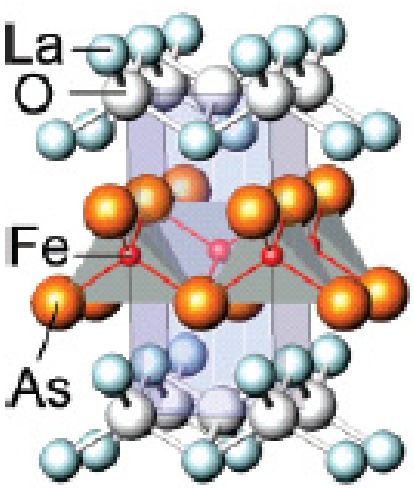
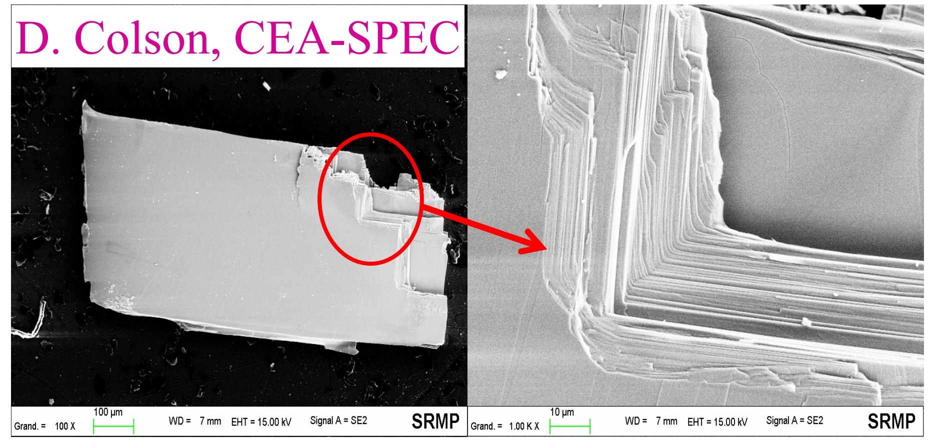
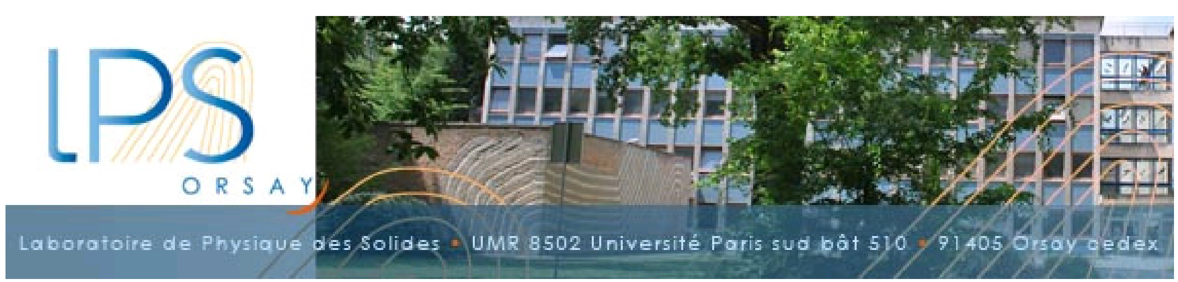
Iron pnictides superconductors (discovered in march 08)

View of the electronic structure with photoemission (ARPES)





Véronique Brouet
Laboratoire de Physique des Solides d'Orsay



Outline

- Why study these systems ?

=> High temperature superconductivity (up to 56K)

=> Exotic superconducting pairing, possibly involving magnetic fluctuations.

- A complicated electronic structure, unusual in the context of correlated systems

=> 5 Fe bands near the Fermi level, giving rise to small hole and electron pockets

=> Angle-resolved photoemission allows to map the dispersion of the different bands

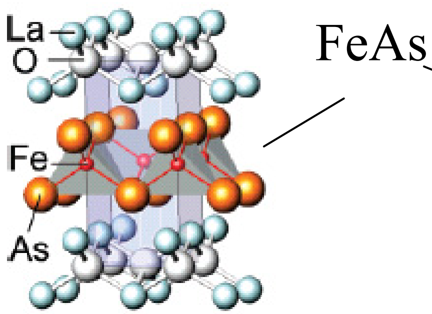
- ARPES study of superconducting and magnetic properties

=> Different superconducting gaps for the different bands

=> Reconstruction of the Fermi Surface in the magnetic state, compared with nesting properties of the Fermi Surface.

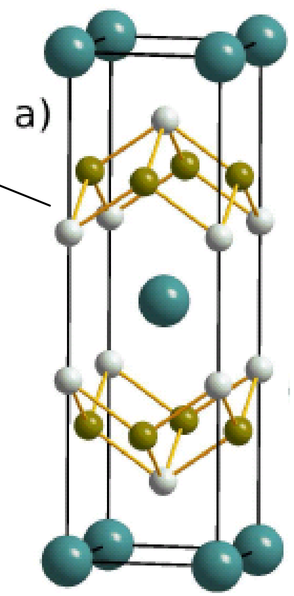
The discovery of iron pnictides superconductors

$LaO_{1-x}F_xFeAs$



Tc up to 56K
(march 2008)

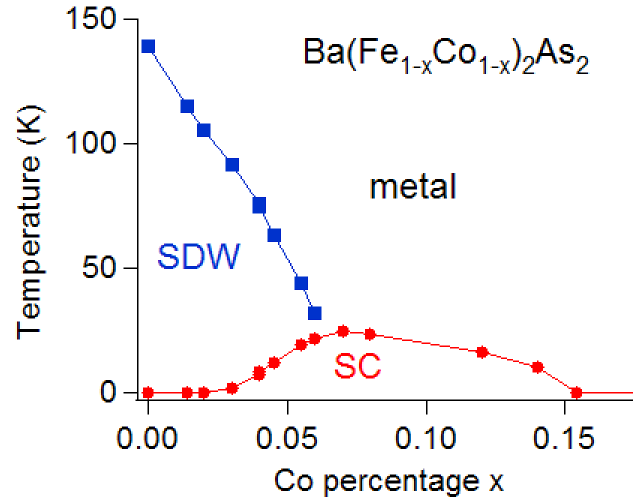
$BaFe_2As_2$

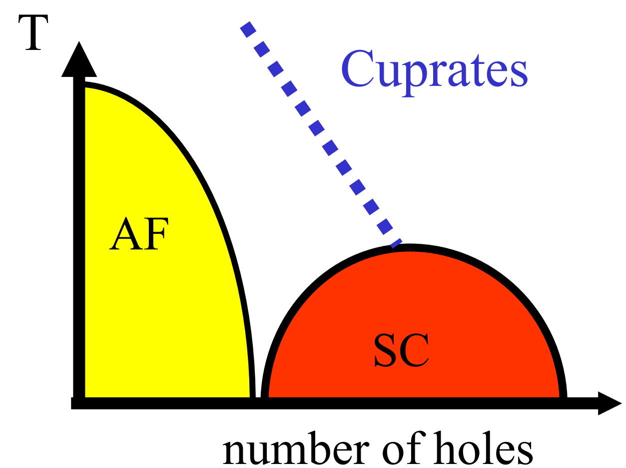


Doping

K instead of Ba => hole doping

Co instead of Fe => electron doping



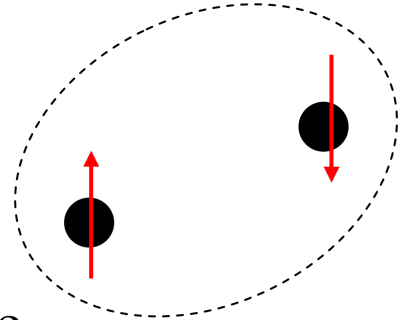


=> Origin of superconductivity ? Relationship with magnetism ?

=> Relationship with other high temperature superconductors, like cuprates ?

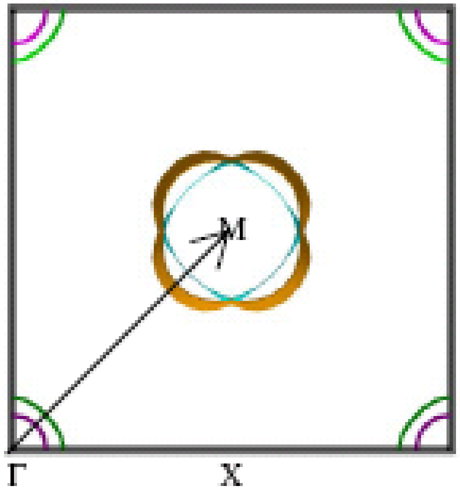
Origin of the superconducting pairing ?

• Electron-phonon coupling seems to be too weak (λ=0.2) to induce superconductivity at such high temperatures



• Could superconductivity be mediated by spin fluctuations ?

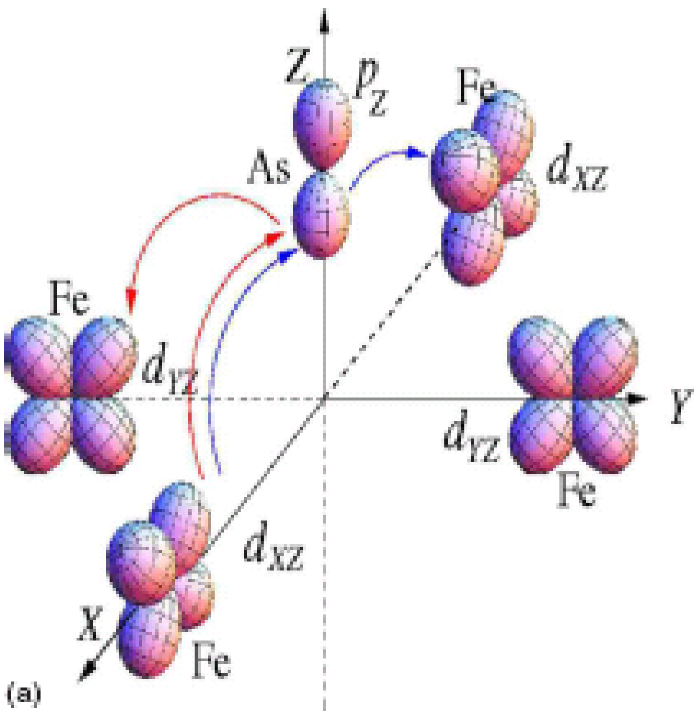
Proposal :
Unconventional superconductivity mediated by spin fluctuations.
=> extended s-wave pairing with a sign reversal between hole and electrons sheets.



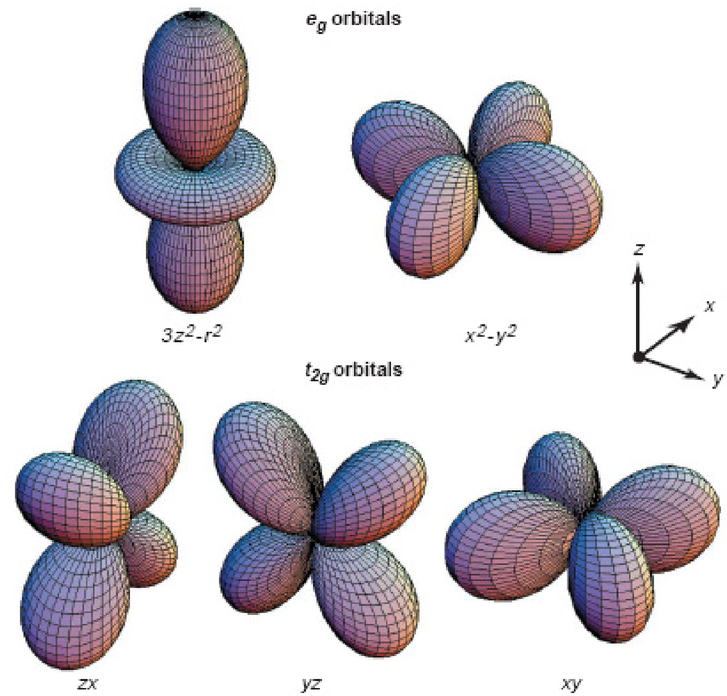
I. I. Mazin, D. J. Singh, M. D. Johannes and M. H. Du, PRL 2008

The undoped compound is a compensated semi-metal with small hole and electron FS pockets

