Iron pnictides as a new playground for ARPES investigations

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SOLEIL synchrotron, CASSIOPEE beamline

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Sample synthesis

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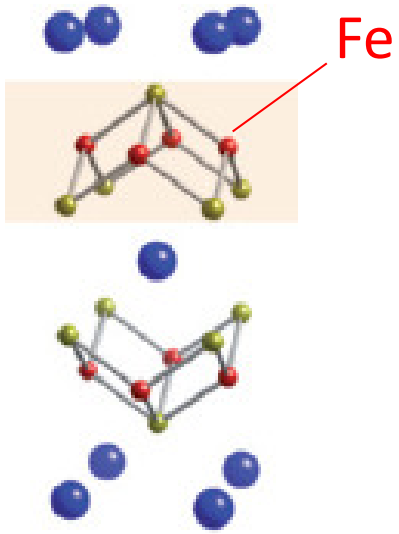
SPEC, CEA-Saclay, France

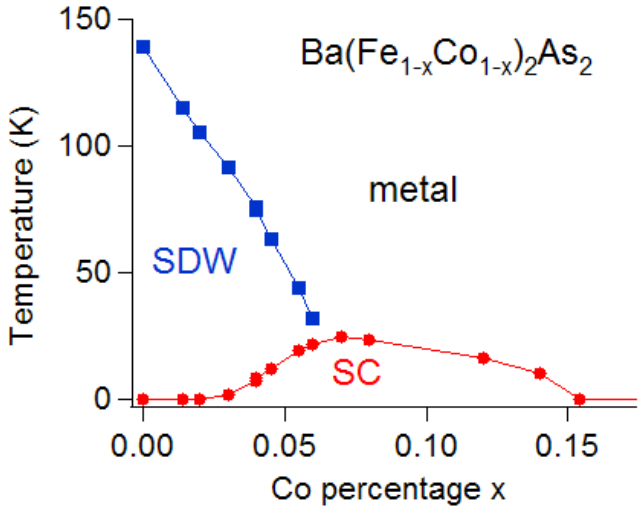
FeTe : Enrico Giannini, *University of Geneva, Switzerland*

New iron based superconductors

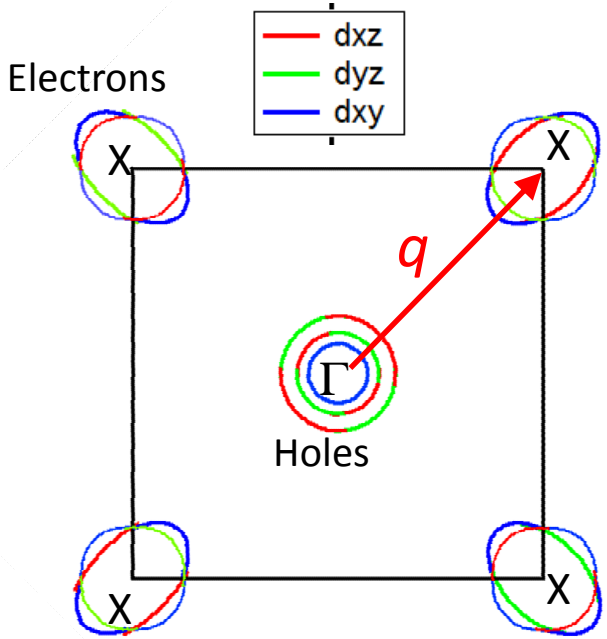
$BaFe_2As_2$



Superconductivity and magnetism



Fermi Surface



Fe^{2+} : 6 electrons for 5 orbitals

=> Are they correlated metals ?

=> What are the roles of the different orbitals ?

Outline

How to resolve the different orbitals ?

Specifities about ARPES in the 2 Fe unit cell

Intraband interactions : do dxy and dxz/dyz bands have similar properties ?

- Orbital dependent renormalization in $Ba(Fe,Co)_2As_2$ and LiFeAs
- Orbital dependent lifetimes ?

Interband interactions : “Shrinking” of the Fermi Surface

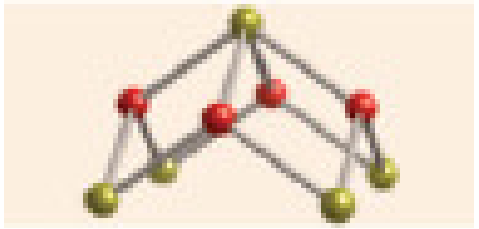
- May change the number of carriers by a factor 2

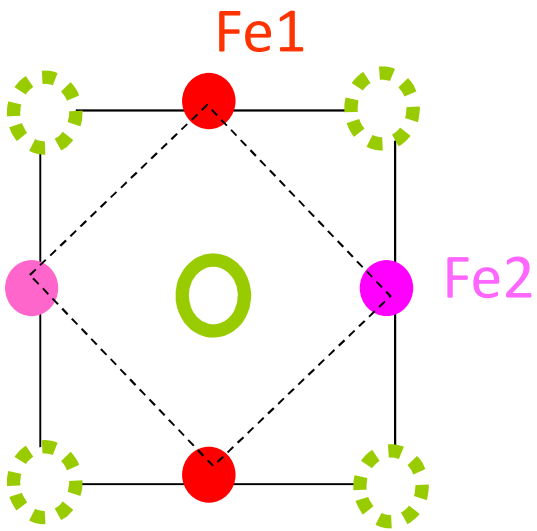
Strongly correlated case : bad metallic behavior in FeTe

- Large (60meV) “pseudogap” on the electron pocket in paramagnetic phase
- Relation to pseudogap observed above superconducting state ?

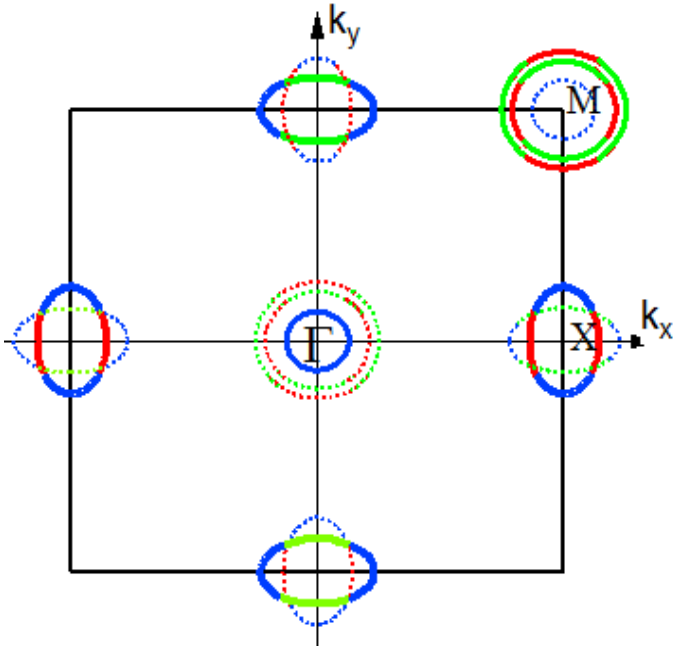
Specifities about ARPES in the 2 Fe unit cell

2 Fe unit cell





FS in 1 Fe BZ
with folded bands

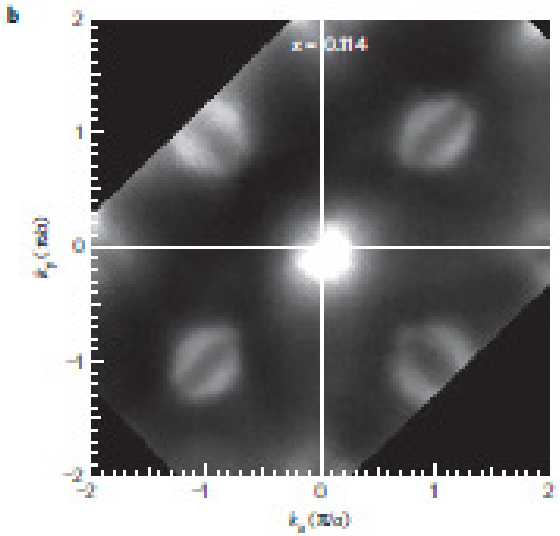


Should ARPES see 1 or 2 electron pockets ?

1 or 2 electron pockets ?

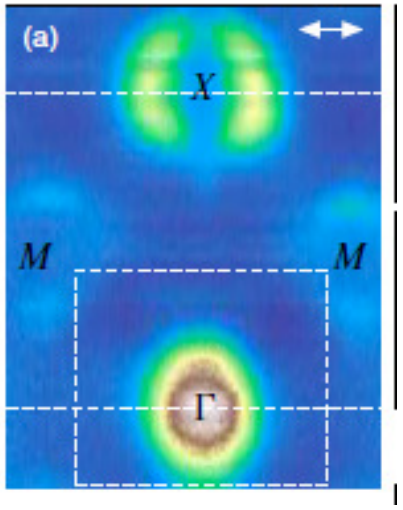
$Ba(Fe_{0,9}Co_{0,1})_2As_2$

Liu, Kaminski et al.,
Nature Physics 2010



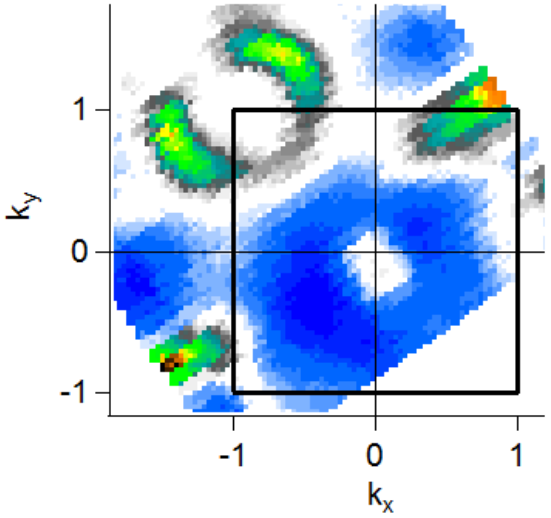
$EuFe_2As_{1,56}P_{0,44}$

Thirupathaiah, Fink et al.,
PRB 2009



$Ba(Fe_{0,9}Co_{0,3})_2As_2$

Brouet et al.,
PRB 2009

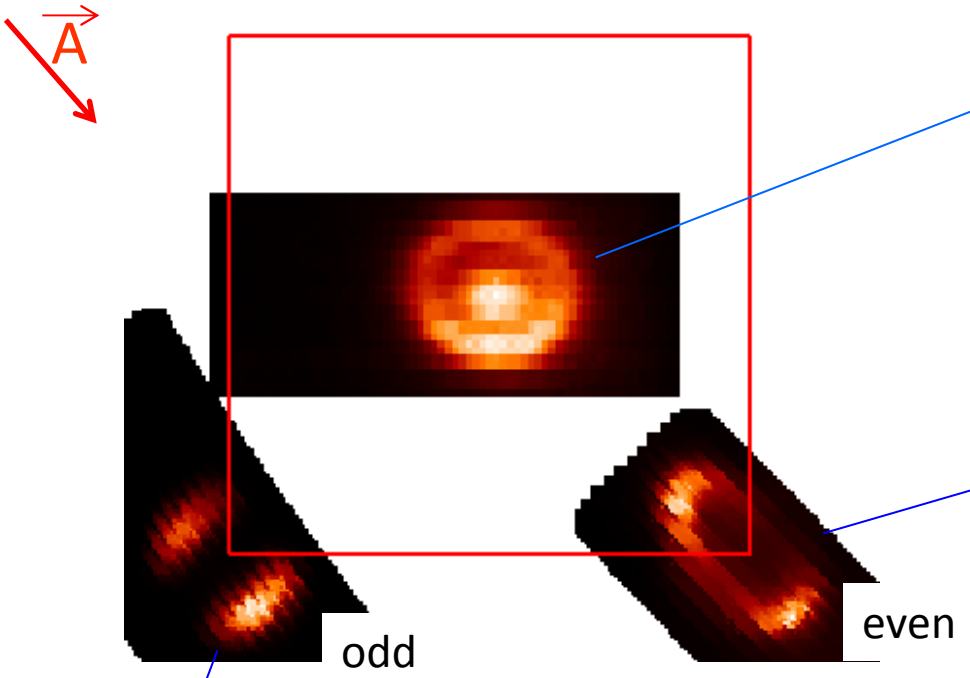


And many others…

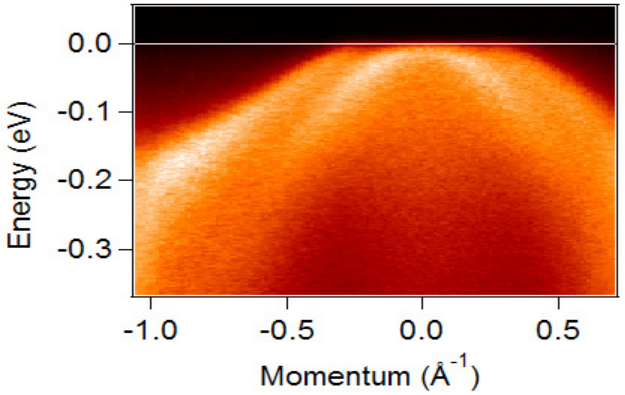
….. half a pocket !

