ARPES investigation of the bad metallic behavior in $Fe_{1.06}Te$

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SOLEIL synchrotron, CASSIOPEE beamline

Amina Taleb-Ibrahimi, Patrick Le Fèvre, François Bertran

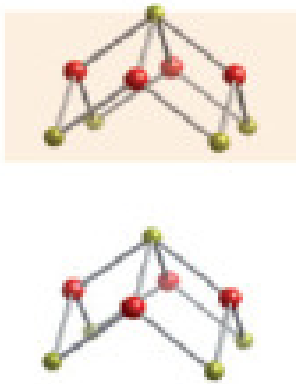
Sample synthesis

FeTe : Enrico Giannini, *University of Geneva, Swizerland*

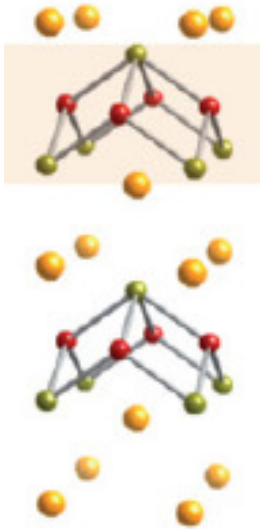
Pnictides : Dorothée Colson, Anne Forget, Florence Rullier- Albenque
SPEC, CEA-Saclay, France

A new family of correlated systems

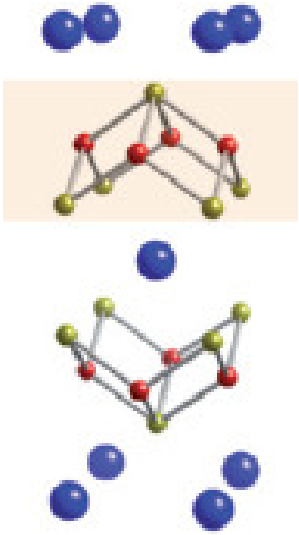
FeTe



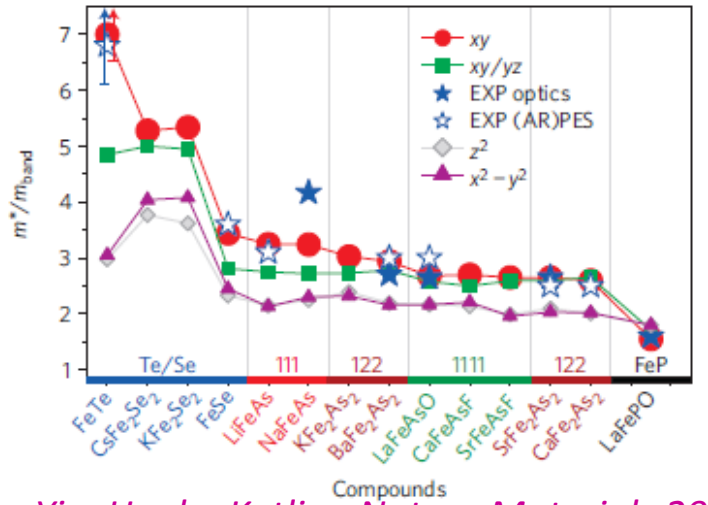
LiFeAs



$BaFe_2As_2$



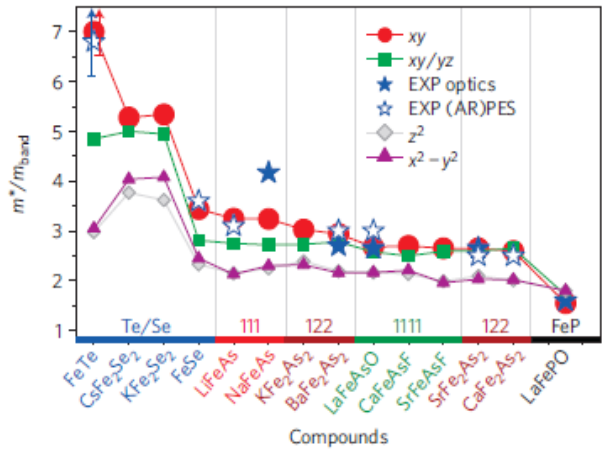
Effective masses calculated by DMFT



Yin, Haule, Kotliar, Nature Materials 2011

A new family of correlated systems

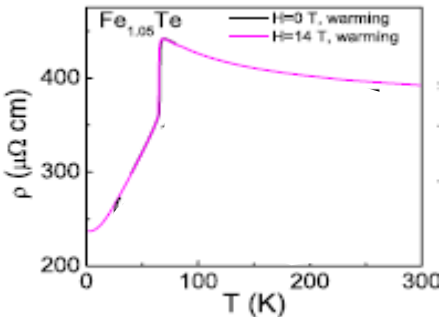
Effective masses calculated by DMFT

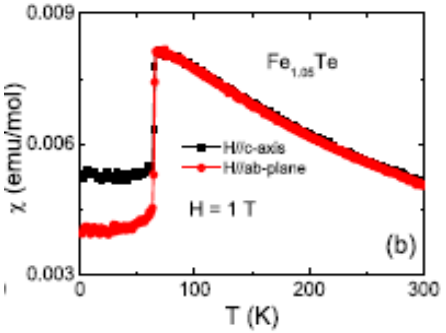


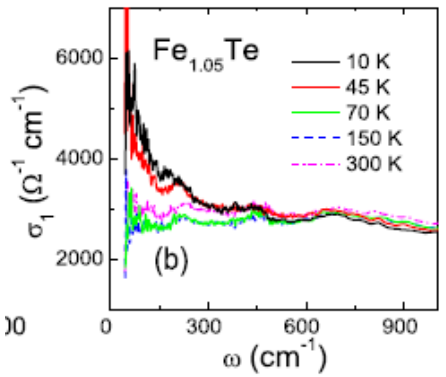
Yin, Haule, Kotliar, Nature Mat. 2011

FeTe is the most correlated case and behaves as a « bad metal » quite different from $BaFe_2As_2$.

FeTe

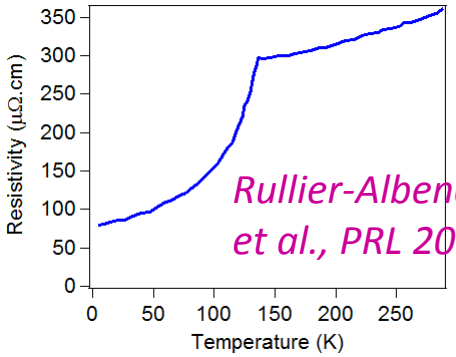




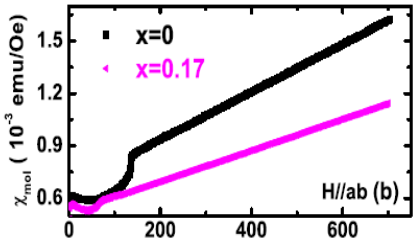


Chen et al., PRB 2009

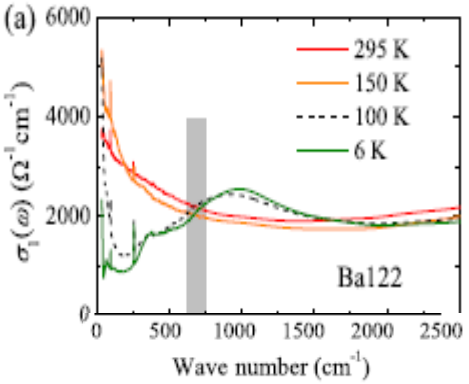
$BaFe_2As_2$



Rullier-Albenque et al., PRL 2009



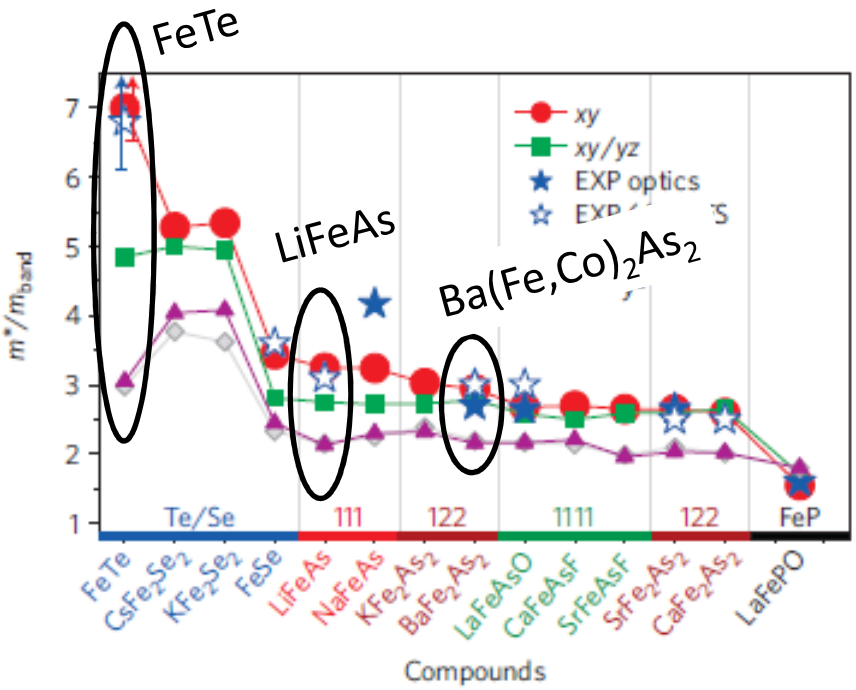
Wang et al., New J. Phys. 2009



Moon et al., PRL 2012

Outline

What can we learn with ARPES about the strength and nature of electronic correlations ? How do they evolve from family to family ?



=> Imaging the different bands of the electronic structure and defining renormalization values for each orbital

Orbital differentiation in LiFeAs

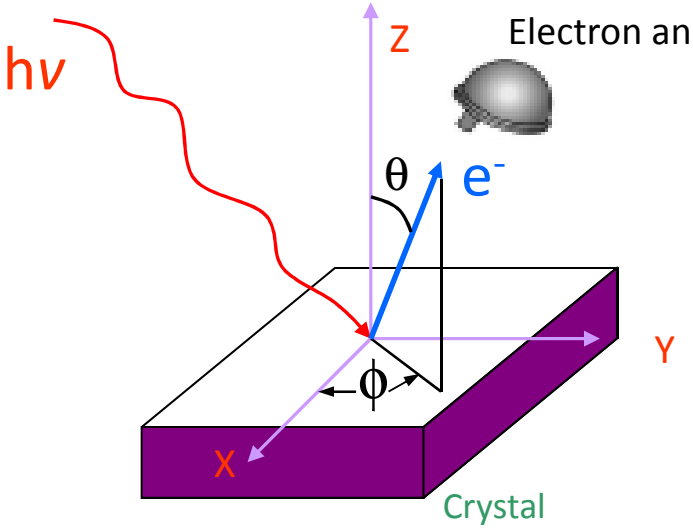
=> Characterizing the « bad metallic state » in FeTe.

There is a large « pseudogap » (60meV) in the paramagnetic state of FeTe.

Spin-freezing regime ?

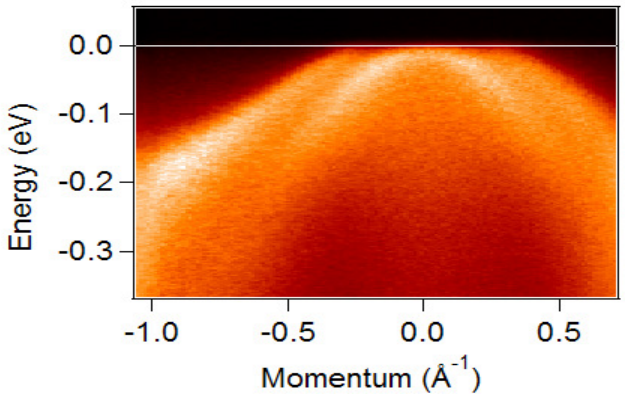
Are pseudogaps ubiquitous in pnictides ?

