What can ARPES tell U about electronic correlations in the Fe-based superconductors?

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ピアー　リシャー
芮夏岩

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ICTP Meeting, Trieste
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Collaborators

ARPES

IOP, CAS (H. Ding Lab)
Tohoku University (Takahashi Lab)
Renmin University (S. C. Wang Lab)
PSI (M. Shi Lab)

Samples

(Where everything begins)

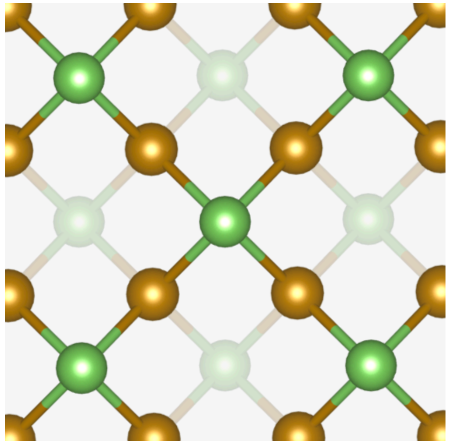
IOP, CAS (X.-L. Chen Lab)
IOP, CAS (C.-Q. Jin Lab)
IOP, CAS (G.-F. Chen Lab)
IOP, CAS (J.-L. Luo Lab)
Peking University (N. L. Wang Lab)
Nanjing University (H.-H. Wen Lab)
Zhejiang University (G.-H. Cao Lab)
Zhejiang University (Z.-A. Xu Lab)
Zhejiang University (M.-H. Fang Lab)
USTC (X.-H. Chen Lab)
Rice, (P.-C. Dai Lab)
ONL (A. Safa-Sefat Lab)
UC-Irvine (Z. Fisk Lab)
BNL (G.-D. Gu Lab)
BNL (C. Petrovic lab)
KIT (C. Meingast lab)
Etc…

Theory

IOP, CAS (Z. Fang Group)
IOP, CAS (X. Dai Group)
IOP, CAS (X.-X. Wu Group)
Tsinghua University (Z. Y. Weng Group)
Purdue and IOP, CAS (J. P. Hu Group)
Boston College (Z. Wang Group)
Rutgers (G. Kotliar and K. Haule Groups)
E. Polytechnique, Paris (S. Biermann Group)
Shanghai Jiaotong (W. Ku Group)
+ instructive discussions with others

Electronic correlations

Local or non-local?



Duality of the 3*d* electrons in bridged systems
(super-exchange)

Long timescale: the electrons are itinerant and do participate in the transport properties.

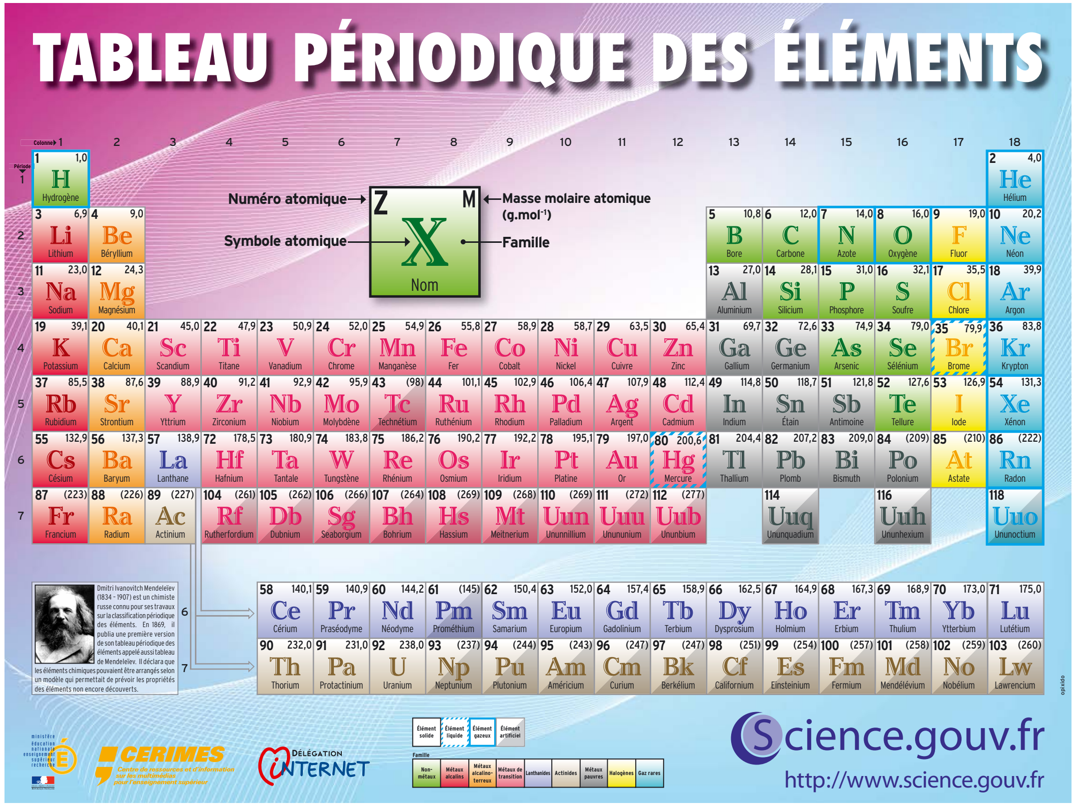
Short timescale: the electrons are “atomic-like”.

Outline

1. Filling the 3*d* shell of the 122 materials: local physics.
2. The nature of the superconducting pairing in the Fe-based superconductors: short-range physics.
3. Non-Fermi liquid behavior induced by low-energy interactions in doped LiFeAs: non-local physics.
4. Coherent to incoherent crossover in KFe_2As_2: not-sure-yet physics.
5. Conclusions

Filling the 3*d* shell of the 122 materials

Motivations

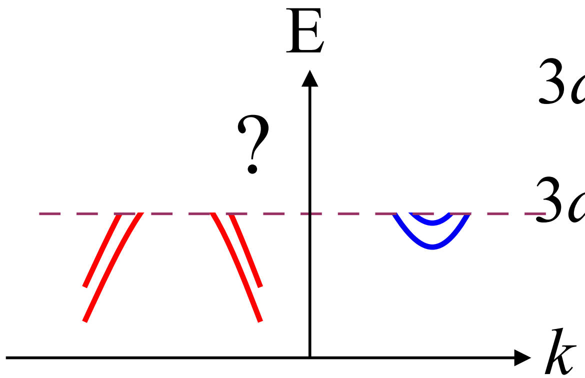


New Journal of Physics
The open-access journal for physics

Coherence–incoherence crossover in the normal state of iron oxypnictides and importance of Hund's rule coupling

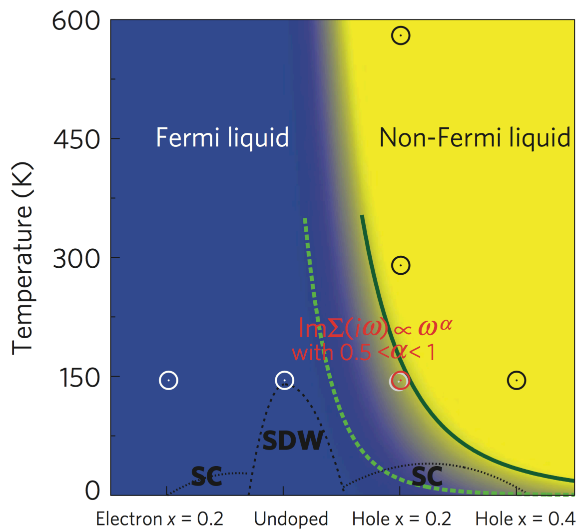
K Haule[1] and G Kotliar
Department of Physics, Rutgers University, Piscataway, NJ 08854, USA
E-mail: haule@physics.rutgers.edu

New Journal of Physics **11** (2009) 025021 (13pp)
Received 16 December 2008
Published 27 February 2009
Online at http://www.njp.org/
doi:10.1088/1367-2630/11/2/025021



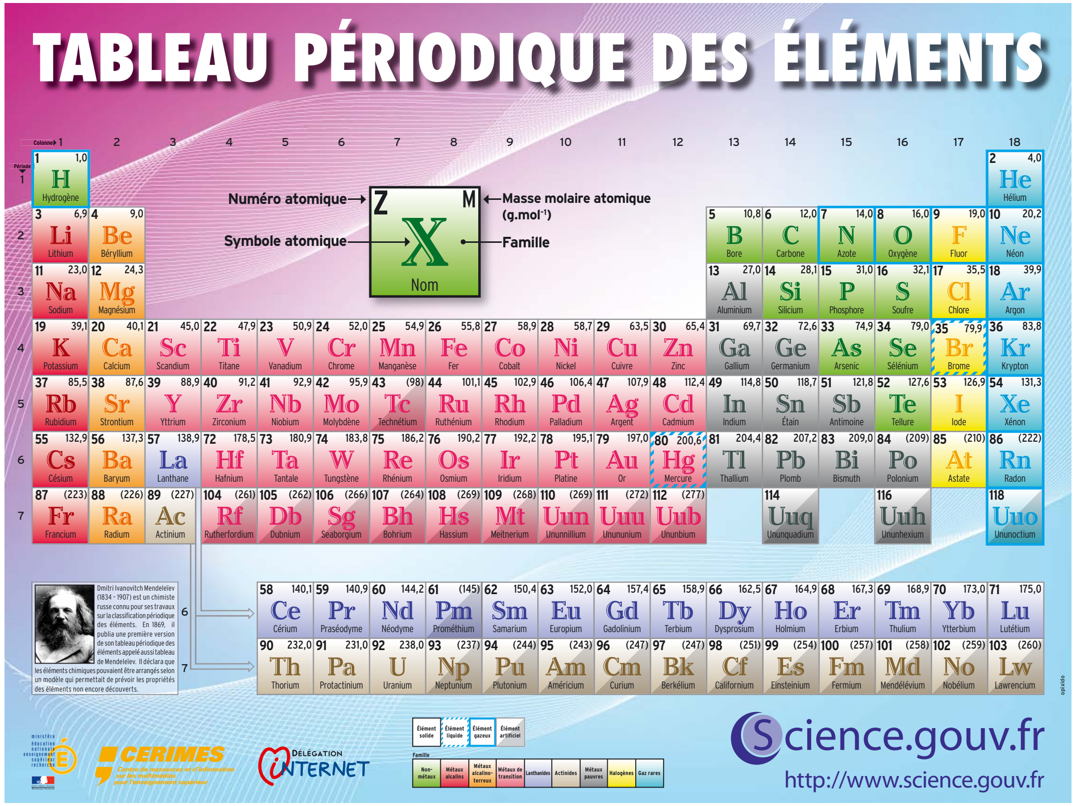
$3d^7$ Co^{2+}

$3d^6$ Fe^{2+}



Werner *et al.*, Nature Phys. **8**, 331 (2012)

Motivations



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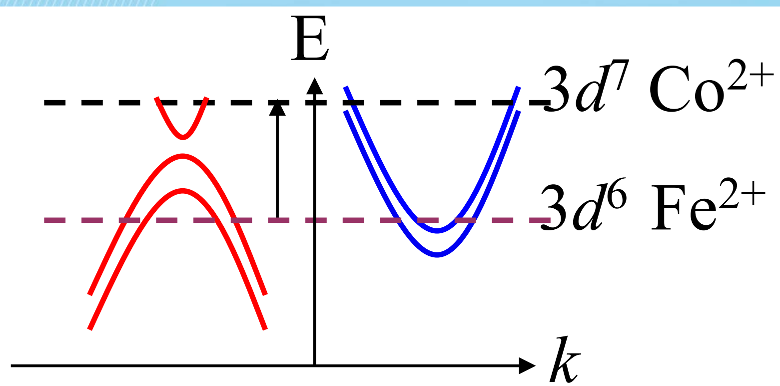
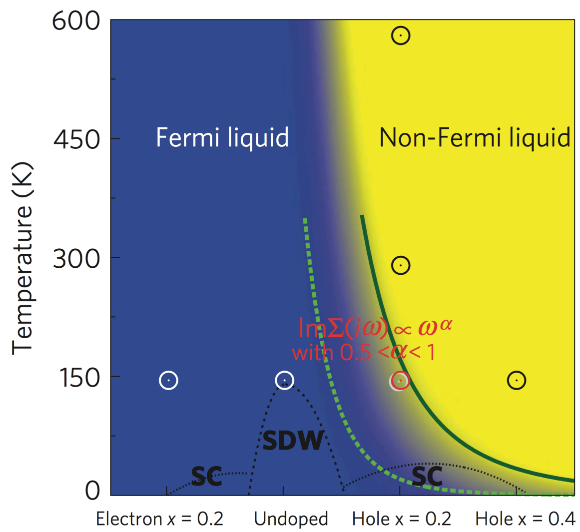
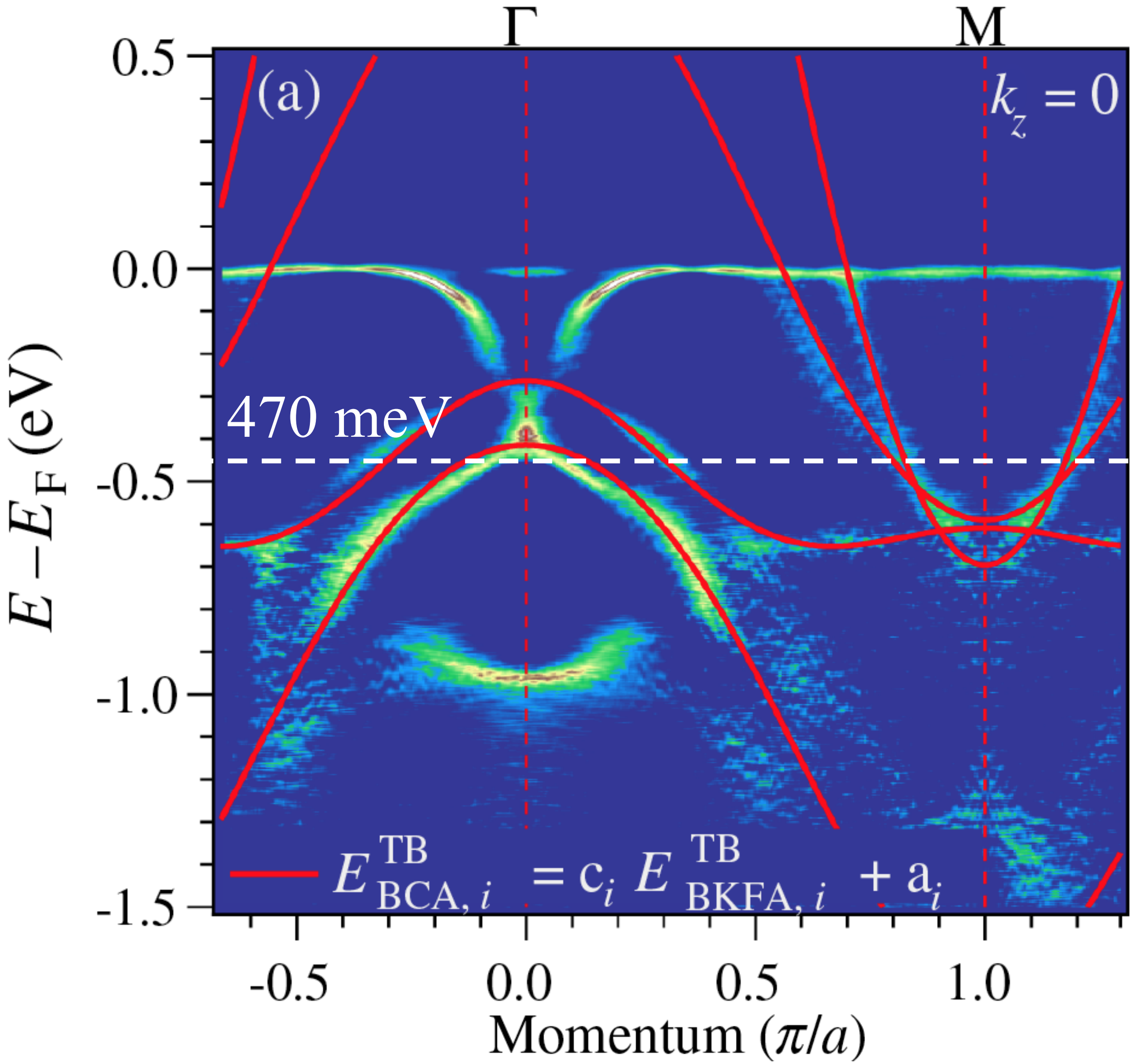