ARPES in Co-doped $BaFe_2As_2$

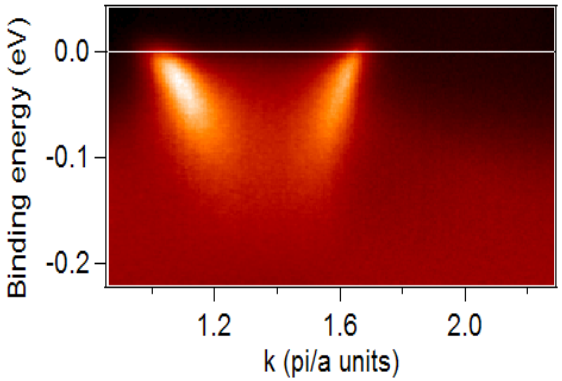
Fermi Surface (34eV, k_z=1)



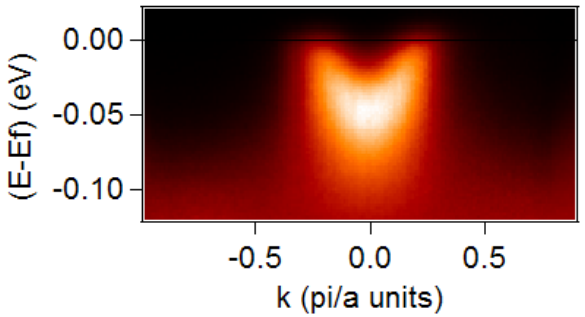
Hole pockets

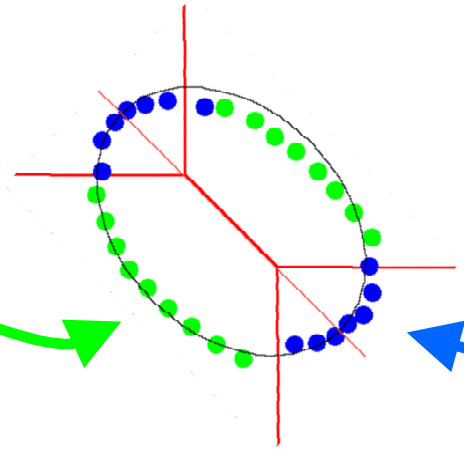


Even electron pocket (dxy)



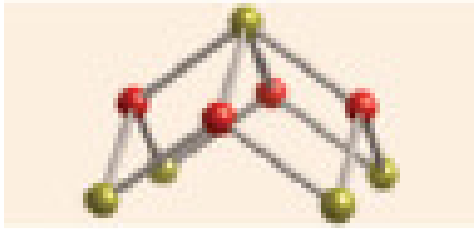
Odd electron pocket (dxz/dyz)



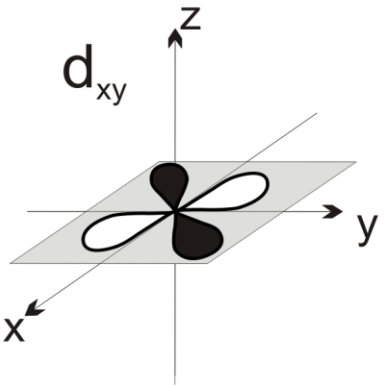


Folding in the 2Fe BZ

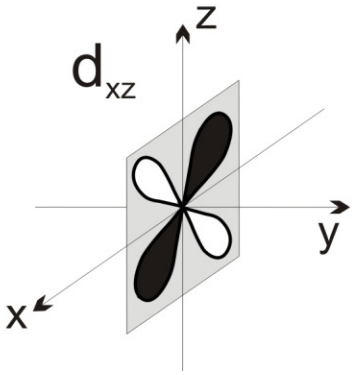
The ARPES intensity of folded bands is proportional to the symmetry breaking potential



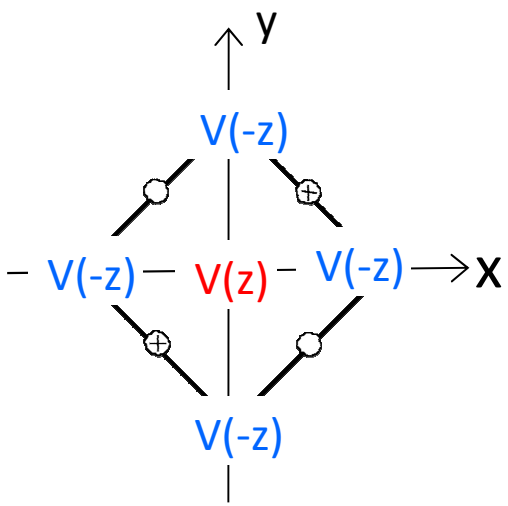
Here, As potential is strong !



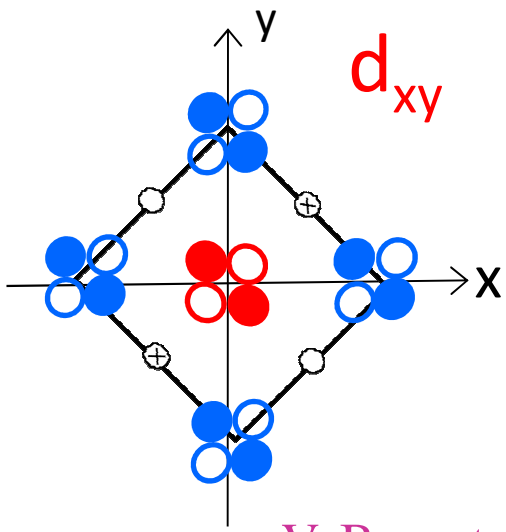
=> All Fe sites look equivalent

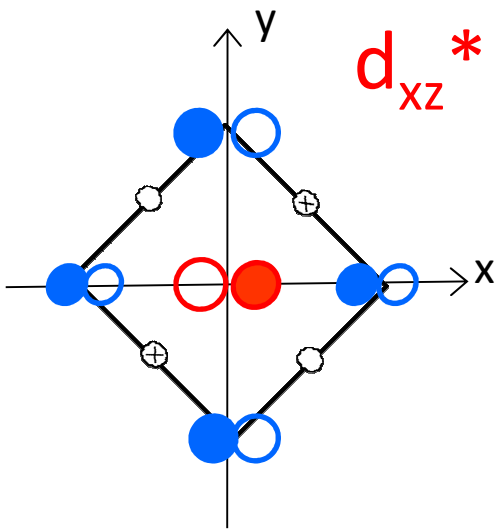


$\Rightarrow$ All Fe sites equivalent if A and B are dephased by π



But only the sign with respect to z change between the 2 sites



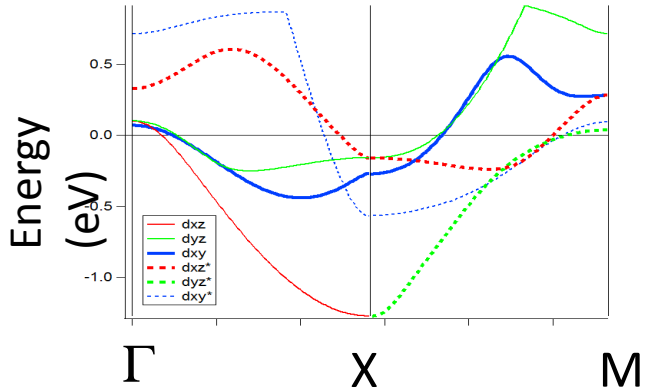


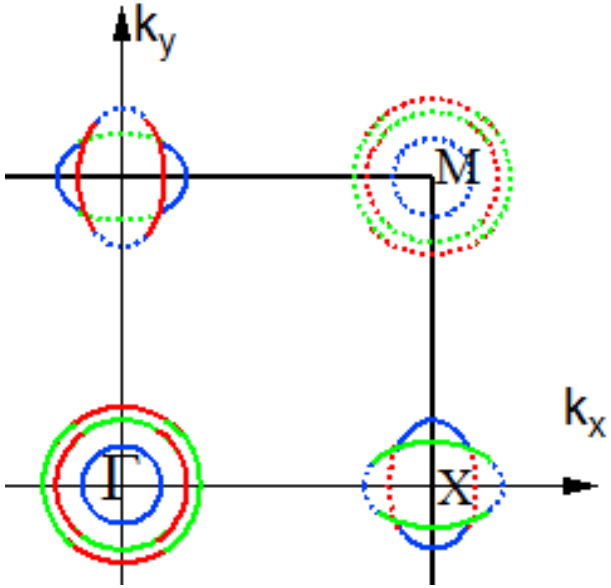
V. Brouet et al., PRB 2012

ARPES weights

Electronic structure with in-phase and out-of phase bands

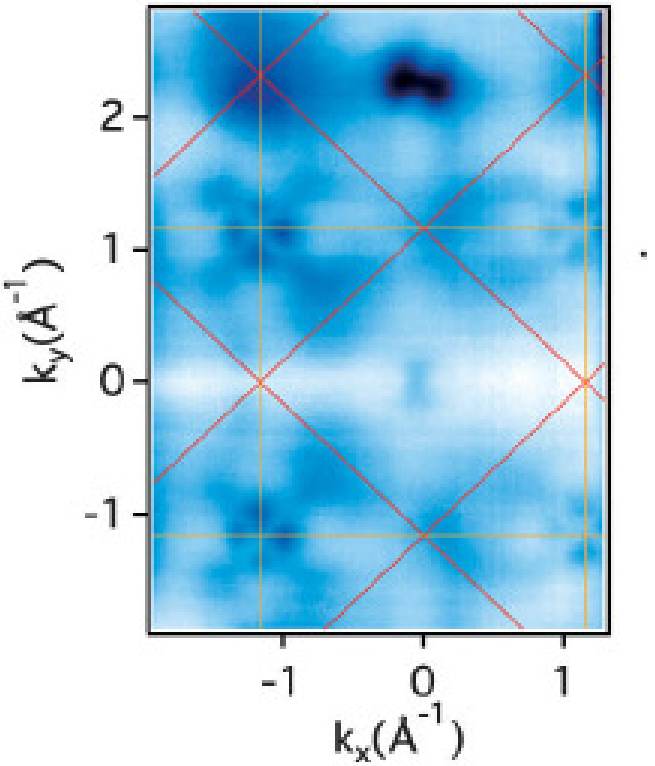
Andersen and Boeri, cond-mat/1011.1658





Inequivalent « Γ » points in adjacent BZ

$FeTe_{0,4}Se_{0,6}$ Fermi Surface



L. Moreschini et al. PRL 14

Direct « unfolding » calculations (Wei Ku's group) predict very well the ARPES weight.

Weight of shadow bands

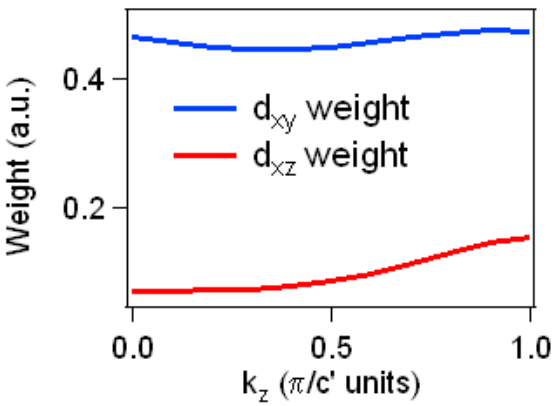
It is proportional to the hybridzation with orbitals of opposite z symmetry

C.H. Lin, PRL 2011

in-phase bands => 1

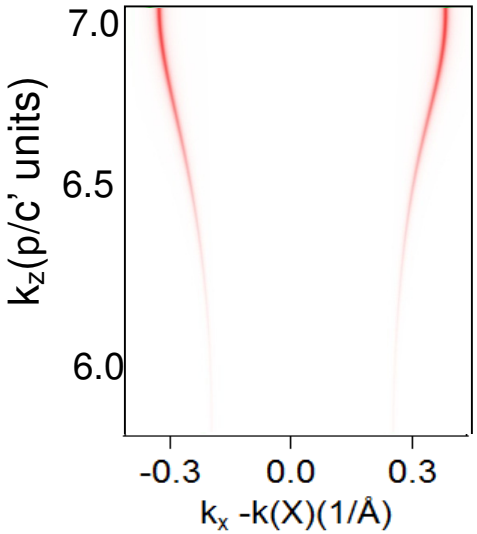
out-of-phase bands => 0, *except if they are hybridized with opposite z symmetry*

Orbital character for dxy* electron band

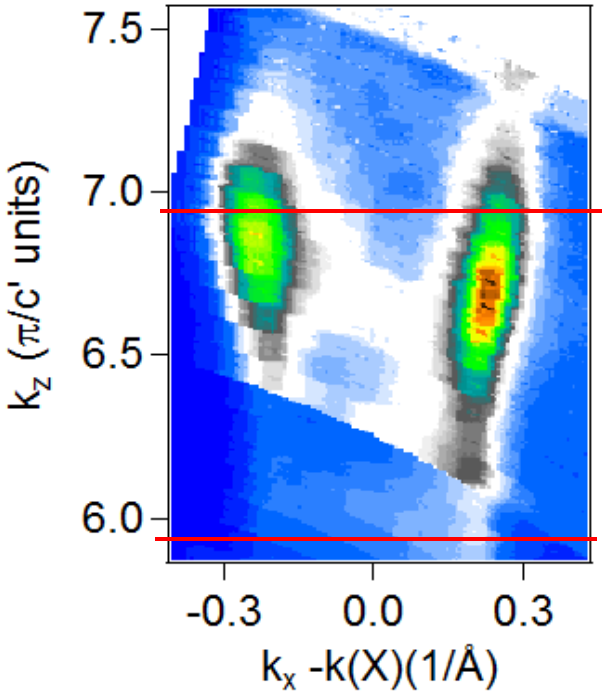


Simulated spectral weight

C.H. Lin, W. Ku



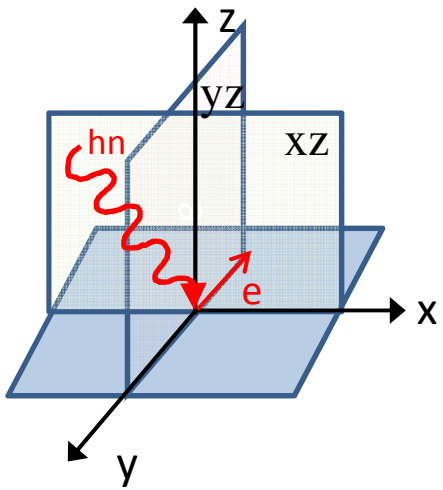
ARPES spectral weight measured at E_F vs k_z

