization and band shift (FS shrinking or blue/red shift)

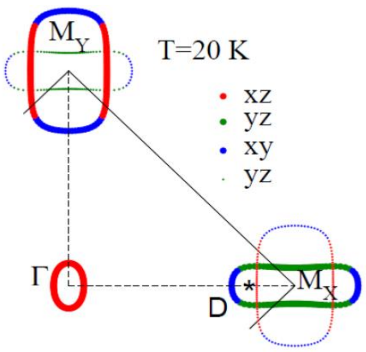
Bare TB + Z-Ren
(High Energy Corrections)



Paramagnetic Shrinking



Nematic phase



- Experimental Paramagnetic FS (3 pocket) obtained via orbital Selective Shrinking + SOC

- At the nematic transition, fluctuations along x and y become different inducing orbital splitting in the yz/xz orbitals

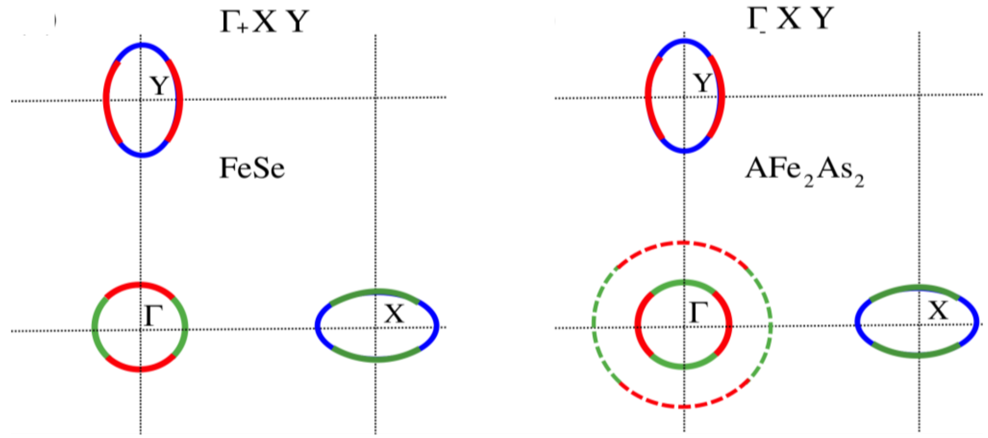
Fanfarillo et al. PRB 94 2016

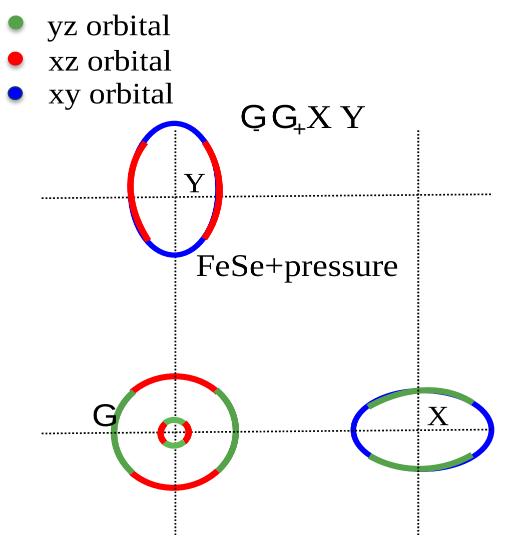
ORBITAL SELECTIVITY AT PLAY:
NEMATICITY & MAGNETISM

- ✓ Orbital Nesting Condition: Distinguish between compounds with similar band nesting condition

- ✓ Orbital Mismatch boosts nematicity while suppressing magnetic order

Orbital mismatch — Orbital nesting





- ✓ The abrupt suppresion in nematicity in FeSe under internal/external pressure could be ascribed to the emergence of the inner hole pocket.