The main orbitals at the Fermi level : Fe d_{XZ} and d_{YZ}



5 Fe 3d orbitals
filled by 6 electrons



Y. Ran et al., Phys. Rev. B **79**, 014505 (2009)

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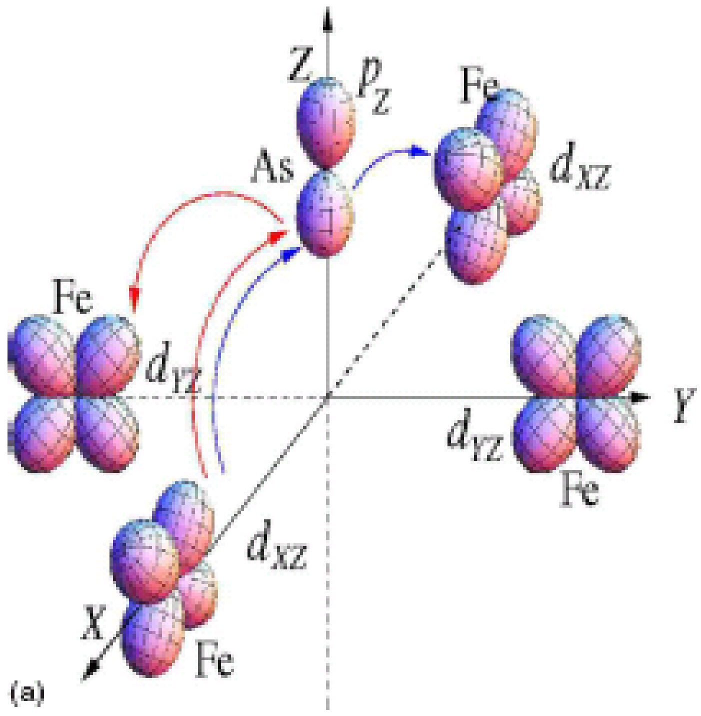
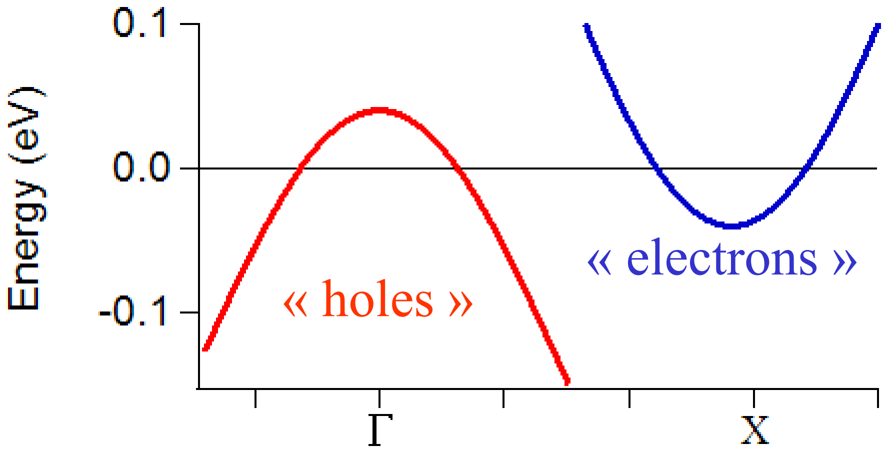
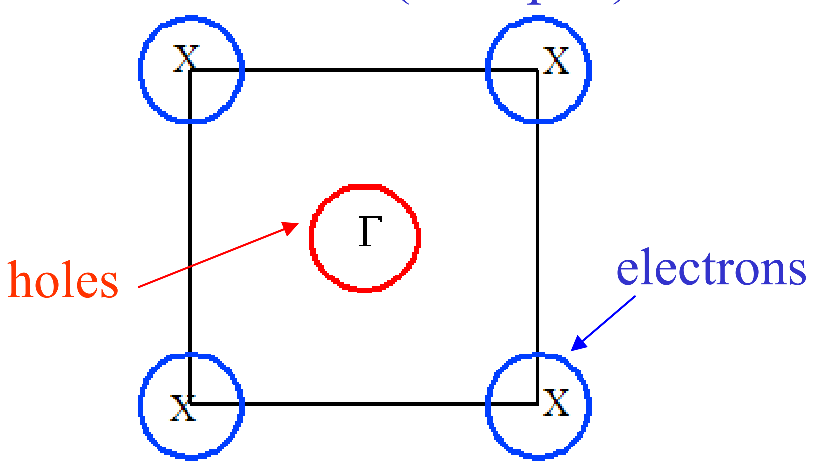


Y. Ran et al., Phys. Rev. B **79**, 014505 (2009)

Band structure along diagonal



Fermi Surface (undoped)



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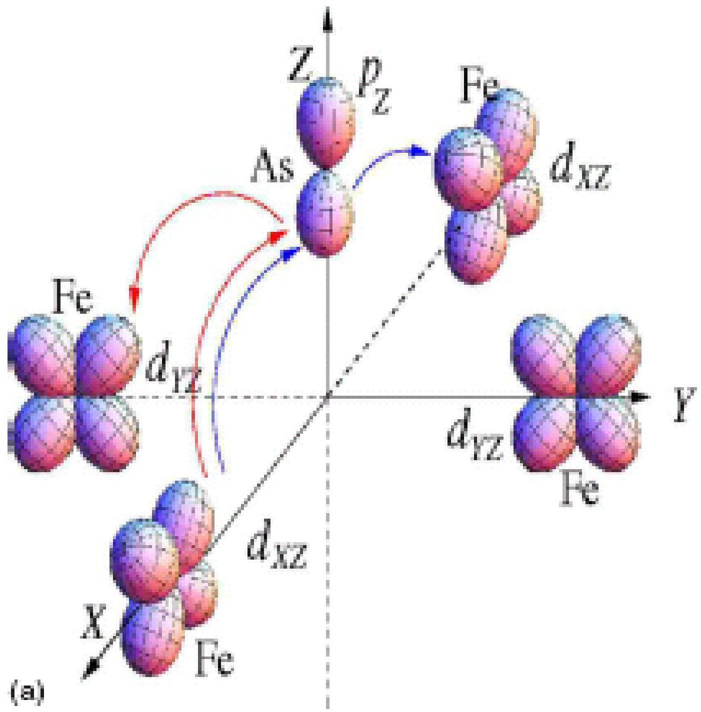

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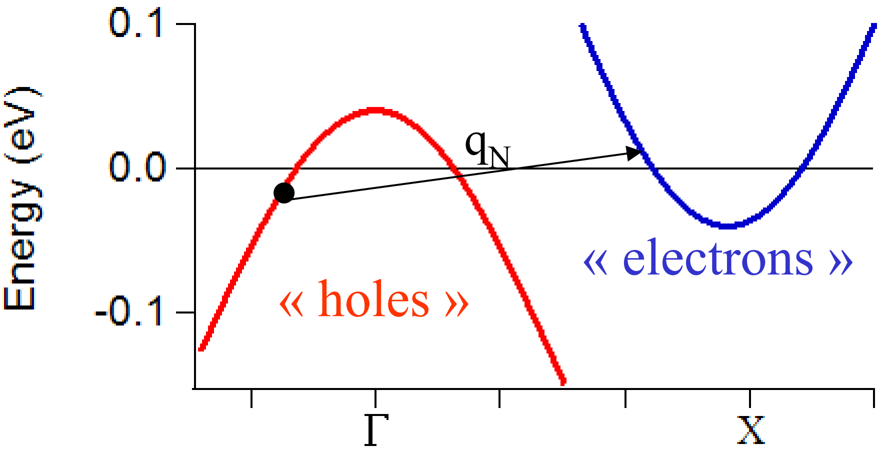

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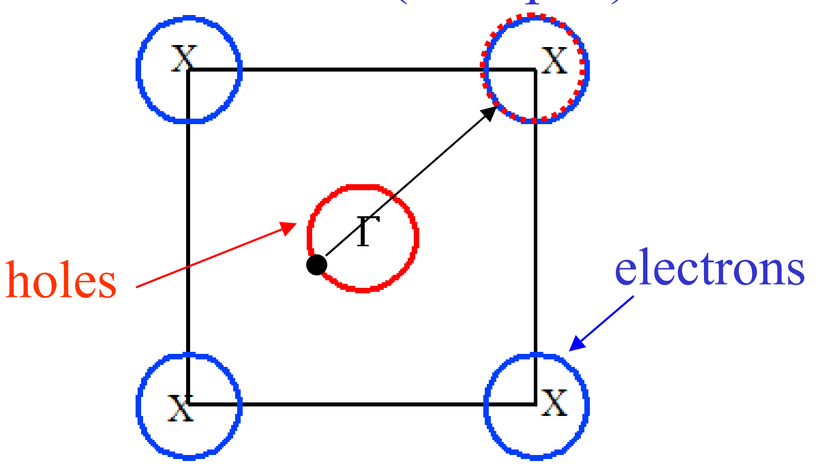
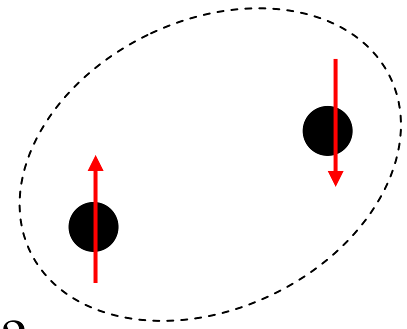


=> Good nesting between hole and electron pockets

Origin of the superconducting pairing ?

• Electron-phonon coupling seems to be too weak (λ=0.2) to induce superconductivity at such high temperatures



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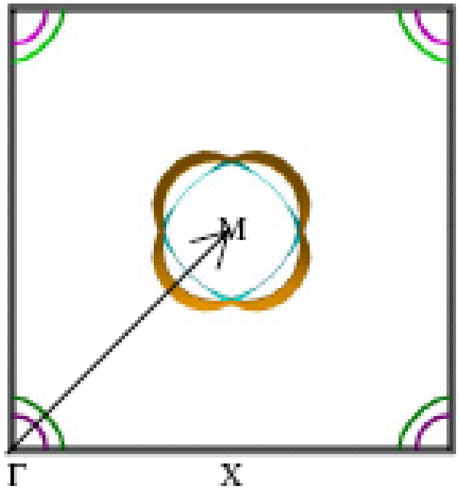
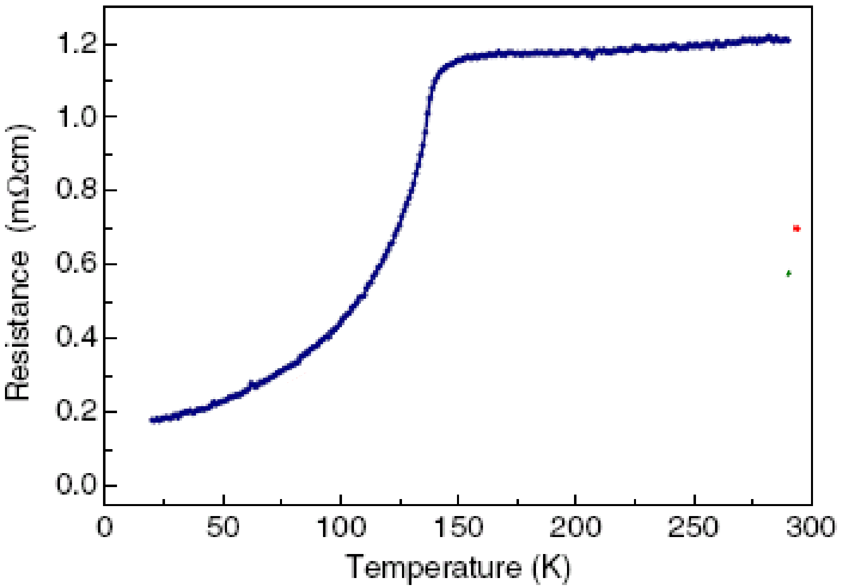


I. I. Mazin, D. J. Singh, M. D. Johannes and M. H. Du, PRL 2008

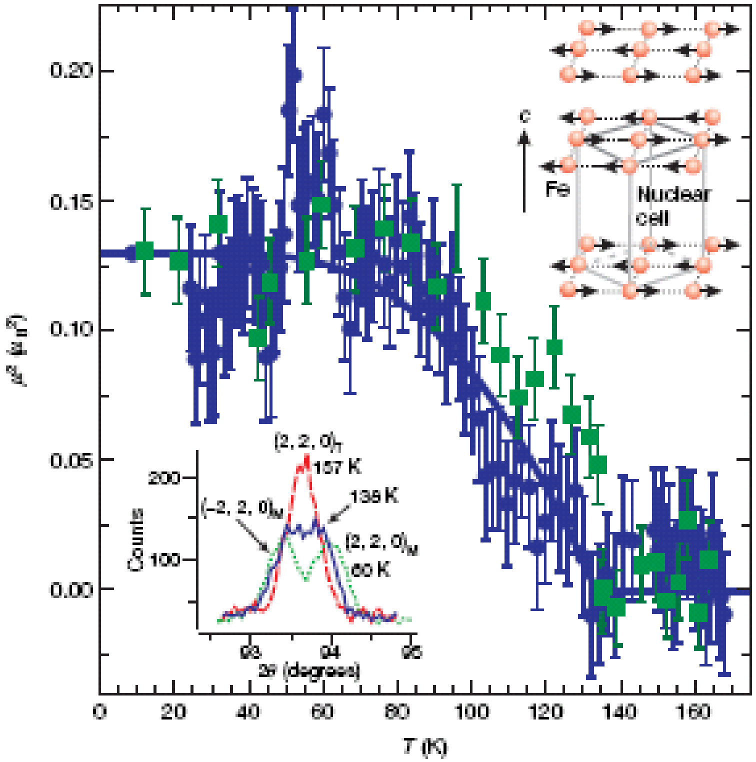
Magnetic transition

Resistivity ($BaFe_2As_2$)



Rotter et al., PRL 2008

Neutrons (LaOFeAs)



q=(π,π)

De la Cruz et al., Nature 2008

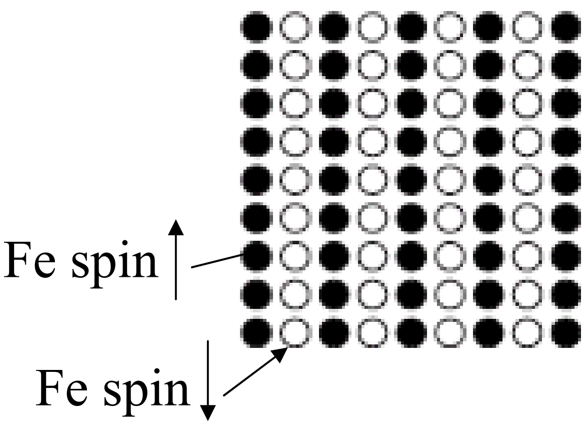
The magnetic phase is metallic with rather small magnetic moments (0.3 - 1 μ_B)

=> this suggests a Spin Density Wave picture

Magnetism : localized or itinerant ?