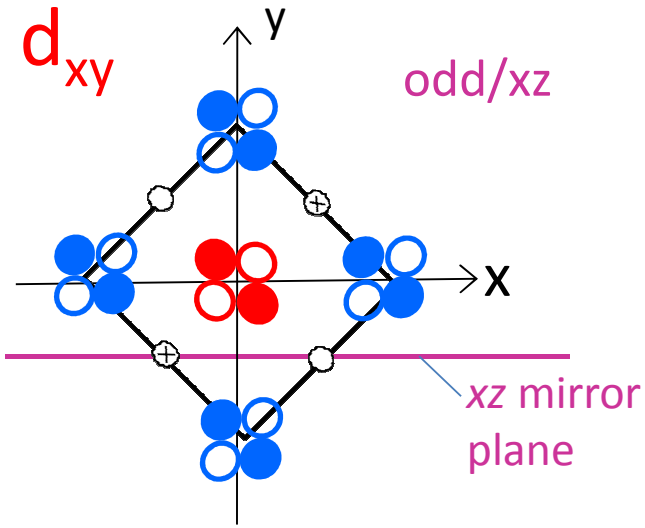


V. Brouet et al., PRB 2012

Band parity

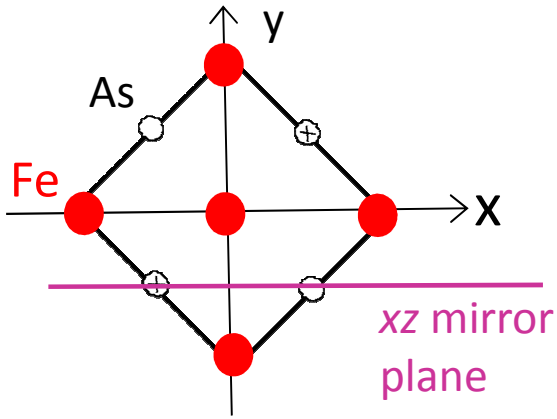
Polarization selection rules

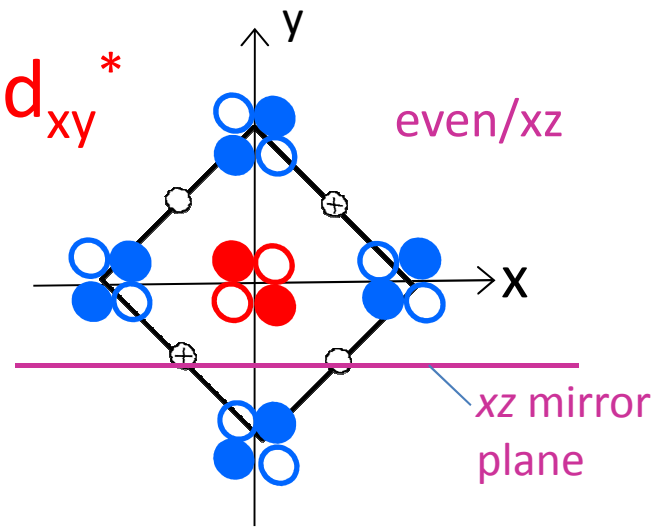




With respect to xz : odd bands

With respect to yz : even bands



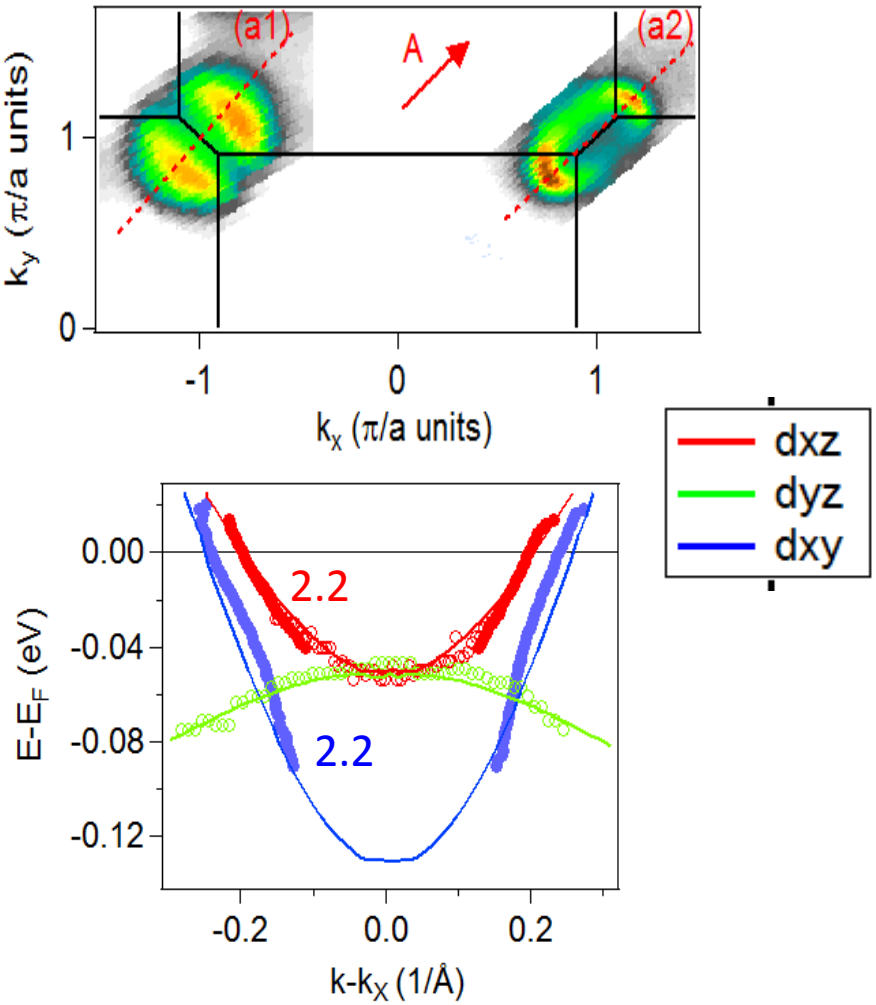


Be careful when applying selection rules in a 2 atom unit cell !!

Intraband interactions :
Do dxy and dxz/dyz bands have similar properties ?

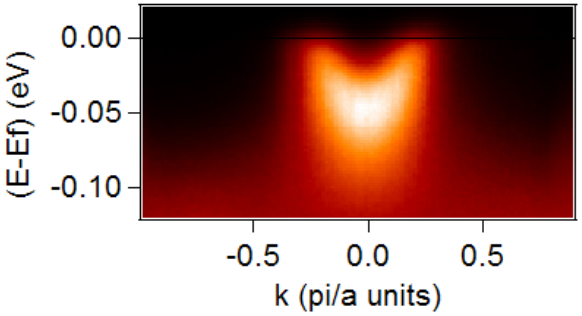
Renormalizations

8% Co doped $BaFe_2As_2$

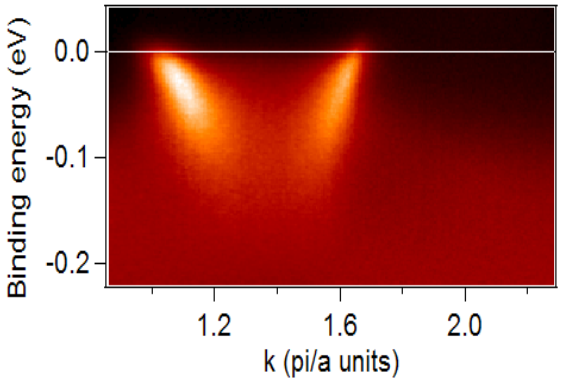


V. Brouet et al., PRL 2013

Odd electron pocket (dxz/dyz)



Even electron pocket (dxy)



Renormalizations

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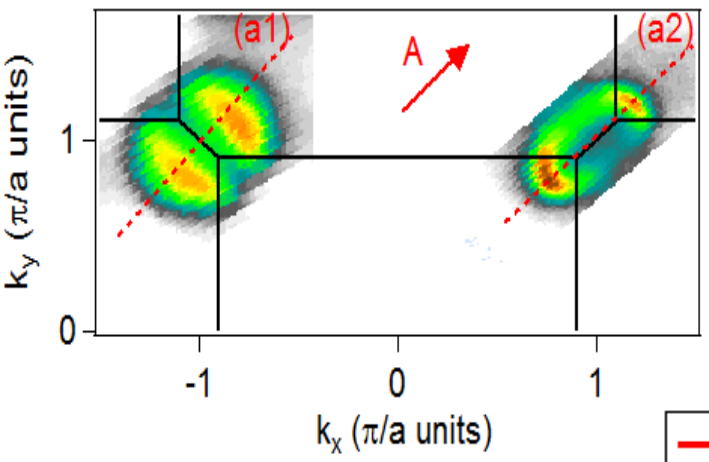
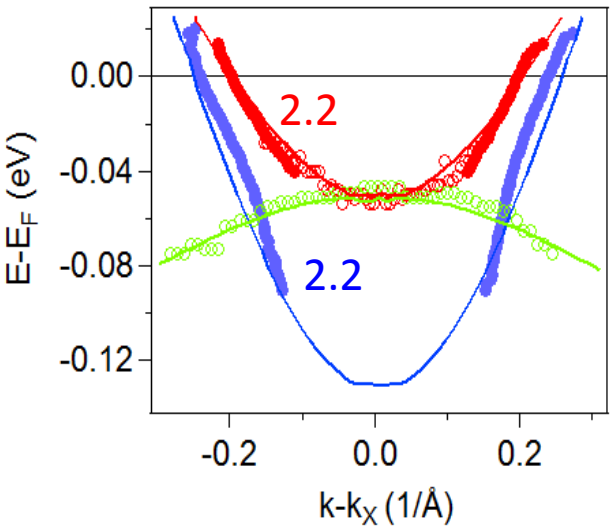
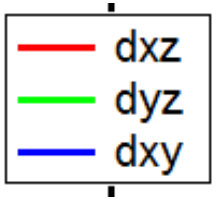
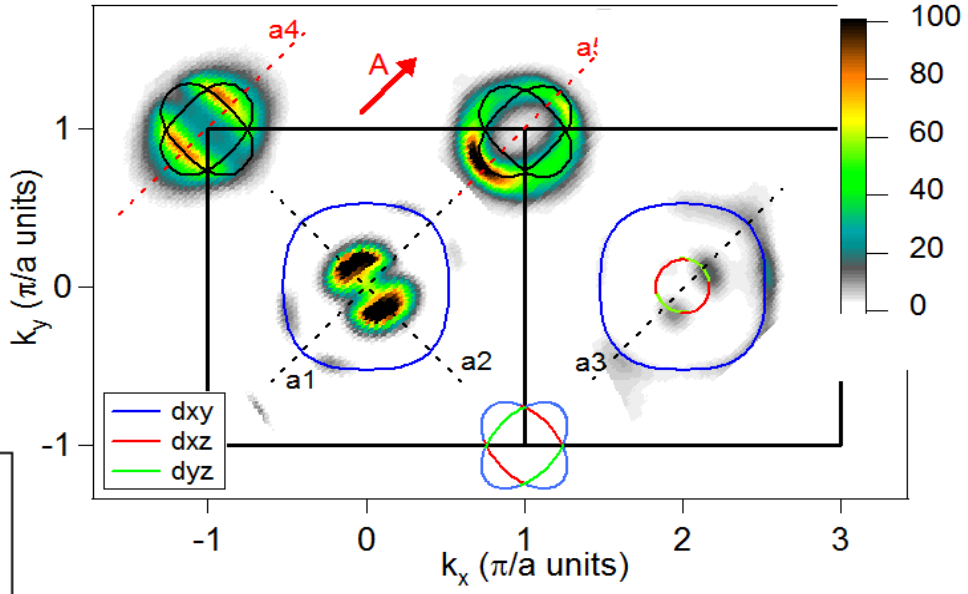
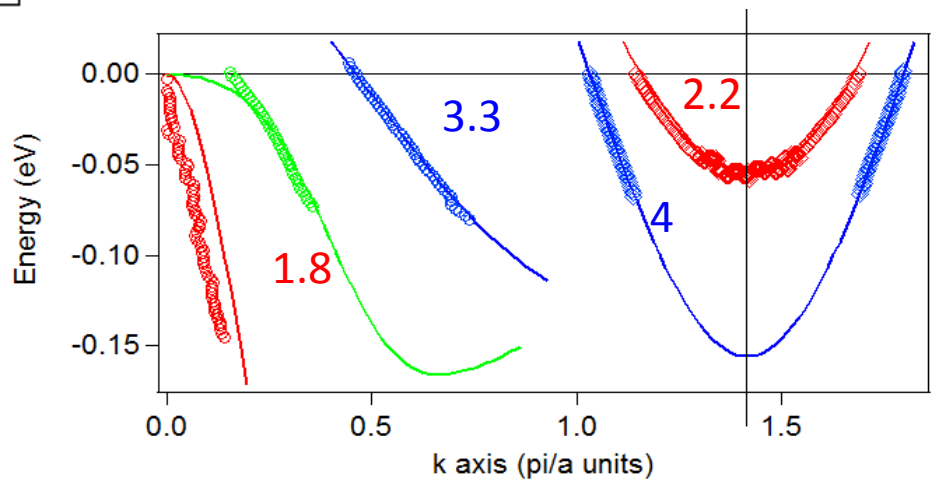






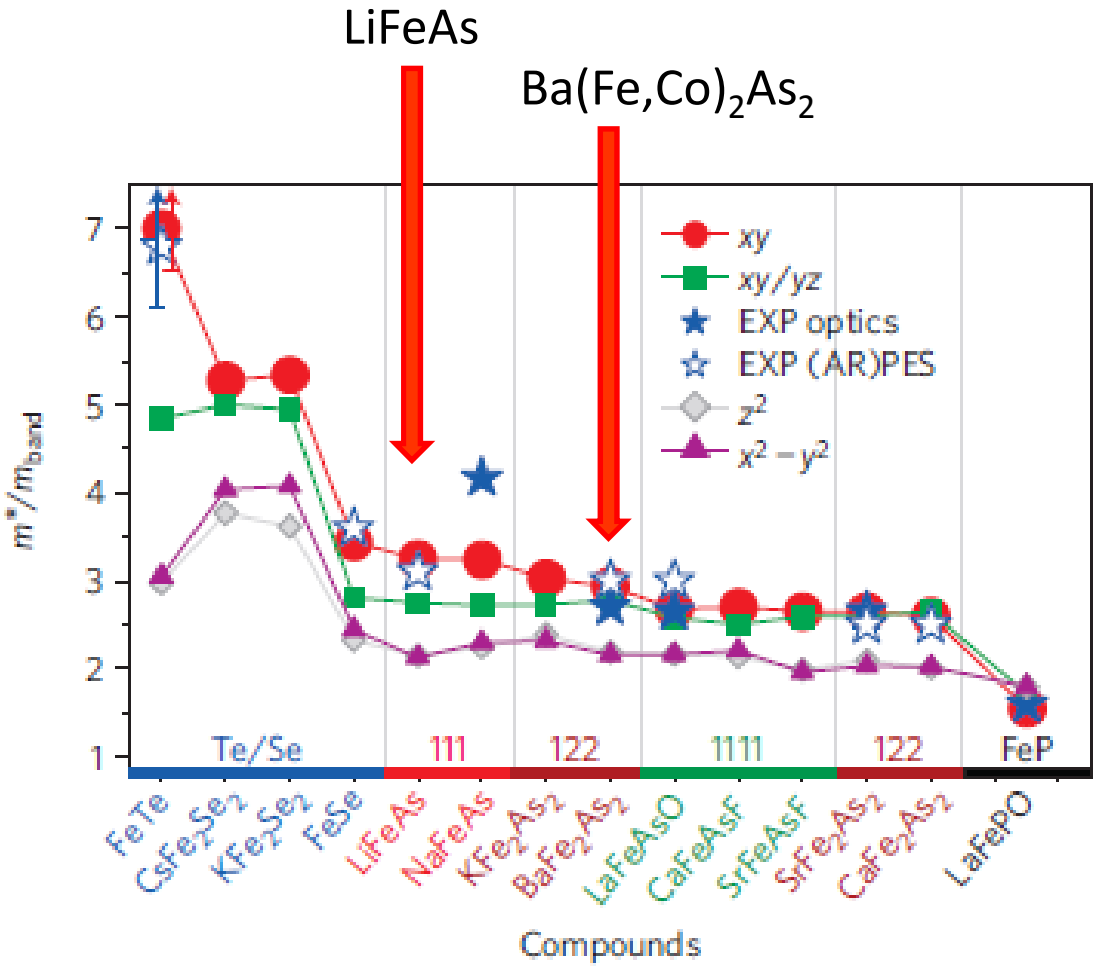
LiFeAs





V. Brouet et al., PRL 2013

Orbital dependent renormalizations predicted by DMFT



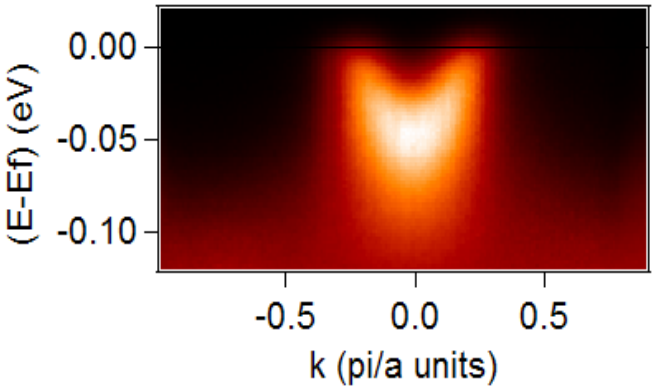
Yin, Haule, Kotliar, Nature Materials 2011