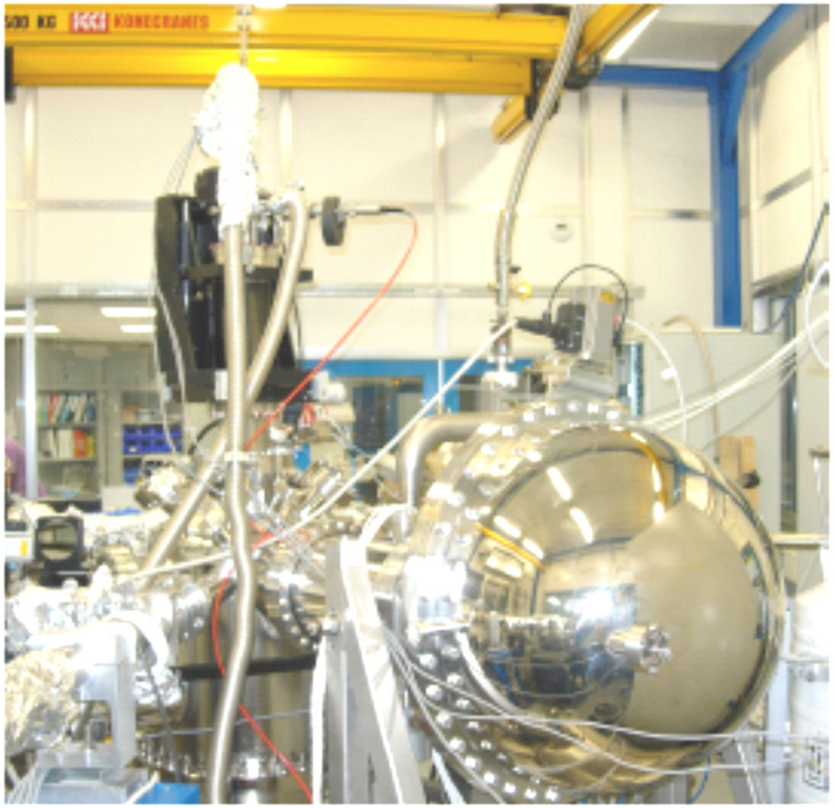
Electronic structure studied by ARPES



$$E_{kin} = h\nu - W - \left|E_B\right|$$

$$\hbar \mathbf{k}_{\parallel} = \sqrt{2mE_{kin}} \sin\theta$$





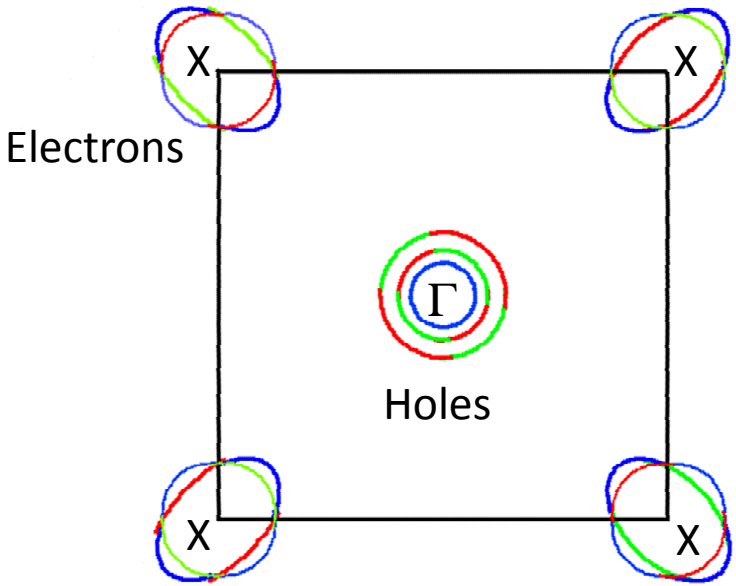
CASSIOPEE beamline, SOLEIL synchrotron

=> 10-100 eV

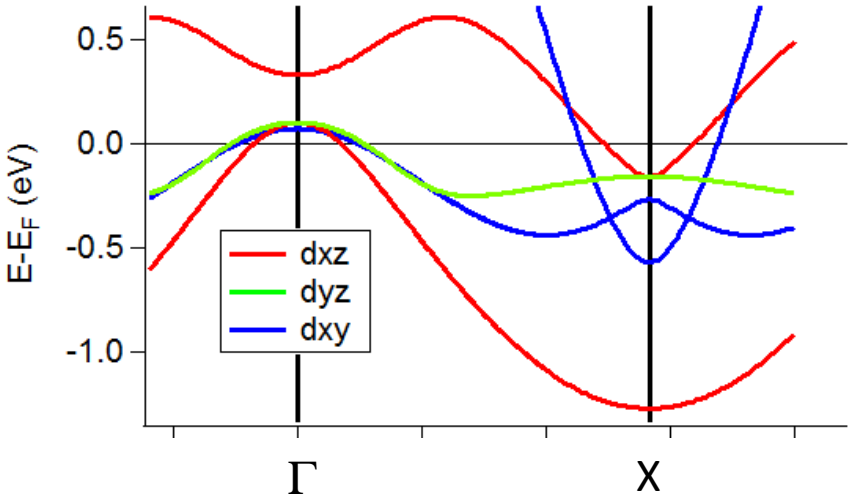
=> high energy and angular resolution

Generic electronic structure expected for iron-based superconductors

Fermi Surface

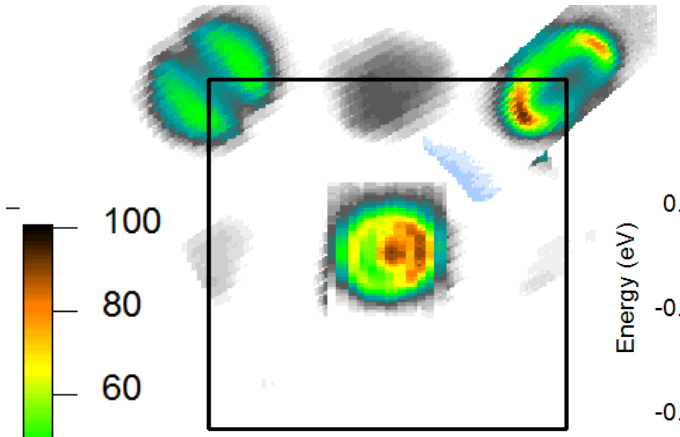


Band dispersion along the diagonal

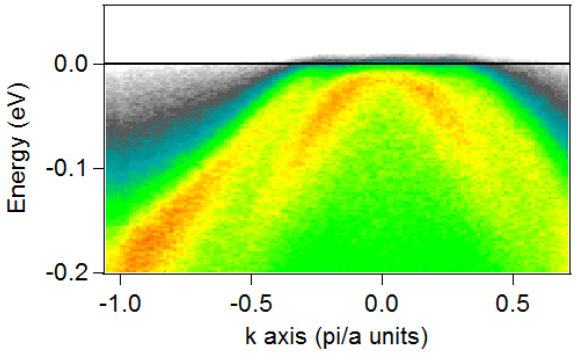


Electronic structure viewed by ARPES

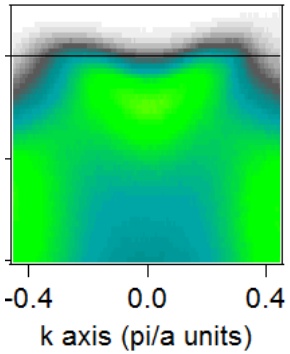
$Ba(Fe_{0.92}Co_{0.08})_2As_2$

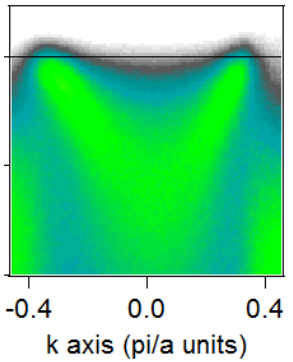


Hole pockets

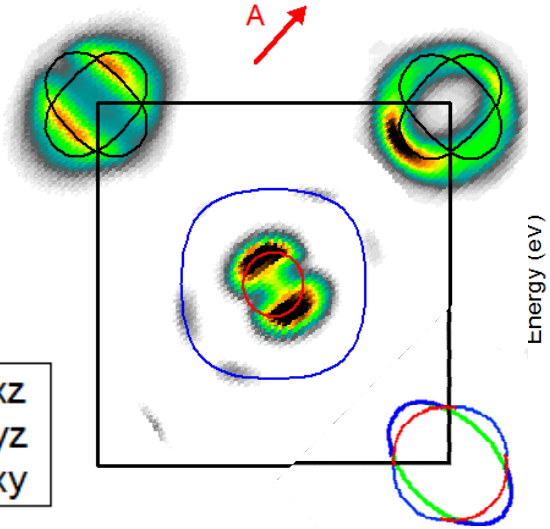


Electron pockets

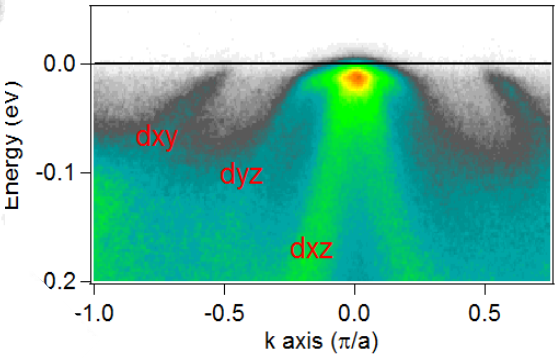




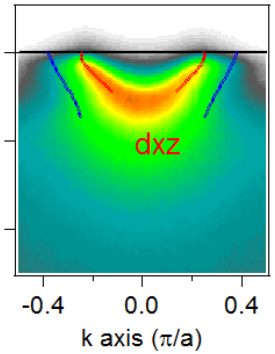
LiFeAs

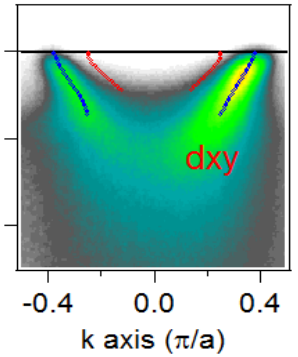


Hole pockets



Electron pockets

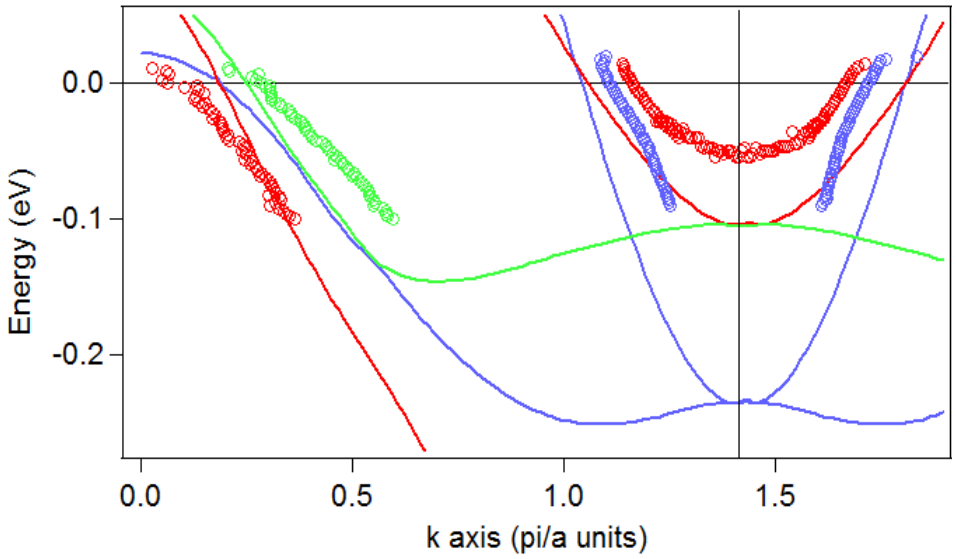




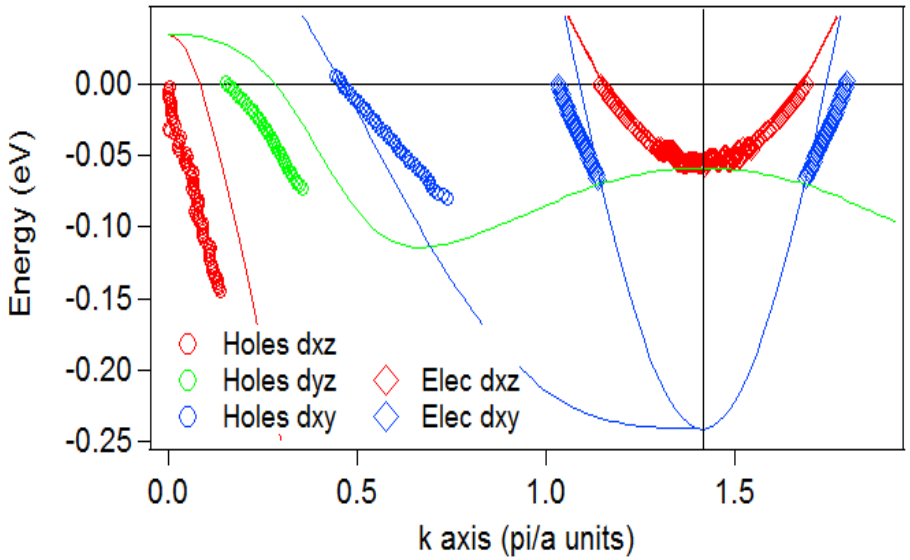
Modulation of intensities => *V. Brouet et al. PRB 2012, L. Moreschini et al. PRL 2014*

ARPES dispersions *vs* band calculations

$Ba(Fe_{0.92}Co_{0.08})_2As_2$ (kz=0.7)



LiFeAs (kz=0)