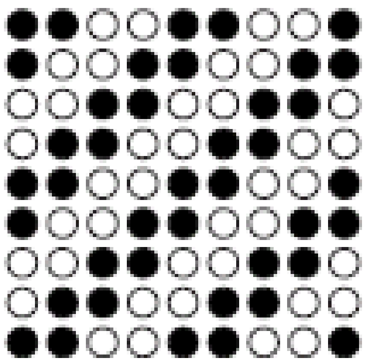
Magnetic structure usually observed in iron pnictides

Consistent with nesting vector OR superexchange interactions (2nd neighbors)



Magnetic structure observed in FeSe family

NOT consistent with Fermi Surface nesting



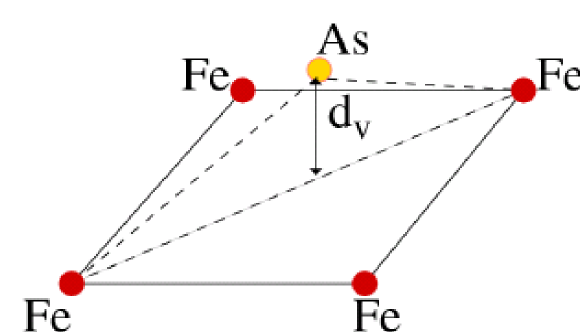
Problems with itinerant approaches

• Systematic overestimation of the magnetic moment by ab initio calculations

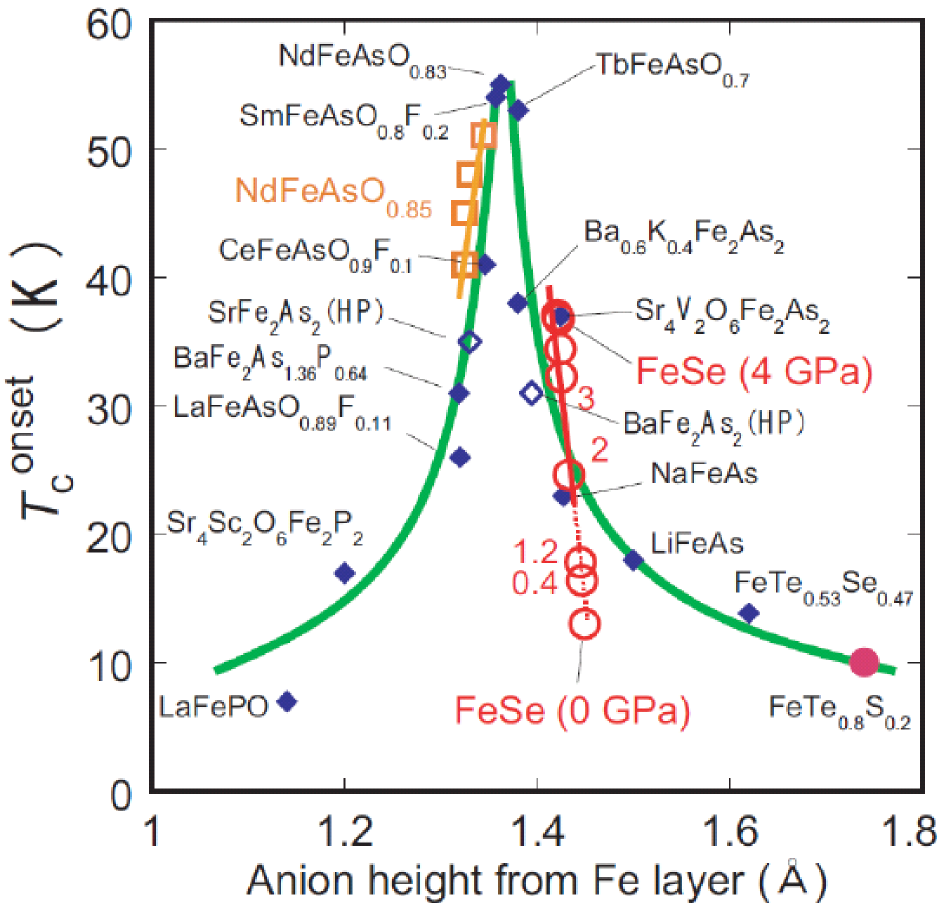
• Also wrong estimation of the As position

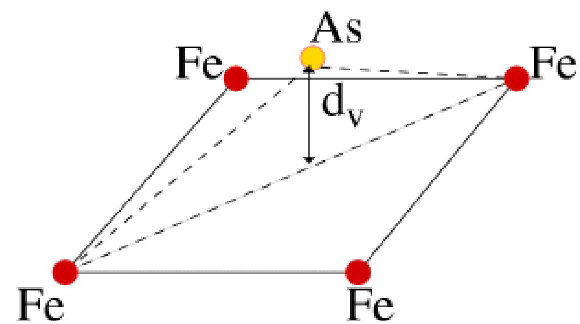
Could the moments be much larger in fluctuating domains ?

cf Mazin and Johannes, Nature Physics 2009



The superconducting temperature seems to scale with the As height !





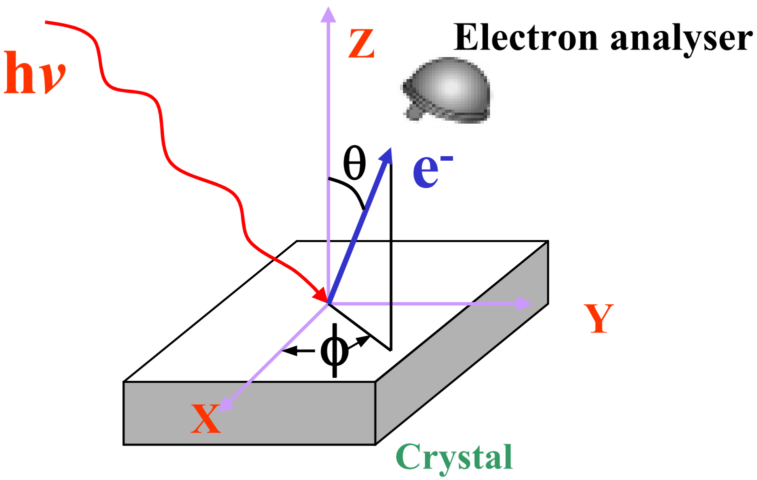
Mizuguchi *et al.*, cond-mat 2010

View of the electronic structure with ARPES

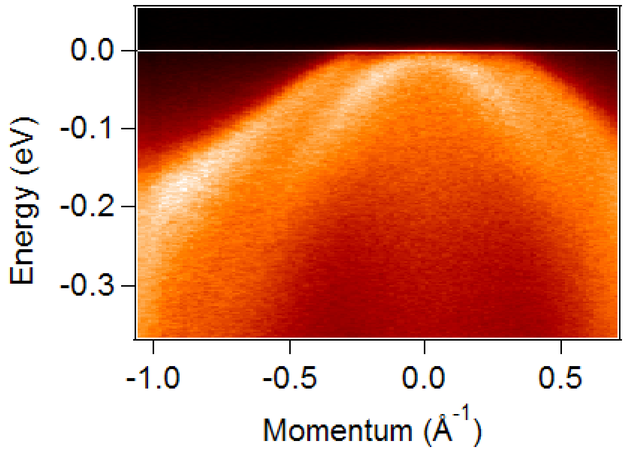
- *How many hole and electron pockets ?*
- *Are they well nested ?*

- *What is the strength of electronic correlations ?*
- *Are there analogies with cuprates ?*

Angle-resolved photoemission



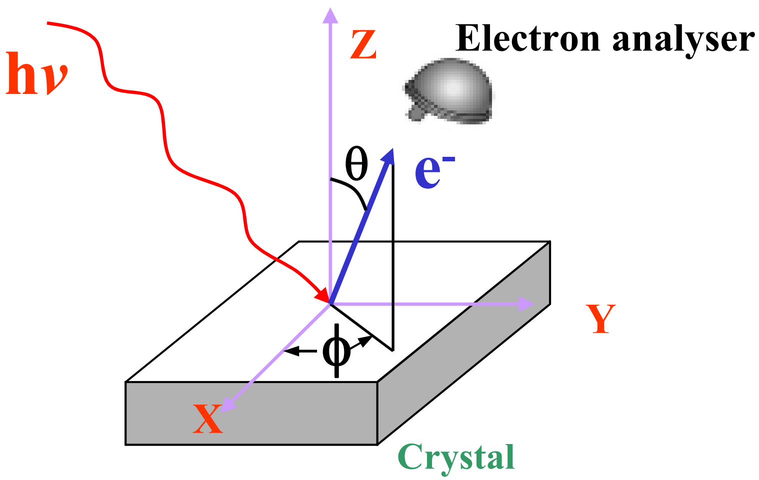
Hole pockets in $Ba(Fe_{0.92}Co_{0.08})As_2$



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

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

Angle-resolved photoemission



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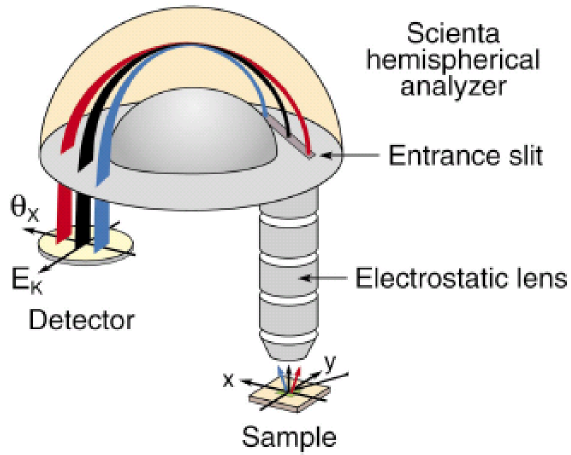

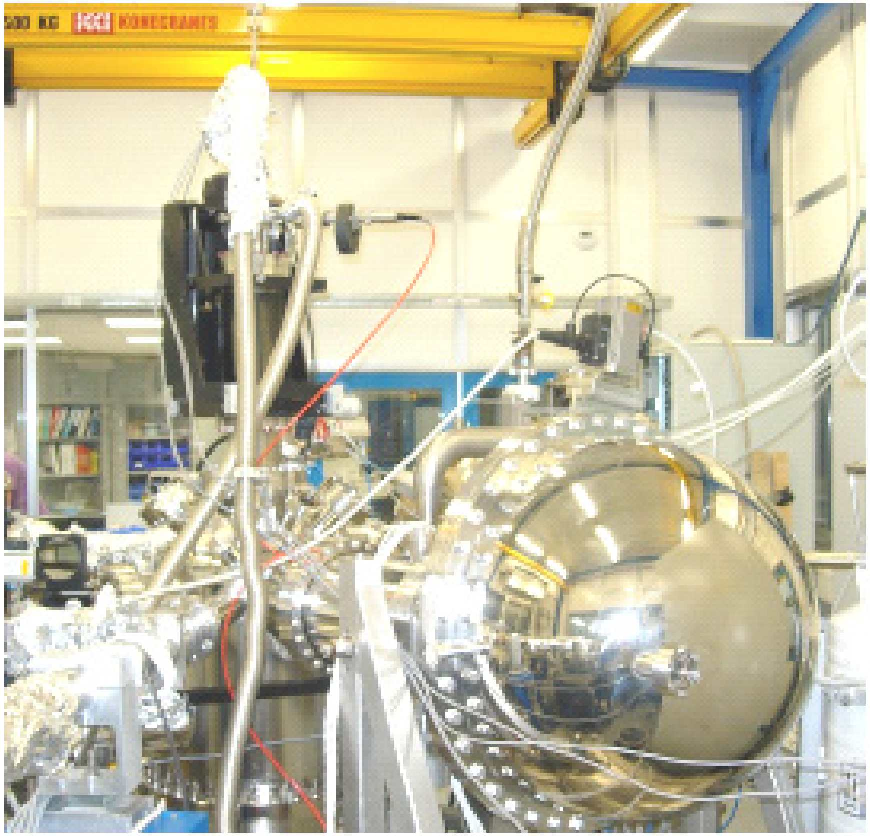

CASSIOPEE beamline, SOLEIL synchrotron

Photons from : Synchrotrons : 10-100eV
He lamp : 21 eV
Laser : 6-7eV

Angle-resolved photoemission

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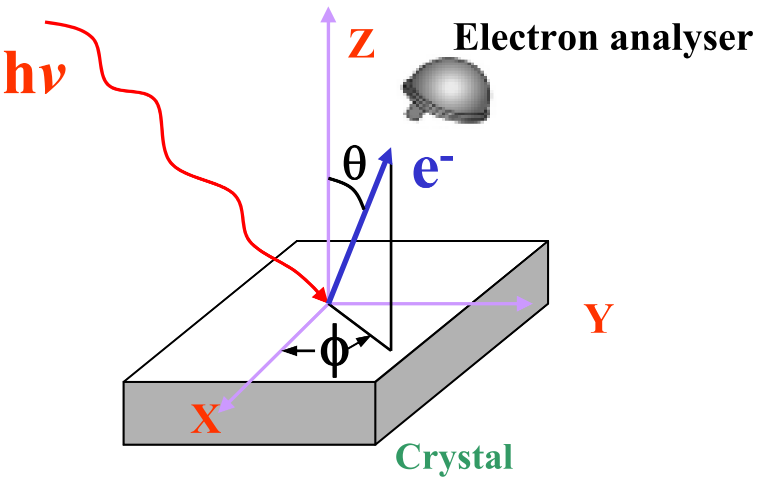