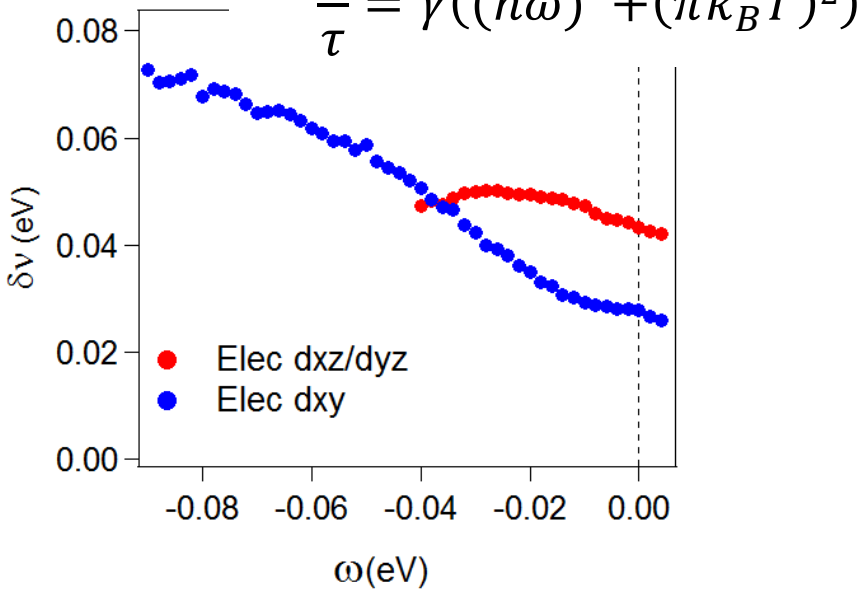
Orbital dependent lifetimes ?

8% Co doped $BaFe_2As_2$

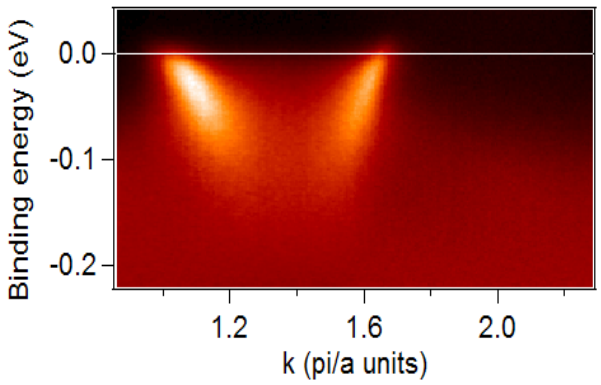
$$\frac{\hbar}{\tau} = \gamma((\hbar\omega)^2 + (\pi k_B T)^2)$$

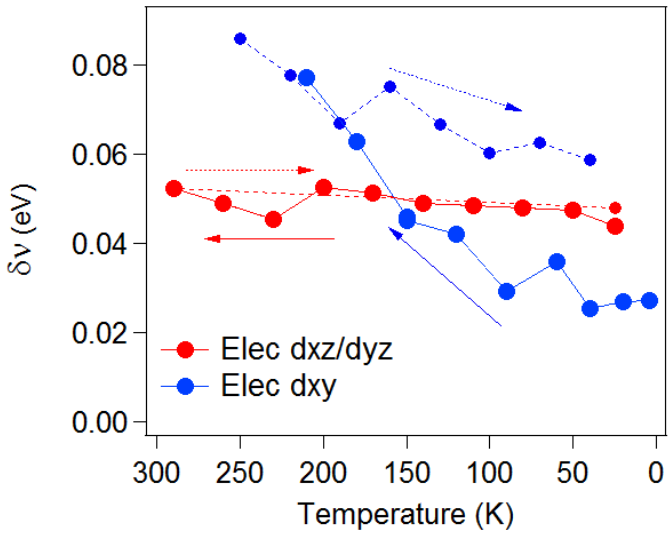
dxz band





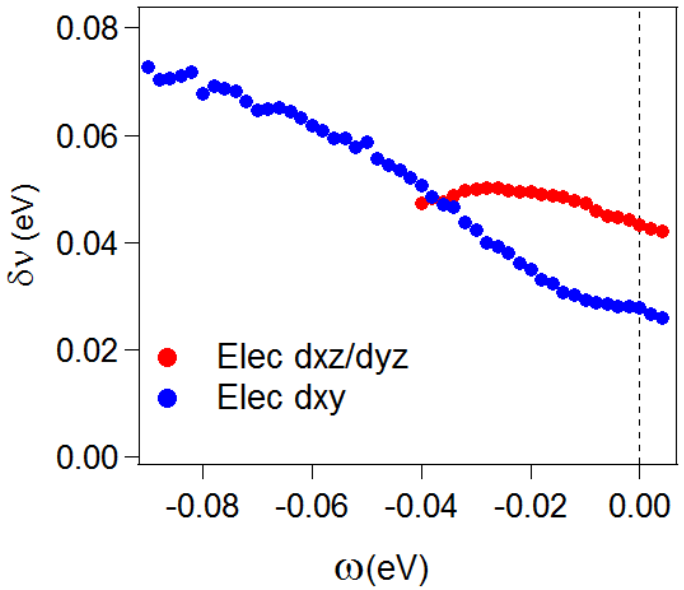
dxy band



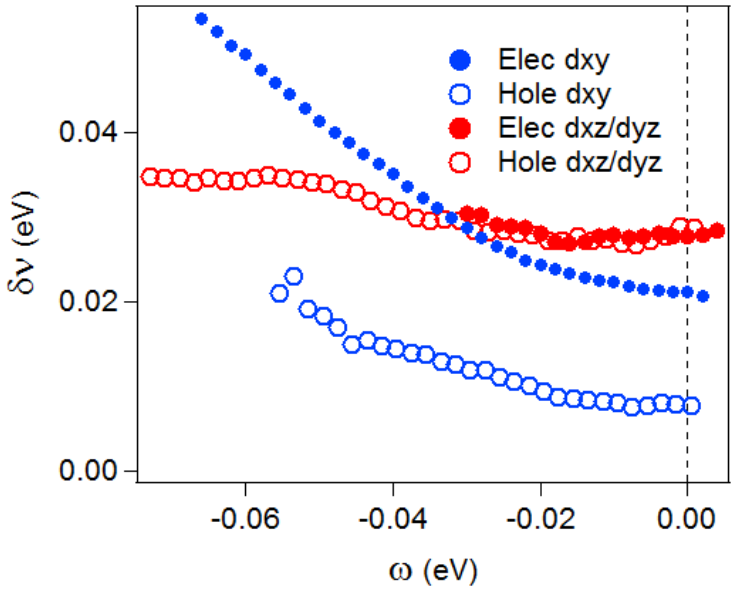


Comparaison between Co-122 and LiFeAs

8% Co doped $BaFe_2As_2$



LiFeAs



⇒ Rule out a contribution from band curvature, as similar effects are found on hole and electrons for LiFeAs.

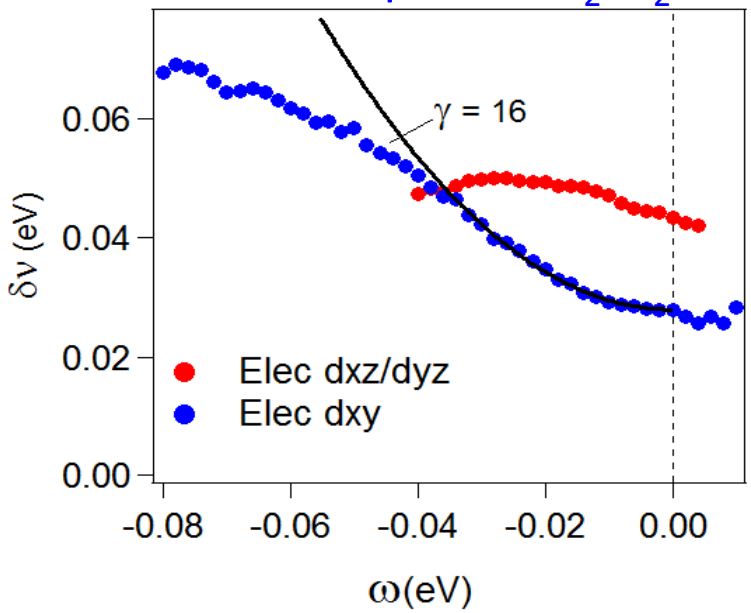
⇒ Rule out a contribution from 3D effects, which are very different in the two cases.

⇒ Rule out a contribution from surface states, which should be very different in the two cases.

Fit to Fermi liquid behavior

$$\frac{\hbar}{\tau} = \gamma((\hbar\omega)^2 + (\pi k_B T)^2)$$

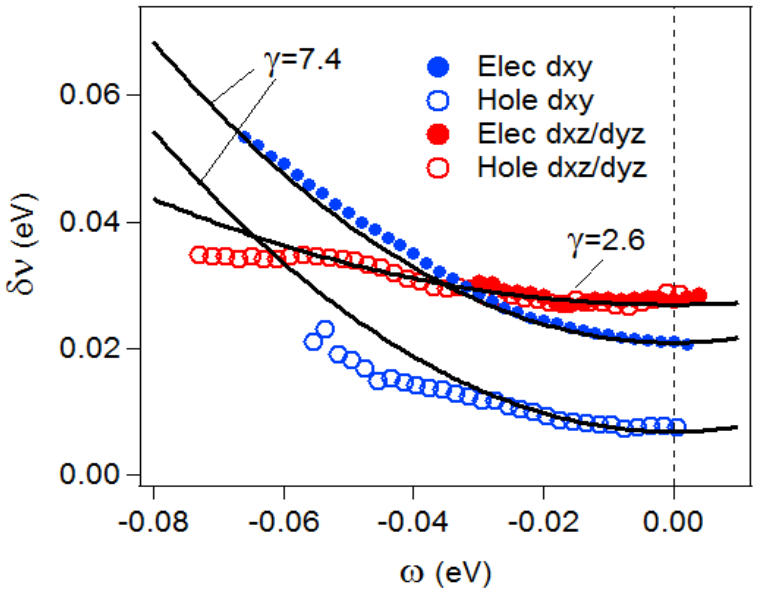
8% Co doped $BaFe_2As_2$

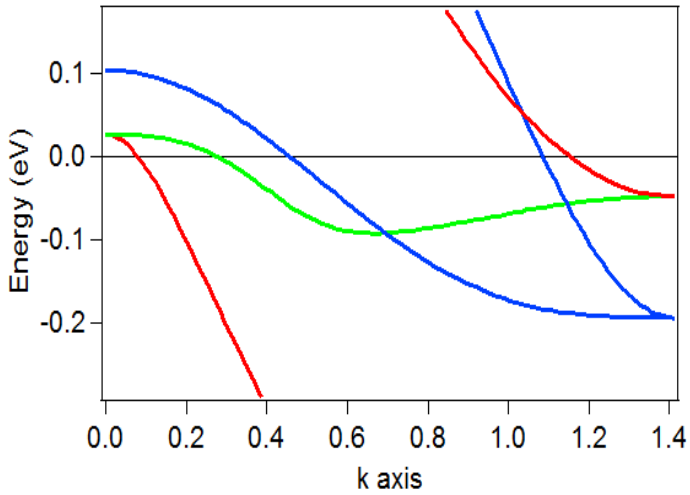


From resistivity in Co-122 ($\rho=AT^2$)=> γ=14

Rullier-Albenque et al., PRL 2009

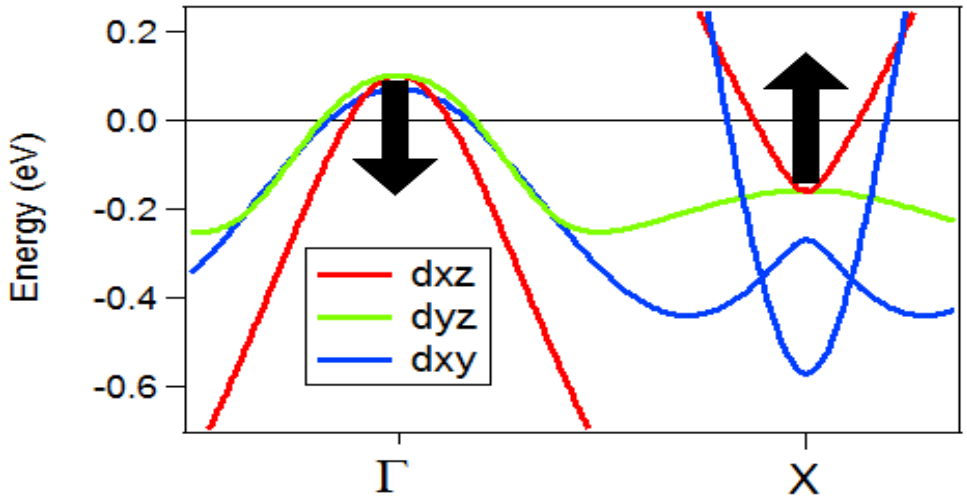
LiFeAs





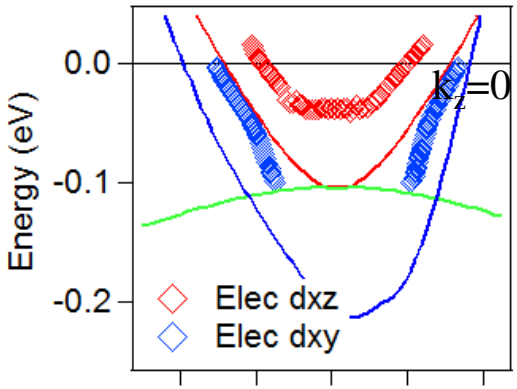
Fermi liquid regim is never reached in the narrow dxz/dyz band ??