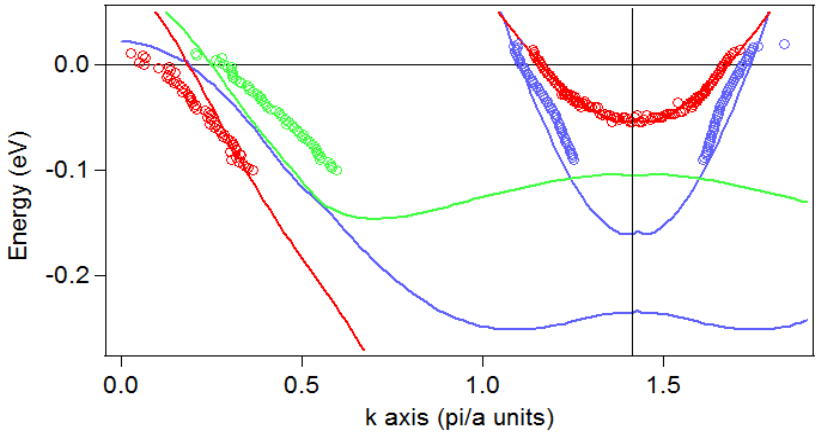
NB : Band calculations are shown renormalized by a factor 2.
=> « modest » correlations

« Shrinking » of FS
=> Smaller hole and electron pockets
=> Driven by interband transitions
=> Brouet et al., PRL 13

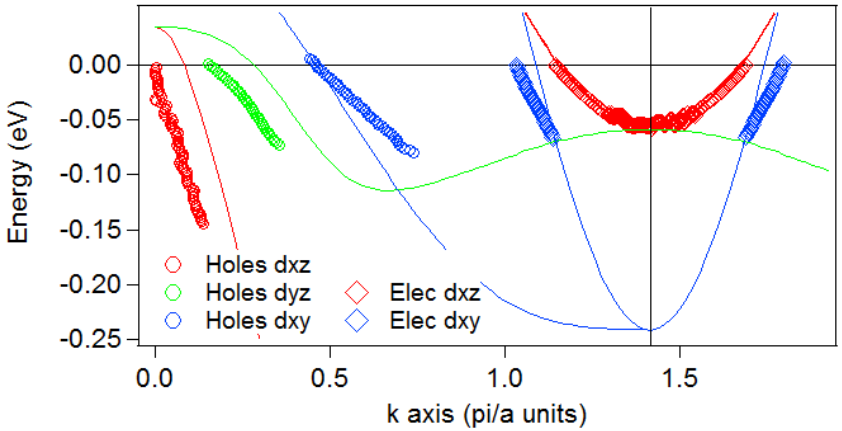
Orbital polarization
=> Holes are transferred from dxz/dyz to dxy

Renormalization values

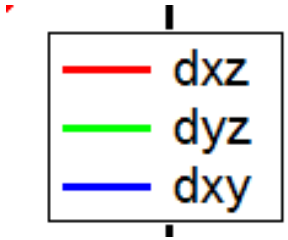
$Ba(Fe_{0.92}Co_{0.08})_2As_2$ (kz=0.7)
Global renormalization of 2 + 130meV shift

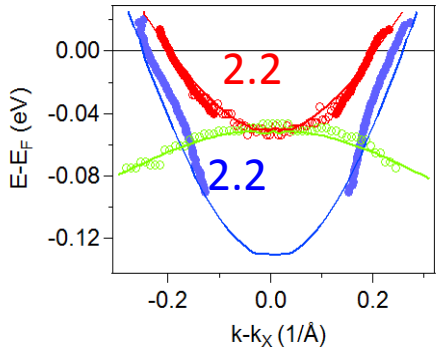


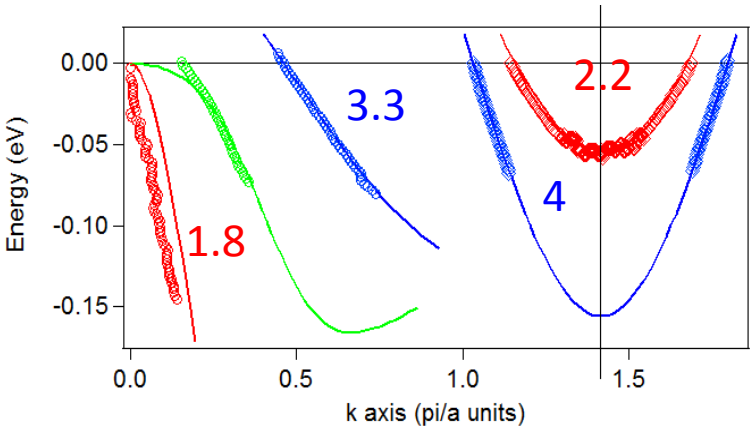
LiFeAs (kz=0)
Global renormalization of 2



With individual shift and normalization







V. Brouet et al., PRL 2013

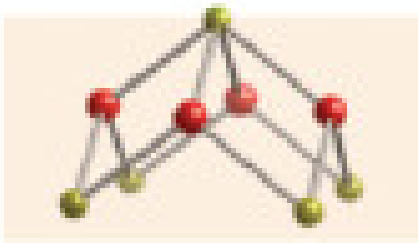
DMFT ~ 2,5 for both

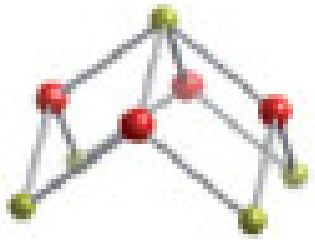
2,5 for dxz/dyz and 3 for dxy

=> In LiFeAs, dxy and dxz/dyz orbitals start to differentiate

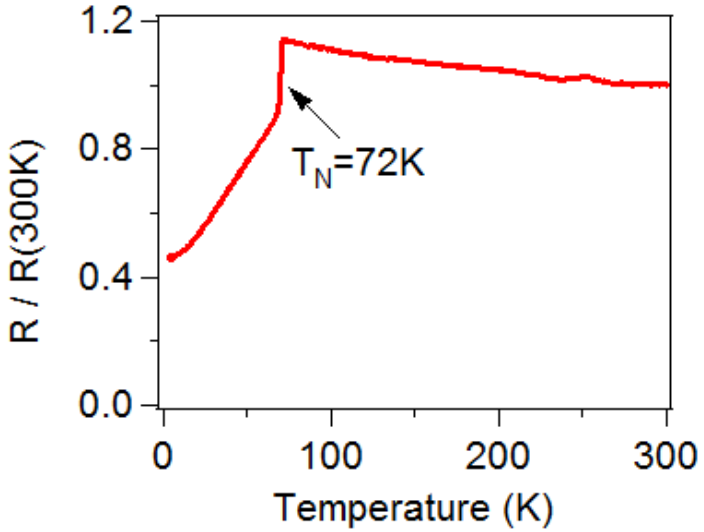
The case of FeTe

$Fe_{1.06}Te$





Resistivity

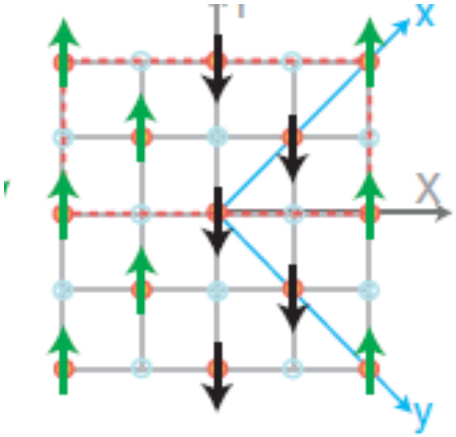


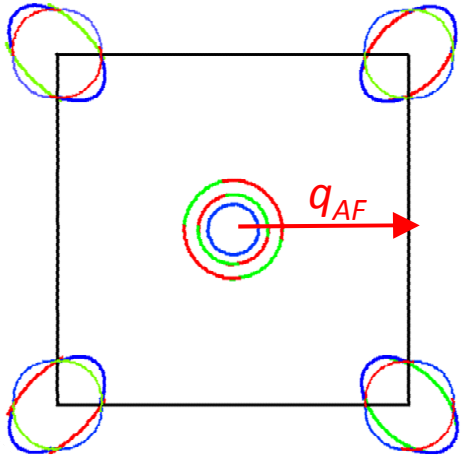
Much larger magnetic moment than Fe pnictides

=> $M=2,1\mu_B$

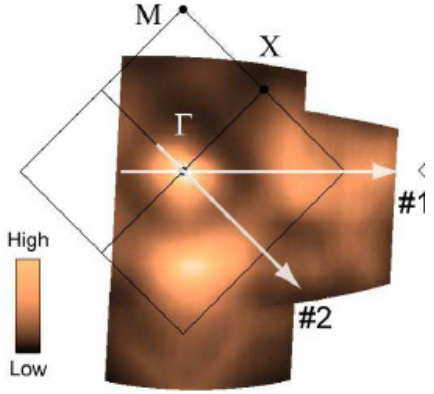
Bao, PRL 2009

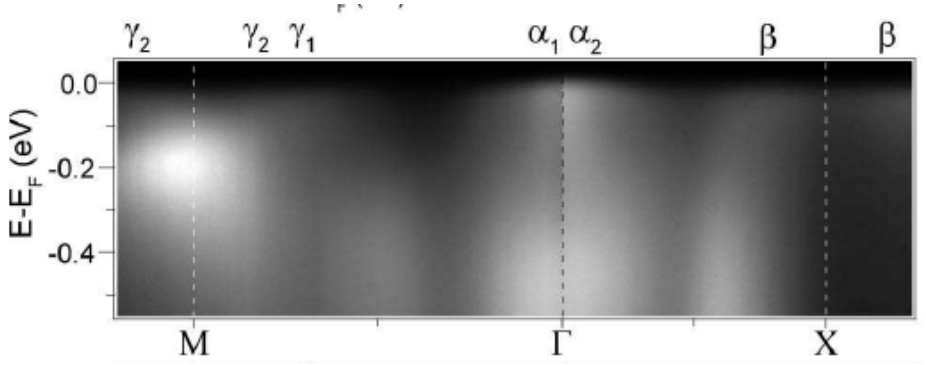
« Double stripe » magnetic structure NOT corresponding to FS nesting



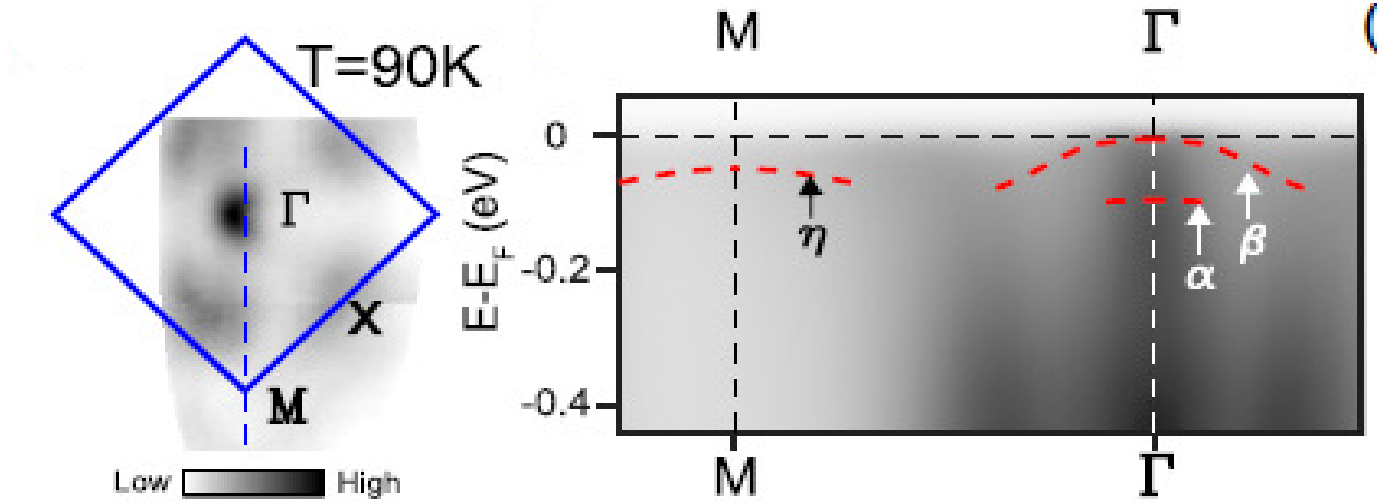


Previous studies of FeTe ($T>T_N$)