Werner *et al.*, Nature Phys. **8**, 331 (2012)

Unoccupied states in ferropnictides



N. Xu *et al.*, PRX **3**, 011006 (2013)

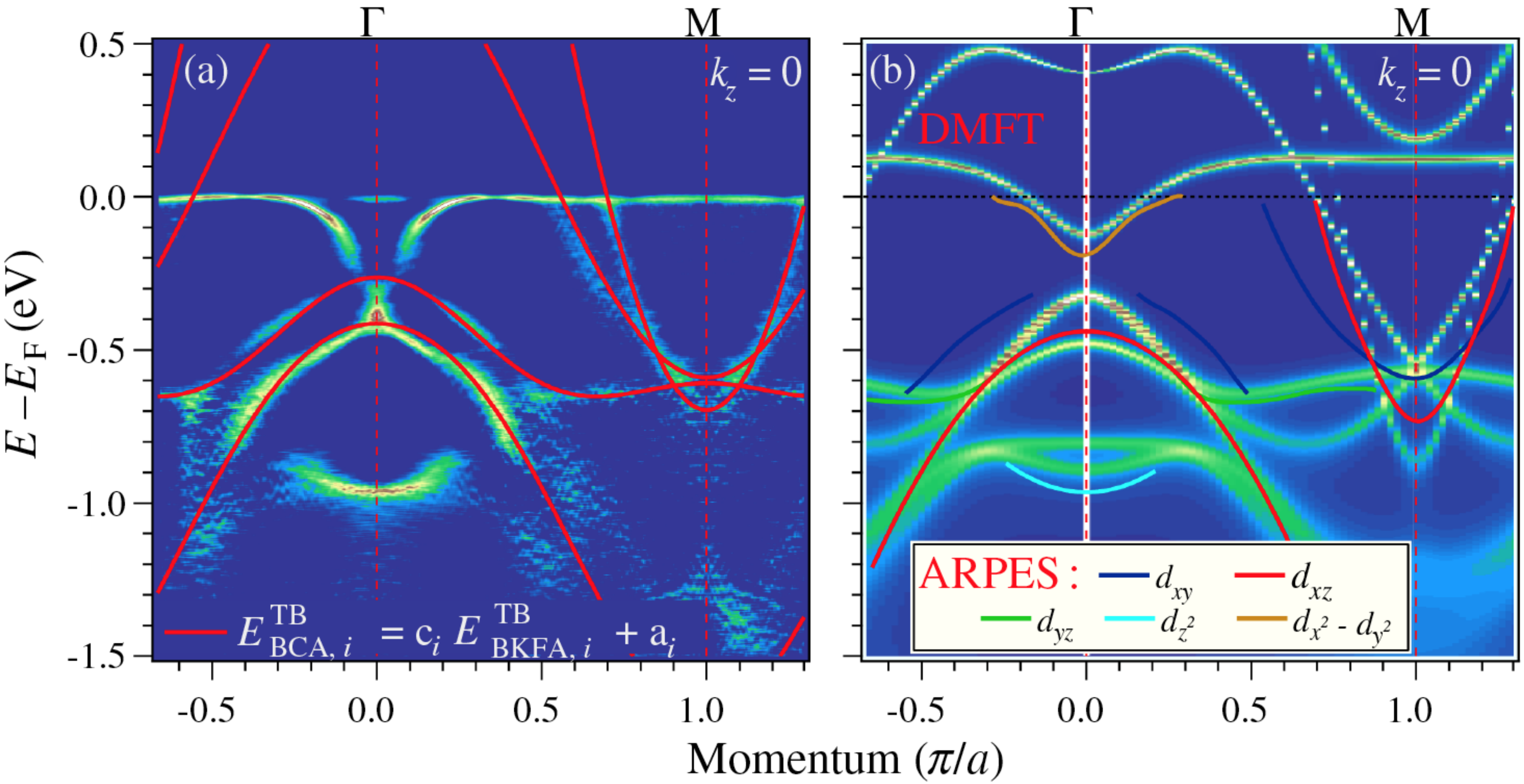
Red curves are fit to optimally-doped (Ba,K)Fe_2As_2 that have been renormalized

d_{xy} (β): x 4

Other bands: x 2

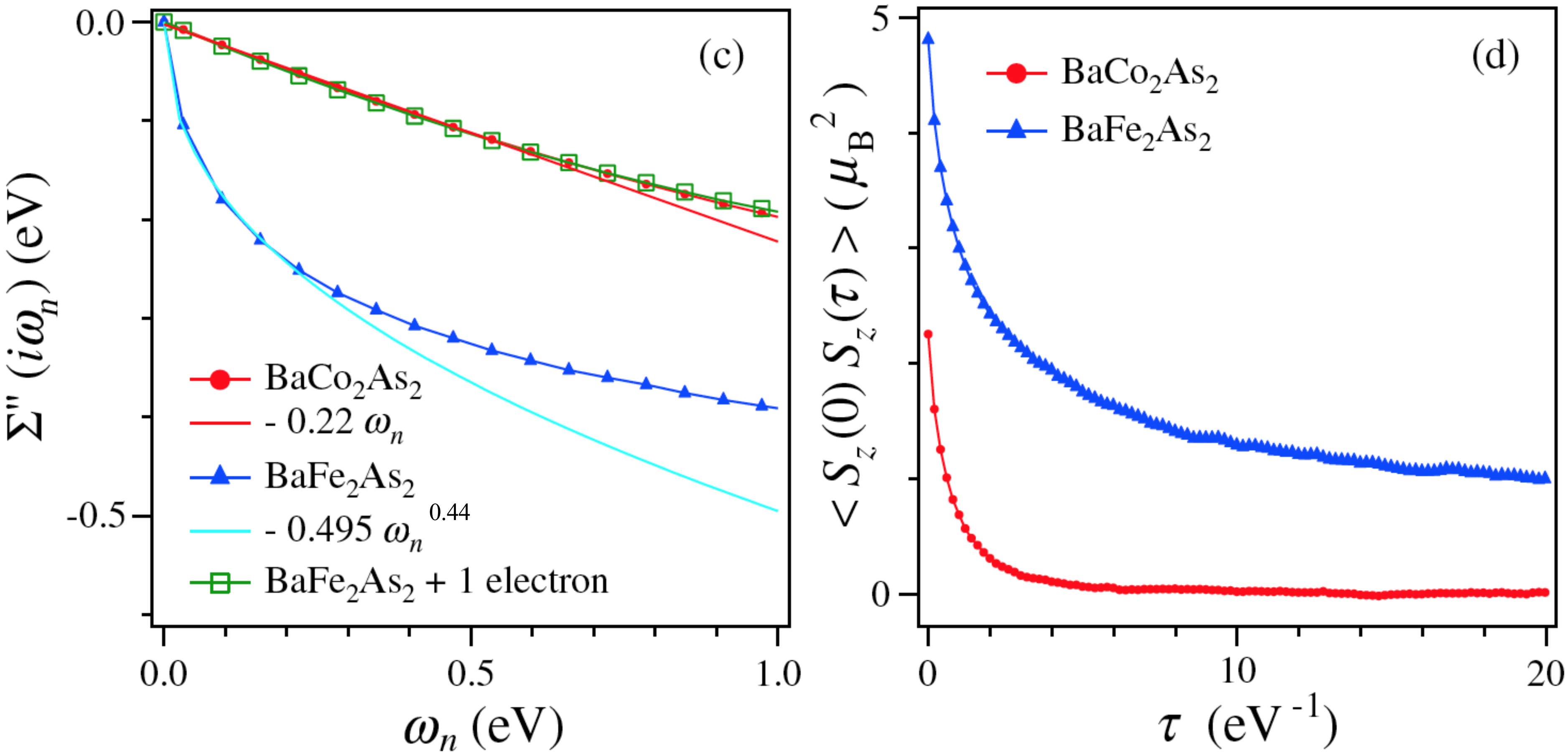
Except for the renormalization, $BaCo_2As_2$ allows the visualization of the unoccupied states in the ferropnictides.

ARPES *vs* DMFT: $BaCo_2As_2$



N. Xu *et al.*, PRX **3**, 011006 (2013)

$BaCo_2As_2$ *vs* $BaFe_2As_2$

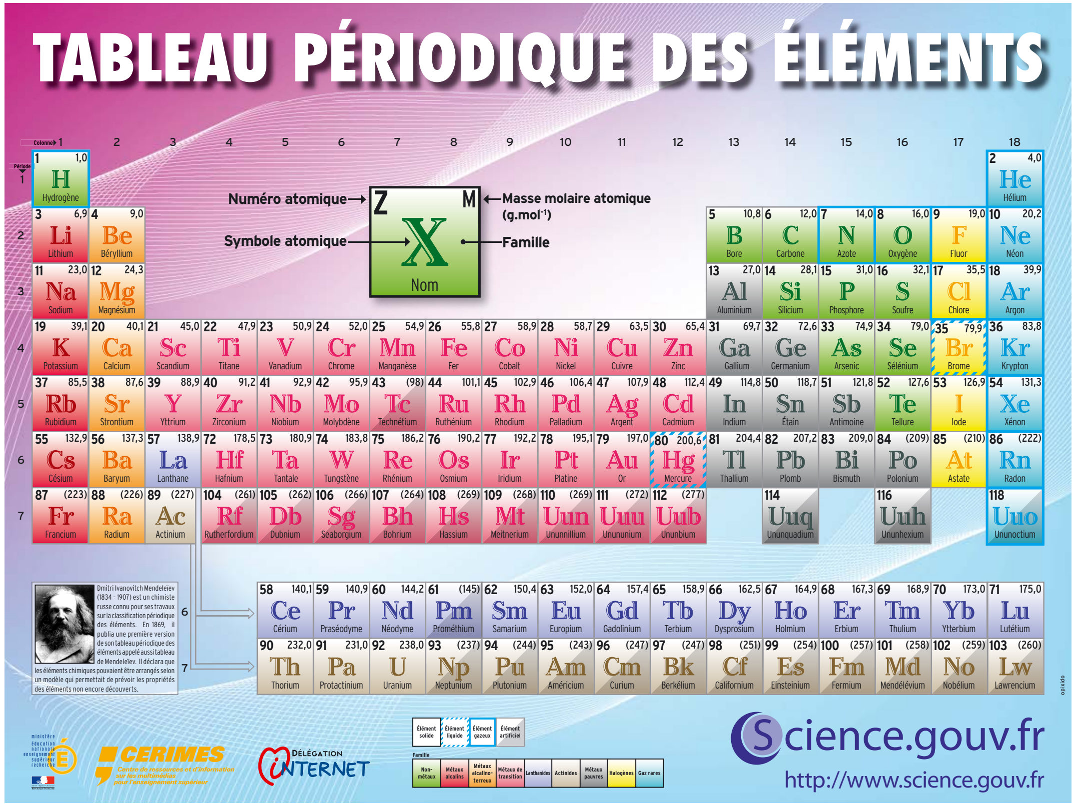


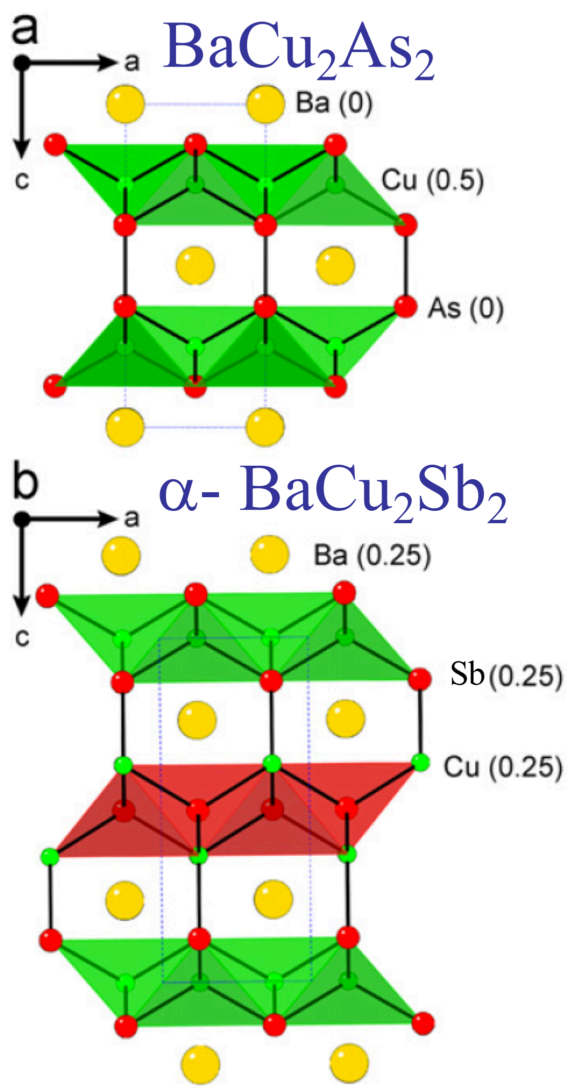
N. Xu *et al.*, PRX **3**, 011006 (2013)