Interband interactions :
“Shrinking” of the Fermi Surface



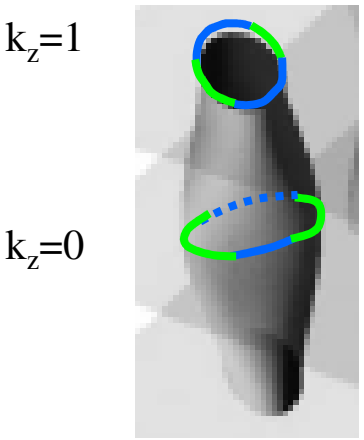
Large shrinking in Co-doped 122

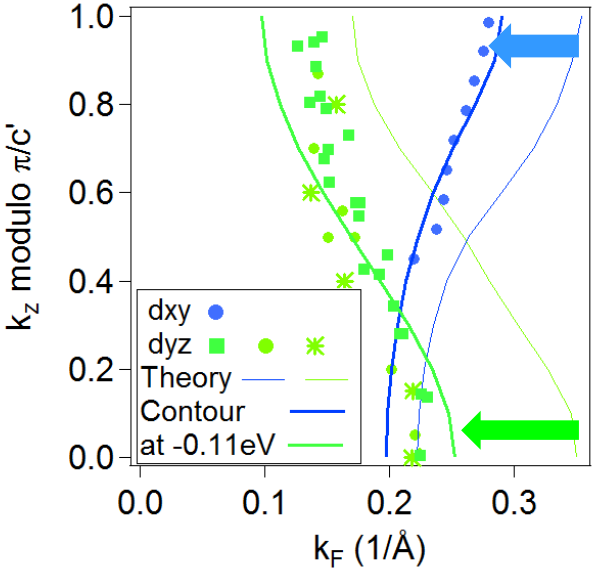
Calculated bands must be shifted up by 100meV to fit the data



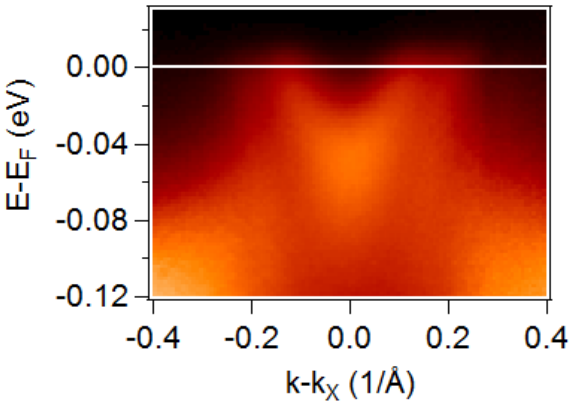
=> The number of electrons is reduced by a factor 2 compared to calculations

3D view of the shrinking

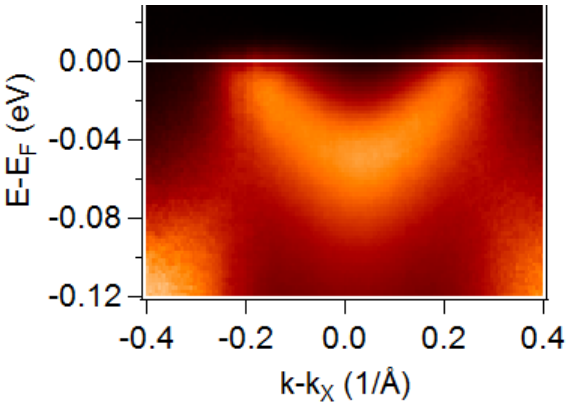




k_z=0

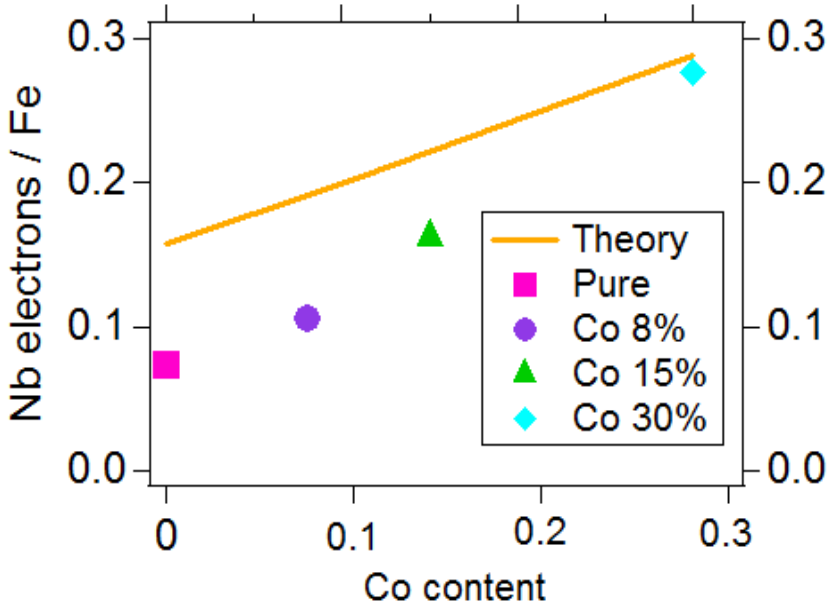


k_z=1

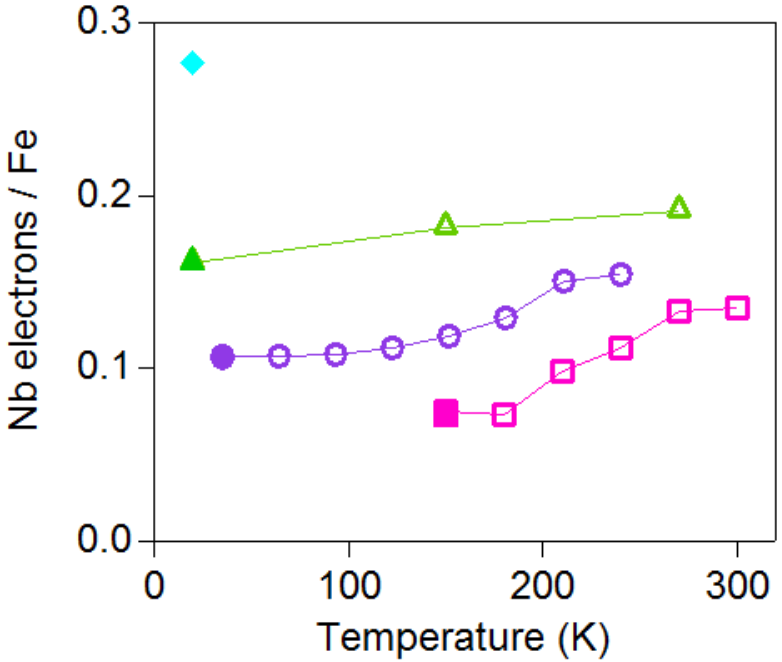


Nb of electrons vs doping and temperature

Nb electrons vs Co content



Nb of electrons vs temperature

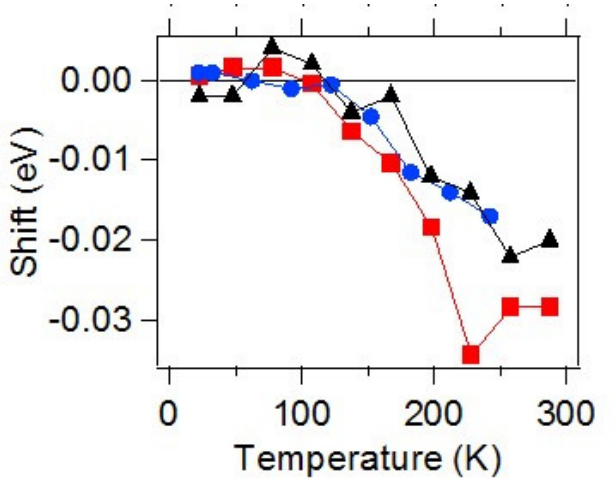


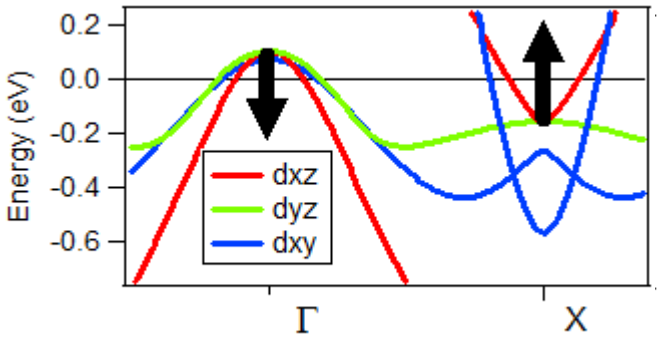
V. Brouet et al., PRL 2013

=> Impact on other properties like resistivity or susceptibility should be taken into account