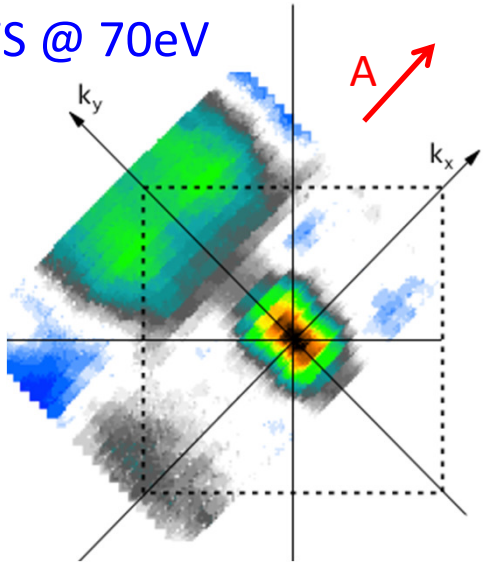
Zhang, DL Feng et al. PRB 2012



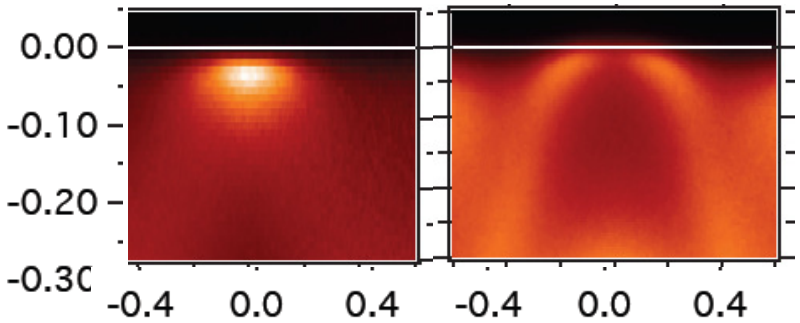
Liu, ZX Shen et al PRL 2013

FeTe Fermi Surface (80K)

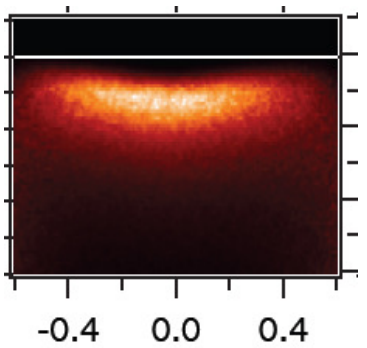
FS @ 70eV



dxz/dyz hole pockets



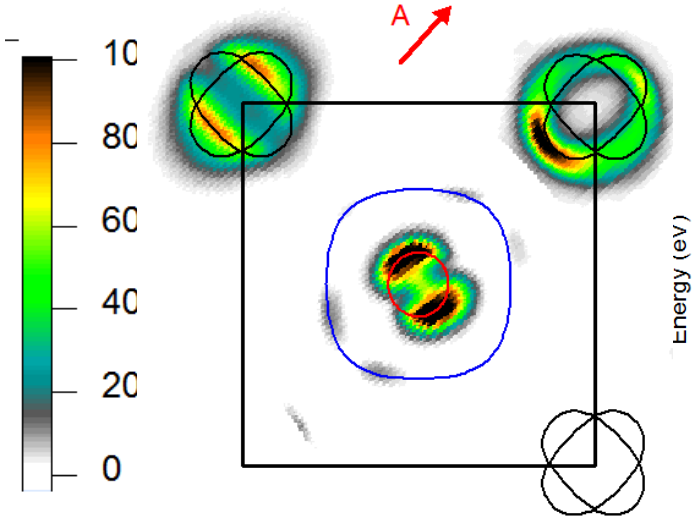
dxz/dyz electron pocket



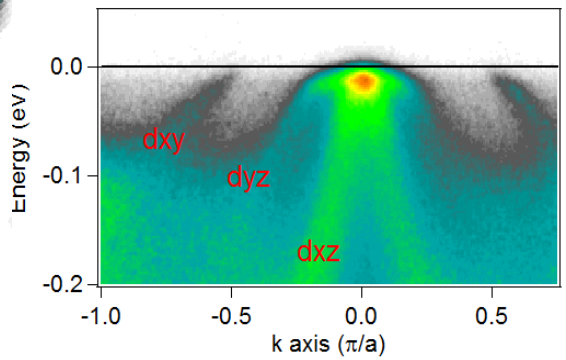
⇒ No trace of d_{xy} band

⇒ Strange shape for electron pocket !

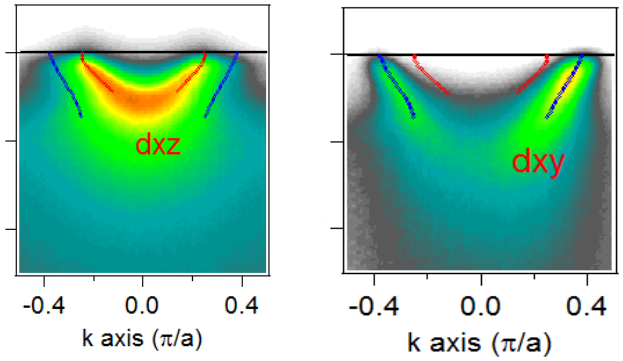
LiFeAs



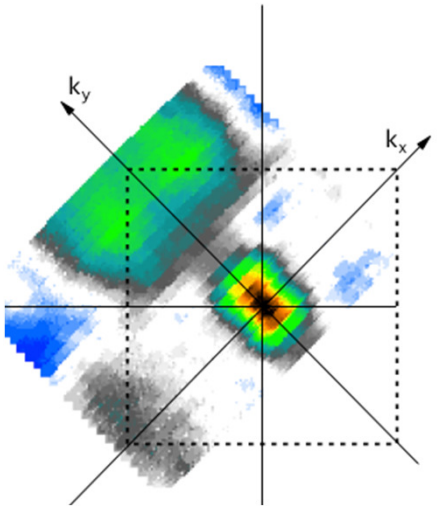
Hole pockets



Electron pockets

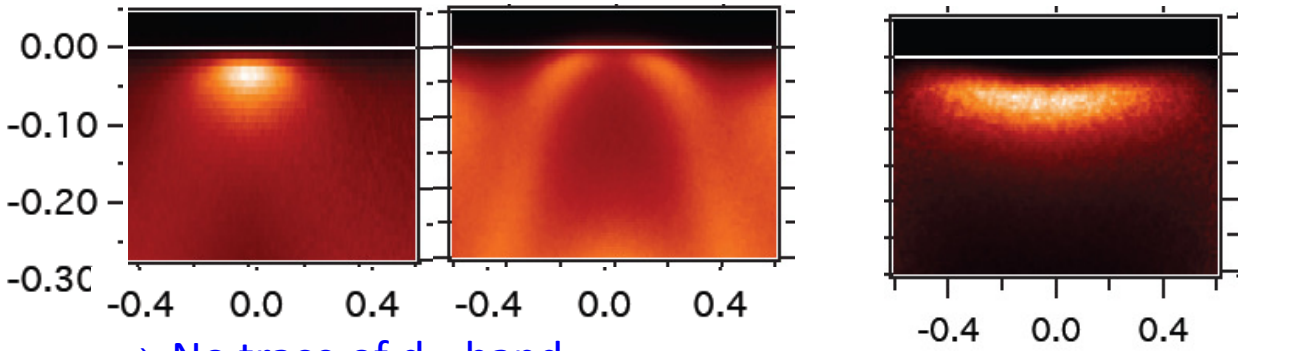


FeTe Fermi Surface (80K)



dxz/dyz hole pockets

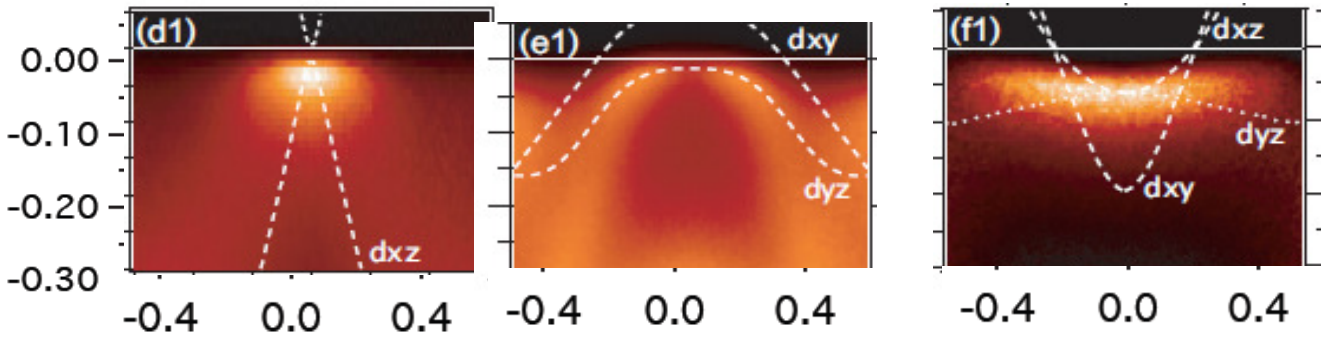
dxz/dyz electron pocket



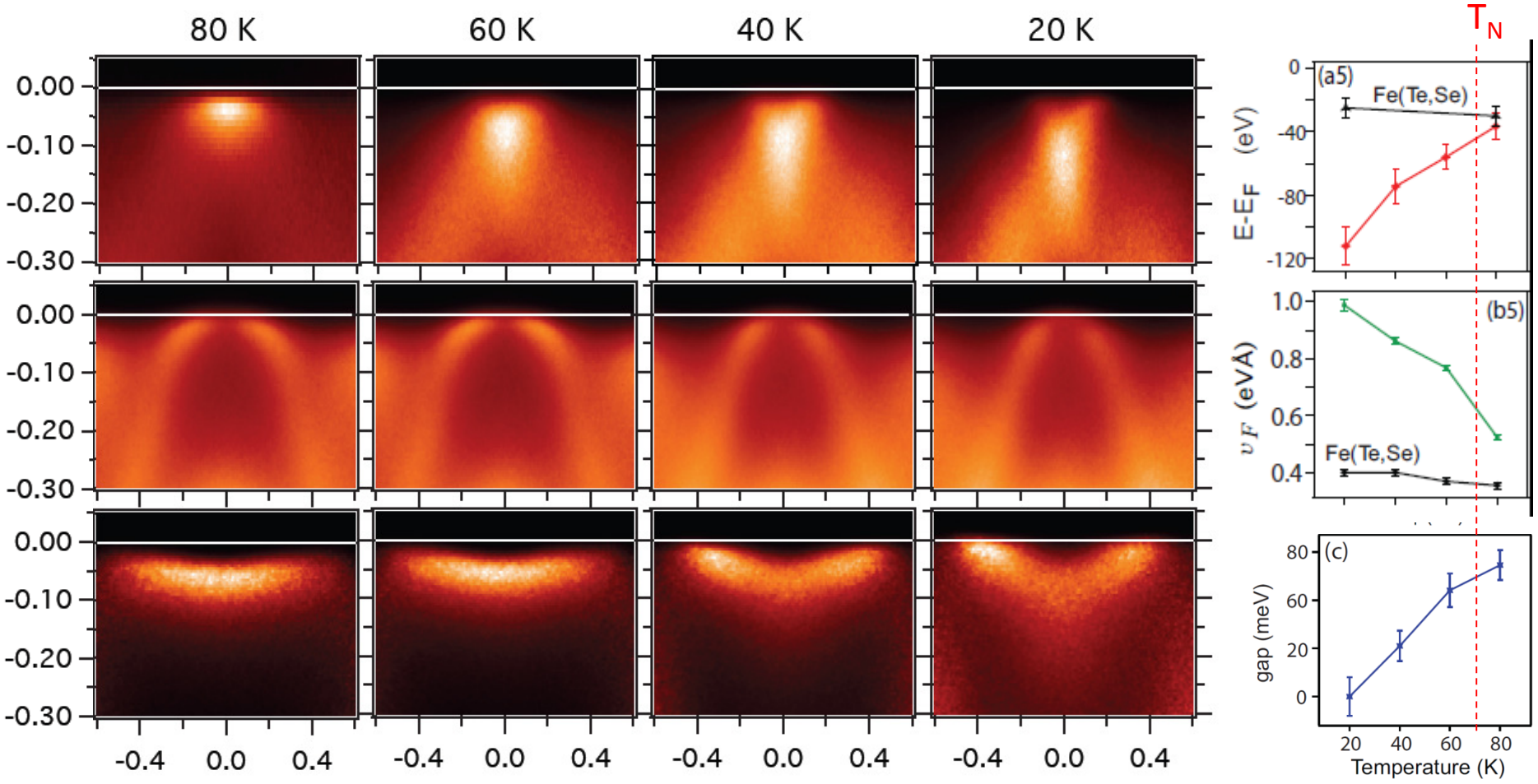
$\Rightarrow$ No trace of d_{xy} band

$\Rightarrow$ Strange shape for electron pocket !