$BaCo_2As_2$ = $BaFe_2As_2$+1 electron

Local physics seems very important

Let’s go for Cu

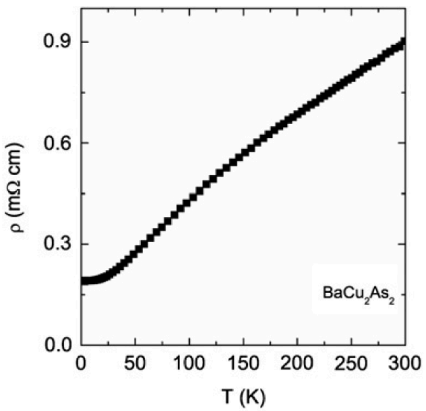




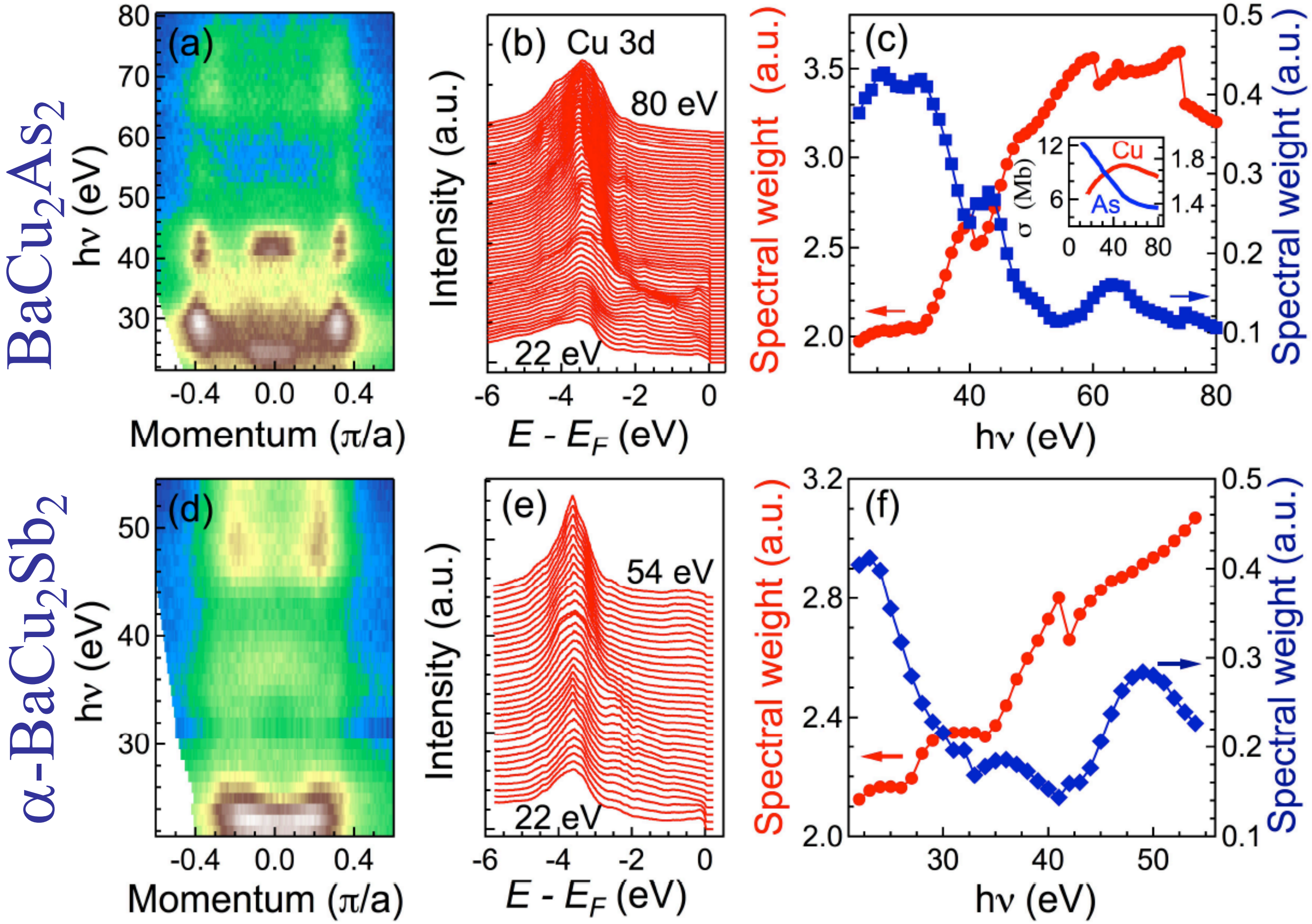
B. Saparov and A. S. Sefat, J. Solid State Chem. **191**, 213 (2012)

What about Cu?

It should be Cu $3d^9$, like in the cuprates, right?



Cu $3d^{10}$



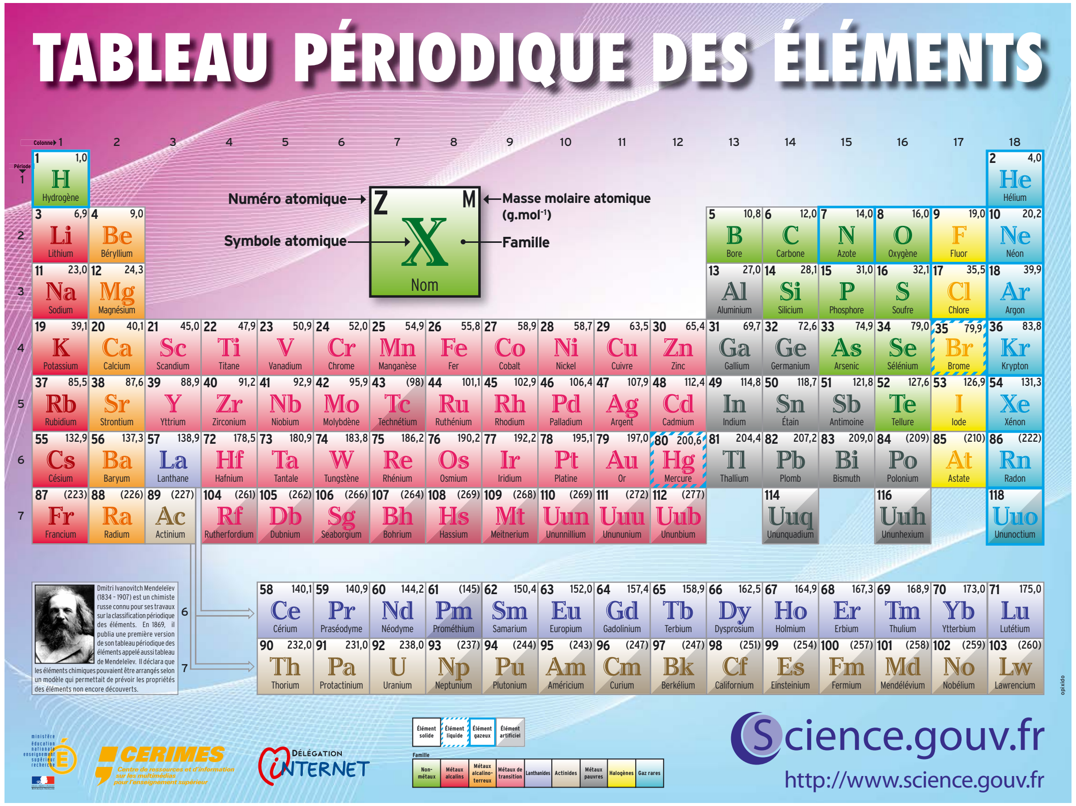
k_z dispersion weak or absent

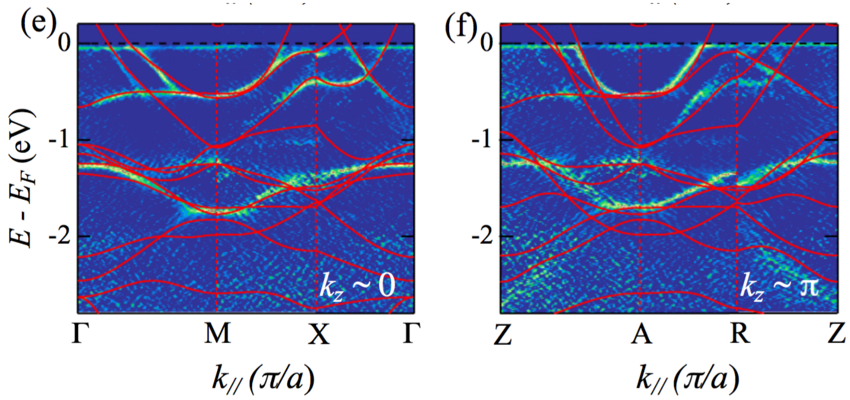
E_F states [-4, -3]

The Cu 3*d* states are located well below E_F

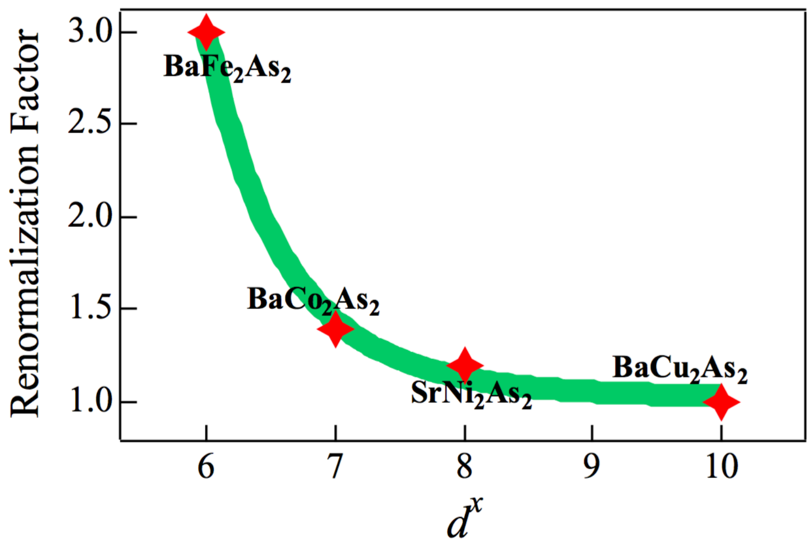
S.-F. Wu *et al.*, Phys. Rev. B **91**, 235109 (2015)