Sensitivity to temperature

Shift vs T

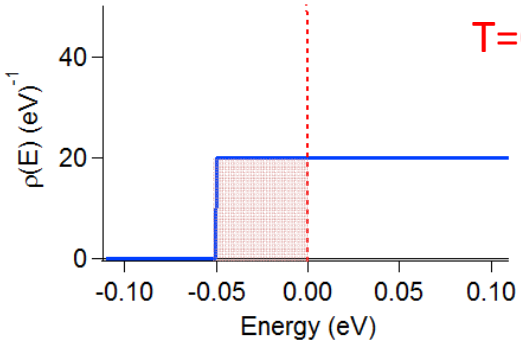


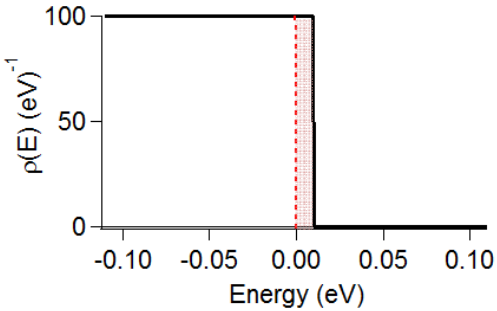


Electron bands

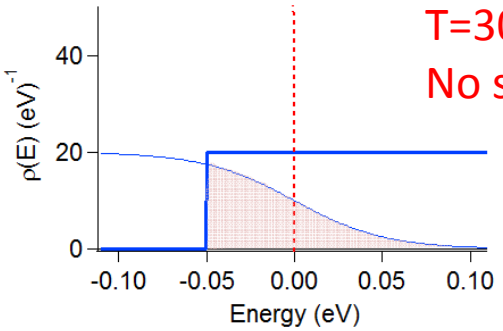
Hole bands

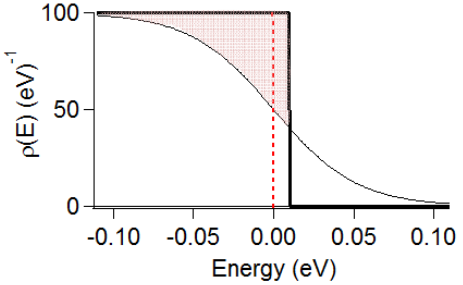
T=0



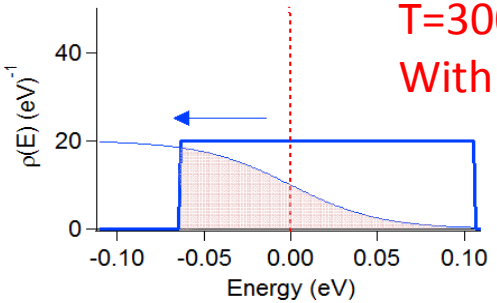


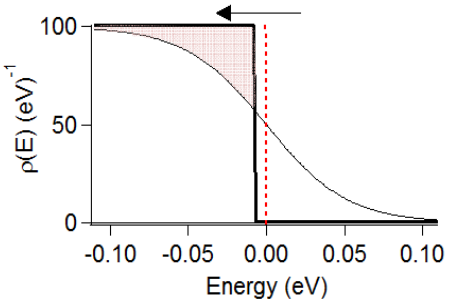
T=300K
No shift





T=300K
With shift

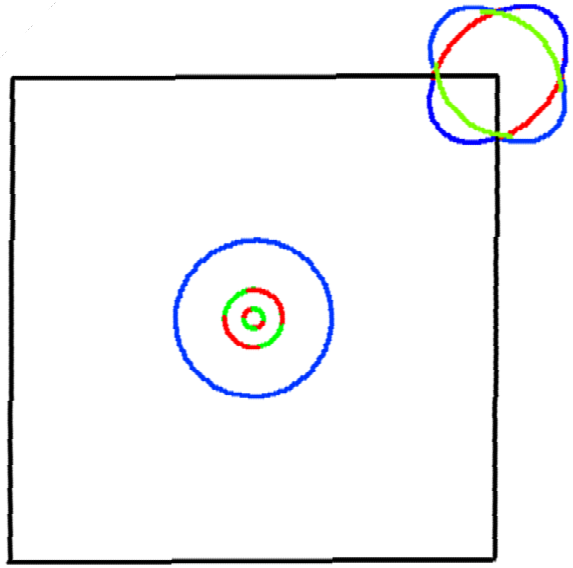




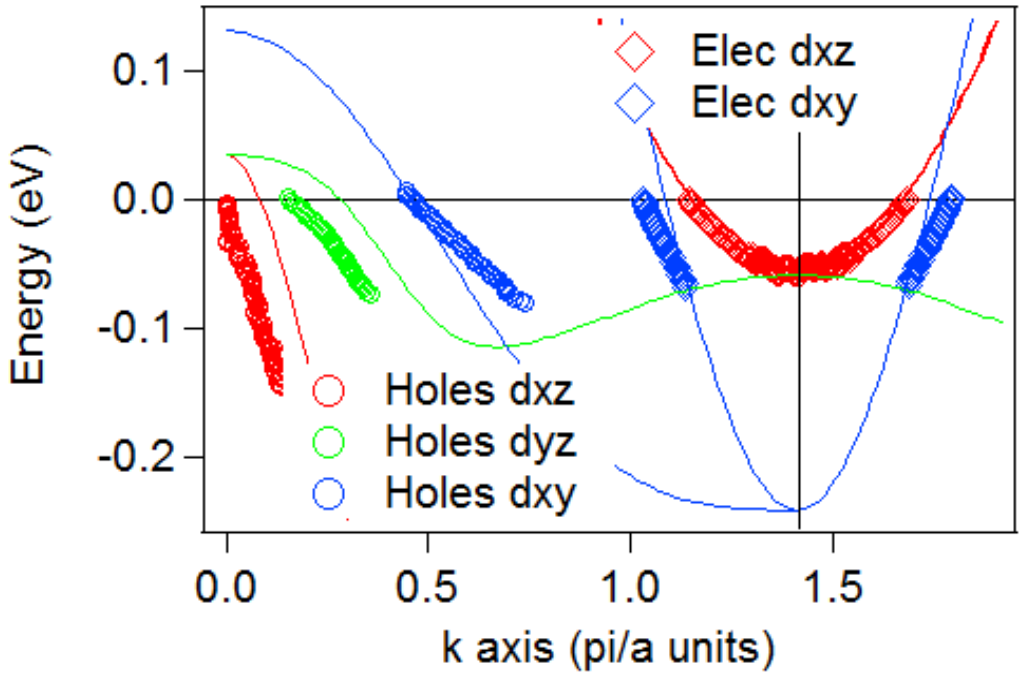
V. Brouet et al., PRL 2013

No shrinking in LiFeAs

Reduced nesting in LiFeAs

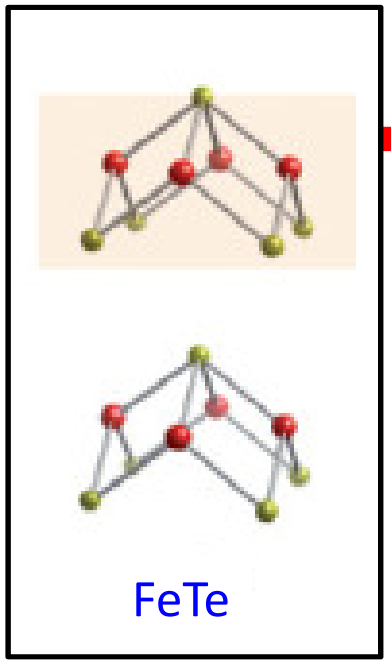


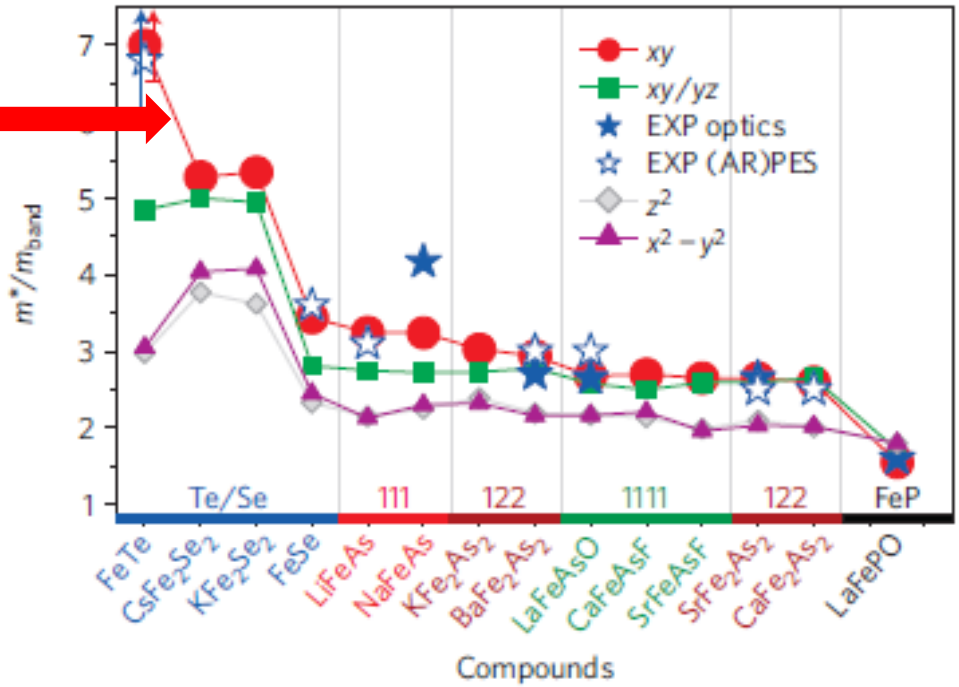
ARPES dispersion compared to calculated structure divided by 2



=> Supports the idea of *Ortenzi et al (PRL 10)* of interband interactions (for example mediated by spin fluctuations) which will be weaker in LiFeAs due to poorer nesting.

Strongly correlated case : bad metallic bahvior in FeTe

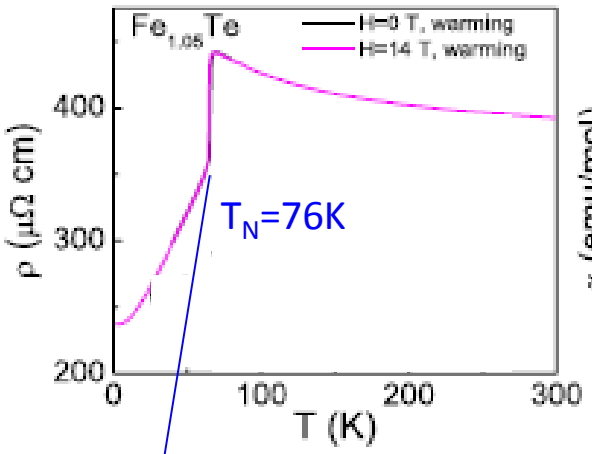




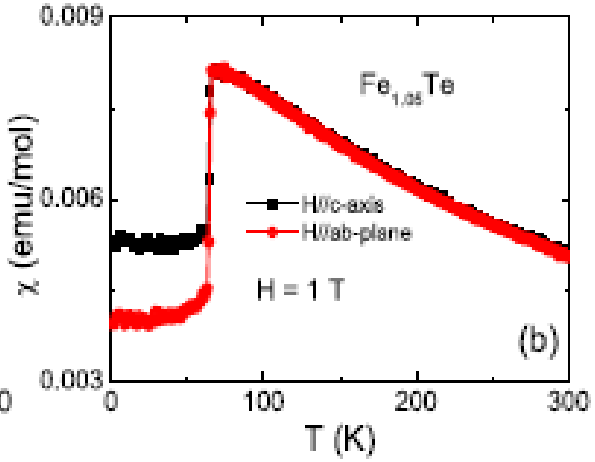
Yin, Haule, Kotliar, Nature Materials 2011

Bad metallic behavior in FeTe

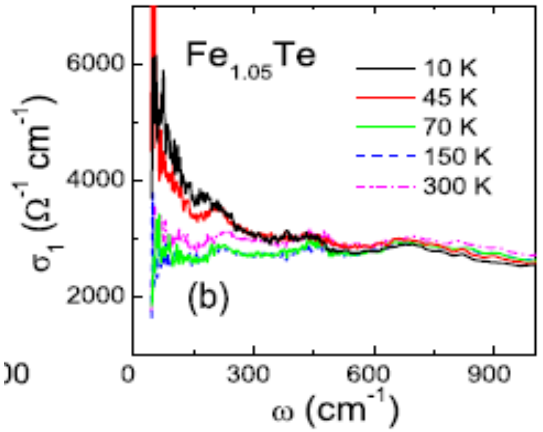
Resistivity



Susceptibility

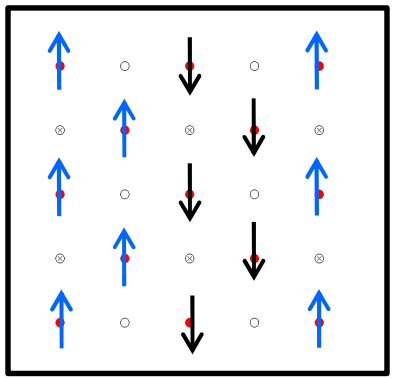


Optical conductivity

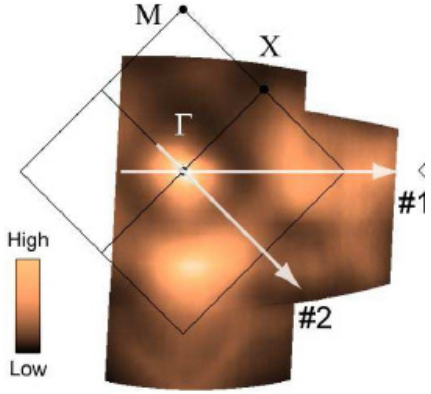


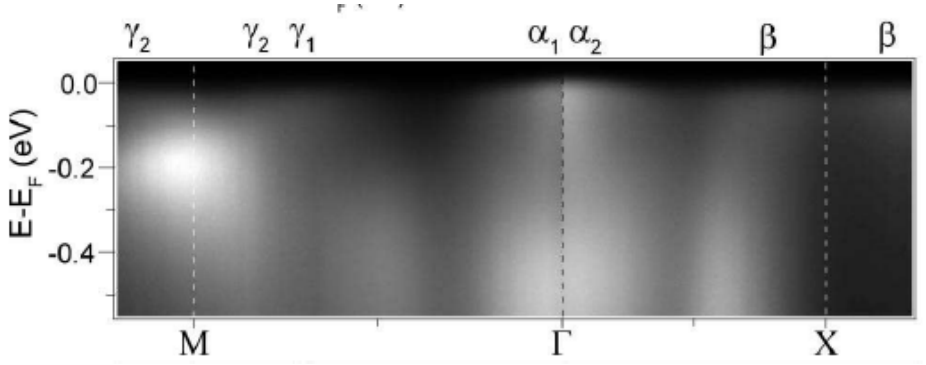
Chen et al., PRB 2009

Magnetic phase
with ($\pi/2$, $\pi/2$) order

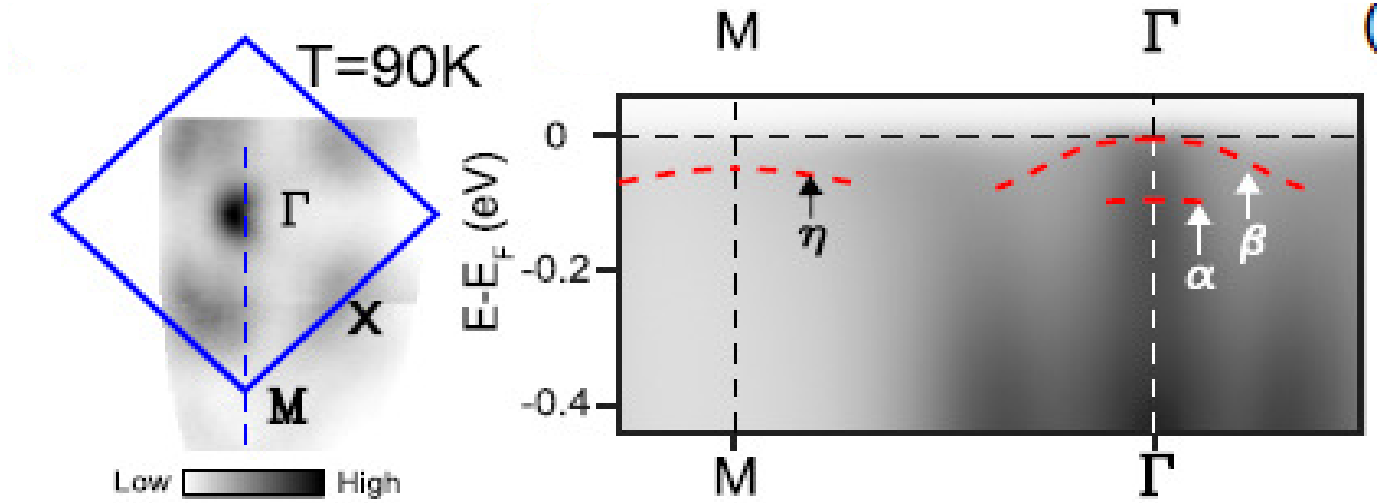


Previous studies of FeTe ($T>T_N$)





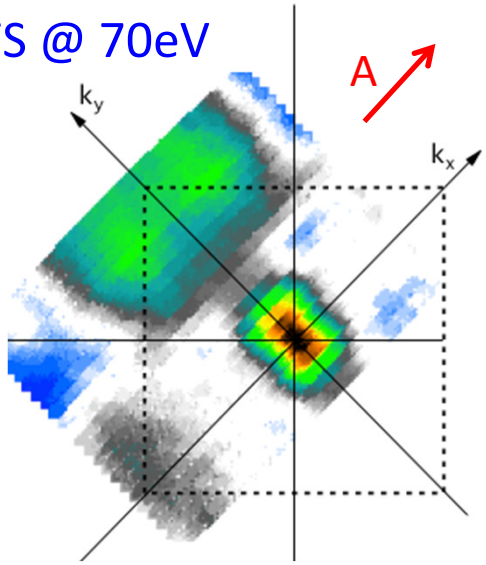
Zhang, DL Feng et al. PRB 2012



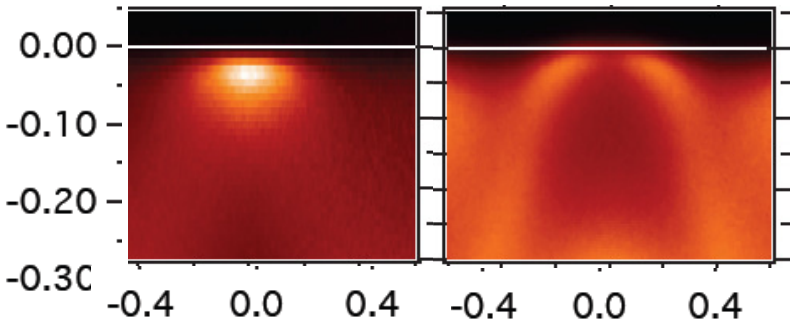
Liu, ZX Shen et al PRL 2013

FeTe Fermi Surface (80K)