Dotted white lines : band calculation shifted and renormalized by 2



FeTe : evolution of the bands with temperature

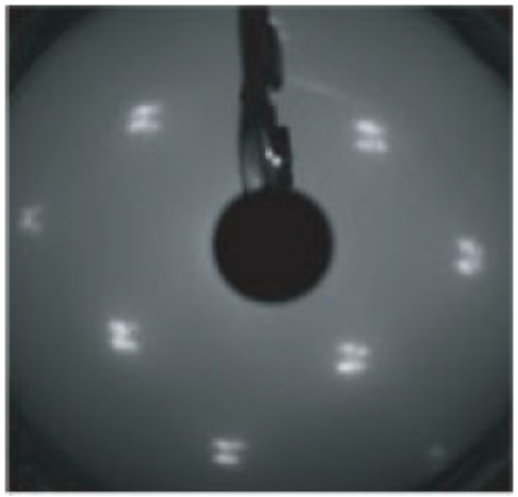


P.H. Lin, V. Brouet et al., PRL 2013

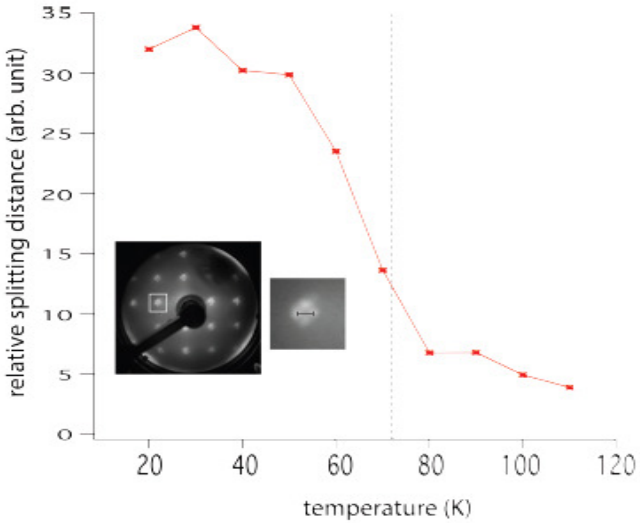
Transition to the magnetic state

80 K

20 K

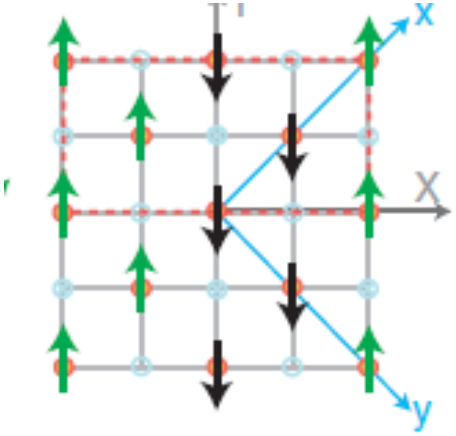


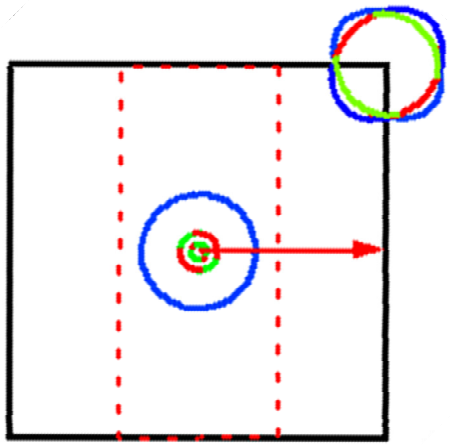
Splitting of LEED spot vs T



LEED evidences a transition to the magnetic monoclinic phase that takes place similarly as in the bulk.

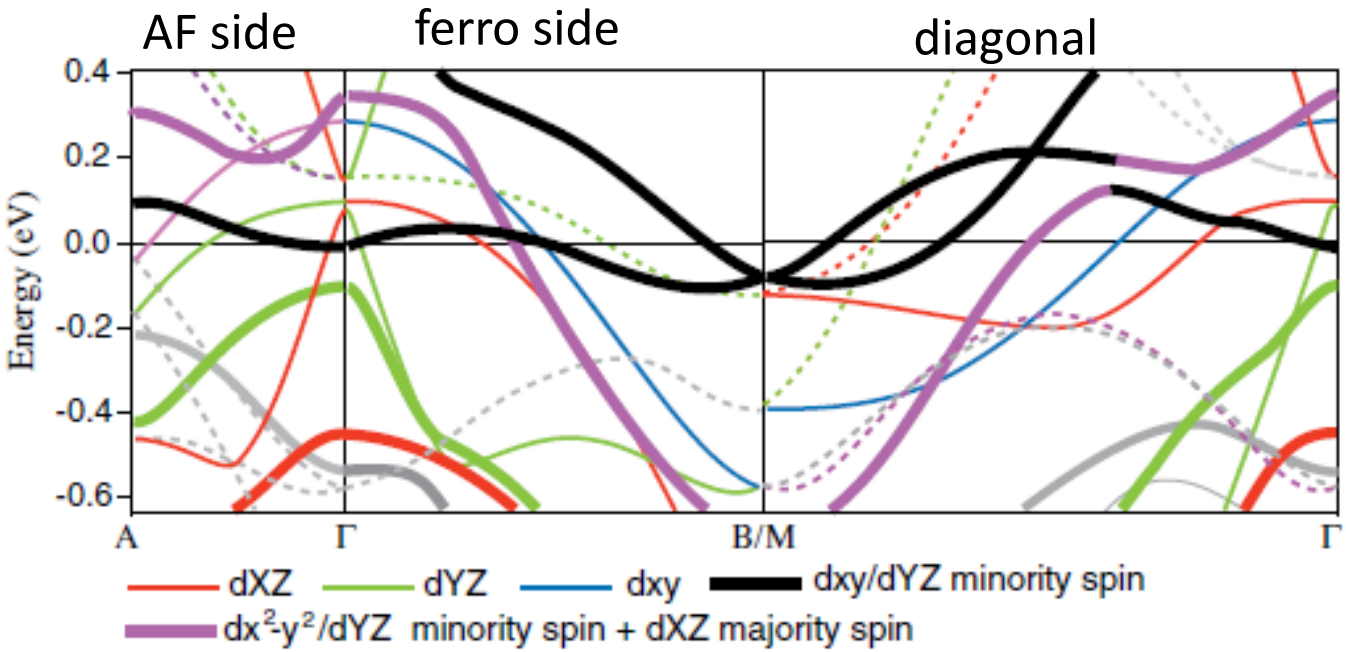
Evolution of the electronic structure in the magnetic state





Q_{AF} does not correspond to FS nesting

Calculation done using Wien2K package, converging to a moment $M=2.2\mu_B$.

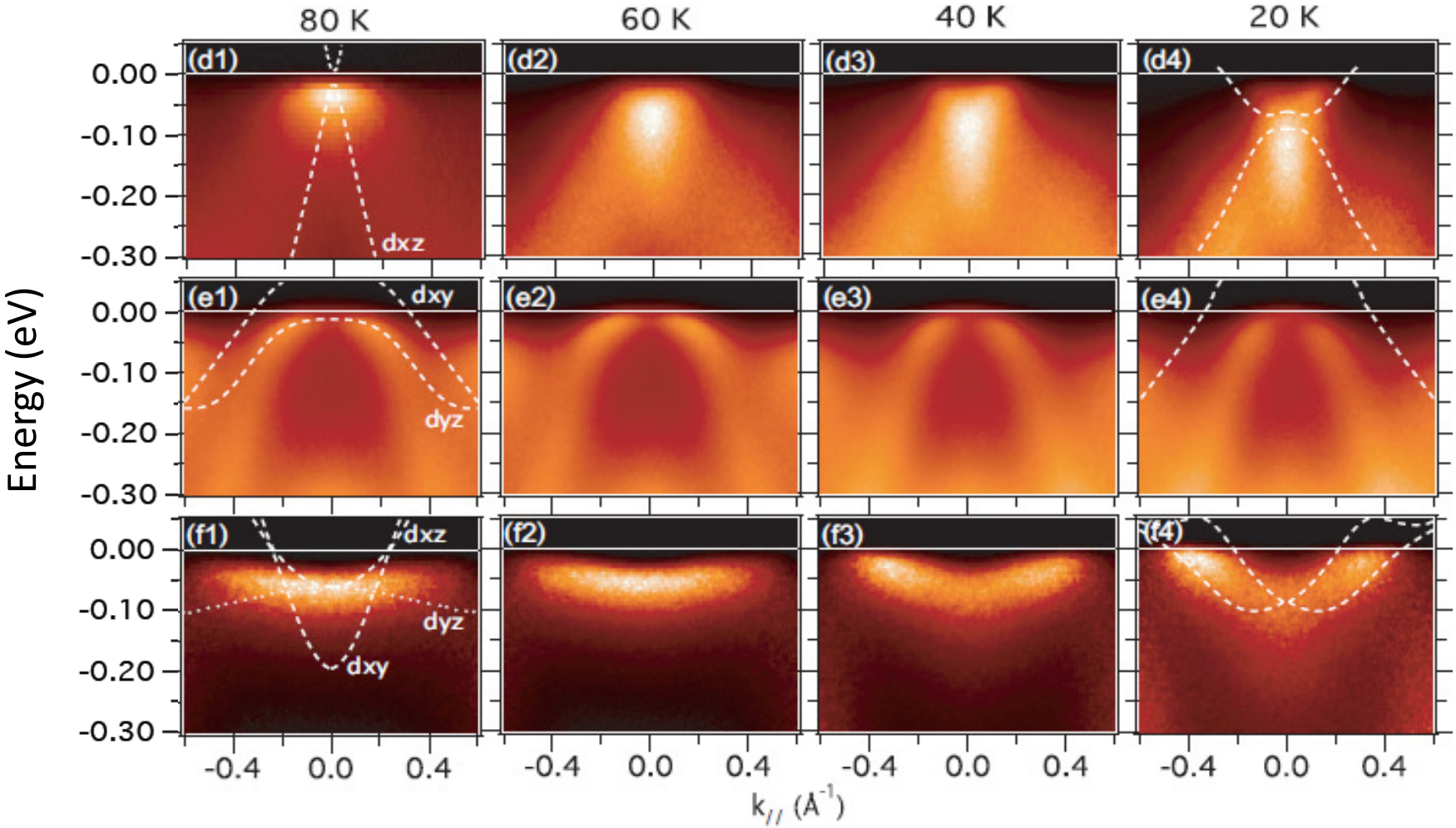


⇒ No gap opening (no FS nesting)

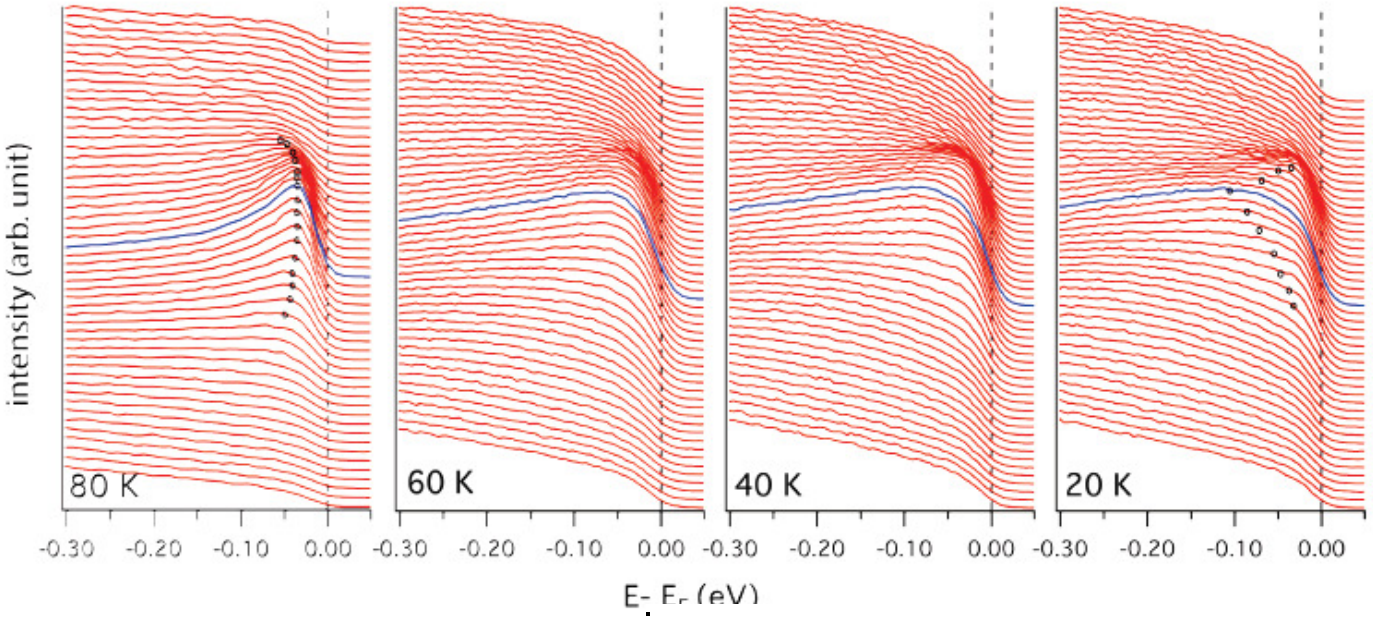
⇒ Large shifts of the bands

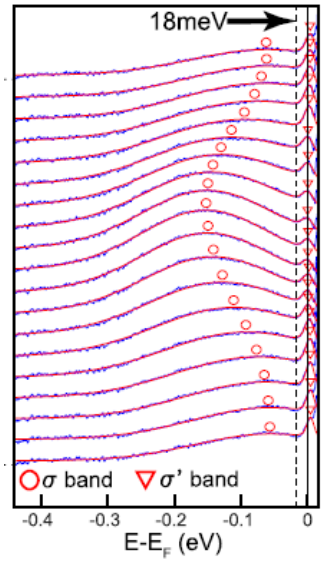
⇒ Rehybridizations into new conduction channels.