Fe→Ni





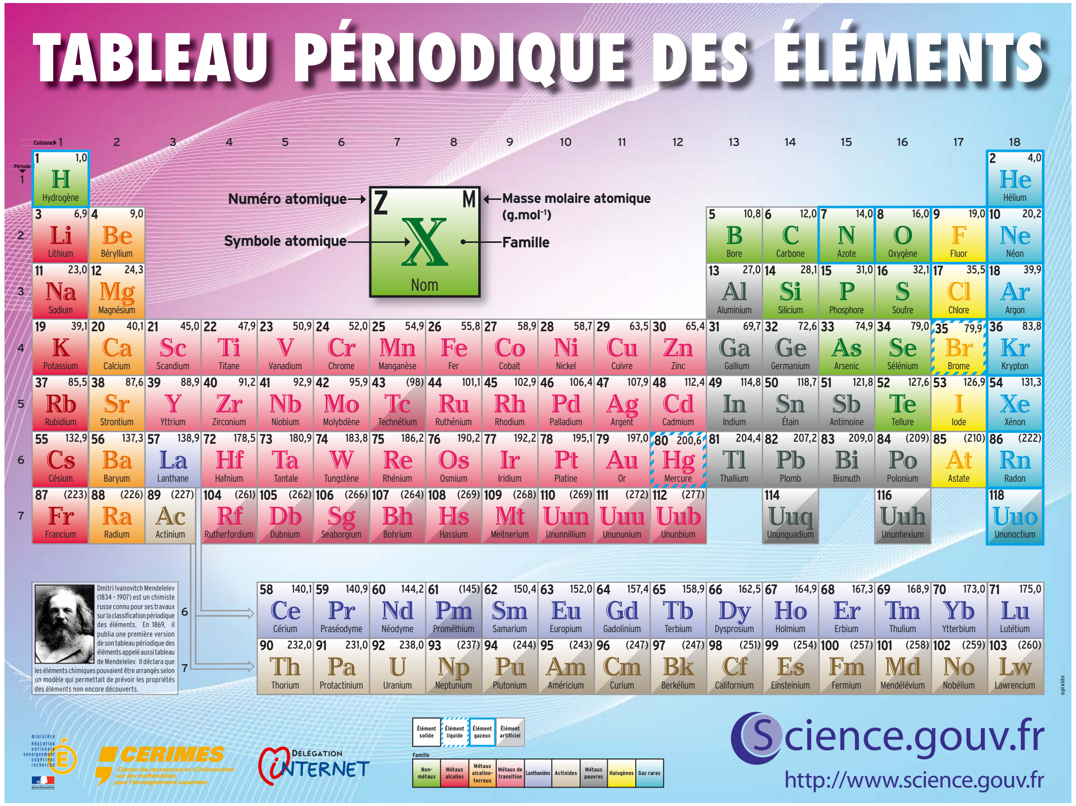
DFT renormalized by 1.1

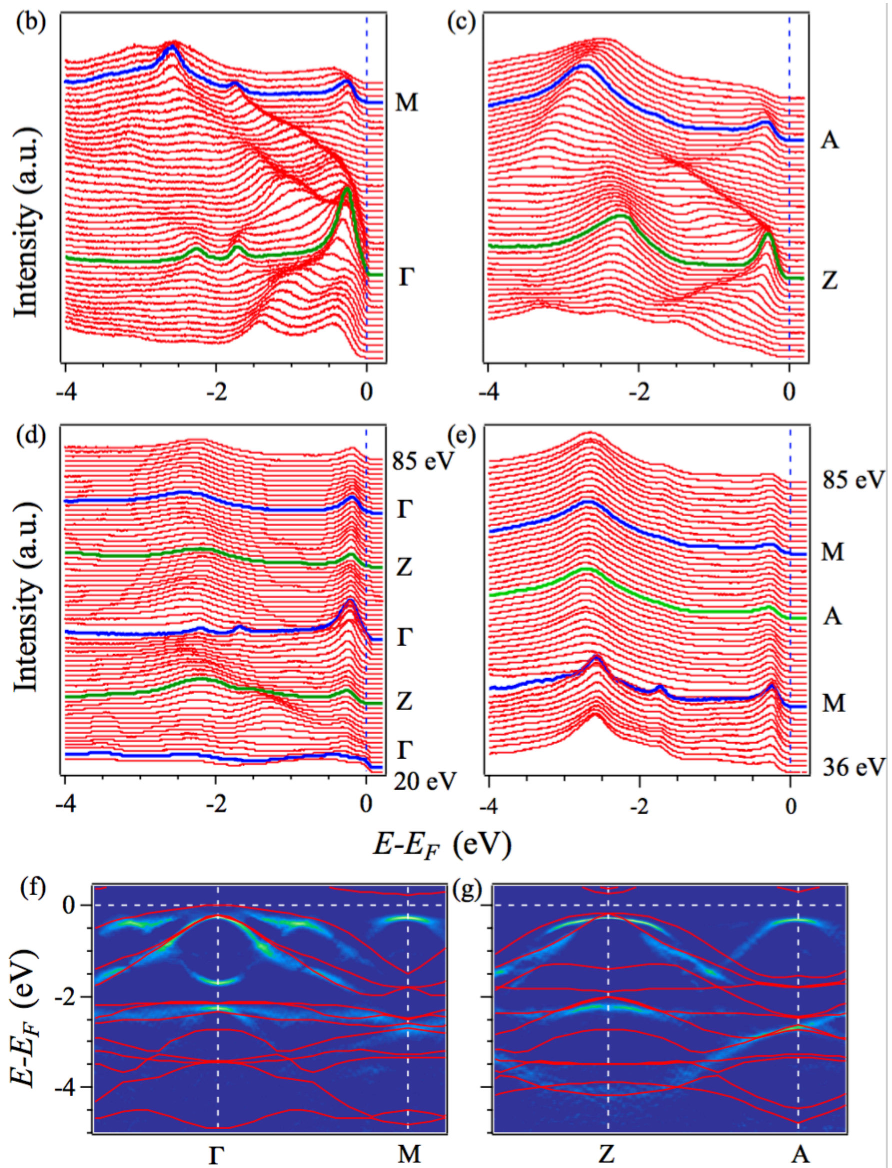


There is a decrease of the band renormalization factor upon filling the 3*d* shell.

L.-K. Zeng *et al.*, PRB **94**, 024524 (2016)

Hole-doping: Fe→Mn





Well-defined features.

No band renormalization.

$T_N = 625$ K

W.-L. Zhang *et al.*, arxiv:1608.06110 (2016), In Press (PRB)

Pairing mechanism in Fe-based superconductors

Nodeless SC gaps

H. Ding, P. Richard *et al.*, EPL **83**, 47001 (2008)

epl A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

August 2008

EPL, **83** (2008) 47001
doi: 10.1209/0295-5075/83/47001

www.epljournal.org

Observation of Fermi-surface–dependent nodeless superconducting gaps in $Ba_{0.6}K_{0.4}Fe_2As_2$

H. DING[1(a)], P. RICHARD[2], K. NAKAYAMA[3], K. SUGAWARA[3], T. ARAKANE[3], Y. SEKIBA[3], A. TAKAYAMA[3], S. SOUMA[2], T. SATO[3], T. TAKAHASHI[2,3], Z. WANG[4], X. DAI[1], Z. FANG[1], G. F. CHEN[1], J. L. LUO[1] and N. L. WANG[1]

[1] *Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences Beijing 100190, China*
[2] *WPI Research Center, Advanced Institute for Material Research, Tohoku University - Sendai*
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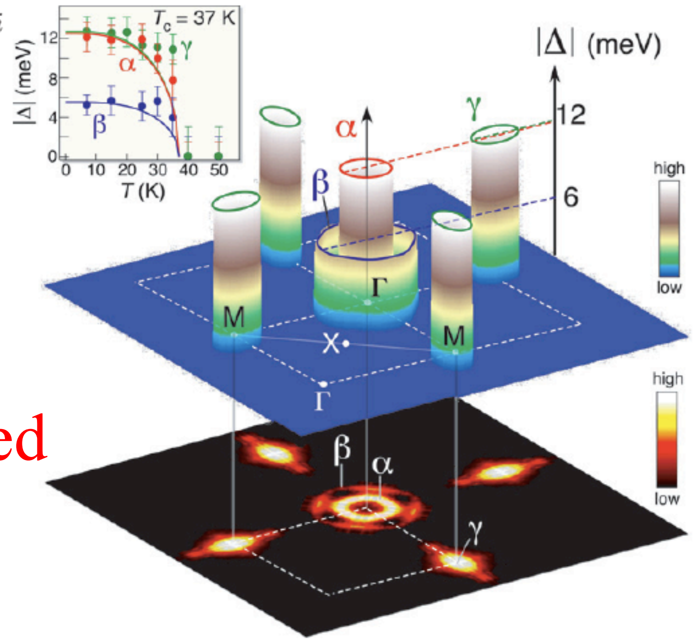
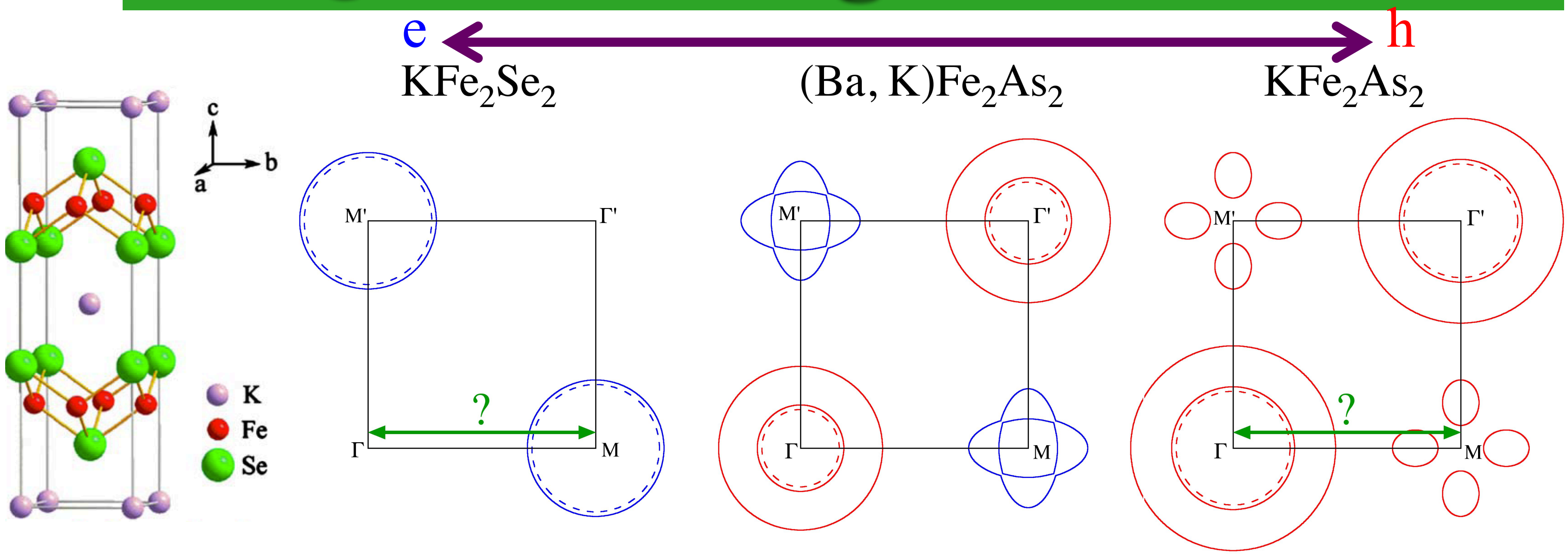
[4] *Department of Physics, Boston College - Chestnut Hill, MA 02467, USA*

received 3 July 2008; accepted 7 July 2008
published online 14 July 2008



Are the pairing interactions better described in the ~~*k* space~~ or in the *r* space?

Quasi-nesting breakdown

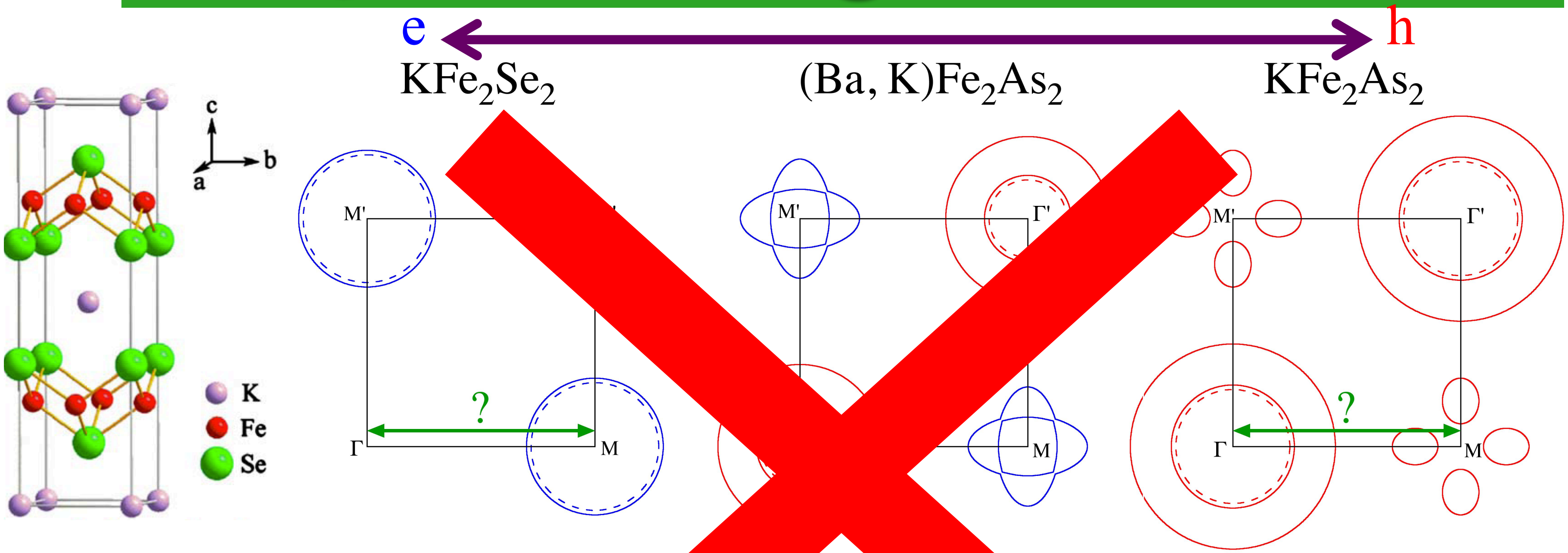


Same crystal structure but totally different Fermi surface topologies

The only way to support a Fermi-surface-driven pairing is to admit that there are at least 3 unconventional (!!!) paring mechanisms for the same crystal structure.

For more details, see our recent review paper:
Richard *et al.*, J. Phys.: Condens. Matter **27**, 293203 (2015)

Quasi-nesting breakdown



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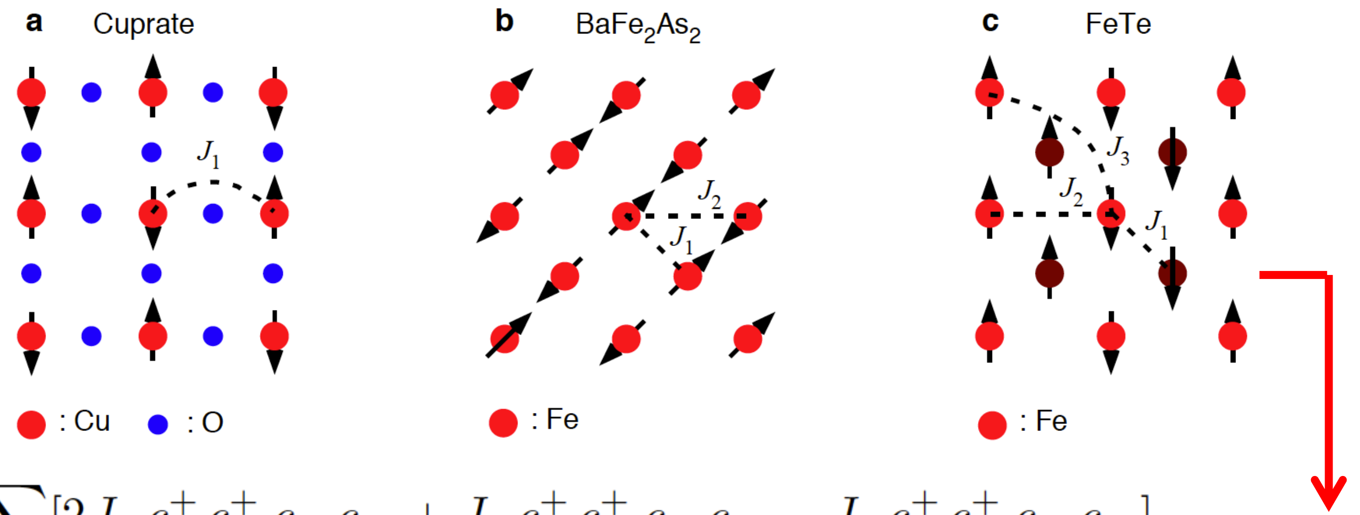
For more details, see our recent review paper:

Richard *et al.*, J. Phys.: Condens. Matter **27**, 293203 (2015)