Fanfarillo et al arXiv 1706.08953

ORBITAL SPLITTING IN THE NEMATIC PHASE

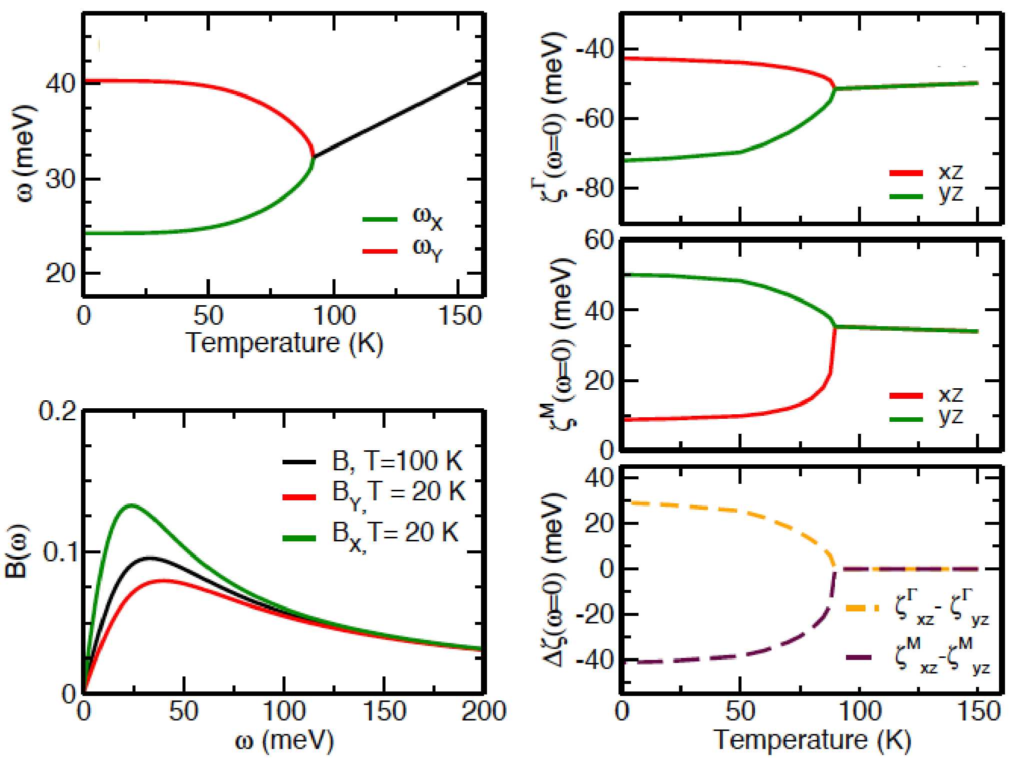
PARAMAGNETIC state:
zx and yz are degenerate

NEMATIC state:
finite splitting between zx and yz

In the nematic phase:

Anisotropic X/Y spin-fluctuation energy

But still similar X-Y Spin-Fluctuation Spectra



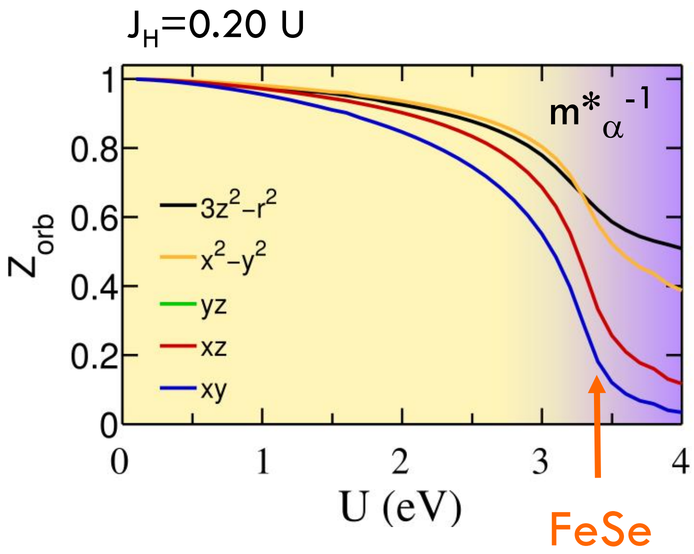
Opposite Sign Orbital splitting at Γ and X/Y are a fingerprints of the "repulsive" nature spin fluctuations:

why the sco is not universally observed in IBS?

Fanfarillo et al. PRB 94 2016

HUND'S PHYSICS IN THE NEMATIC PHASE

- ❑ Can nematicity be induced by electronic correlations due to Hund's coupling?
- ❑ If the nematic phase is induced by other degrees of freedom (e.g. spin fluctuations) do electronic correlations affect the stability of this nematic phase?



m* from ARPES, Quantum oscillations …

- ❑ Are the orbital masses modified by nematicity? How much?
- ❑ Which is the effect of electronic correlations in the band spectrum measured by ARPES in the nematic phase?