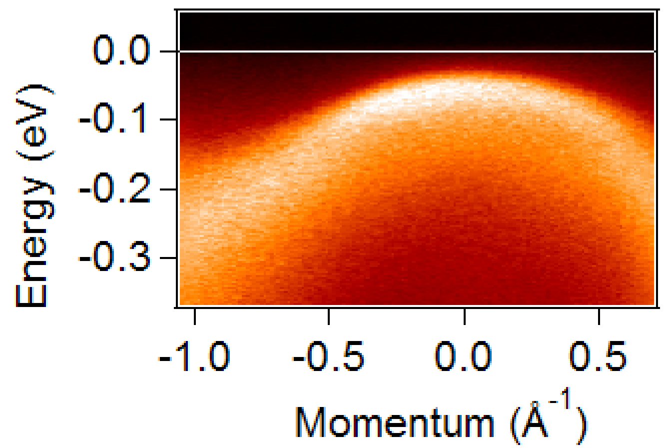

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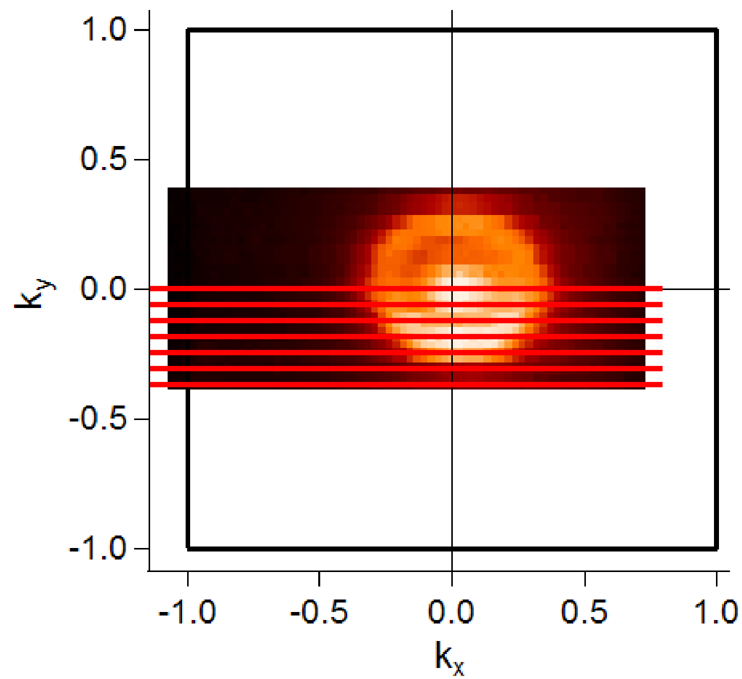
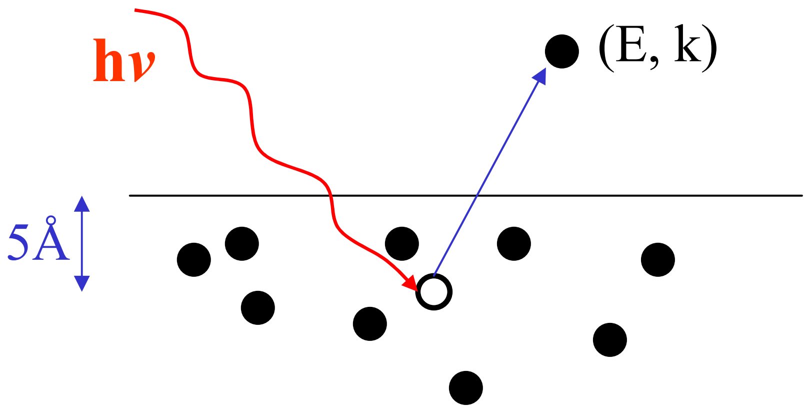


Some aspects of the photoemission theory



Surface :
Work function W, information on $k_\perp$ lost

$$I(k,\omega) = \sum_{i,f} \frac{2\pi}{\hbar} \left| \left\langle \psi_f^N \left| \frac{e}{mc} \vec{A}.\vec{p} \right| \psi_i^N \right\rangle \right|^2 \delta(E_f^N - E_i^N - h\nu)$$

Sudden approximation :

$$\psi_f^N = \varphi_f^k \psi_f^{N-1}$$

$$\left\langle \varphi_f^k \left| \frac{e}{mc} \vec{A}.\vec{p} \right| \varphi_i^k \right\rangle \left\langle \psi_f^{N-1} \left| c_k \right| \psi_i^N \right\rangle$$

Matrix element describing the photoemission process. May depend on *A* and hν.

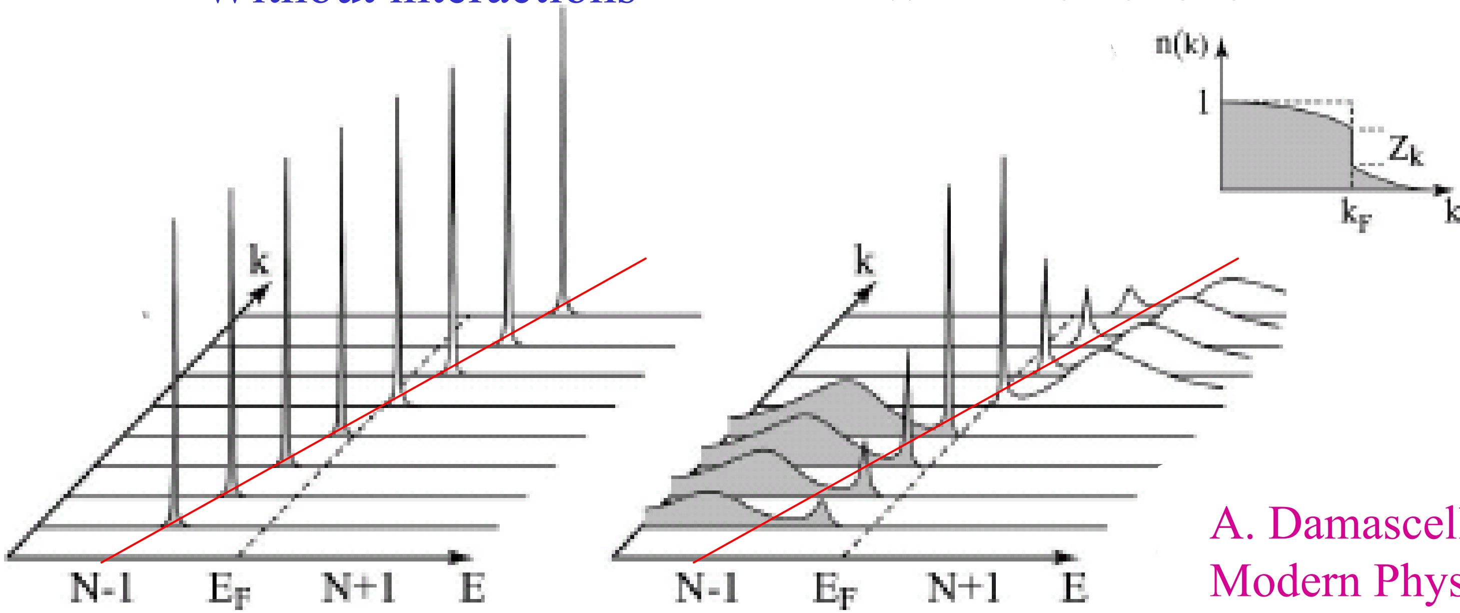
Spectral function A(k,ω)
Interaction effects

Measuring interaction effects

$$I(k,\omega)=\sum_{i,f}\left|M_{i,f}^{k}\right|^{2} f(\omega)A(k,\omega)$$

with $$A(k,\omega)=-\frac{1}{\pi}\frac{\Sigma''(k,\omega)}{\left[\omega-E_k-\Sigma'(k,\omega)\right]^2+\Sigma''(k,\omega)^2}$$

Without interactions | With interactions



A. Damascelli, Rev. Modern Physics 2003

=> Renormalization of the dispersion (« higher effective mass »)

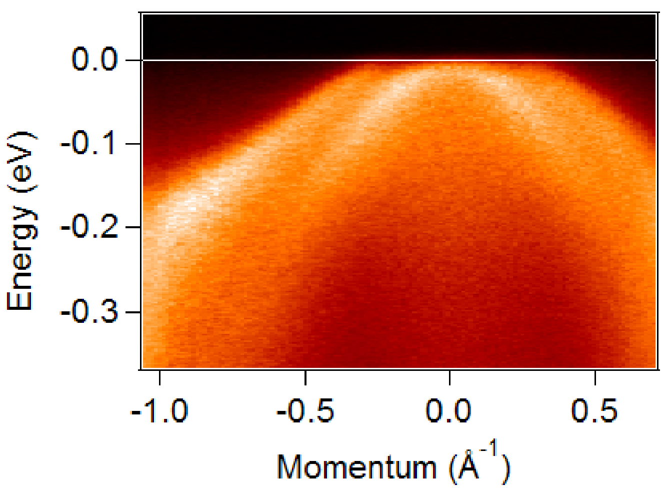
=> Finite linewidth (measurable for a 2D system)

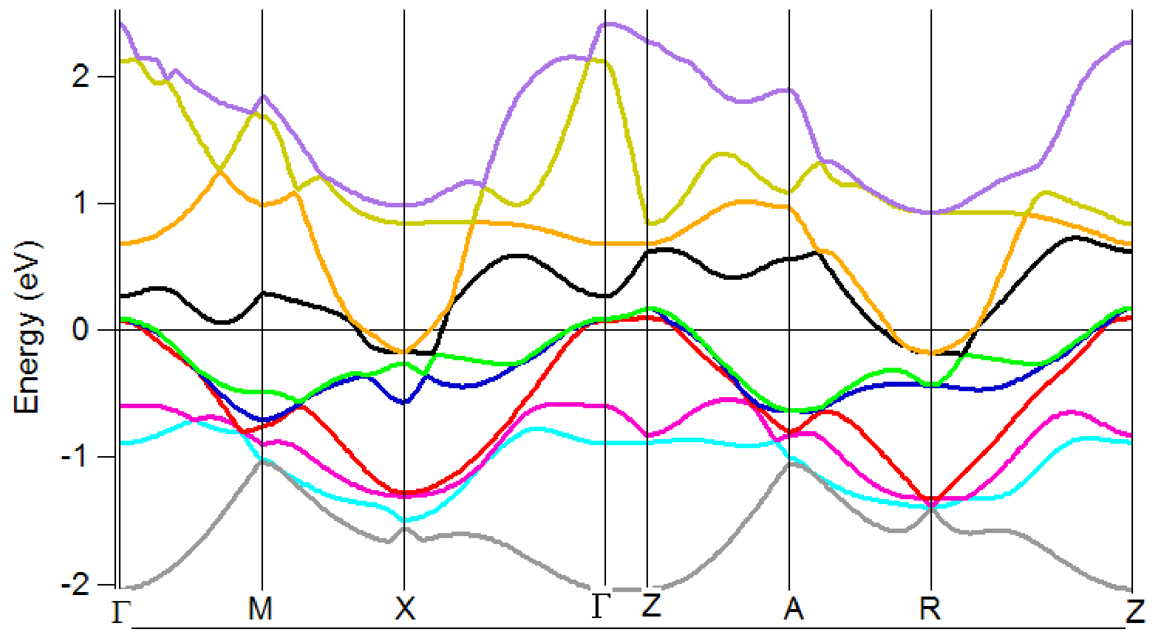
=> Reduced quasiparticle weight Z, transfer of spectral weight to incoherent structures

Estimating the strength of electronic correlations

LDA calculation for $BaFe_2As_2$ *(M. Aichhorn et al.)*

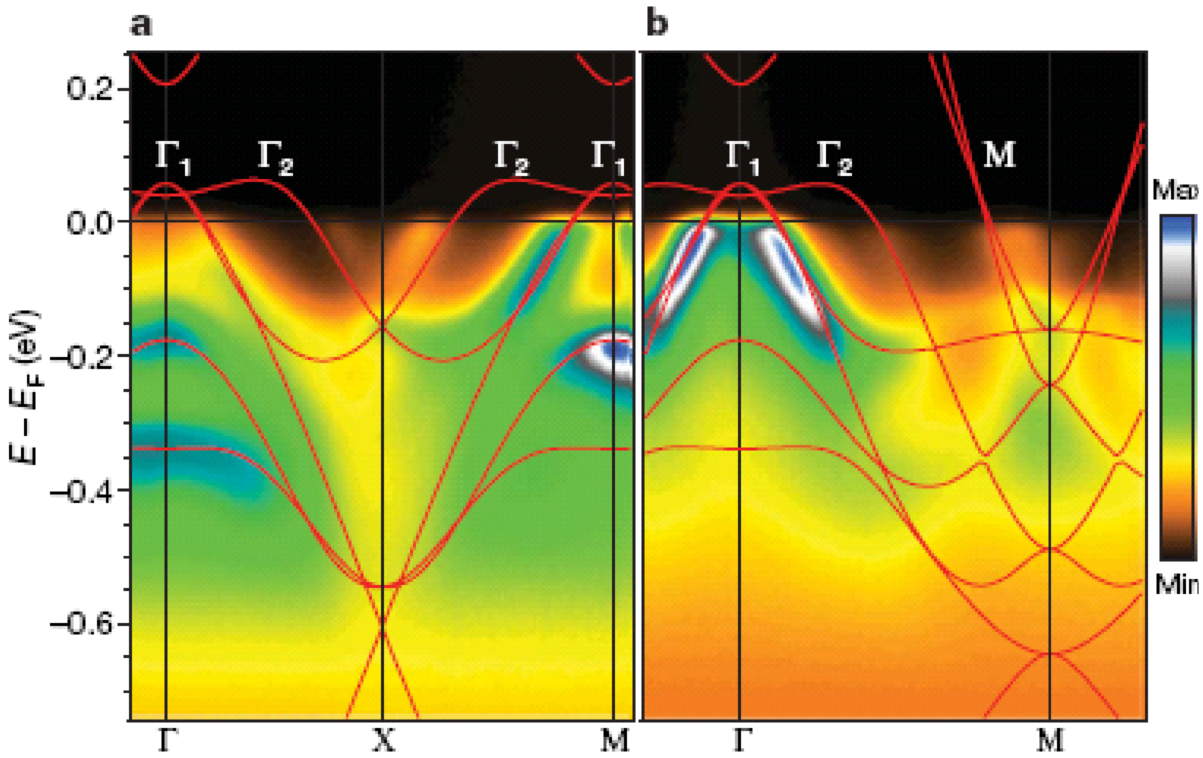
ARPES in $Ba(Fe,Co)_2As_2$
around Γ





Estimating the strength of electronic correlations

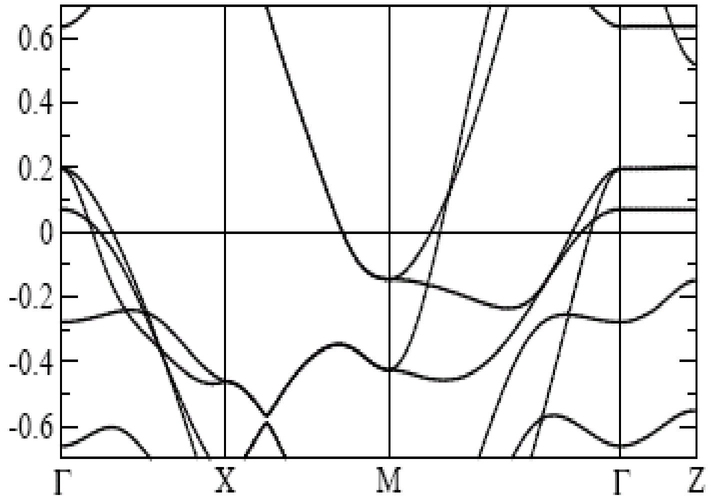
LaFeOP - D.H. Lu, Z.-X. Shen et al., Nature 2008