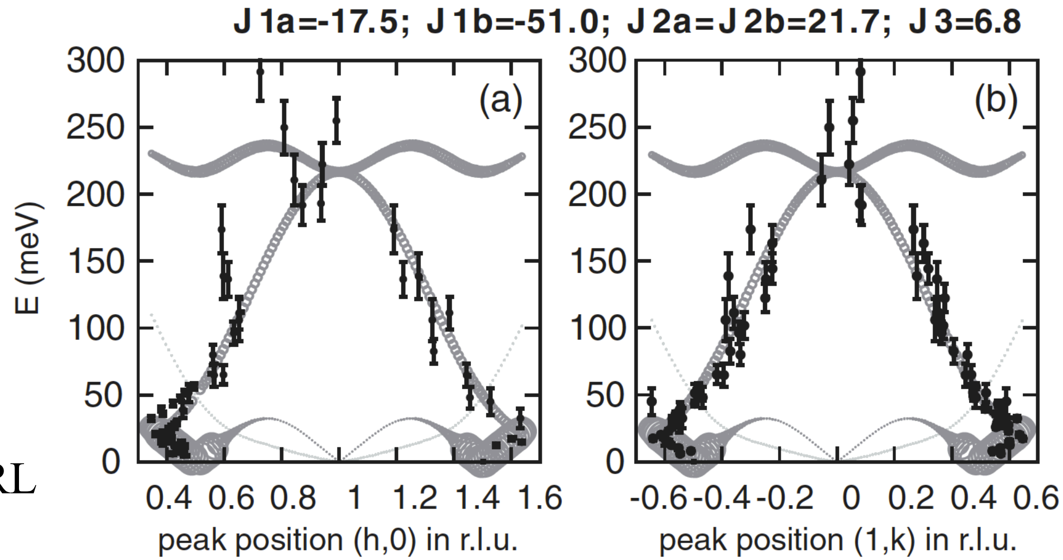
Local magnetic interactions

J.-P. Hu and H. Ding., Sci. Rep. **2**, 00381 (2012)



$$J_{ij}\vec{S}_i \cdot \vec{S}_j = \frac{1}{4}\sum_{\sigma}[2J_{ij}c^+_{i\sigma}c^+_{j\sigma}c_{j\bar{\sigma}}c_{i\bar{\sigma}} + J_{ij}c^+_{i\sigma}c^+_{j\sigma}c_{j\sigma}c_{i\sigma} - J_{ij}c^+_{i\sigma}c^+_{j\bar{\sigma}}c_{j\bar{\sigma}}c_{i\sigma}]$$

Magnetism can be characterized by the J_1-J_2-J_3 model in cuprates, pnictides and chalcogenides



Lipscombe *et al.*, PRL **106**, 057004 (2011)

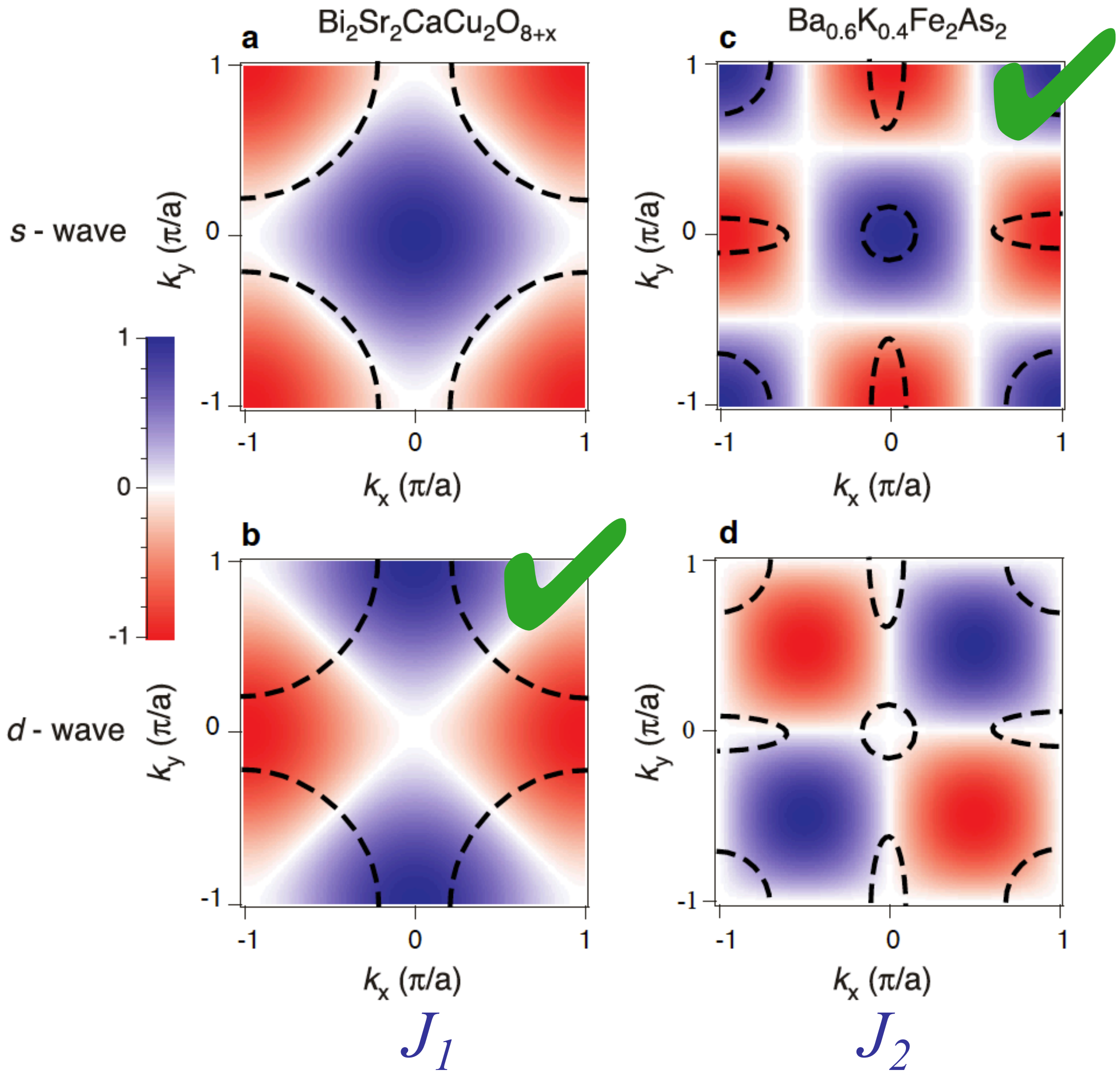
Recipe for a high-T_c SC

J.-P. Hu and H. Ding., Sci. Rep. **2**, 00381 (2012)

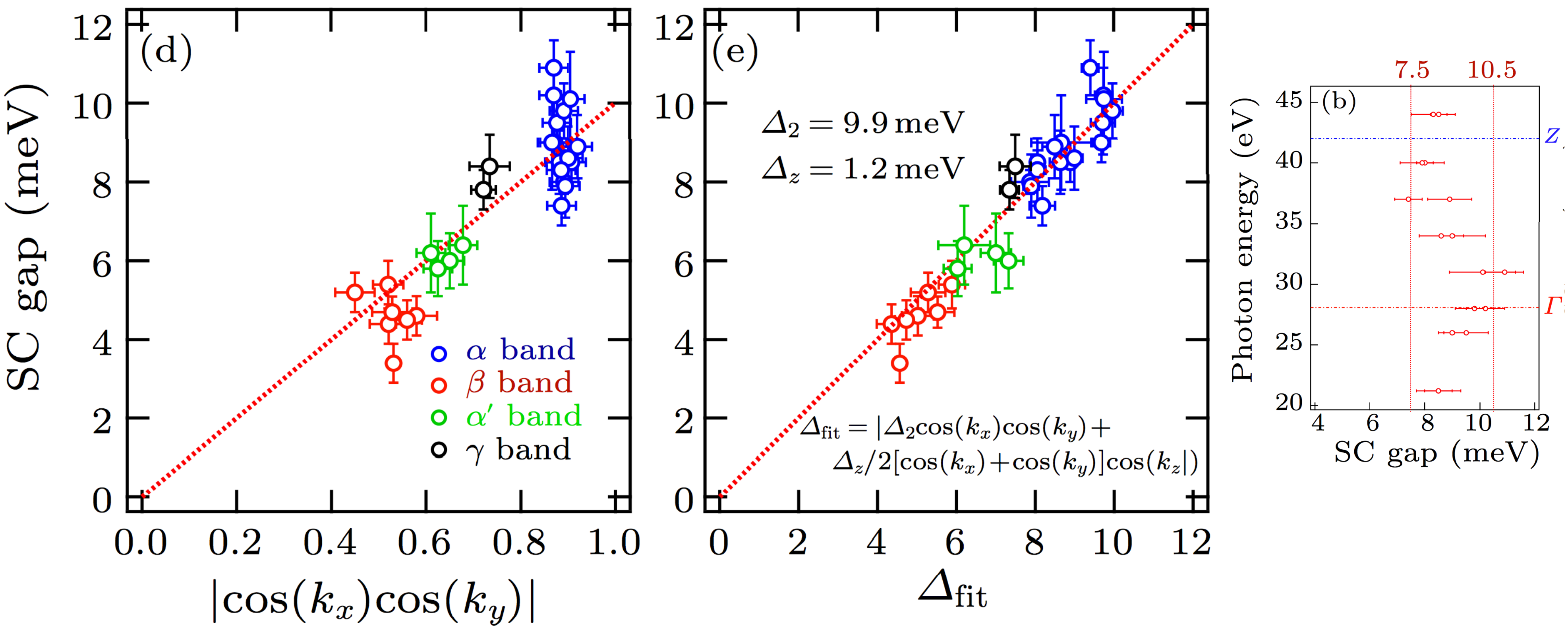
Global gap functions

AF couplings & gap form
J_1: *s*-wave $(cosk_x + cosk_y)/2$
J_1: *d*-wave $(cosk_x - cosk_y)/2$
J_2: *s*-wave $cosk_x cosk_y$
J_2: *d*-wave $sink_x sink_y$
J_3: *s*-wave $(cos2k_x + cos2k_y)/2$
J_3: *d*-wave $(cos2k_x - cos2k_y)/2$

The form of the different functions simply comes from the Fourier transform of Dirac functions representing the position of the atoms in real space.



$Ca_{0.67}Na_{0.33}Fe_2As_2$



Y.-B. Shi *et al.*, CPL **37**, 067403 (2014)

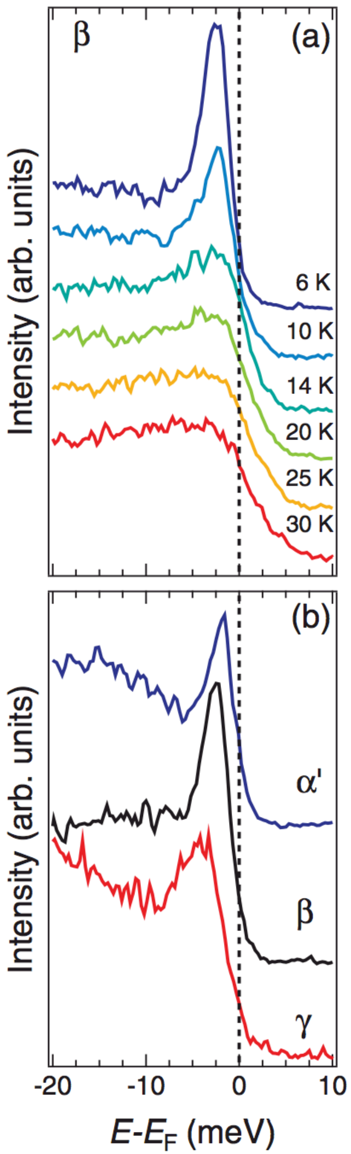
$J_2/J_z = 7$

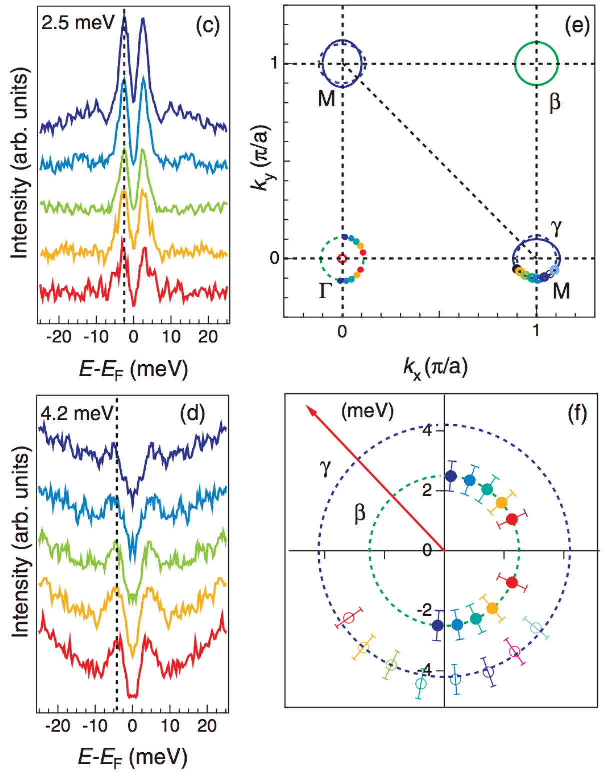
$\Delta_2/\Delta_z = 8.3$

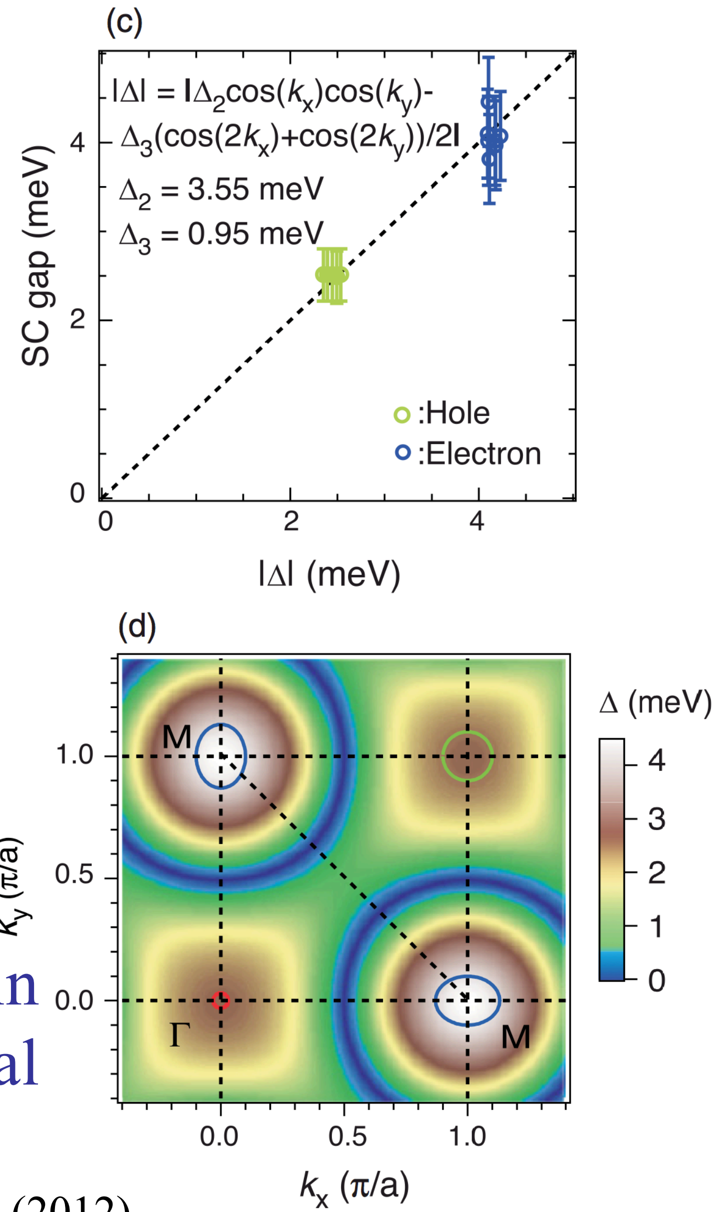
The SC gap obeys a strong coupling derived formula!