HUND'S PHYSICS IN THE NEMATIC PHASE

Compute the Response of the system to orbital perturbations modulated in k-space when orbital correlation are included

$$\delta H^{m}_{A_{1g}/B_{1g}} = \sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) \pm n_{yz}(\mathbf{k})) f_m(\mathbf{k}) h_m$$

Onsite ferro-orbital OFO

$h_{OFO} = \delta\epsilon \qquad f_{OFO}(\mathbf{k}) = 1$

ε_{zx}, ε_{yz}, $\delta\varepsilon$

Sign-change orbital order SCO

$h_{SCO} = \delta t' \qquad f_{SCO}(\mathbf{k}) = \cos k_x \cos k_y$

Lift the degeneracy of the second neighbor hopping

d-wave bond order DBO

$h_{DBO} = \delta t \qquad f_{DBO}(\mathbf{k}) = (\cos kx - \cos ky)/2.$

Lift the degeneracy of the nn hopping

Orbital Nematic Parameter:

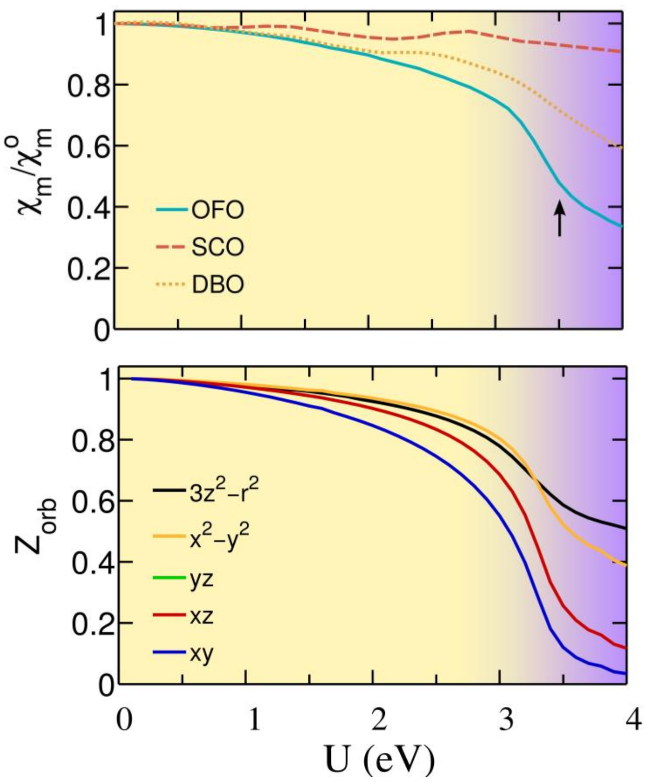
$$\Delta_m = -\langle \textstyle\sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) \pm n_{yz}(\mathbf{k})) f_m(\mathbf{k}) \rangle$$

Linear response:

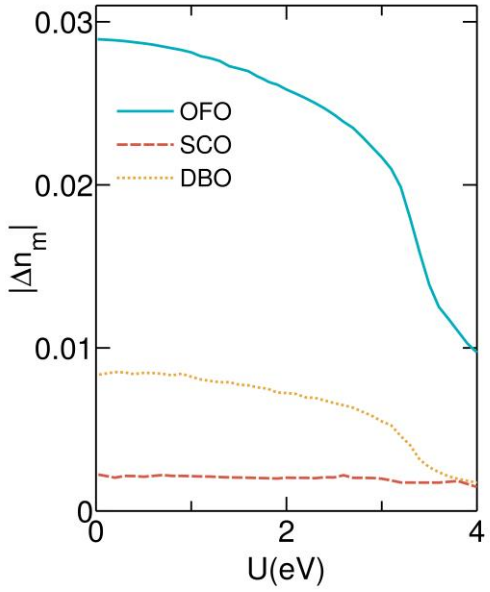
$$\chi_m = \left.\frac{\delta \Delta_m}{\delta h_m}\right|_{h_m \to 0}$$

HUND'S PHYSICS & NEMATIC ORDER

Fanfarillo et al. PRB 95 (2017)



- ❑ Can electronic correlations due to Hund's coupling induce nematic order?
  - ✓ NO! No divergence = no phase transition



- ❑ Do electronic correlations affect the stability of this nematic phase?
  - ✓ YES! In the Hund's Metal correlations select the possible orbital orders