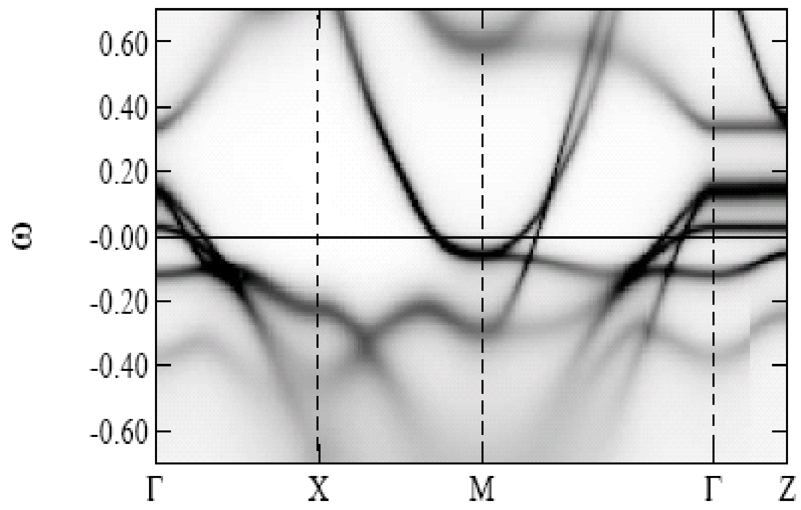


=> Band structure renormalized by factor 2

This renormalization agrees well with calculations including correlation effects

LaFeOAs - M. Aichhorn *et al.*, PRB 2009

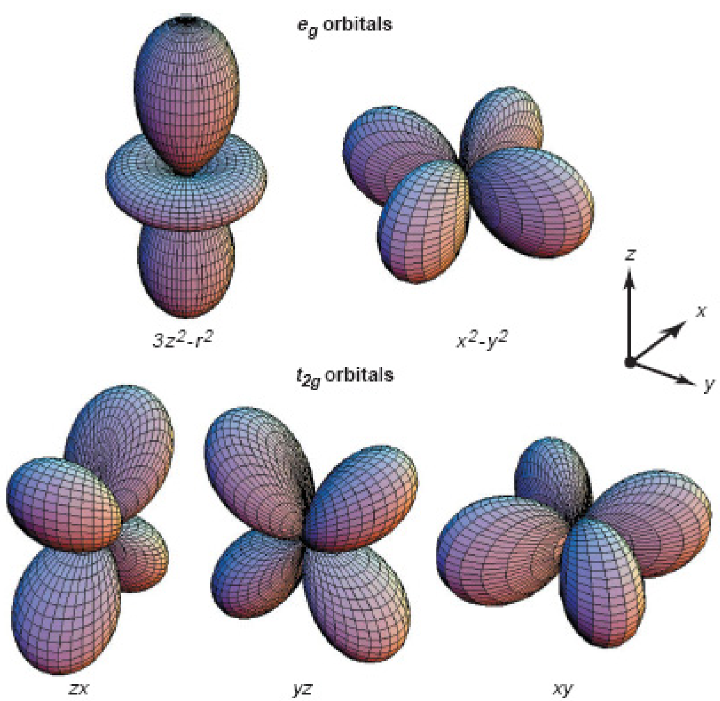


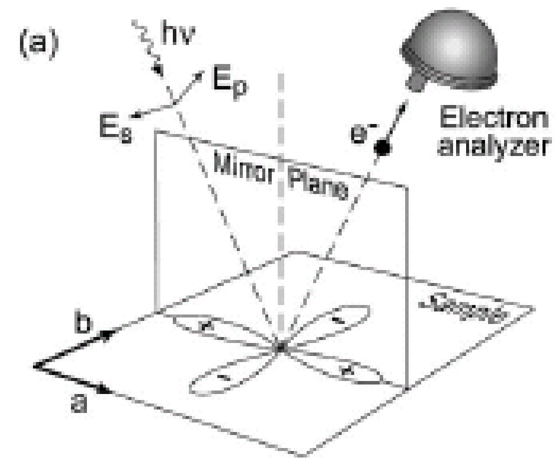


• The degree of correlations may change significantly between different families => m*/m = 2 to 4
• Different behaviors for bands with different orbital symmetries

Probing the symmetry of orbitals with ARPES

Fe 3d orbitals





$$\langle \phi_f^{\mathbf{k}} | \mathbf{A}\cdot\mathbf{p} | \phi_i^{\mathbf{k}} \rangle \begin{cases} \phi_i^{\mathbf{k}} \text{ even} & \langle + | + | + \rangle \Rightarrow \mathbf{A} \text{ even} \\ \phi_i^{\mathbf{k}} \text{ odd} & \langle + | - | - \rangle \Rightarrow \mathbf{A} \text{ odd.} \end{cases}$$

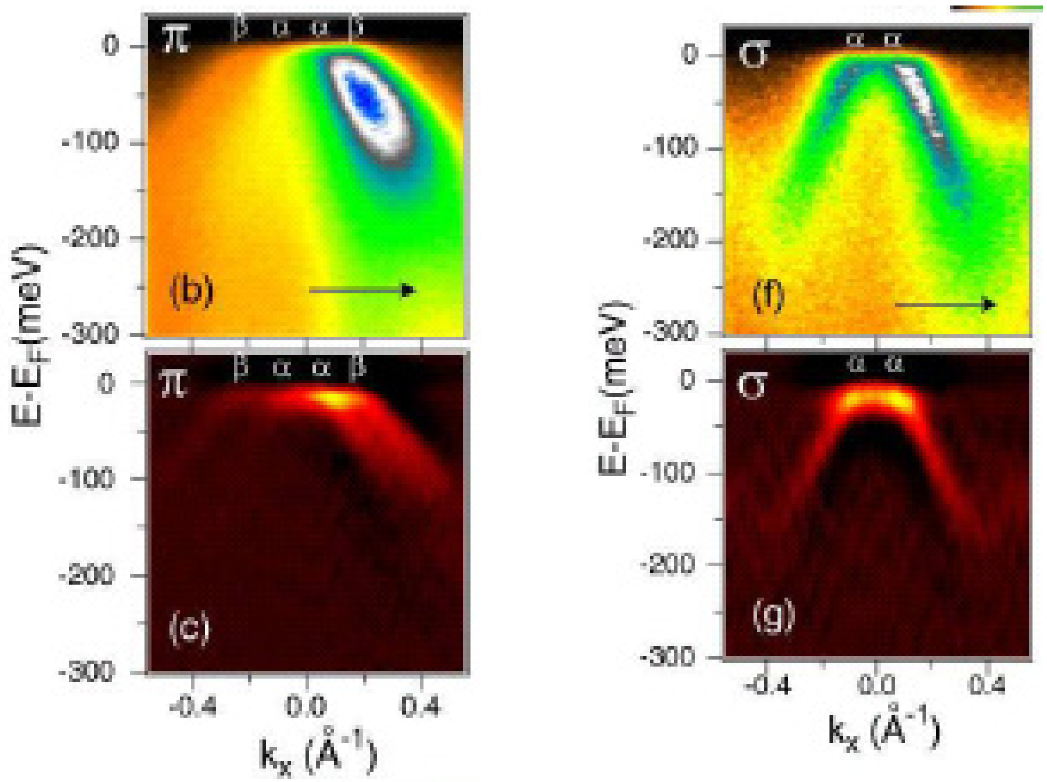
A. Damascelli et al.,
Rev. Mod. Physics 2003

Horizontal polarization => even orbitals
Vertical polarization => odd orbitals

Probing the symmetry of orbitals with ARPES

$Ba(Fe,Co)_2As_2$

« even » « odd »



Zhang, Feng et al. cond-mat 2009

=> The inner pocket is doubly degenerated, with odd and even symmetries (probably d_{XZ} and d_{YZ}).

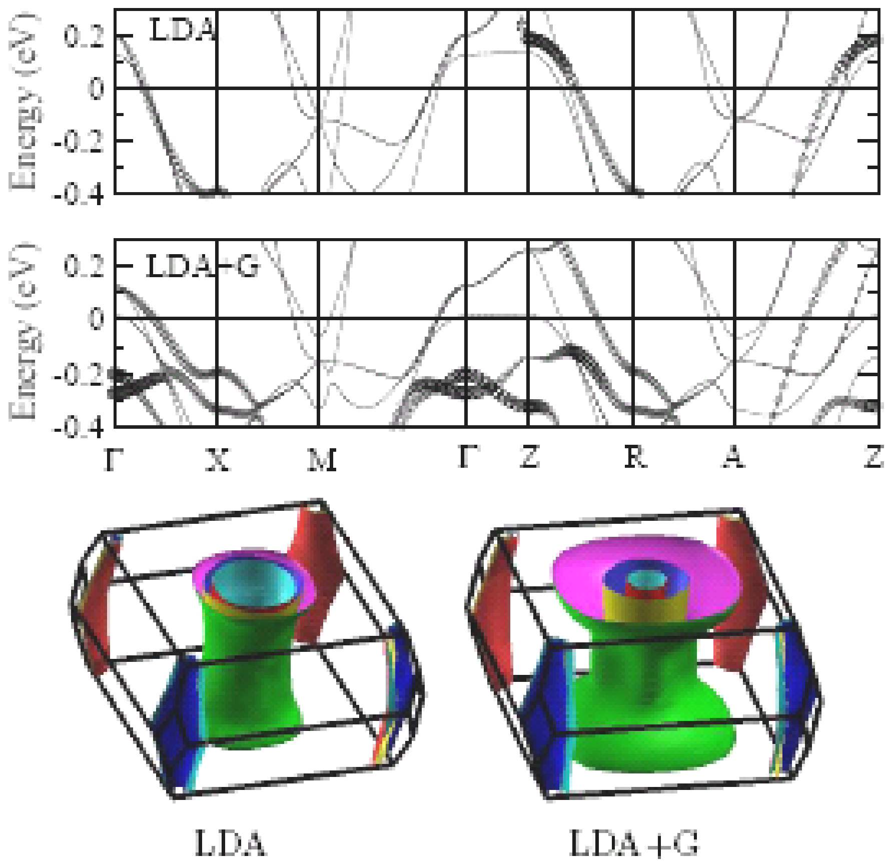
=> The outer pocket is mainly even : could have strong d_z^2 character.

S. Thirupathaia *et al.*, B. Mansart *et al.*

Correlations may enhance the contribution of the d_z^2 band

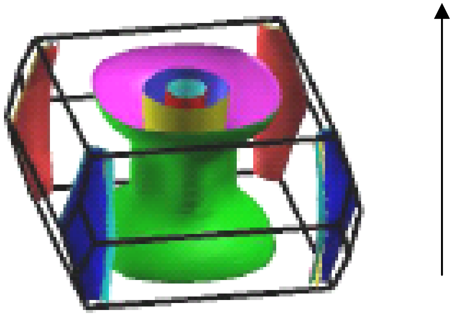
Gutzwiller density functional calculations ($Ba_{0.6}K_{0.4}Fe_2As_2$)

Wang et al., cond-mat/0903.1385



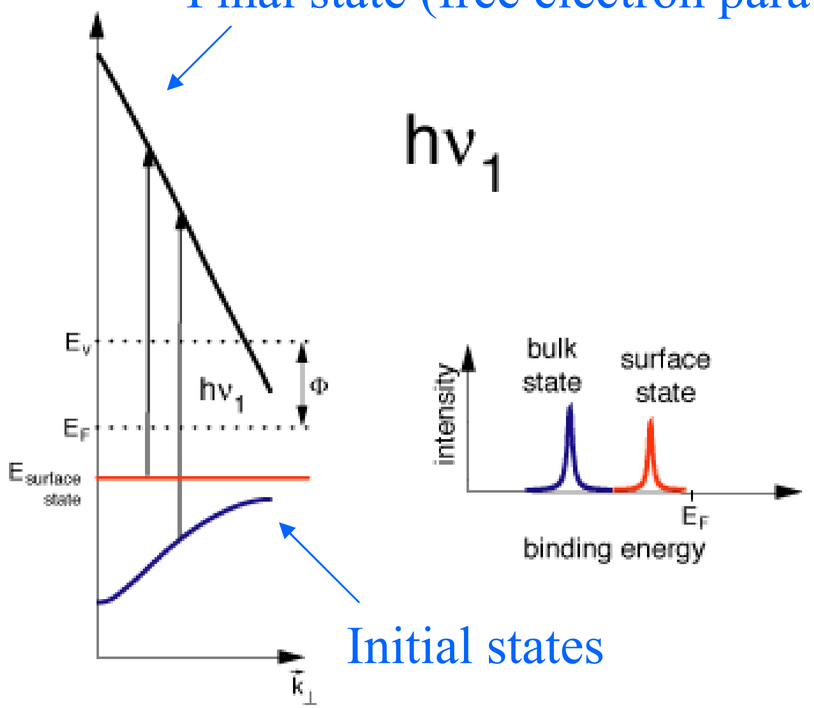
=> Consequences for the electronic properties ?