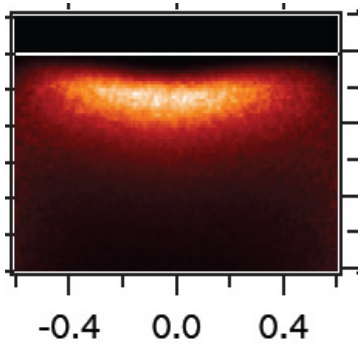
FS @ 70eV



dxz/dyz hole pockets



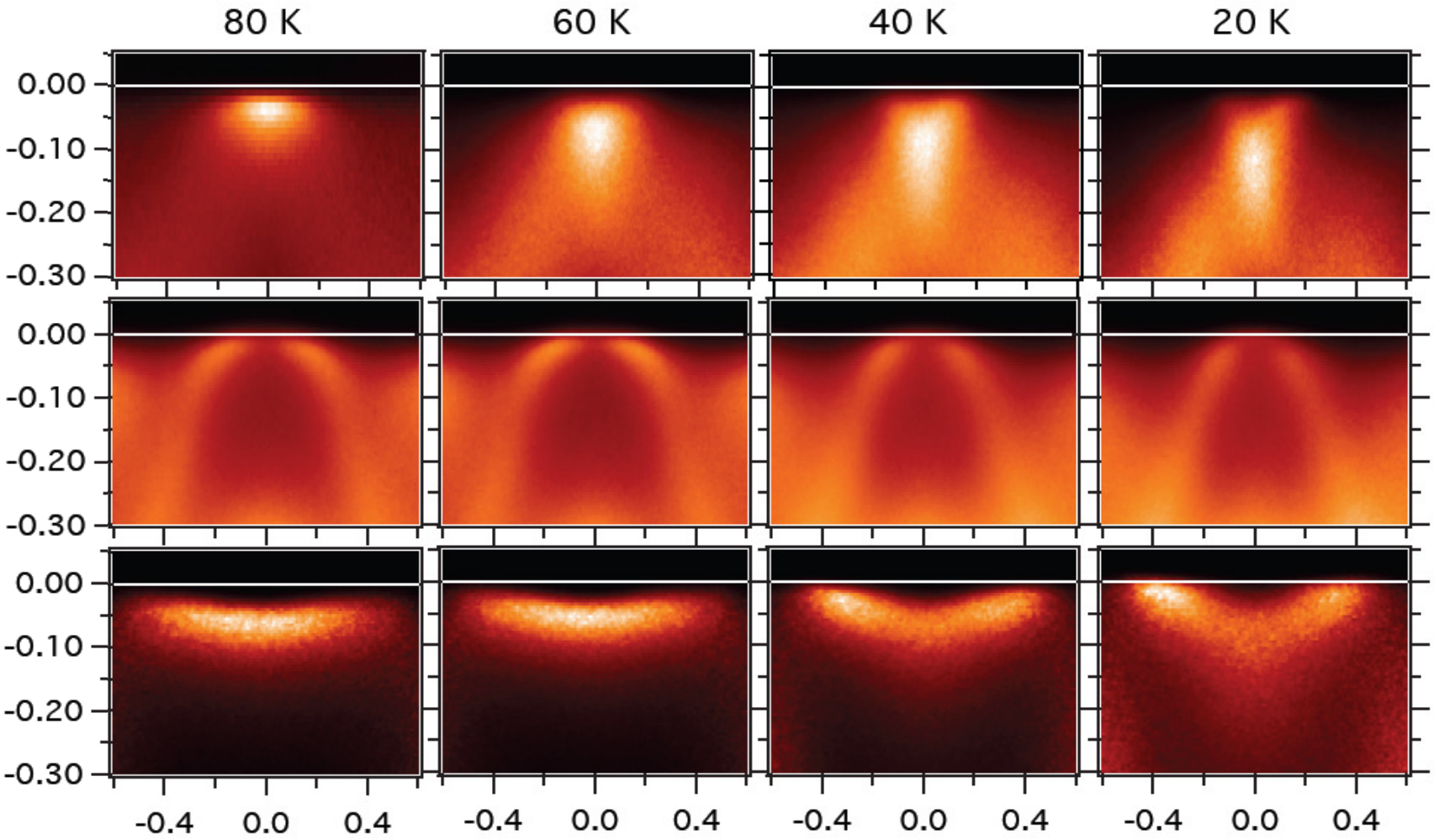
dxz/dyz electron pocket



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

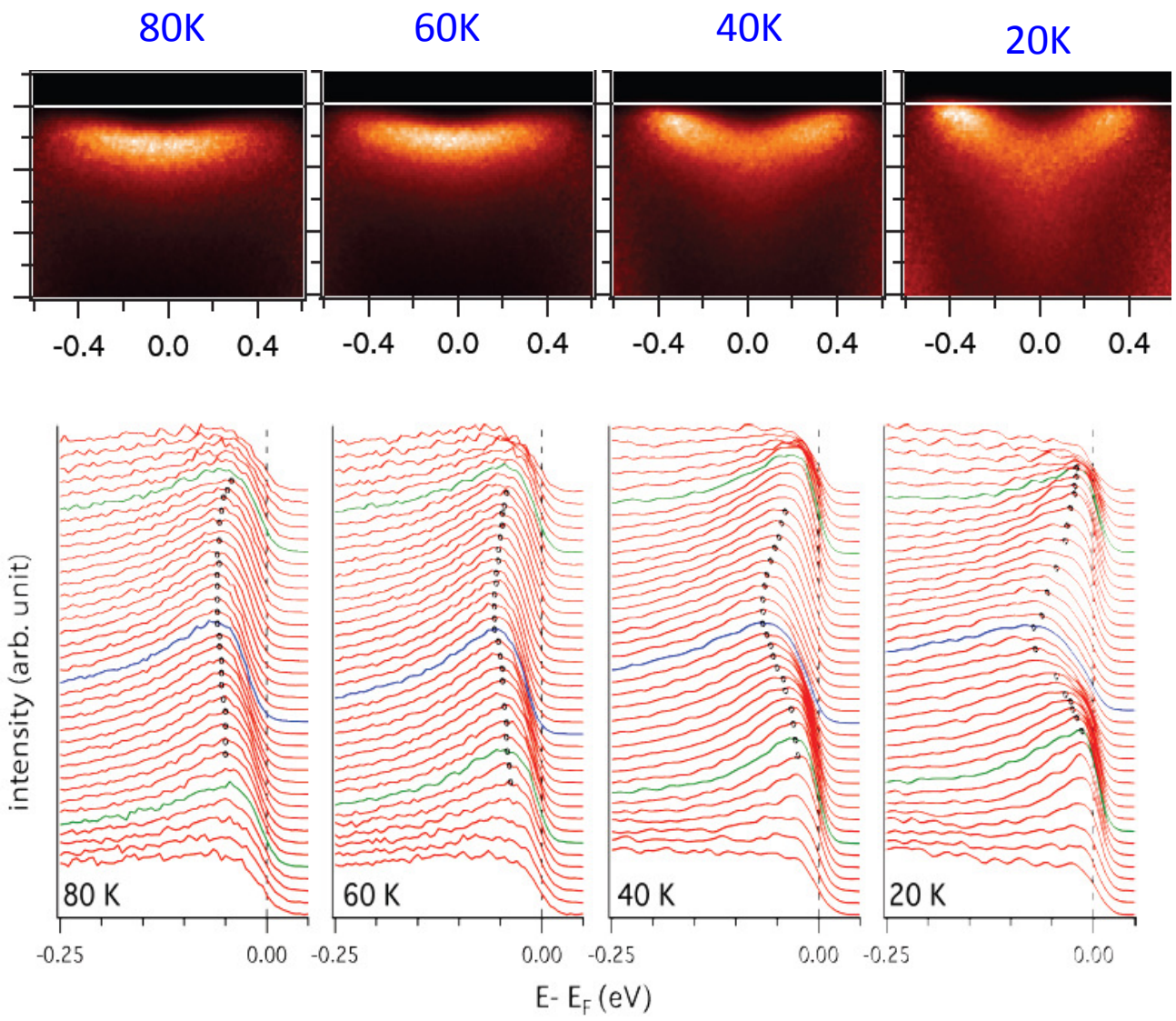
$\Rightarrow$ Strange shape for electron pocket !

FeTe : evolution of the bands with temperature

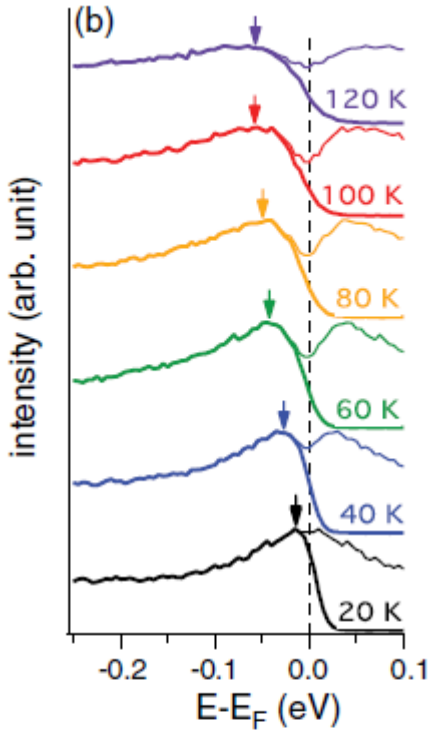


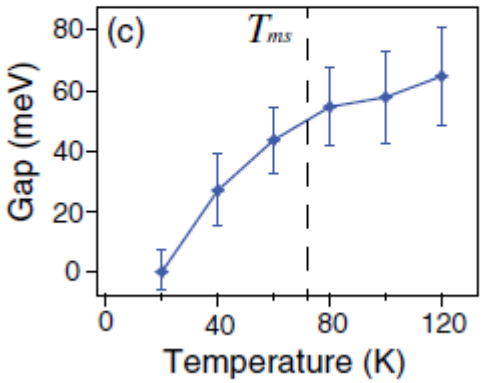
P.H. Lin, V. Brouet et al., PRL 2013

« Pseudogap » on the electron pocket



Spectra at k_F





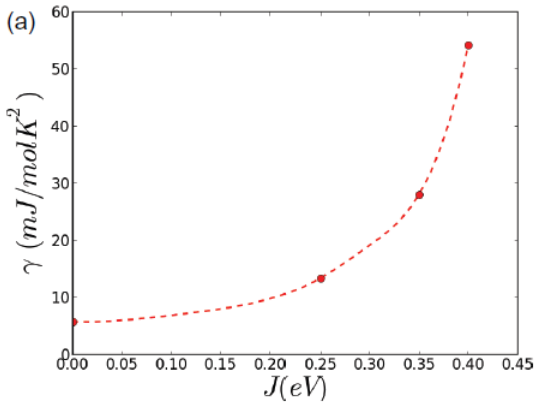
Can it be understood theoretically ?

« Hund's metals »

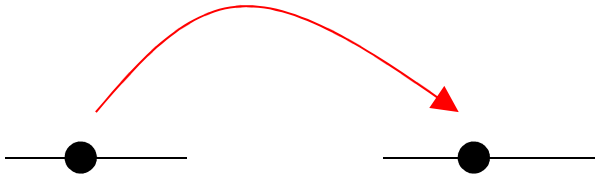
J – not U – is responsible for the mass enhancement

Haule and Kotliar,
New J. Of physics 2009

Specific heat coefficient γ vs J

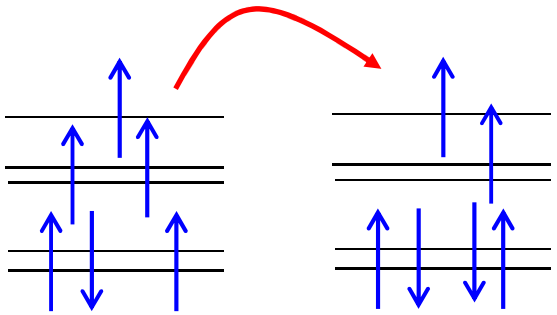


Electronic correlations are usually governed by Coulomb repulsion U



controlled by U

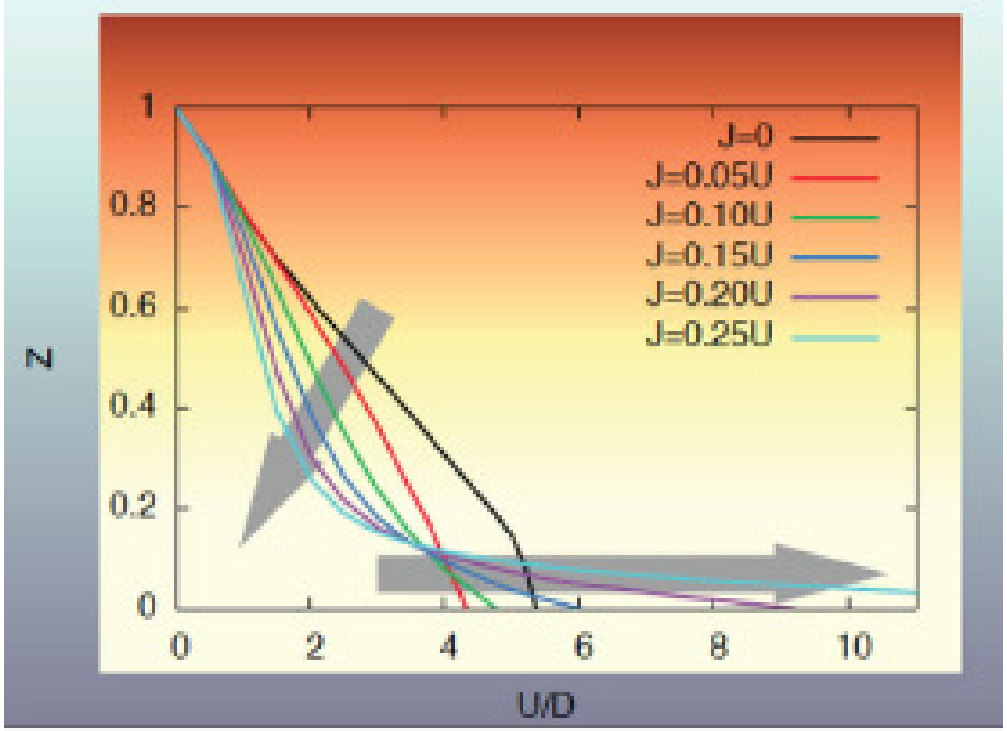
In iron-based superconductors Hund's couplings play a major role.