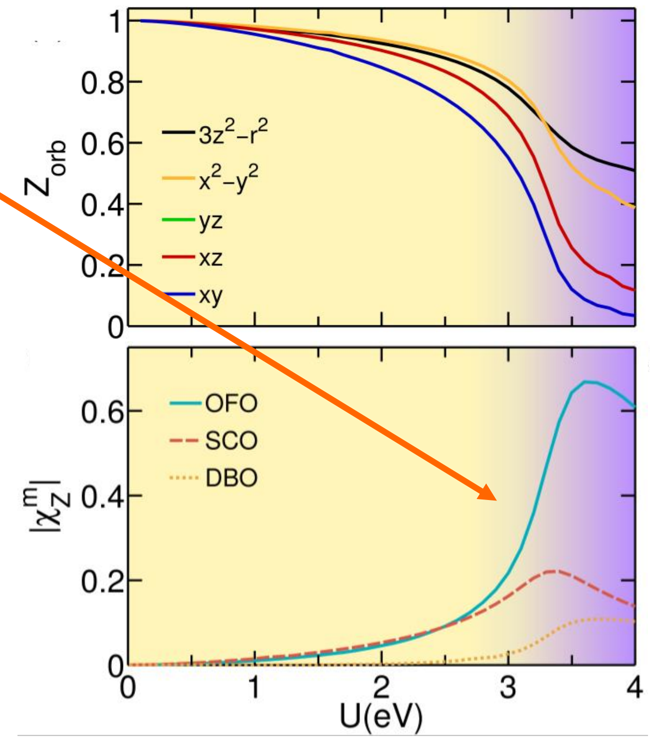
Only orbital orders that do NOT create large occupation unbalance survive to the correlations

ENHANCED NEMATICITY & HUND METAL PHASE

New route to nematicity:
anisotropy in the orbital effective mass

$$\chi_Z^m(U) = \left.\frac{\delta(Z_{zx} - Z_{yz})}{\delta h_m}\right|_{h_m \to 0}$$

Enhanced response at the entrance of the Hund Metal.



- ❑ Are the orbital masses modified by nematicitity?
  - ✓ YES! Anisotropy in the orbital mass is induced by the orbital order perturbations
- ❑ How much?
  - ✓ Few %! 1-10% for realistic parameters for IBS

Fanfarillo et al. PRB 95 (2017)

EFFECT ON THE BAND STRUCTURE

PARAMAGNETIC state:
zx and yz are degenerate

NEMATIC state:
finite splitting between zx and yz

Splittings between zx & yz bands at Γ and M in the nematic phase in absence of correlations

$$Sp_{\Gamma}^{OFO}(U=0) = 2\delta\epsilon \qquad Sp_{M}^{OFO}(U=0) = 2\delta\epsilon$$

$$Sp_{\Gamma}^{SCO}(U=0) = 2\delta t' \qquad Sp_{M}^{SCO}(U=0) = -2\delta t'$$

$$Sp_{\Gamma}^{DBO}(U=0) = 0 \qquad Sp_{M}^{DBO}(U=0) = 2\delta t$$

$Sp_{\Gamma}^{m} / Sp_{M}^{m}$:
- OFO= 1
- SCO= -1
- DBO= 0

EFFECT ON THE BAND STRUCTURE

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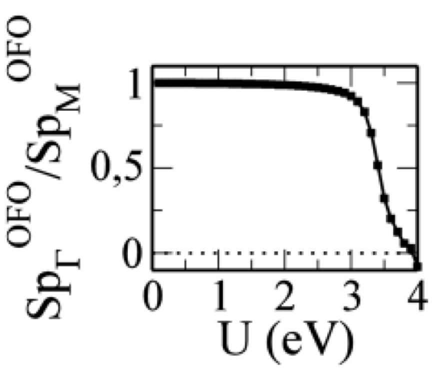
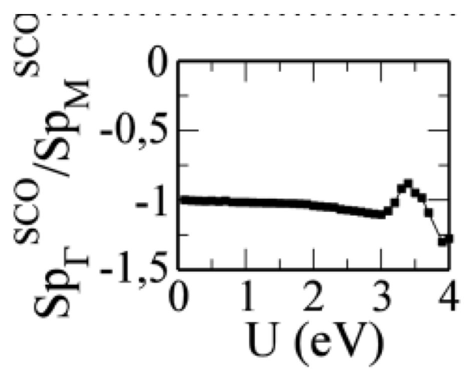
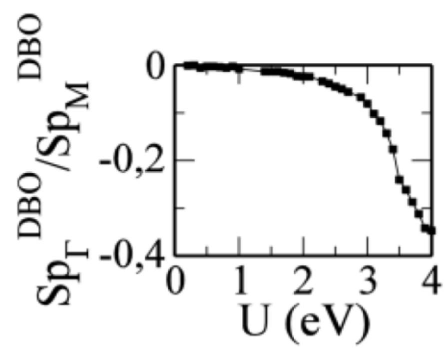
$$Sp_\Gamma^{DBO}(U=0) = 0 \qquad Sp_M^{DBO}(U=0) = 2\delta t$$