Probing 3D effects in ARPES

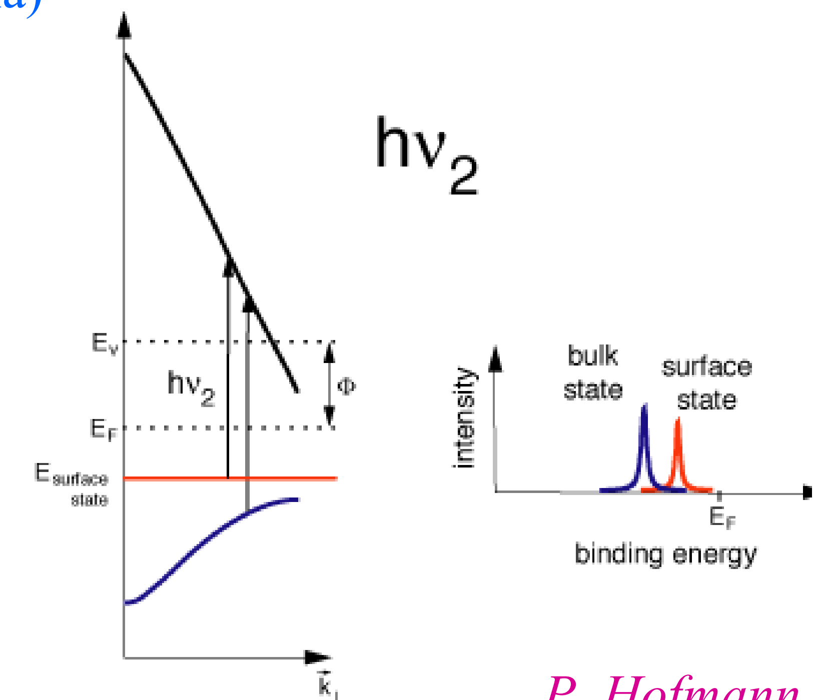


$$k_{\perp} = \frac{\sqrt{2m}}{\hbar}\sqrt{h\nu - W + V_0}$$

Final state (free electron parabola)



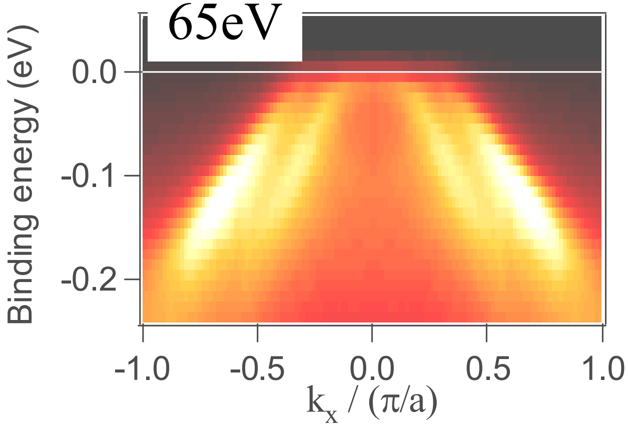
Initial states

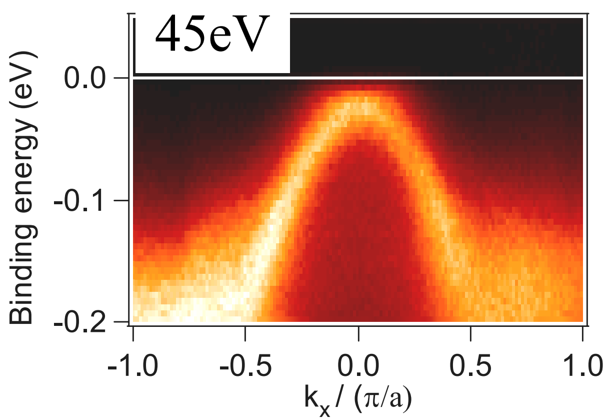


P. Hofmann

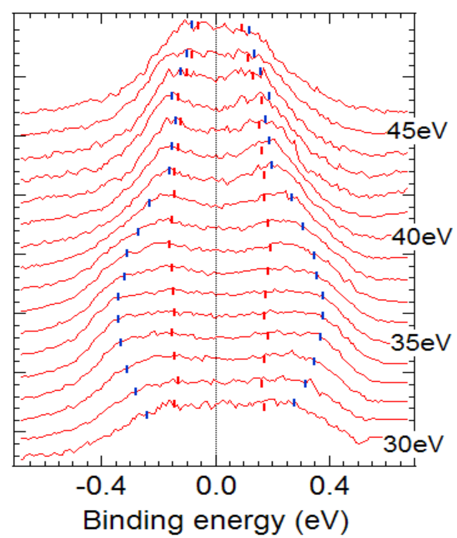
3D effects on the hole pockets

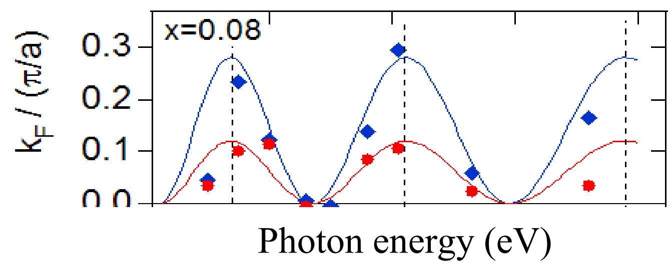
There are strong variations of the hole pockets with photon energy

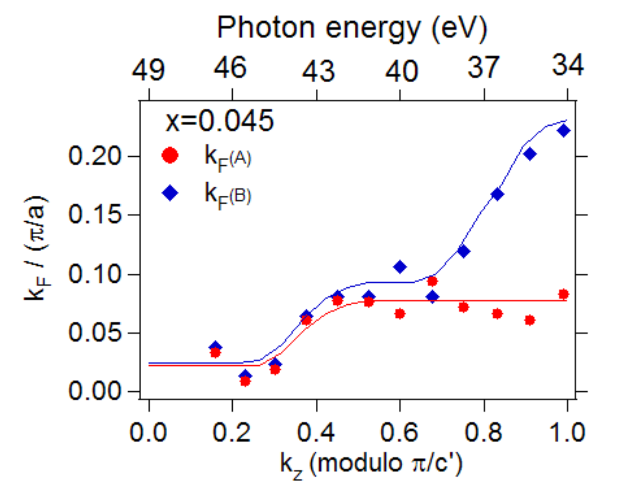




Oscillations with kz periodicity

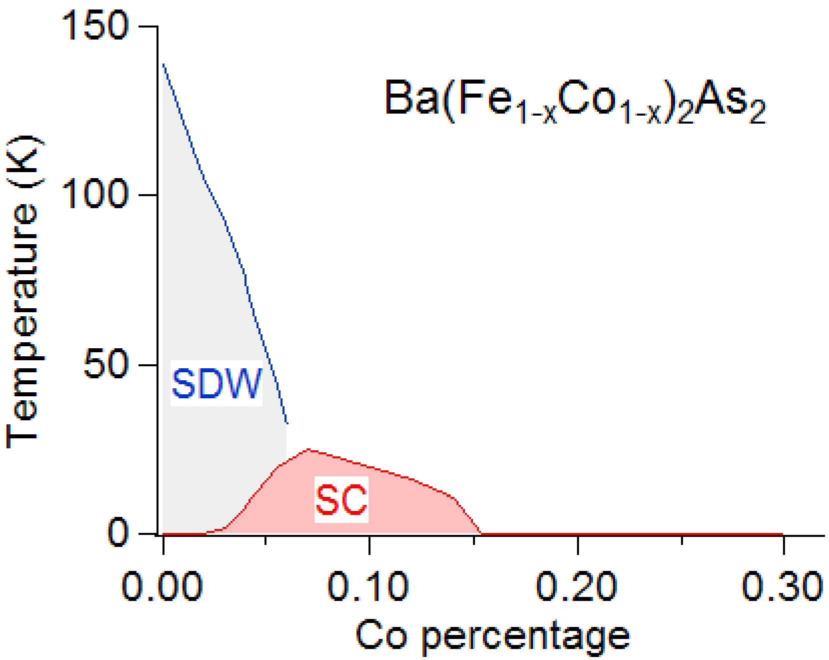


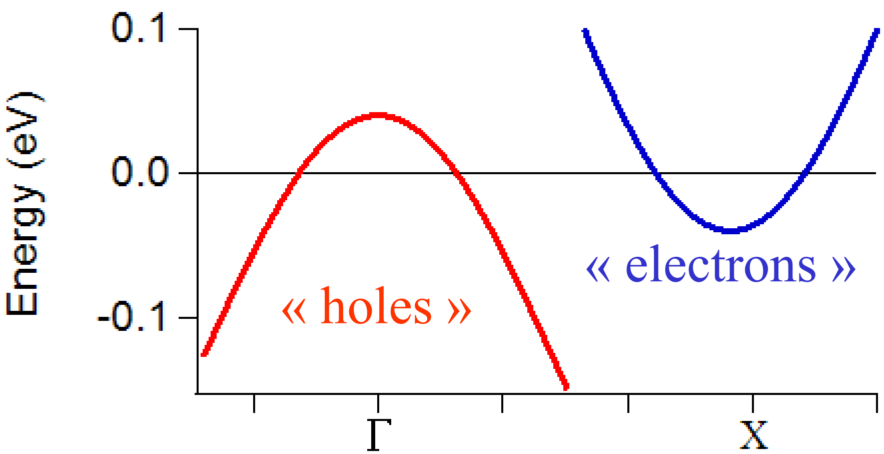


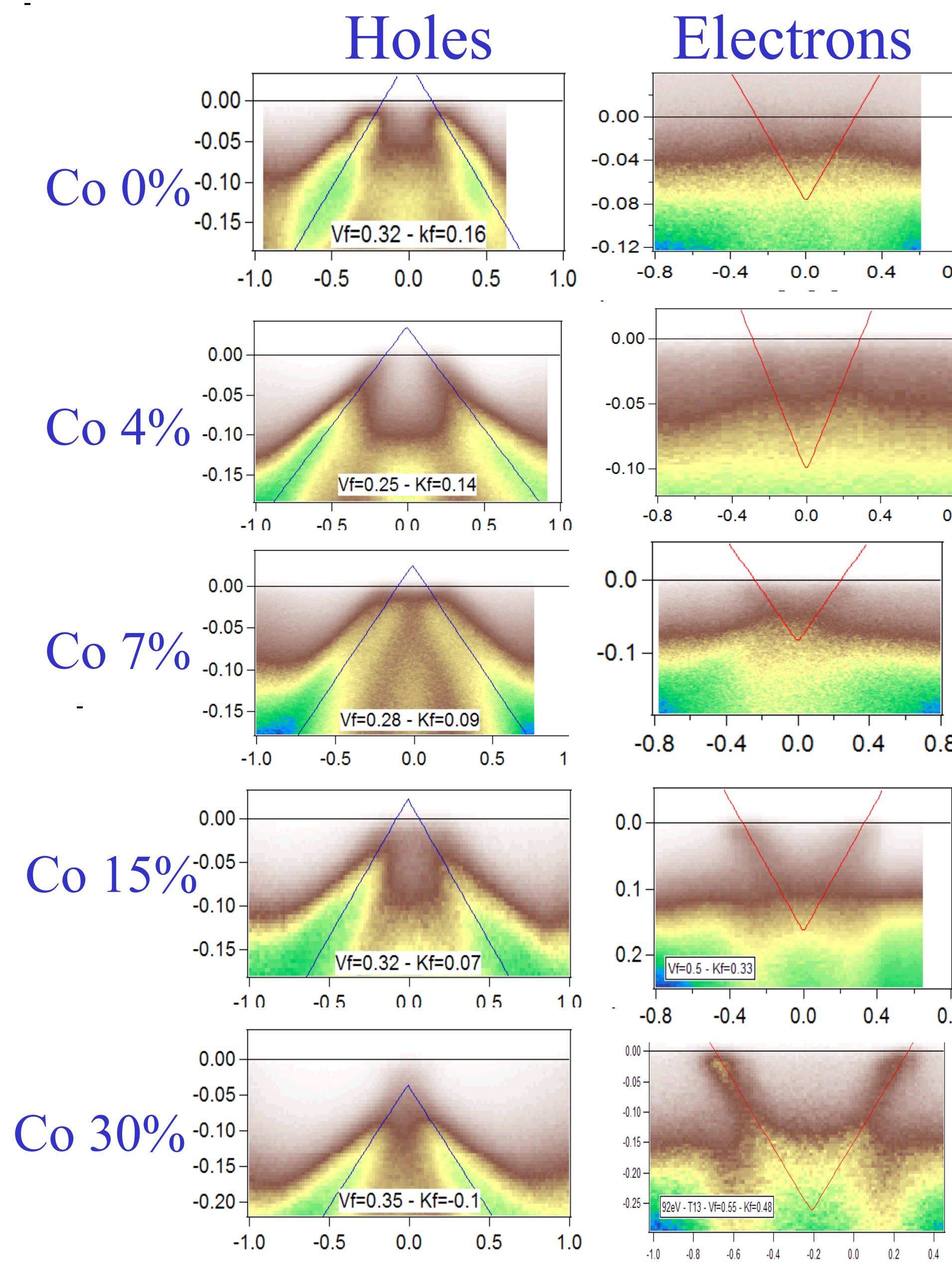


=> Significant 3D effects in this family (unlike for example in cuprates)