$FeTe_{0.55}Se_{0.45}$: gap asymetry

T_c = 14.5 K







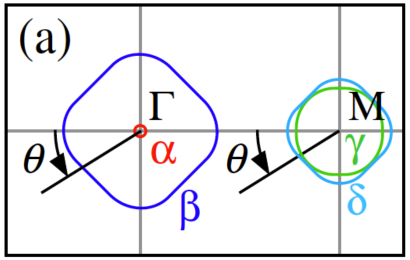
Δ_2/Δ_3 = 3.7 compares quite well with J_2/J_3 = 3.2

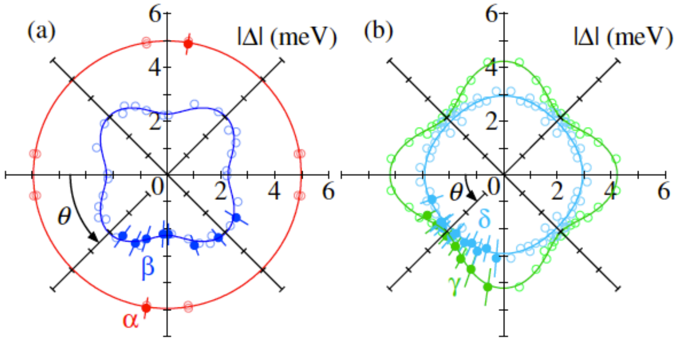
The absence of band at Γ in KFe_2Se_2 has no fundamental importance

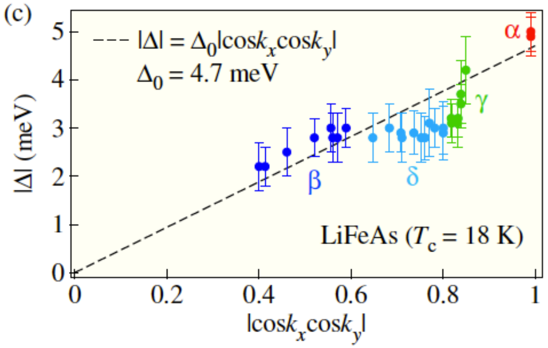
H. Miao, P. Richard *et al.*, PRB **85**, 094506 (2012)

Orbital anti-phase $S_{\pm}$

LiFeAs

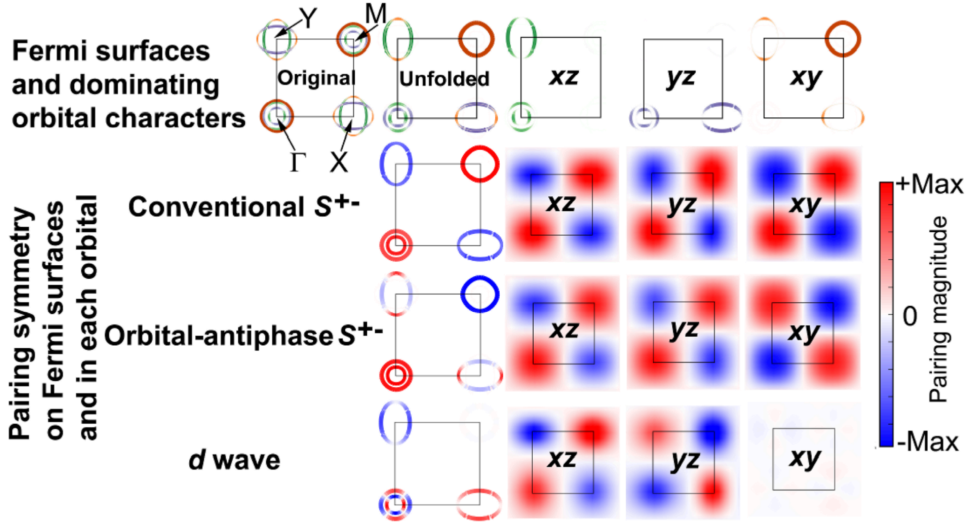


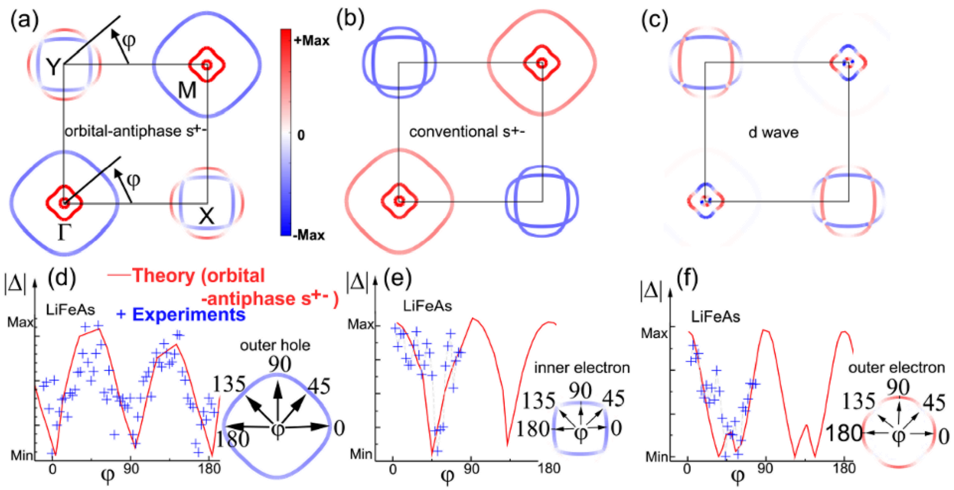




Umezawa *et al.*, PRL **108**, 037002 (2012).

See also Borisenko *et al.*, Symmetry **4**, 00251 (2012).

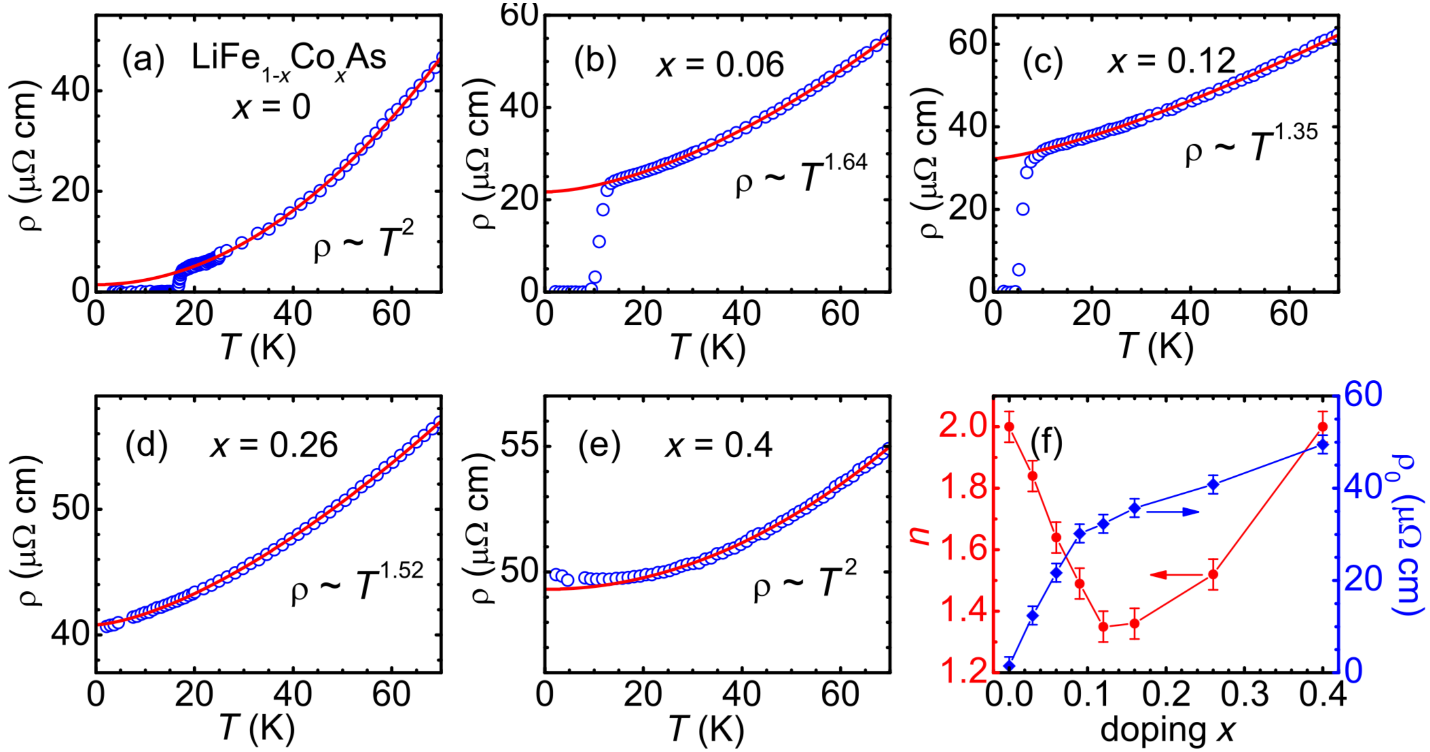




Z. P. Yin, K. Haule and G. Kotliar, Nature Phys. **10**, 845 (2014)

Non-Fermi liquid behavior in doped LiFeAs

Electrical resistivity

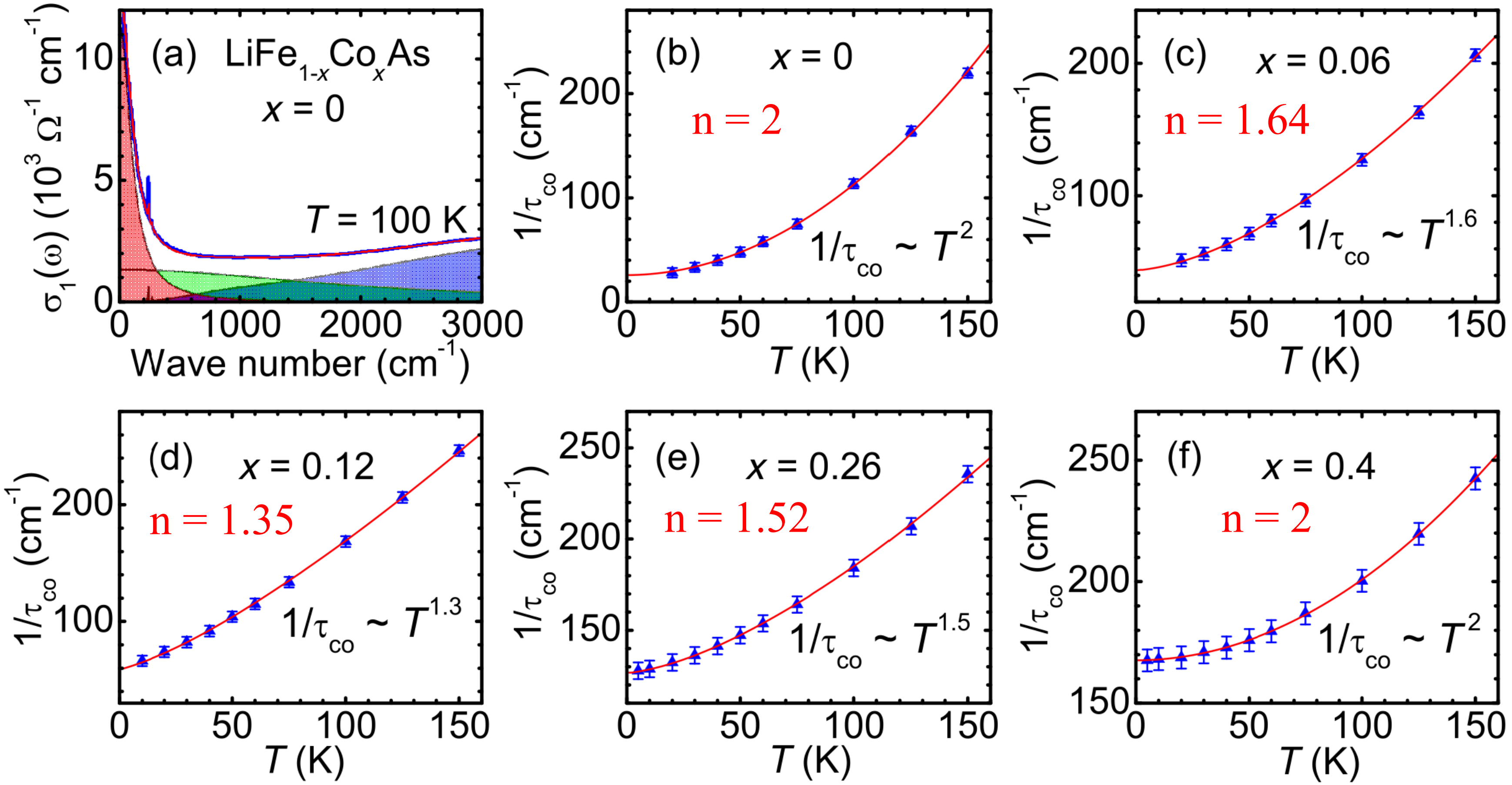


LiFeAs shows the T^2 dependence of a Fermi liquid. The exponent decreases down to nearly 1.3 with Co doping but increases towards 2 for further doping.