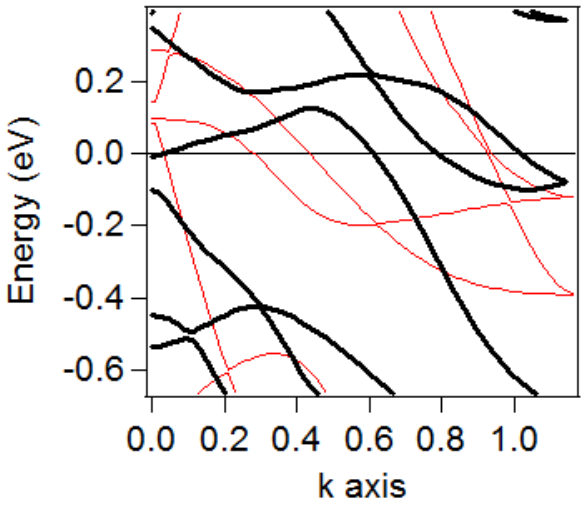
FeTe : evolution of the bands with temperature

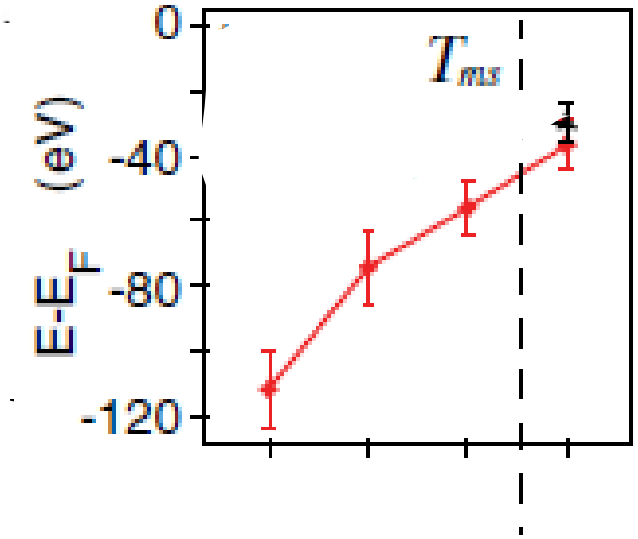


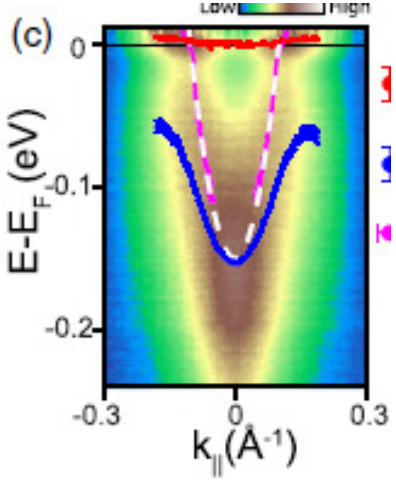
Hole/electron pocket near Gamma





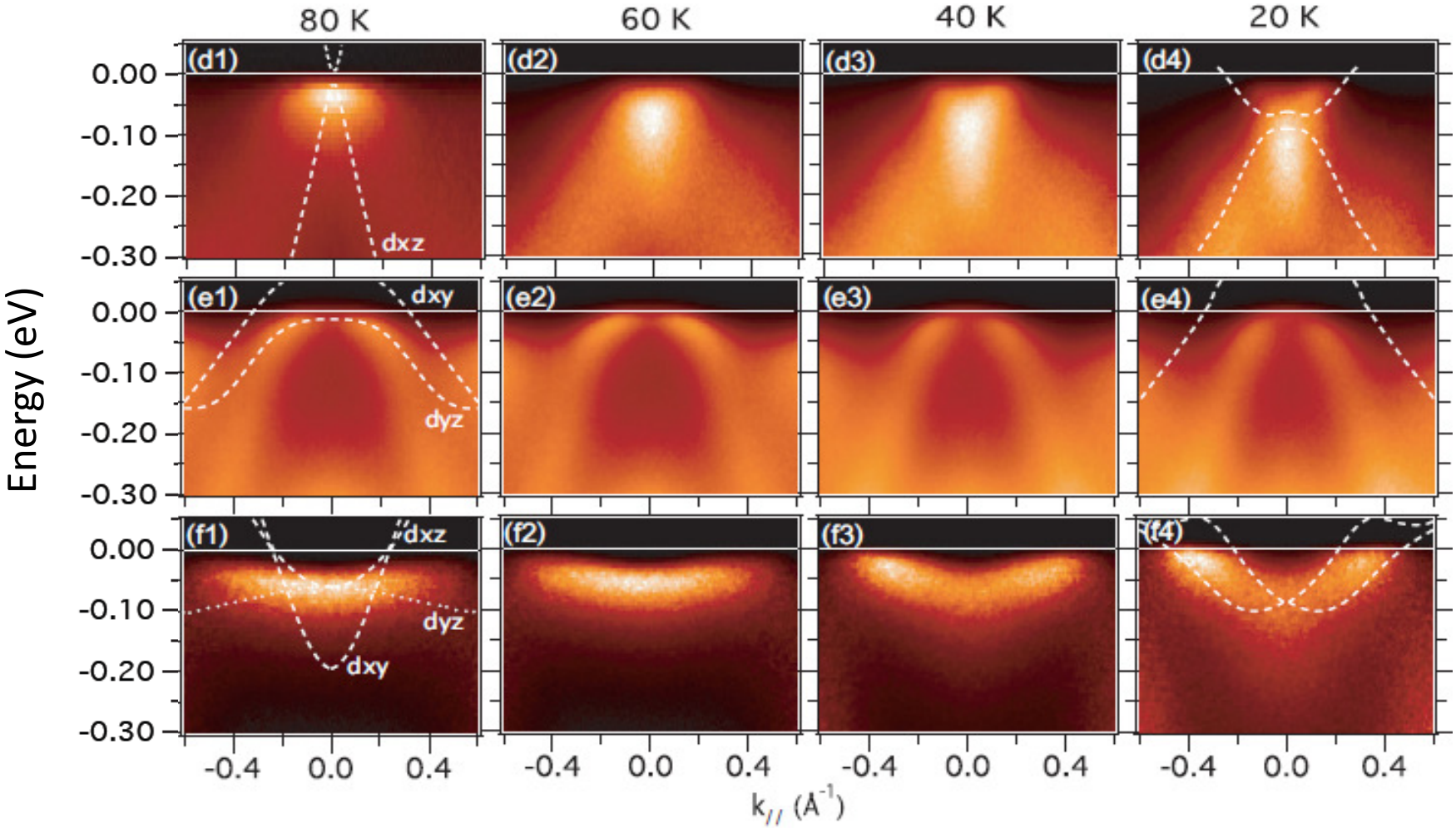




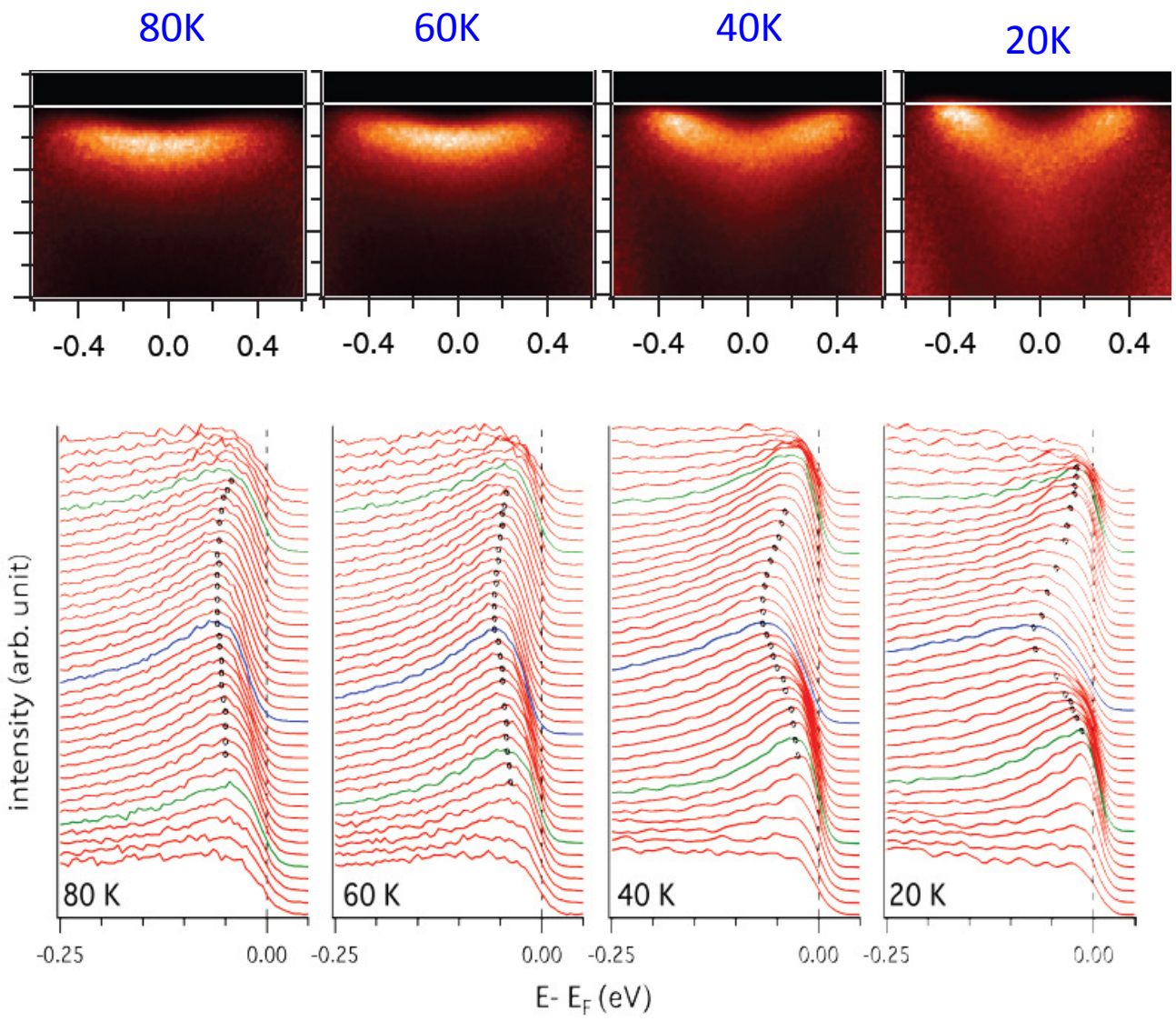


Liu et al PRL 2013

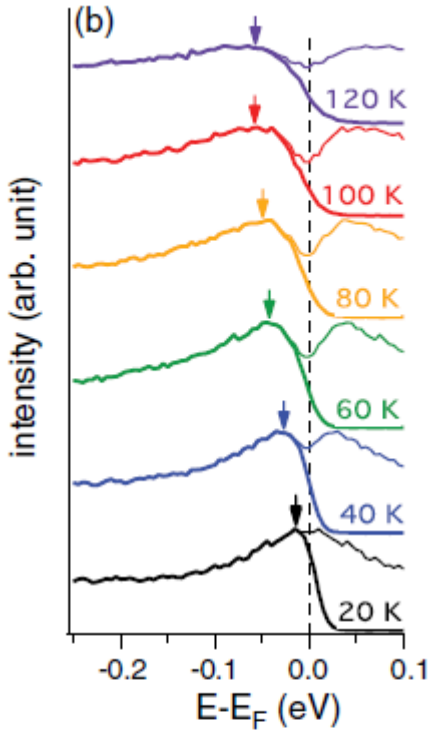
FeTe : evolution of the bands with temperature