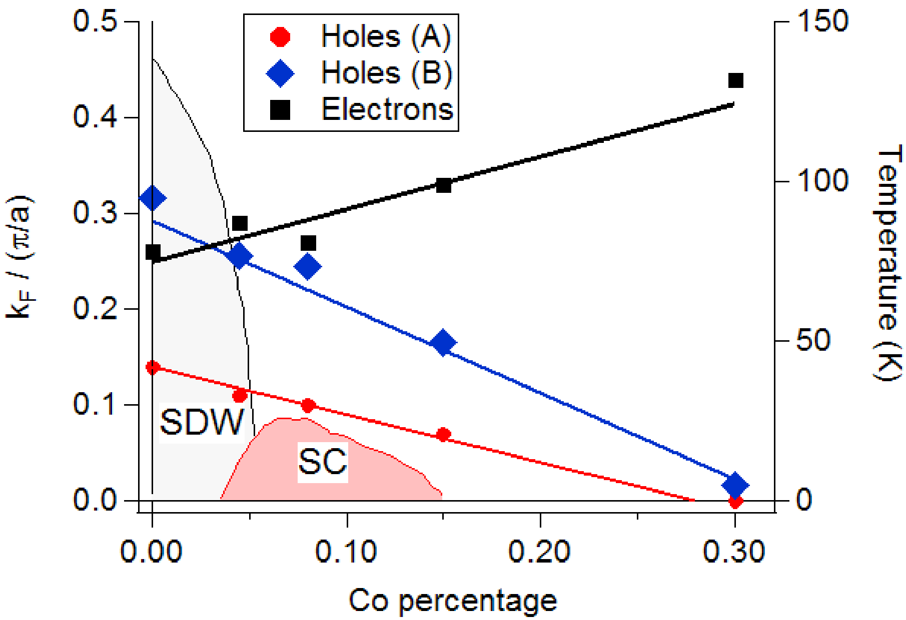
Evolution with electron doping : $Ba(Fe_{1-x}Co_x)_2As_2$

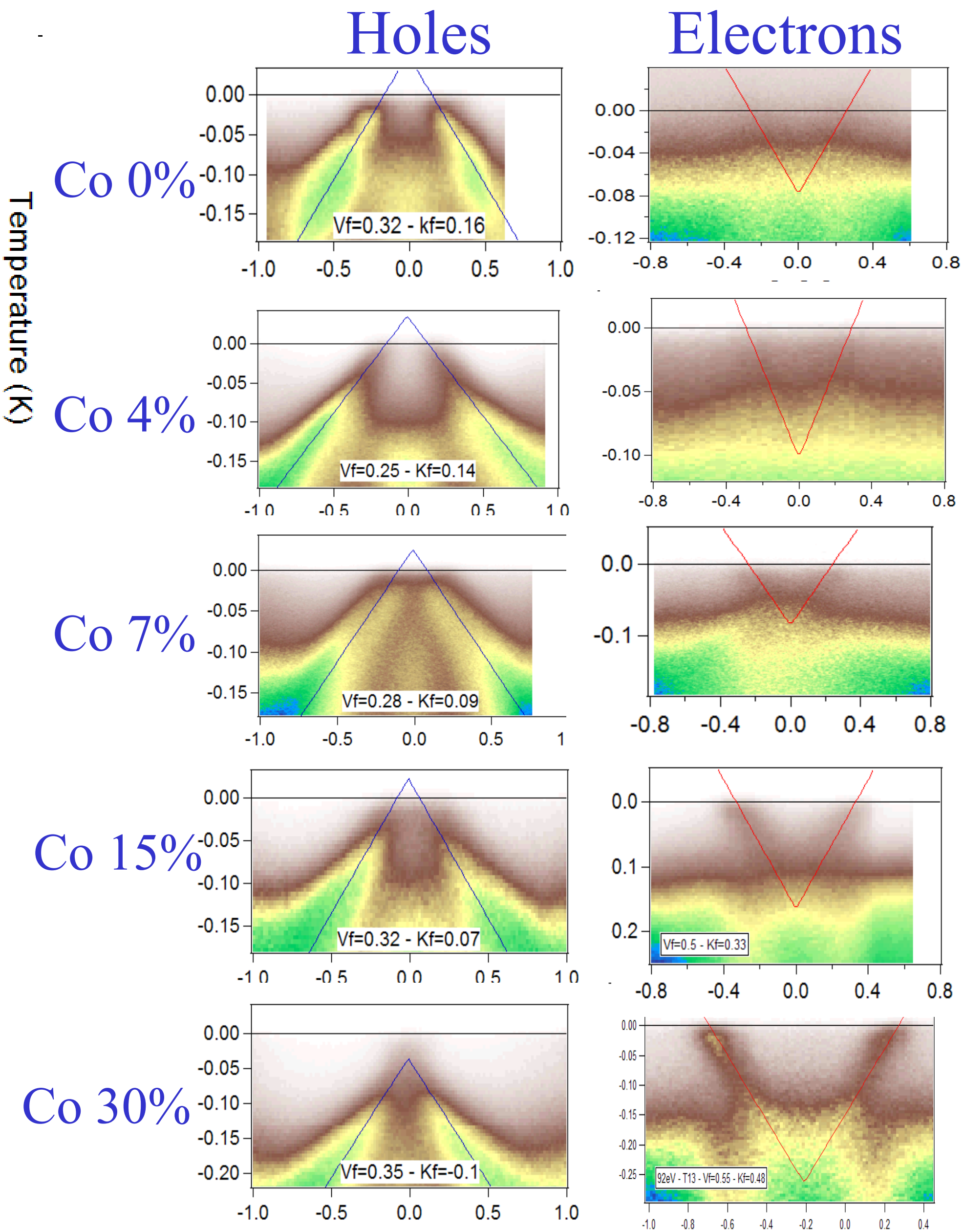






Evolution with electron doping : $Ba(Fe_{1-x}Co_x)_2As_2$



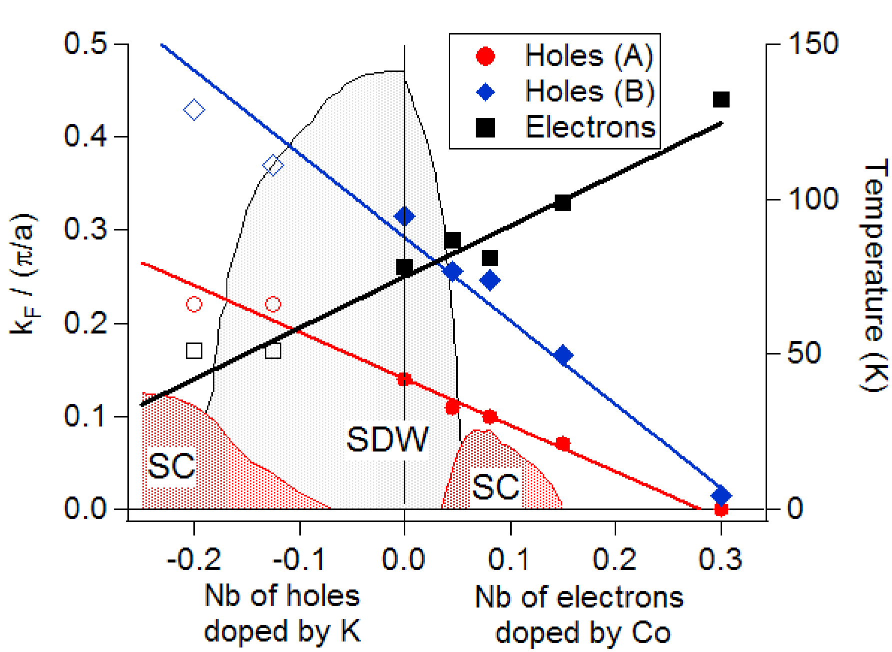


=> A rigid band filling can be applied

=> « Best » nesting between the electron and outer hole band at k_z=1

V. Brouet et al., PRB 2009

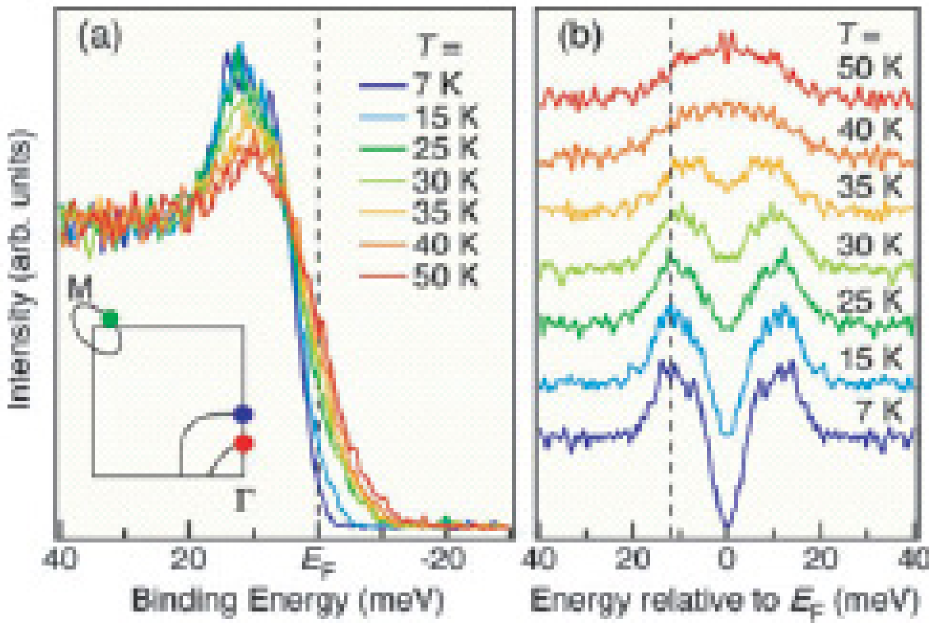
Exploring the magnetic and superconducting properties with ARPES

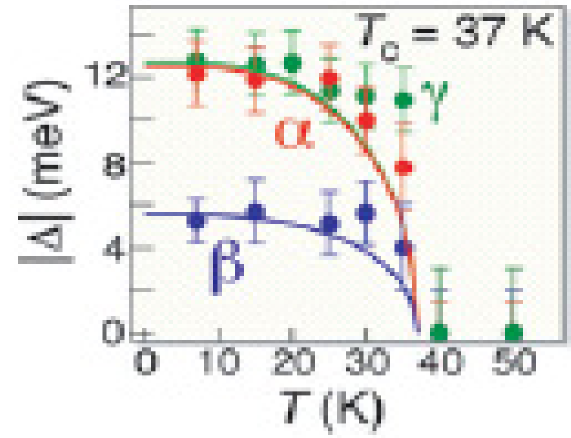


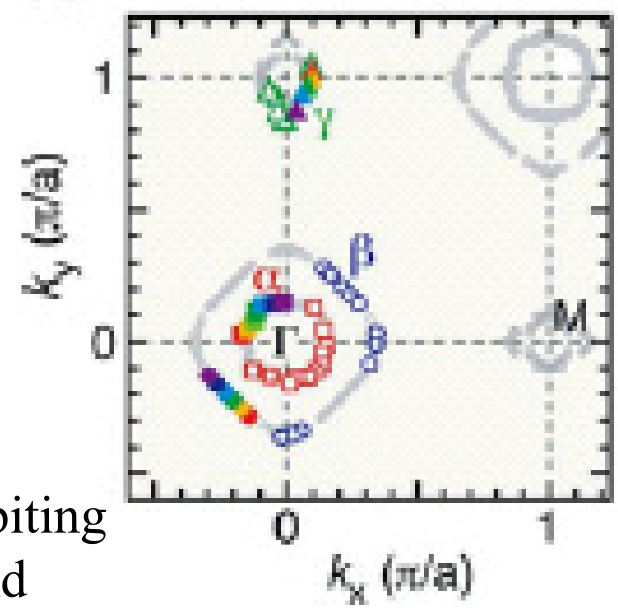
=> Value and symmetry of the superconducting gap on the different bands ?

=> Role of nesting in the formation of the magnetic state ?