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

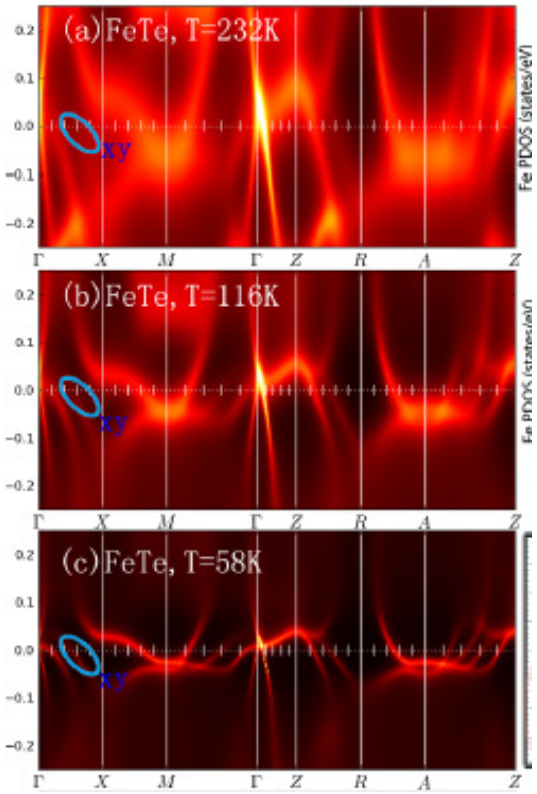
$\Rightarrow$ J decreases the quasiparticle weight but destabilizes the Mott transition.

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

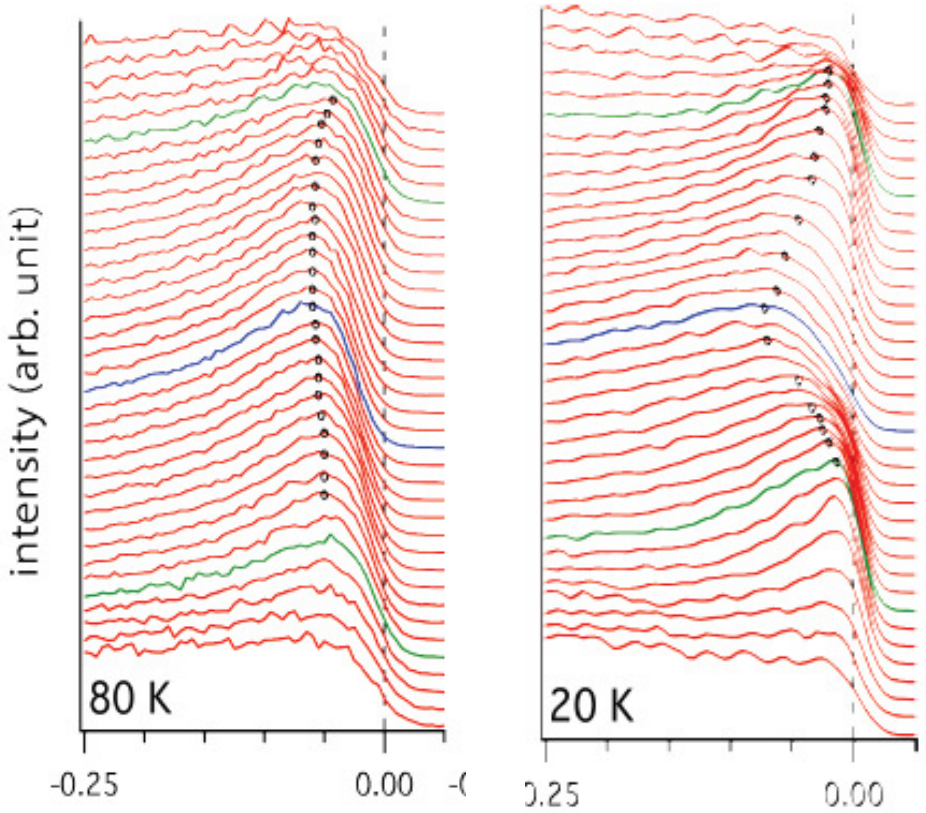
Is a pseudogap expected in the « spin freezing » regime ?

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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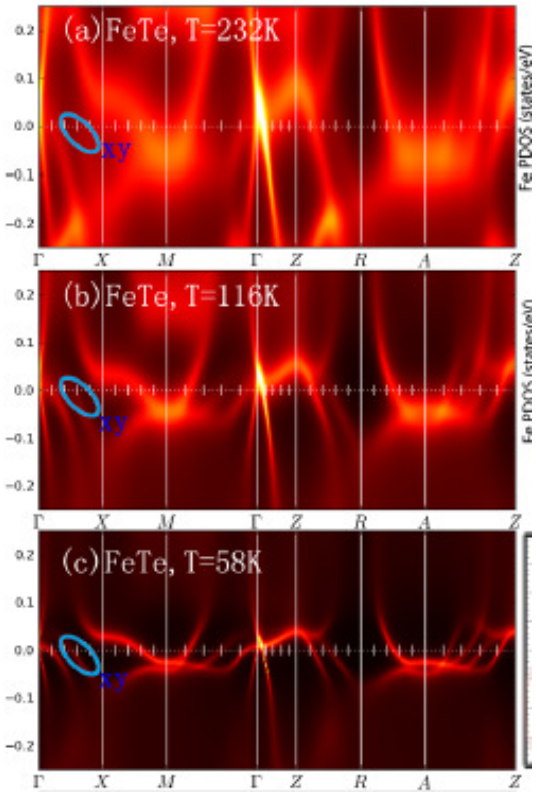
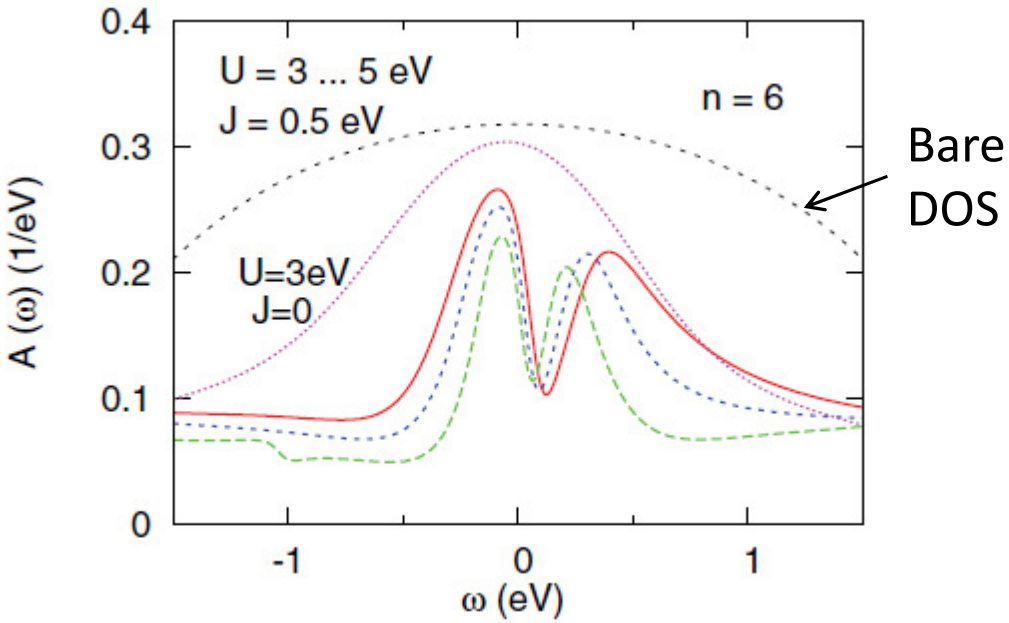


Yin, Haule, Kotliar, PRB 2012

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

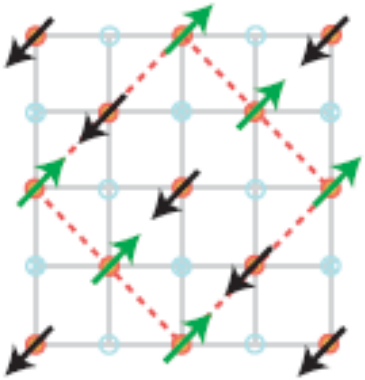


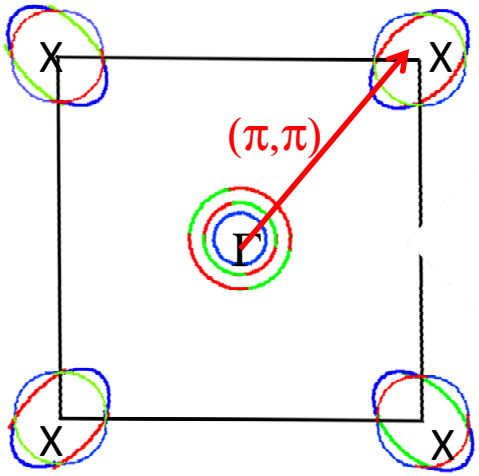
Liebsch, PRB 2011

(π, π) and (π, 0) fluctuations

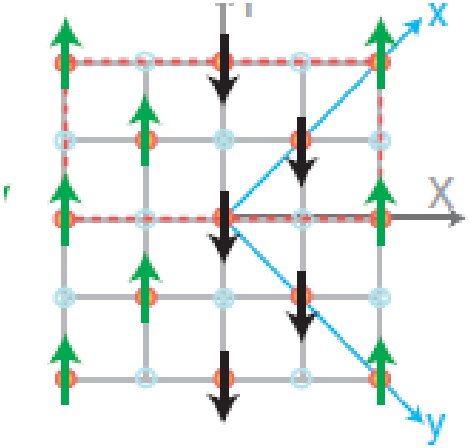
One characteristic of the FeTe pseudogap is that it only develops on the electron pocket.

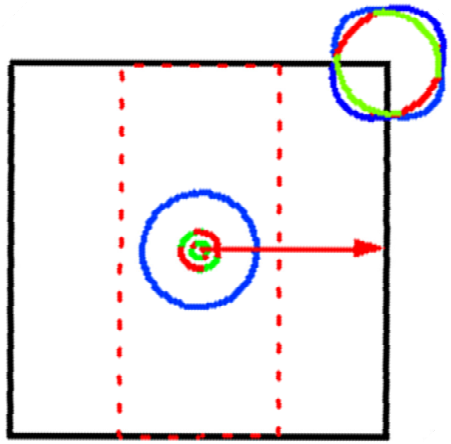
(π, π) fluctuations (FePn)

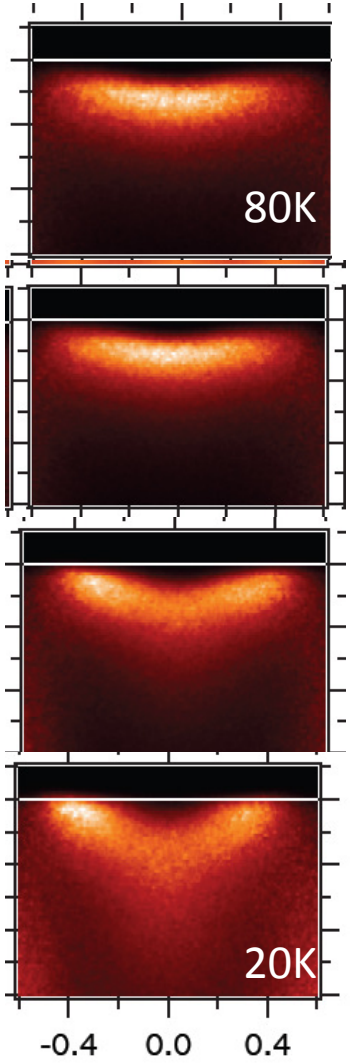




(π, 0) fluctuations (FeTe)

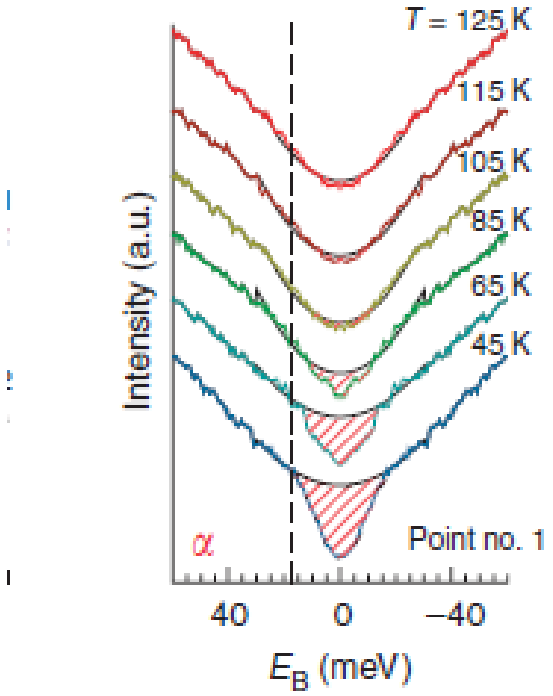






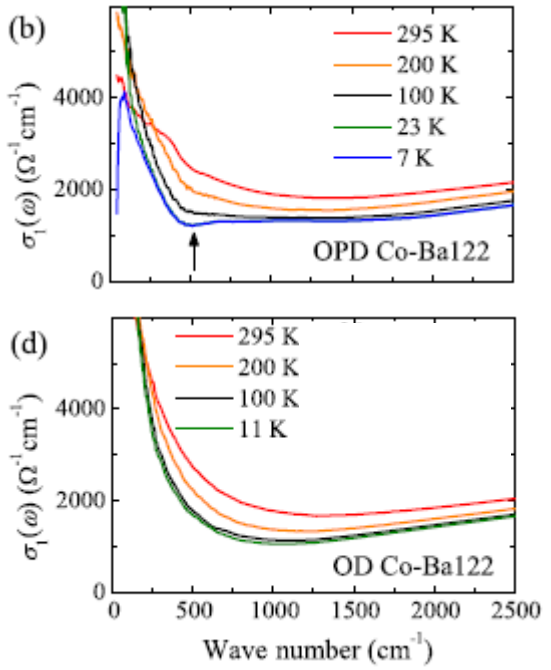
Are « pseudogaps » a general feature of iron-based superconductors ?

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.

- Lifetimes behavior are intrinsically different on dxz/dyz and dxy, possibly due to the narrow bandwidth of dxz/dyz.

- There is a large doping and temperature dependent « shrinking » of the Fermi Surface in 122.

  It is favored by good nesting, suggesting the role of interband transitions

- 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.

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

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