Sp_Γ^m / Sp_M^m:
- OFO= 1
- SCO= -1
- DBO= 0

Splittings between zx & yz bands at Γ and M in the nematic phase in presence of correlations

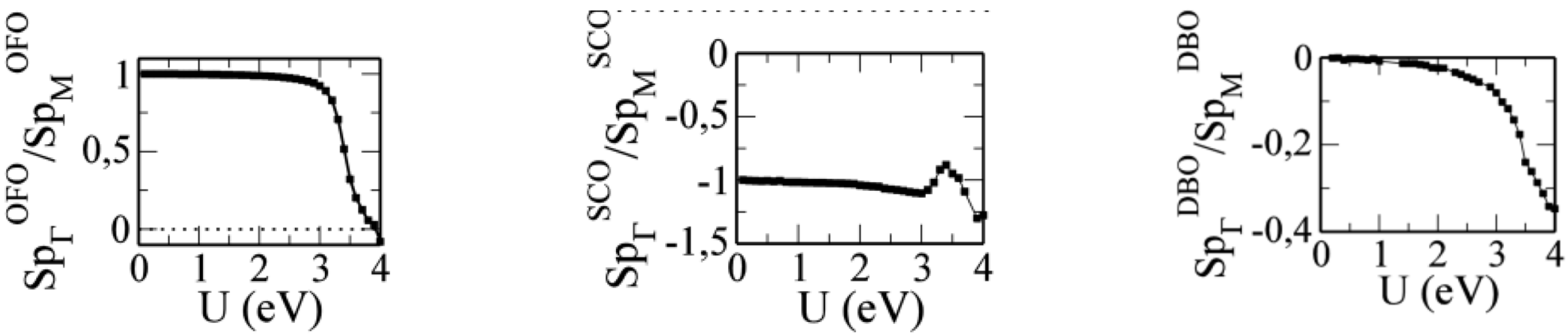






EFFECT ON THE BAND STRUCTURE

Splittings between zx & yz bands at Γ and M in the nematic phase in presence of correlations:



- ✓ The ratio between the splittings between zx/yz bands changes with respect to its value in the absence of correlations.

Sp_Γ^m / Sp_M^m — OFO= 1; SCO= -1; DBO= 0

✓ STRONG local correlations modify the orbital splitting

Induce k-dependence & drive sign change

Fanfarillo et al. PRB 95 (2017)

CONCLUSIONS

✓ Orbital Selectivity Emerges from both weak and strong correlated approach in the physics of Iron-Based SC:

- Hund's Metal - Orbital selective doped-Mott physics
- Spin-Mediated Model - Orbital Selective Spin-Fluctuations (OSSF)

✓From Low-Energy Approach:

- OSSF: relevant parameters FS topology (how many pockets?), band nesting AND orbital matching

- Orbital selective Self-Energy:
FS shrinking, orbital splitting in the nematic phase (orbital order parameter-like behavior *without breaking the symmetry in the orbital cannel)*

✓From High-Energy Approach:

- Electronic correlations cannot drives the nematic transition, but constrains the possible orbital orders. Orders that do not create large occupation unbalance survive even in a strong correlated system (as FeSe).

TAKE-HOME MESSAGE & PERSPECTIVES

- ✓ Weak-correlated and Strong-correlated approaches allow to treat he same electronic interactions at different energy scale (high vs low energy renormalization)

- ✓ Analysis in the paramagnetic and nematic phase show that Strong and Weak correlated approaches give consistent results!

- ✓ Work in progress: Orbital selective pairing

- ✓ Final aim: merge the effects of high and low energy renormalization within a unified description