First determination of superconducting gaps in $Ba_{0.6}K_{0.4}Fe_2As_2$





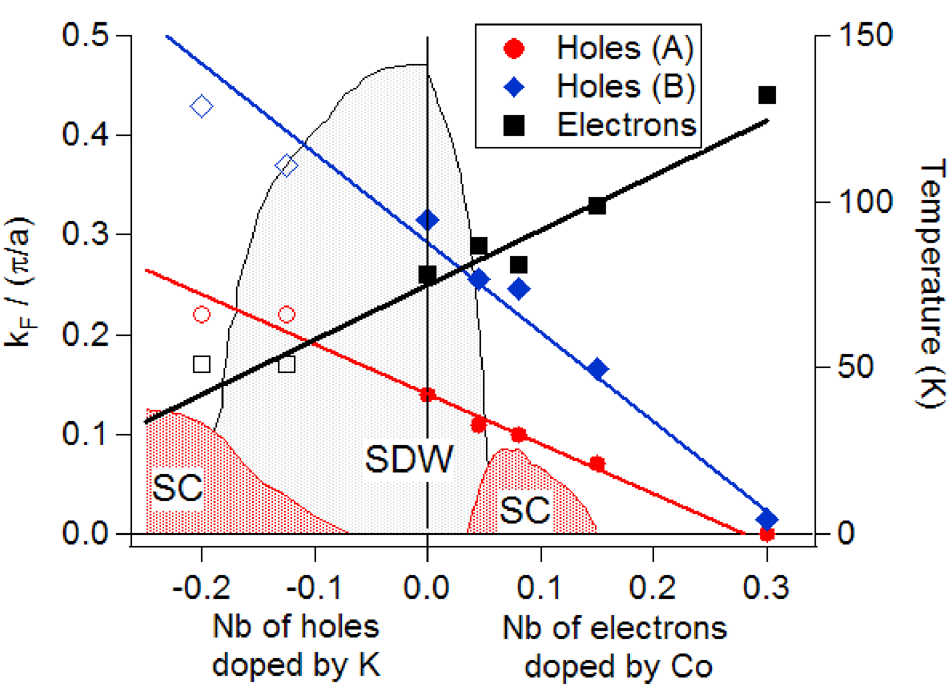


H. Ding et al. Europhysics Letters **83**, 47001 (2008)

=> Nearly isotropic gaps
=> Same values on the hole and electron bands exhibiting the best nestings, smaller value on the other hole band

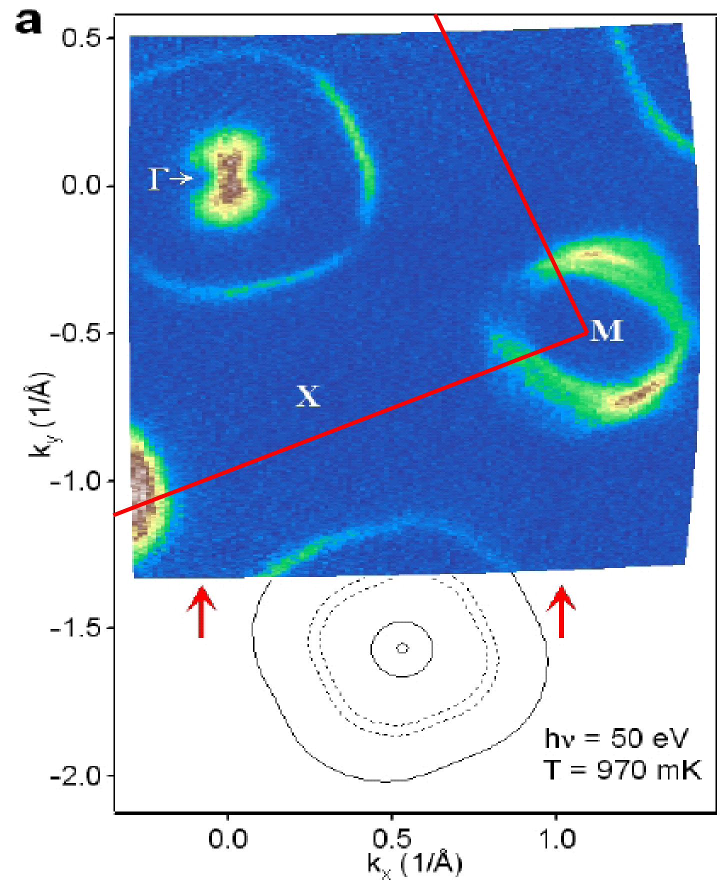
Is « nesting » important for superconductivity ?

$BaFe_2As_2$



Asymmetry between hole and electron sides, as well as the disappearance of superconductivity when the hole band is filled support the importance of interband transitions

LiFeAs



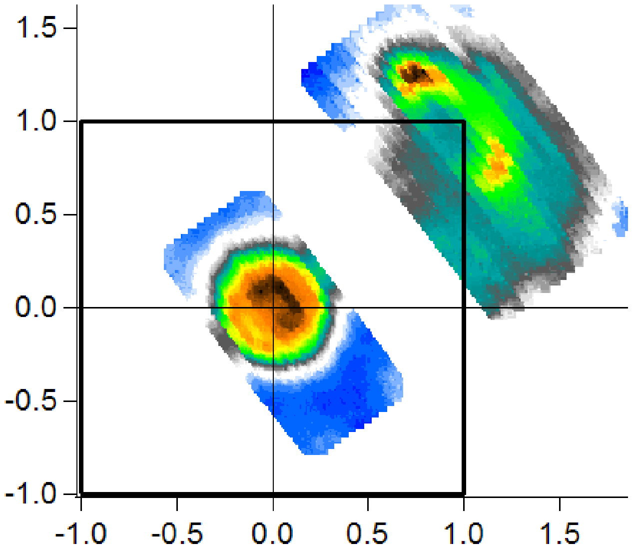
However, in LiFeAs, nesting is completely lost, which does not weaken much superconductivity (T_c=18K)

Borisenko, cond-mat 2010

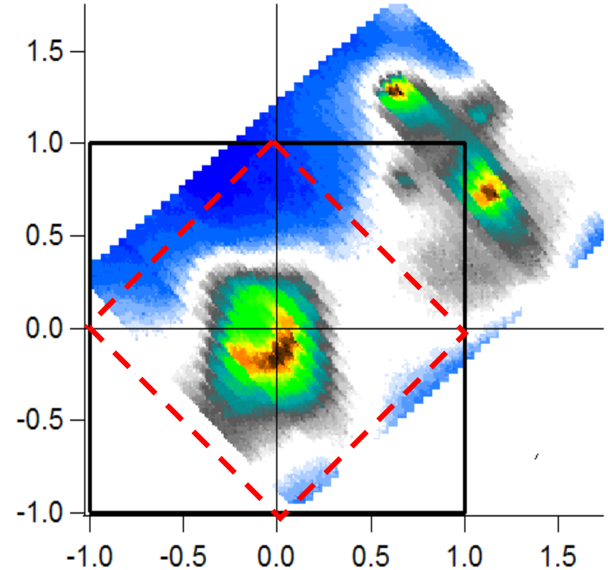
Is « nesting » important for magnetism ?

$BaFe_2As_2$

Fermi Surface above T_N (150K)



Fermi Surface below T_N (150K)



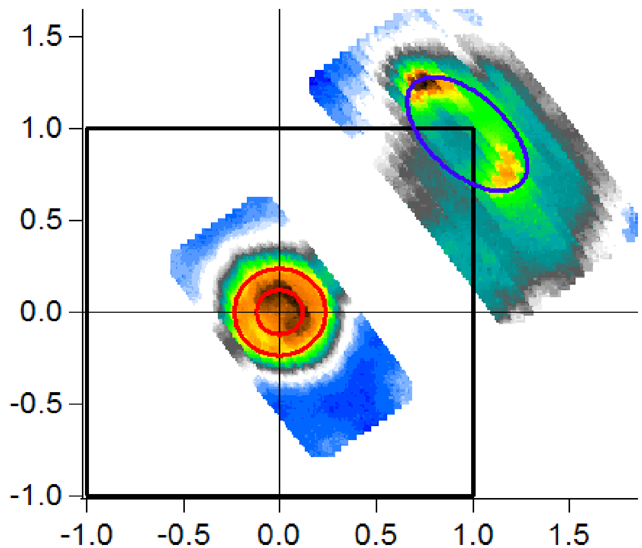
Only small parts of the FS are remaining : « droplets » FS

M.F. Jensen, in preparation

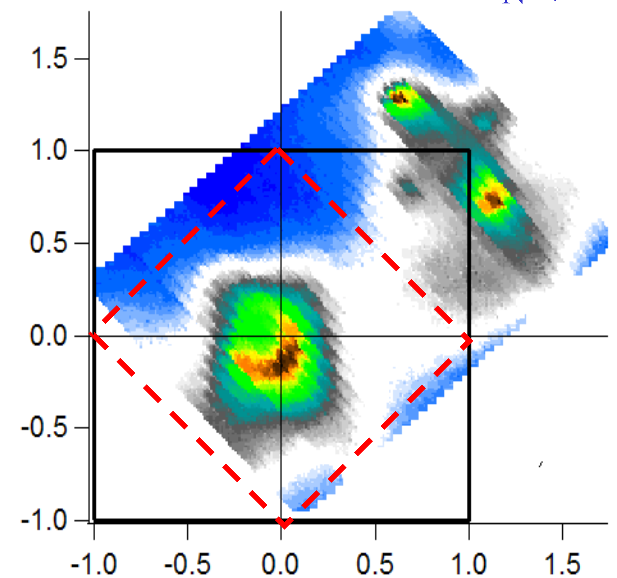
Is « nesting » important for magnetism ?

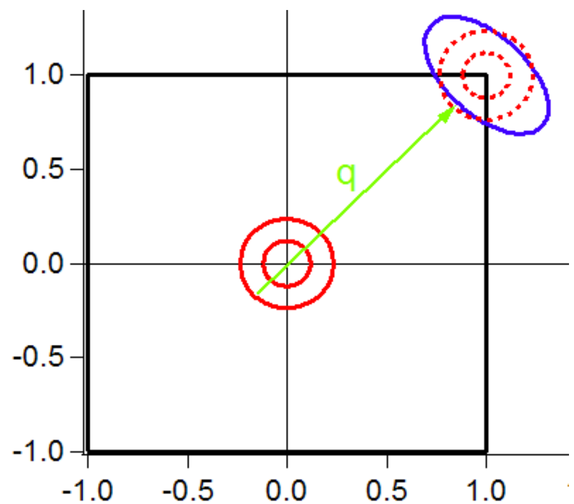
$BaFe_2As_2$

Fermi Surface above T_N (150K)



Fermi Surface below T_N (150K)





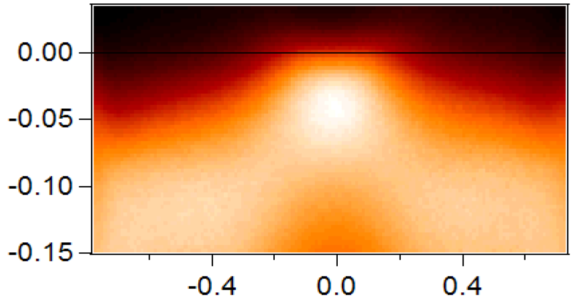
Only small parts of the FS are remaining : « droplets » FS

M.F. Jensen, in preparation

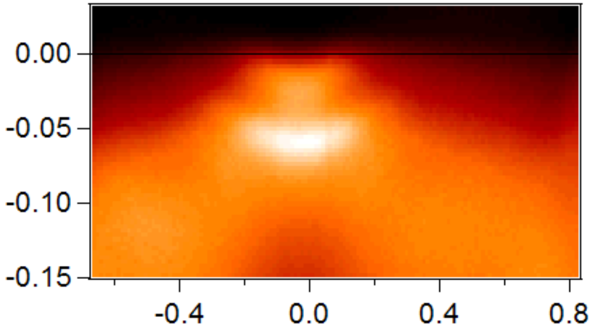
More than a simple folding

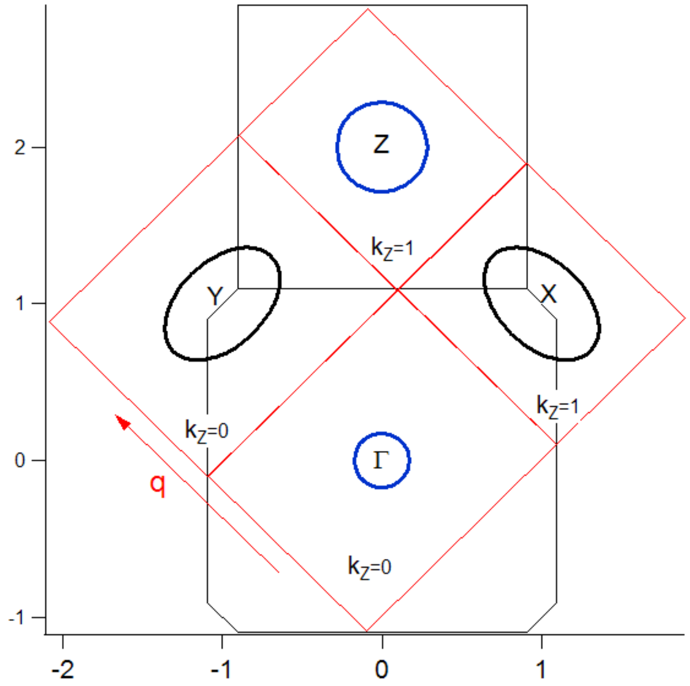
Reconstruction of the electron pockets (splitting)

150 K



20 K





Splitting due to :

- local moments ?
- inequivalency between X and Y (orthorhombicity) ?
- k_z dispersion ?

See also : L.X Yang et al., PRL **102**, 107002 (2009)
M. Yi et al., PRB **80**, 174510 (2009)
S. de Jong et al., cond-mat/0912.3434

Conclusions

- Renormalization of the LDA band structure by a factor 2-3
  => *moderately correlated systems*

- Three hole bands and two electron pockets
  => *one hole band probably with d_z^2 character*

- Significant 3D dispersion

- Rigid-band evolution with doping - *unlike in other families of superconductors like Ba(Fe,Ru)$_2$As$_2$*

- Different superconducting gaps for the different bands

- Significant reconstruction of the electronic structure in the magnetic state.

Collaborators

Maria Fuglsang Jensen, Marino Marsi, Barbara Mansart
LPS Orsay

Amina Taleb-Ibrahimi, Patrick Lefèvre, François Bertran, Alessandro Nicolaou
CASSIOPEE beamline, SOLEIL

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