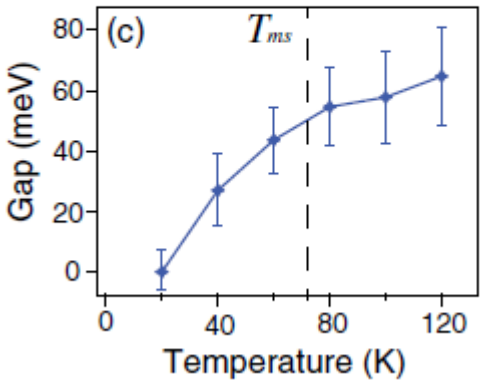


« Pseudogap » on the electron pocket



Spectra at k_F

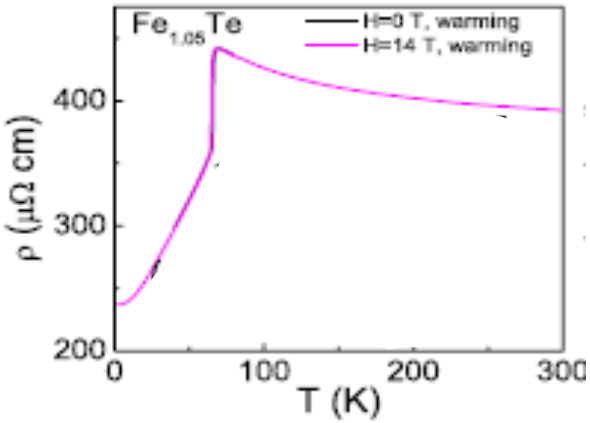




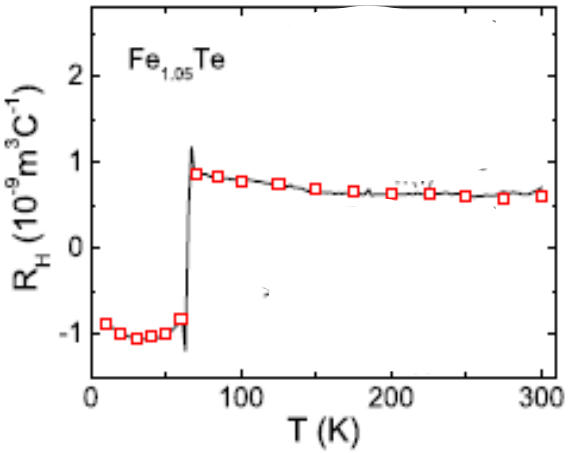
Good agreement with transport

⇒ Good metallic features in the magnetic state contrary to PM state

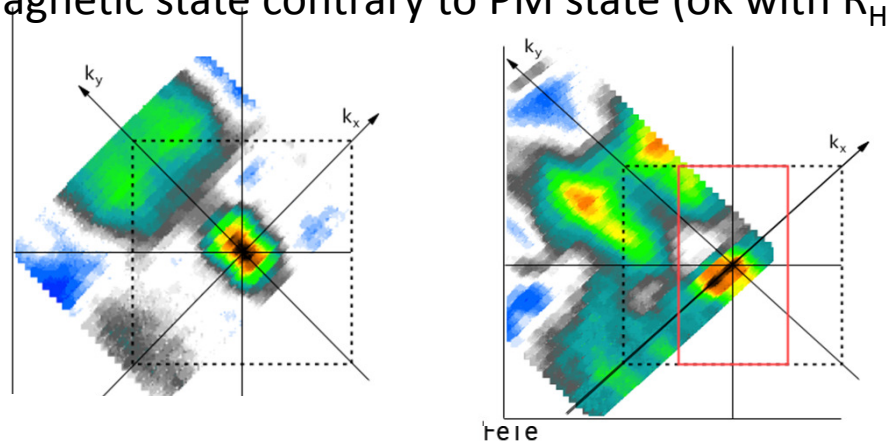
⇒ Dominated by electrons in the magnetic state contrary to PM state (ok with R_H).

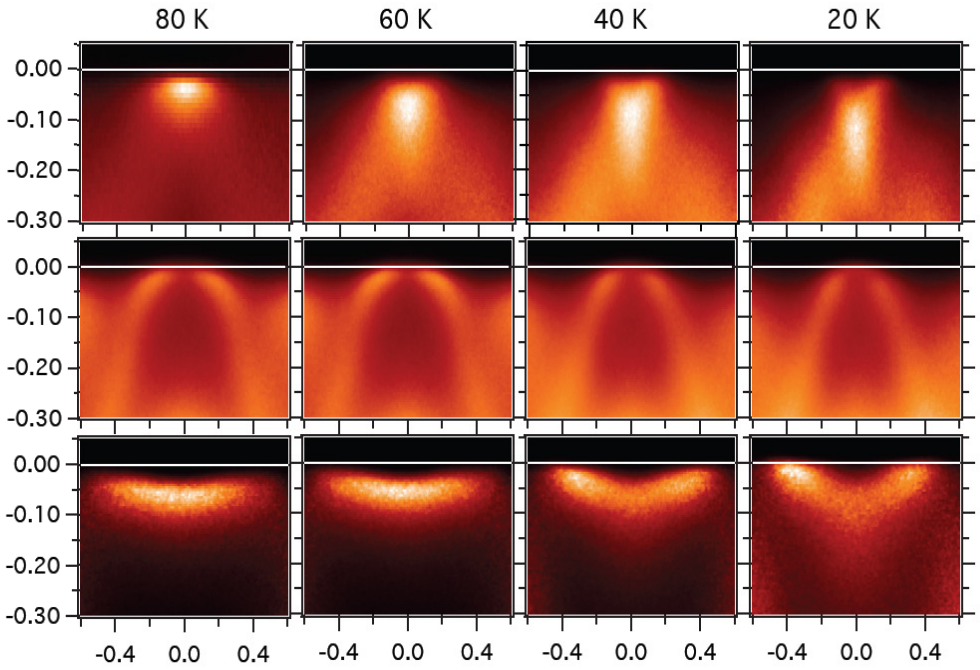


Change of the sign of R_H



Chen et al., PRB 2009





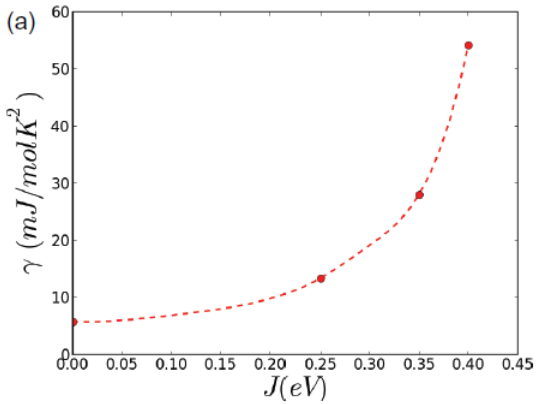
Can it be understood theoretically ?

« Hund's metals »

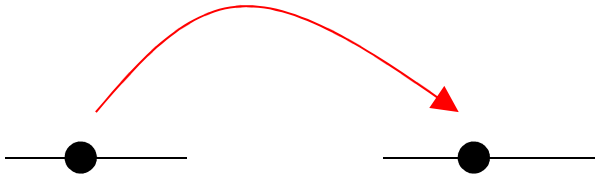
J – not U – is responsible for the mass enhancement

Haule and Kotliar,
New J. Of physics 2009

Specific heat coefficient γ vs J

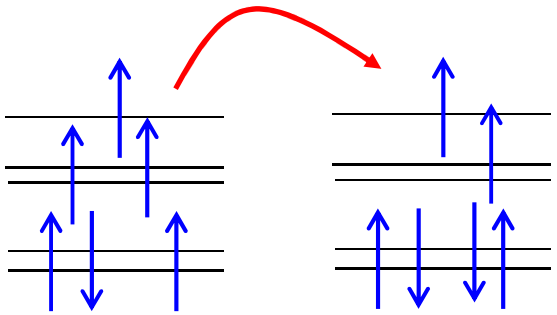


Electronic correlations are usually governed by Coulomb repulsion U



controlled by U

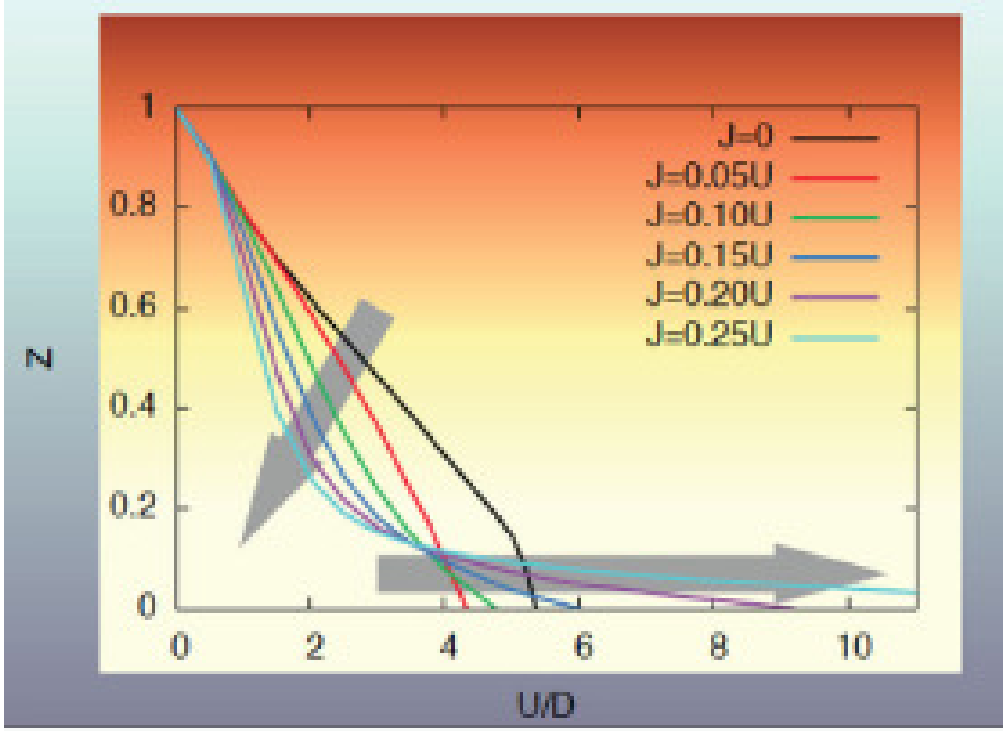
In iron-based superconductors Hund's couplings play a major role.



New type of correlated state ?

Hund's couplings enlarge regions of « bad metallic » behaviors

Quasiparticle weight as a function of U and J



L. deMedici, J. Mravlje, A. Georges, PRL 2011

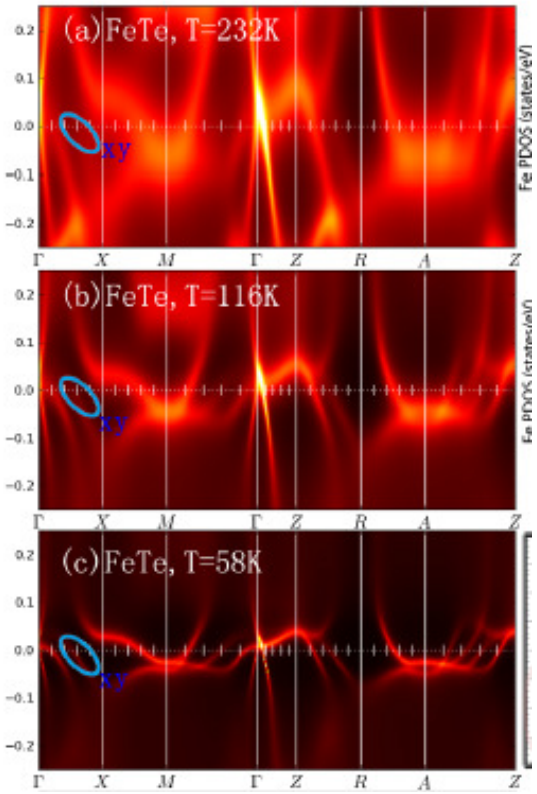
$\Rightarrow$ J decreases the quasiparticle weight but destabilizes the Mott transition.