ρ_0 increases monotonically with doping ⇒ the crossover is not the result of impurities.

Y.-M. Dai *et al.*, Phys. Rev. X **5**, 031035 (2015)

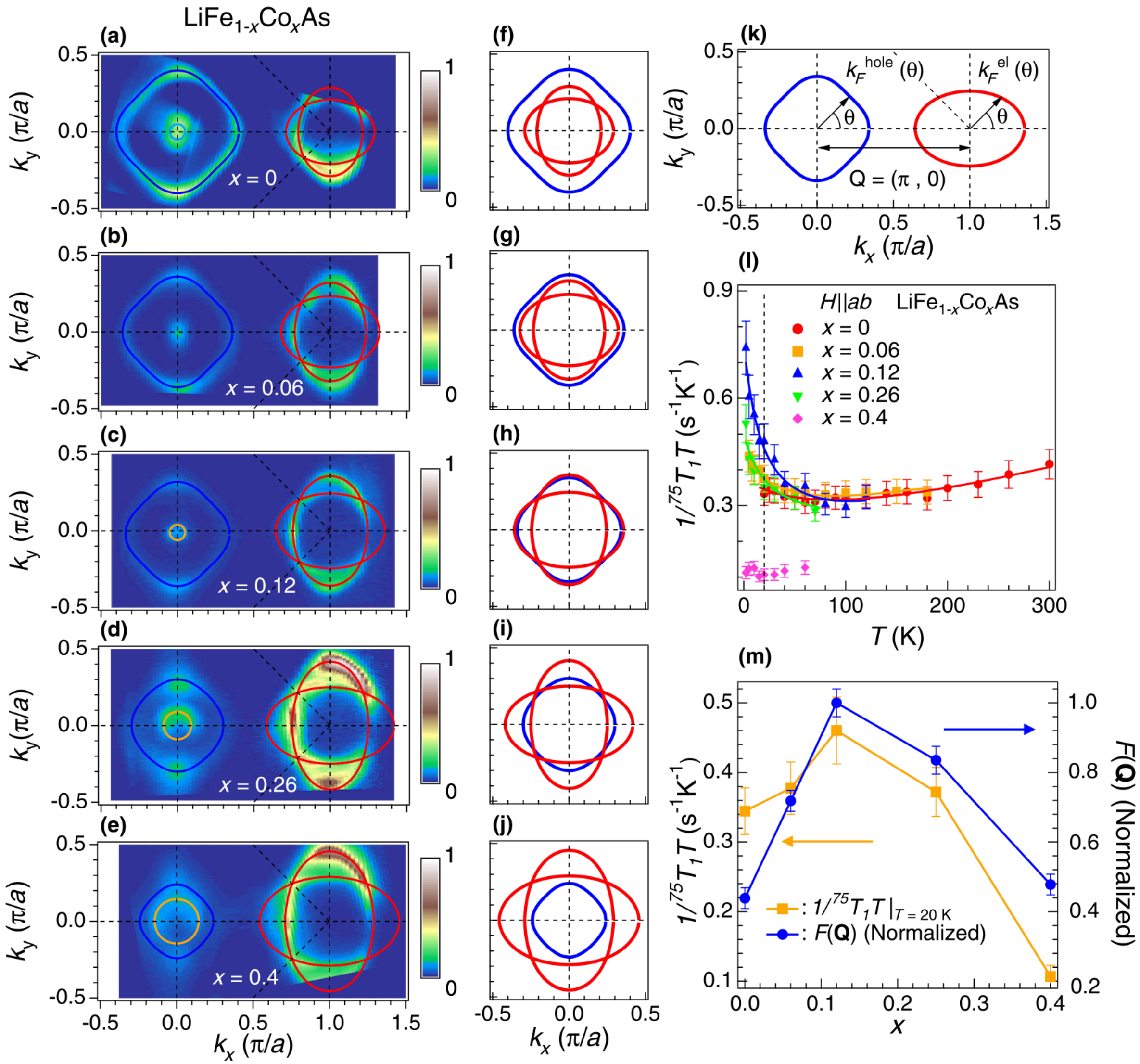
Optical conductivity

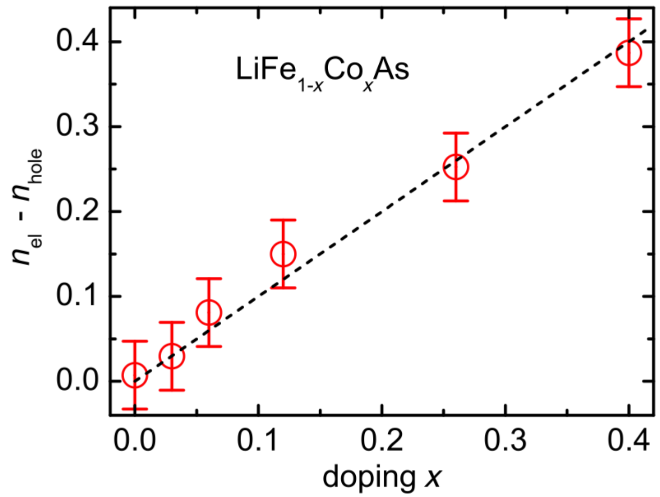


The same exponents are obtained from the real part of the optical conductivity.

Y.-M. Dai *et al.*, Phys. Rev. X **5**, 031035 (2015)

LiFeAs: FL-NFL-FL crossover





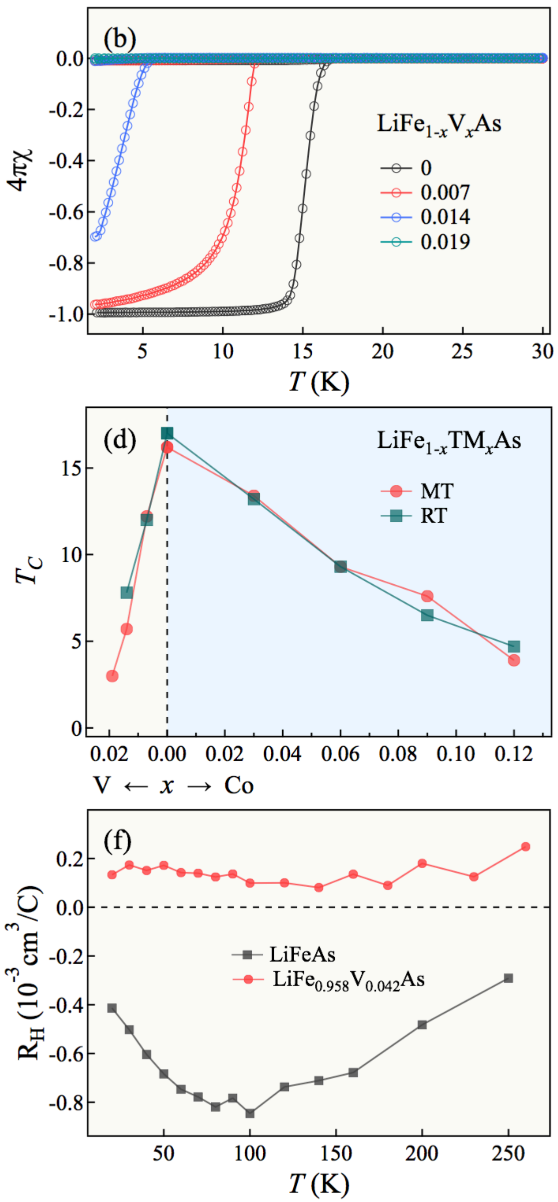
Y.-M. Dai *et al.*, Phys. Rev. X **5**, 031035 (2015)

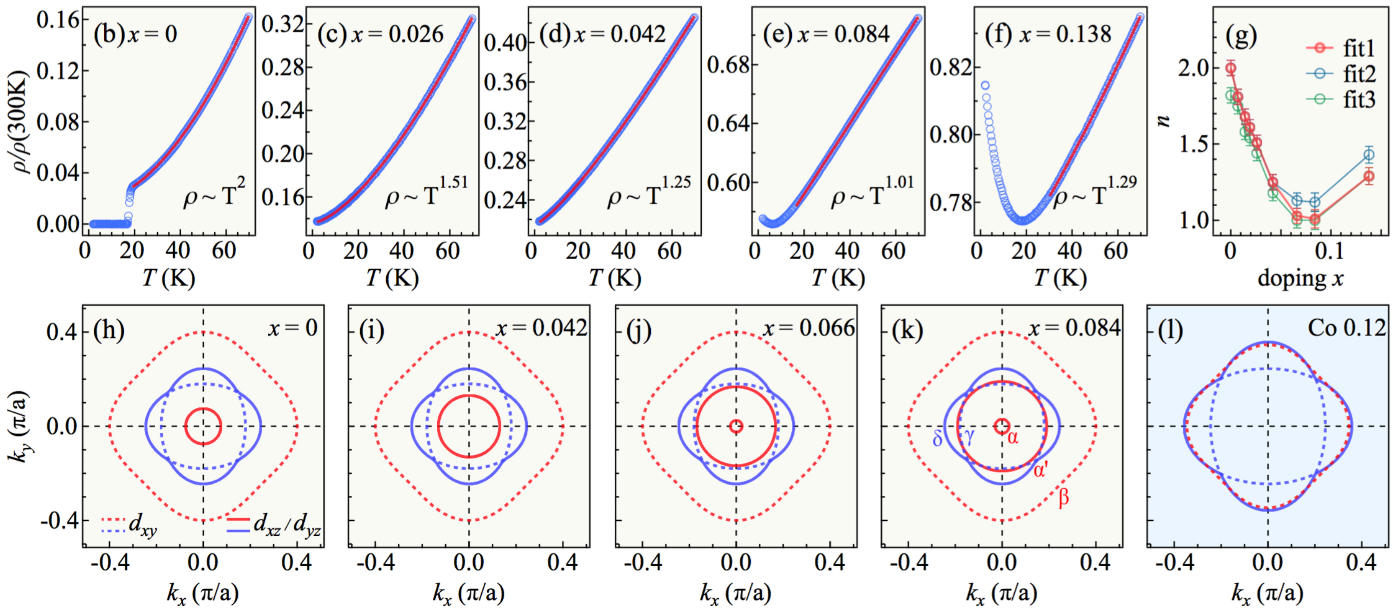
The FS nesting is poor in LiFeAs, it increases with Co-doping up to x = 0.12, and then deteriorates again.

$1/T_1T$ increases rapidly for x = 0.12

$$F(\mathbf{Q}) = \sum_{i,j} \int_0^{2\pi} \frac{1}{\|\mathbf{k}_\mathbf{F}^{\mathrm{el}_i}(\theta) - \mathbf{k}_\mathbf{F}^{\mathrm{hole}_j}(\theta) - \mathbf{Q}\| + \delta} d\theta$$

V-doped LiFeAs





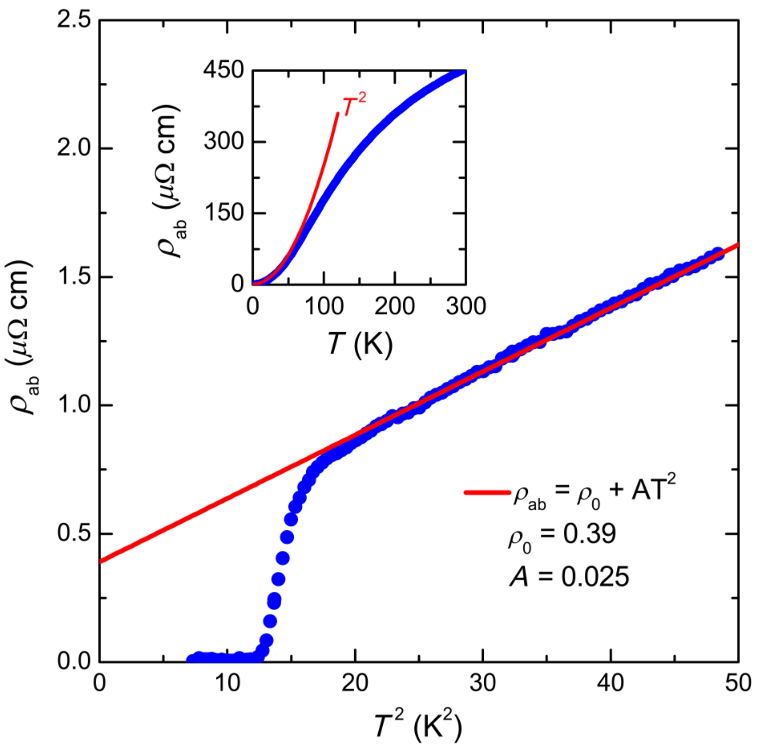
L. Y. Xing *et al.*, Phys. Rev. B **94**, 094524 (2016)

- Hole-doping
- Confirms the nesting-induced NFL scenario
- Inter-orbital scattering is favored