$\Rightarrow$ *Non Fermi liquid behaviors, Spin freezing regime Werner et al., PRL 2008*

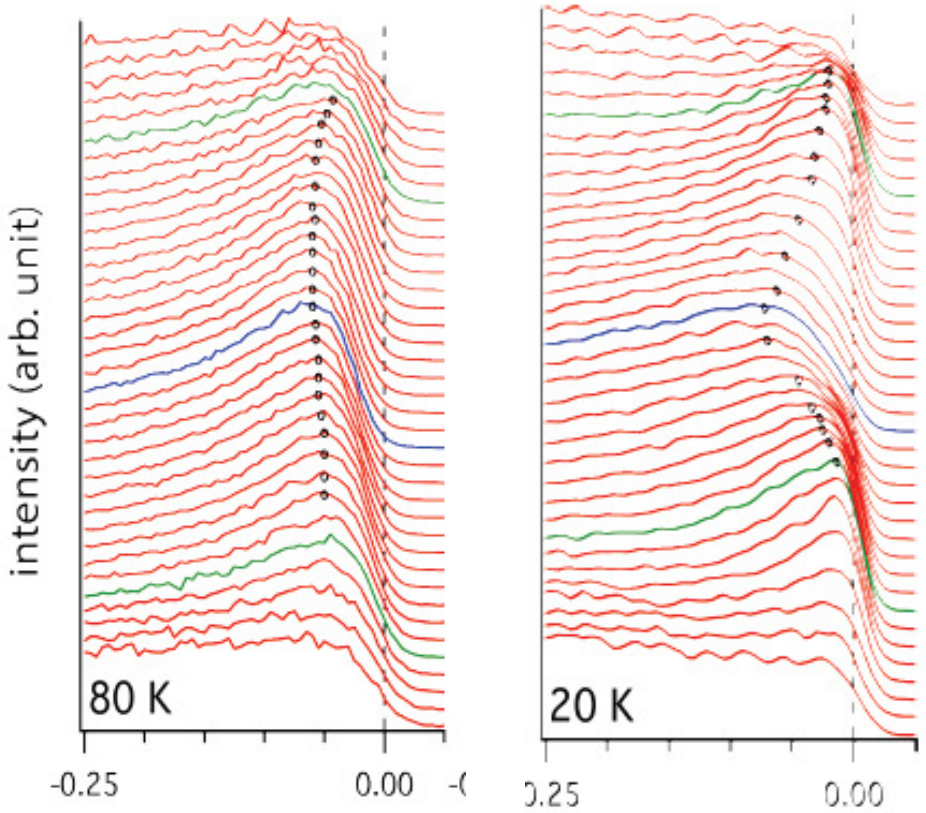
Is a pseudogap expected in the « spin freezing » regime ?

FeTe is expected to be a metals with low coherence temperature.
Fractional power laws for the self-energy.

DMFT simulations for FeTe
at various temperatures



Yin, Haule, Kotliar, PRB 2012



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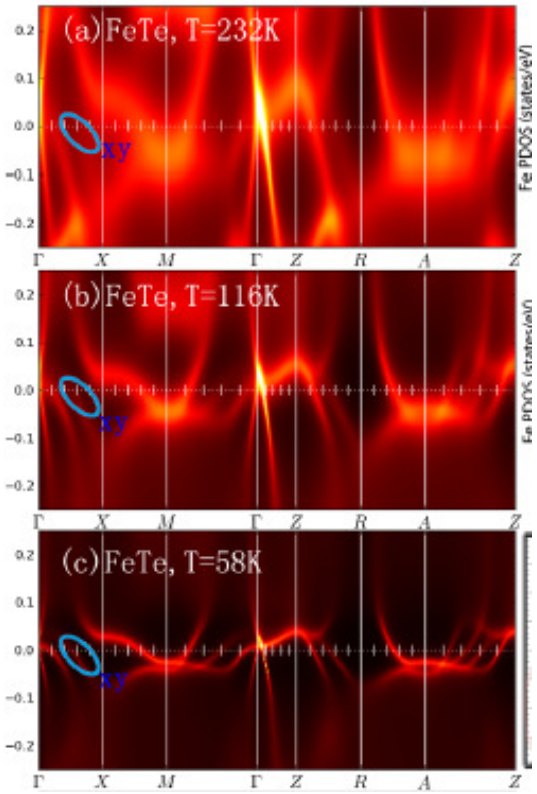
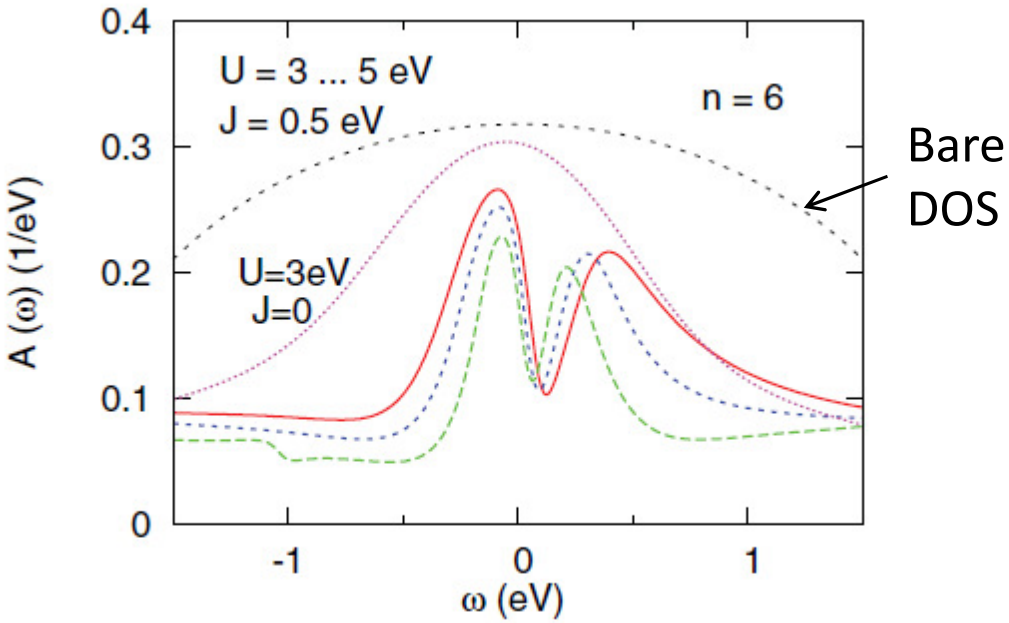


Yin, Haule, Kotliar, PRB 2012

For Liebsch, J opens a pseudogap associated to a collective mode in the self-energy due to spin-fluctuations.

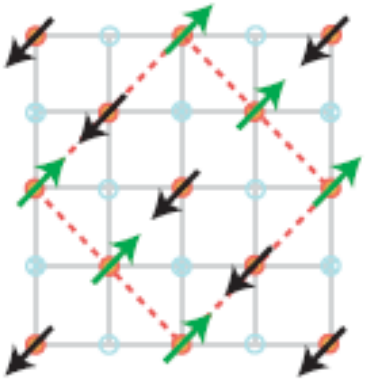


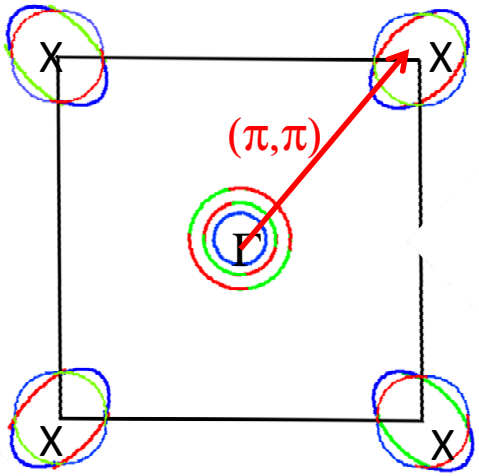
Liebsch, PRB 2011

(π, π) and (π, 0) fluctuations

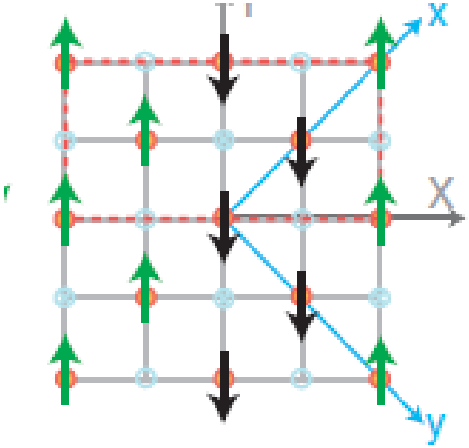
One characteristic of the FeTe pseudogap is that it only develops on the electron pocket.

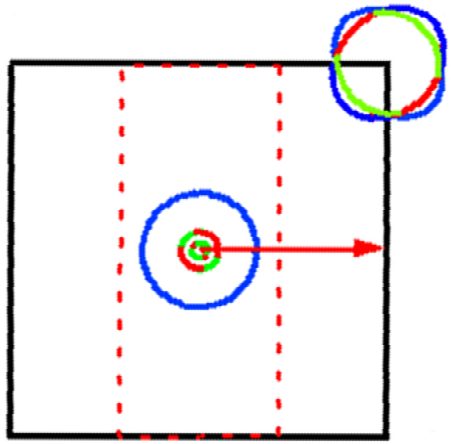
(π, π) fluctuations (FePn)

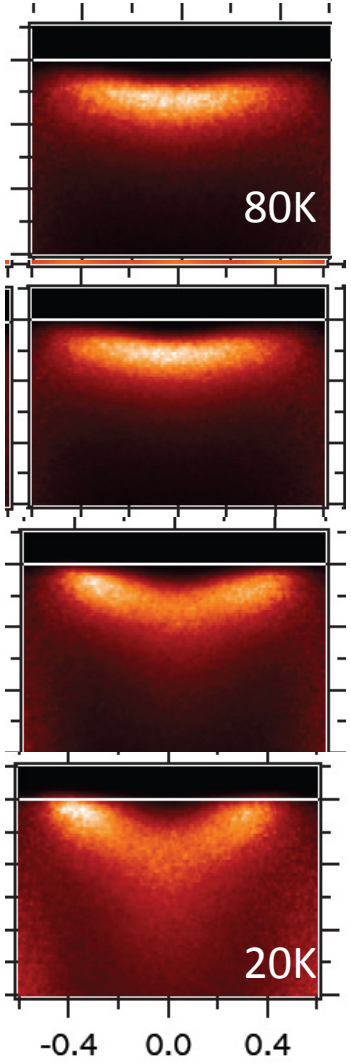




(π, 0) fluctuations (FeTe)

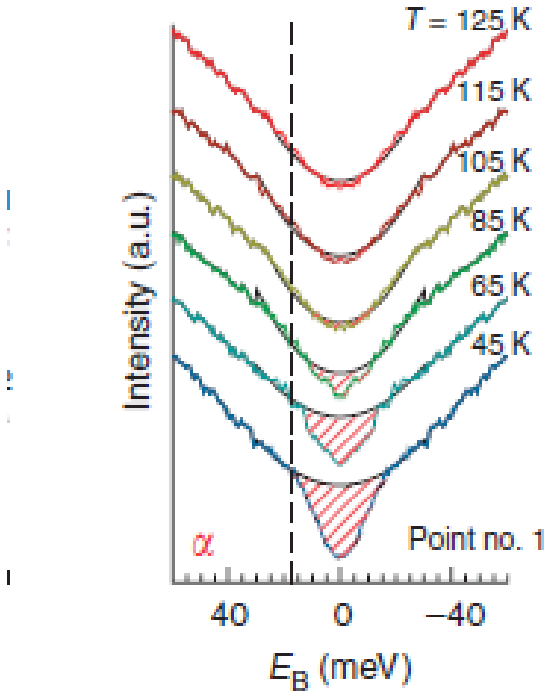






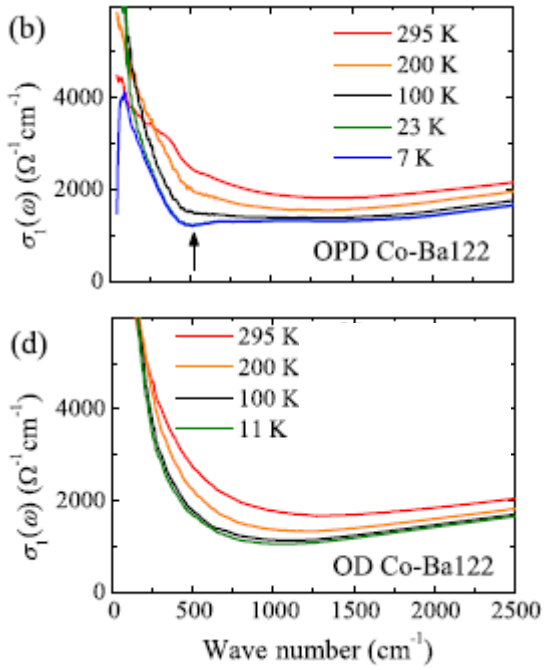
Are « pseudogaps » a general feature of iron-based superconductors ?

For Xu et al. (ARPES study), there is a 18meV PG in $Ba_{0.75}K_{0.25}Fe_2As_2$ related to (π, π) fluctuations.



Xu et al. Nat Com 2011

For Moon et al. (infrared study), there is a PG in underdoped $Ba(Fe,Co)_2As_2$, also connected to (π, π) fluctuations.



Moon et al. PRL 2012

Conclusions

- Correlations develop preferrentially in dxy, which is more renormalized in LiFeAs than dxz/dyz and not detected in FeTe

- A large pseudogap of 60meV on the dxz/dyz elctron pocket characterizes the « bad metallic » phase of FeTe

- It disappears in the magnetically ordered phase.

  $\Rightarrow$ It may be related to (π,π) fluctuations and already present in other iron pnictides

  $\Rightarrow$ It may be emphasized in FeTe due to the larger frozen magnetic moments and the incoherence of dxy.

Thanks to : L. de Medici, S. Bierman, M. Casula, A. Georges and M. Grioni