Coherent to incoherent crossover in KFe_2As_2

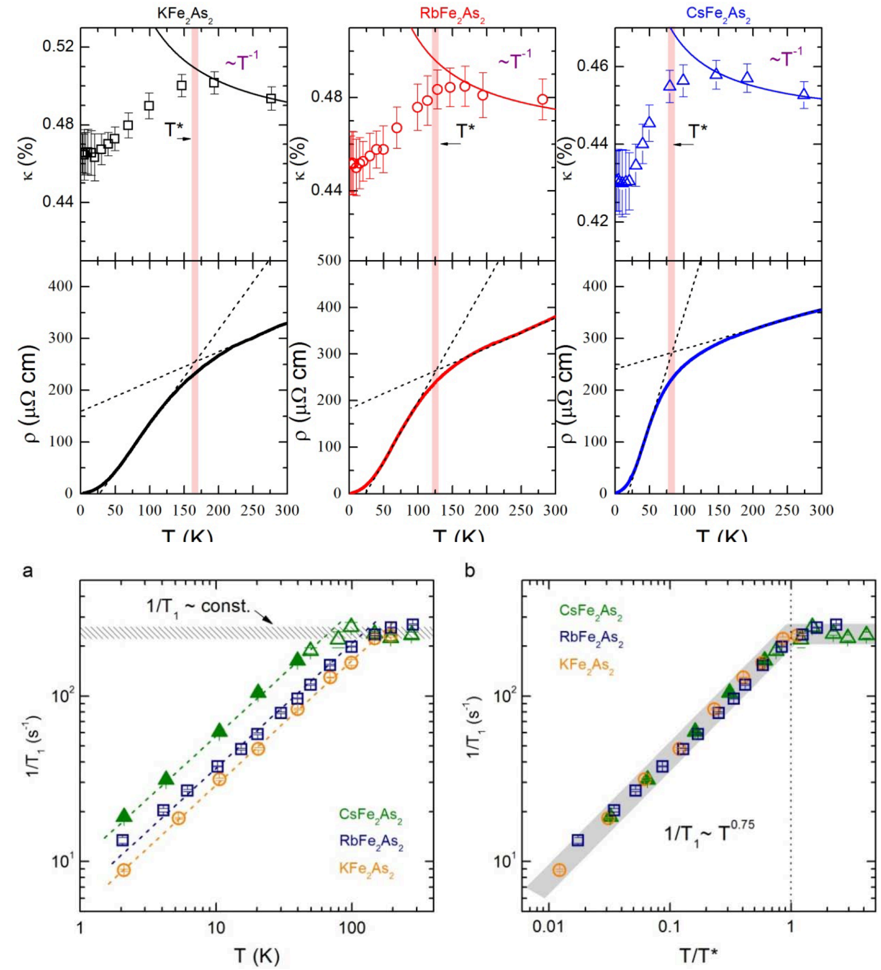
KFe_2As_2: Motivations

F. Hardy *et al.*, PRL 111, 027003 (2013)



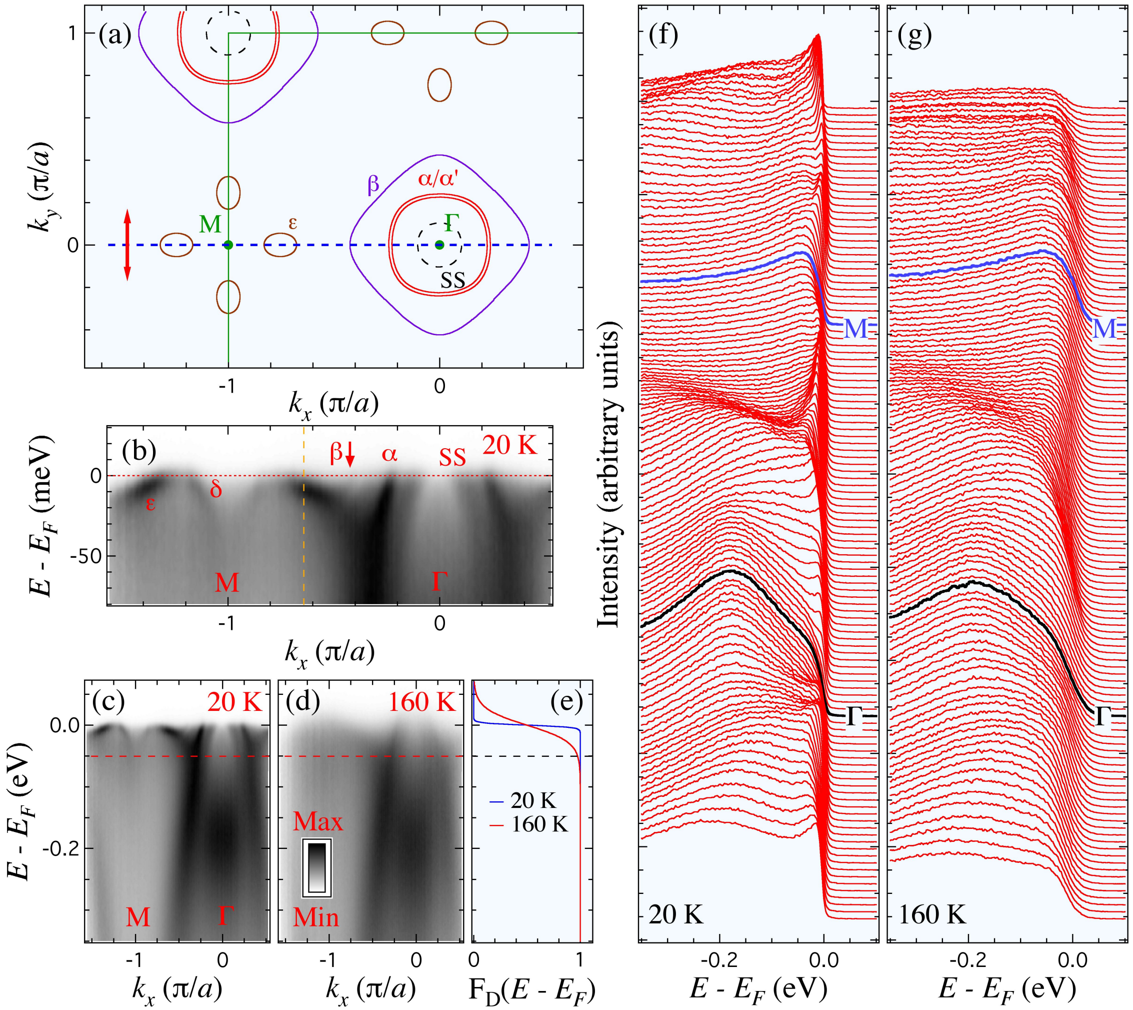
Fermi liquid at low *T*, incoherent state at high *T*.

Y. P. Wu *et al.*, PRL **116**, 147001 (2016)



Coherence-incoherence crossover in KFe_2As_2 at T* = 165 ± 25 K

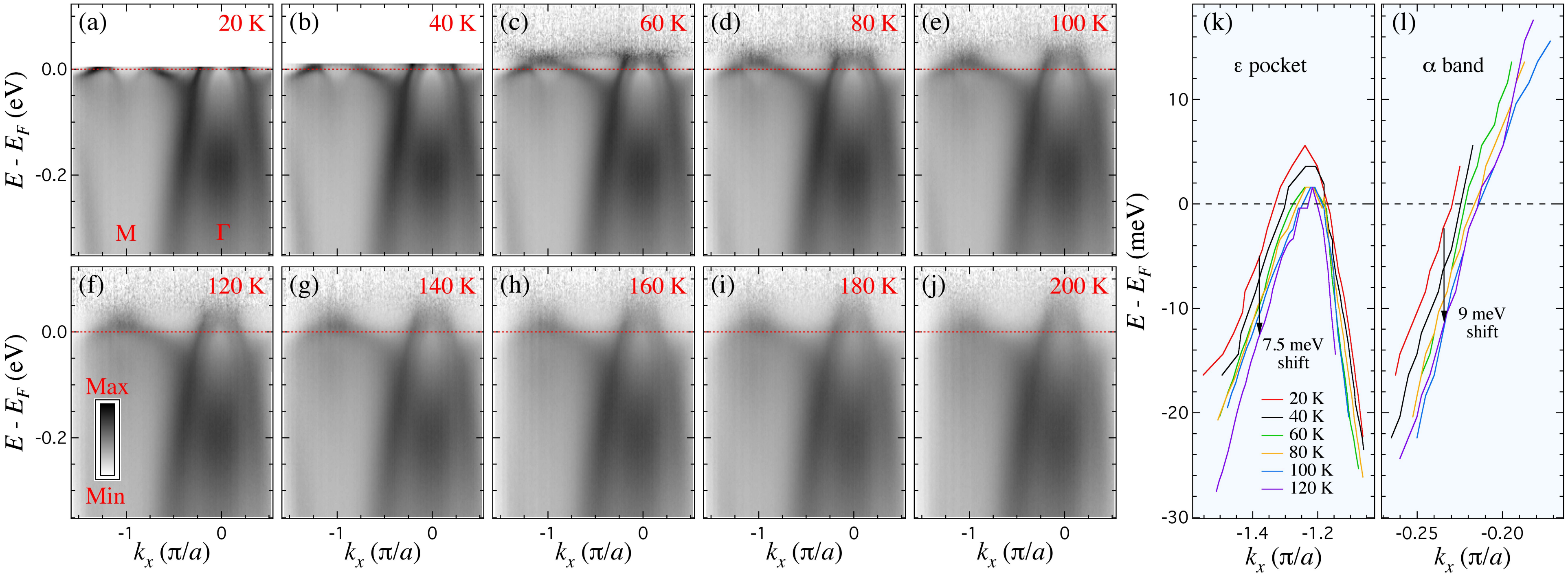
Fermi-Dirac cutoff



P. Richard *et al.*, Unpublished.

Be aware that the electronic states of interest locate within the energy range affected by the Fermi-Dirac cutoff.

Removing the cutoff



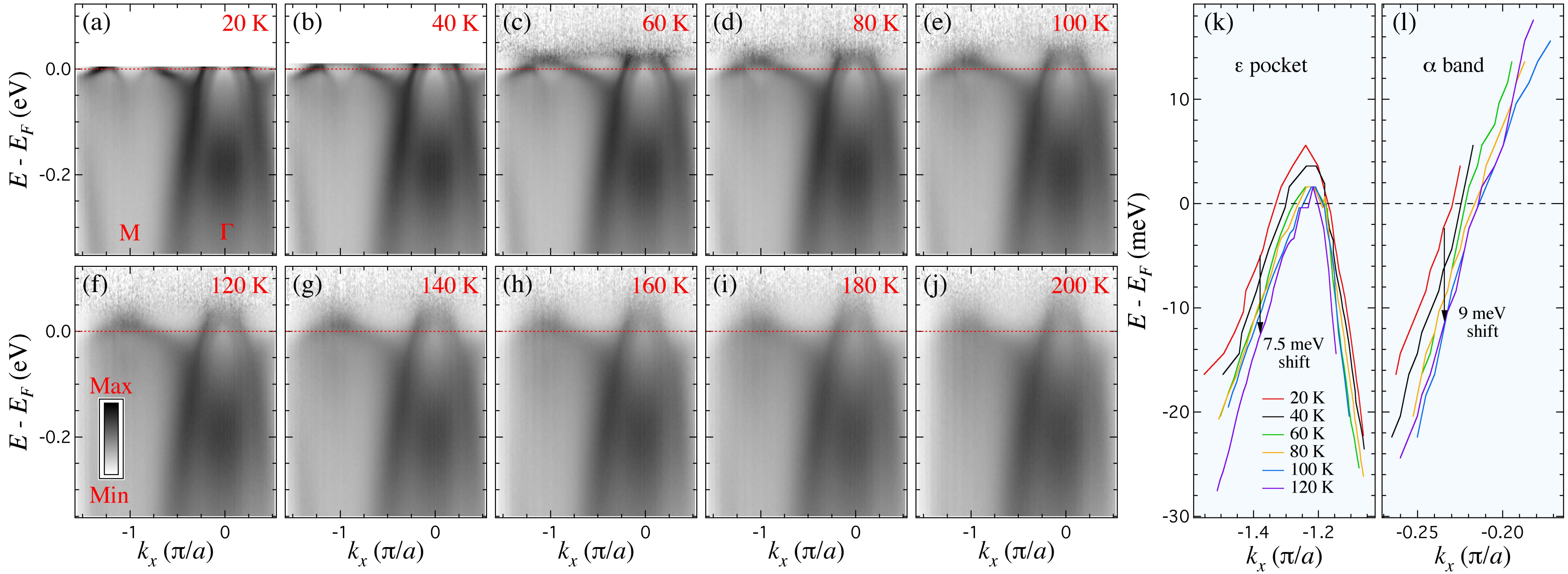
P. Richard *et al.*, Unpublished.

Similar, and even more pronounced chemical potential shift observed in other Fe-based superconductors as a function of temperature.

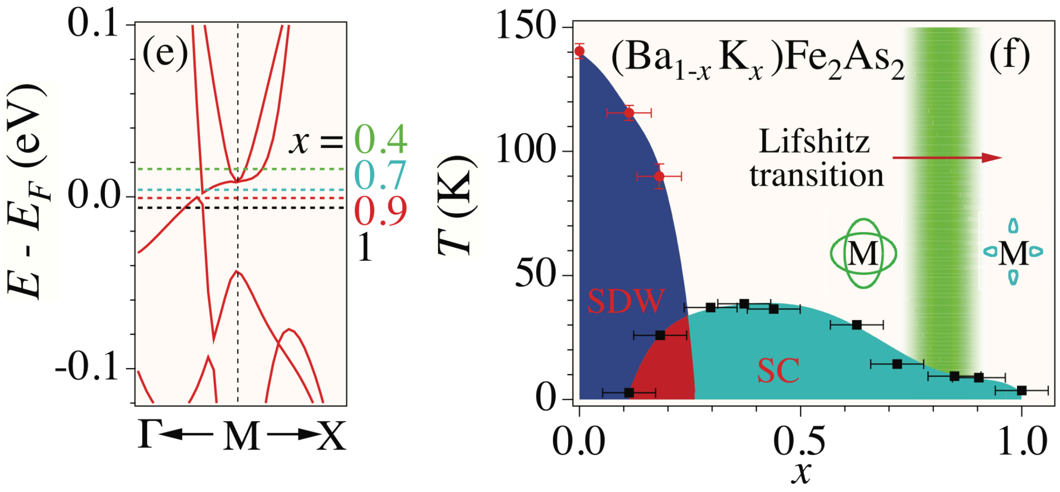
See V. Brouet *et al.* and A. Kaminski *et al.*

… and S. Borisenko's talk

Removing the cutoff



P. Richard *et al.*, Unpublished.

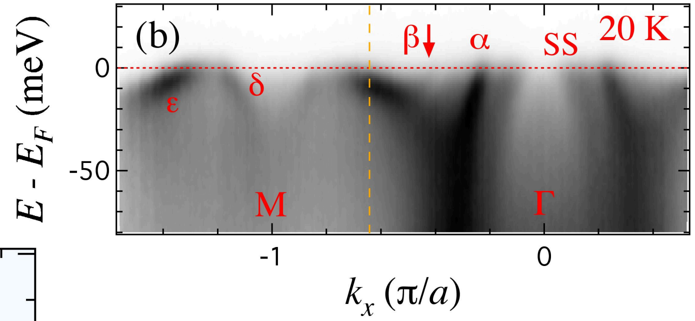


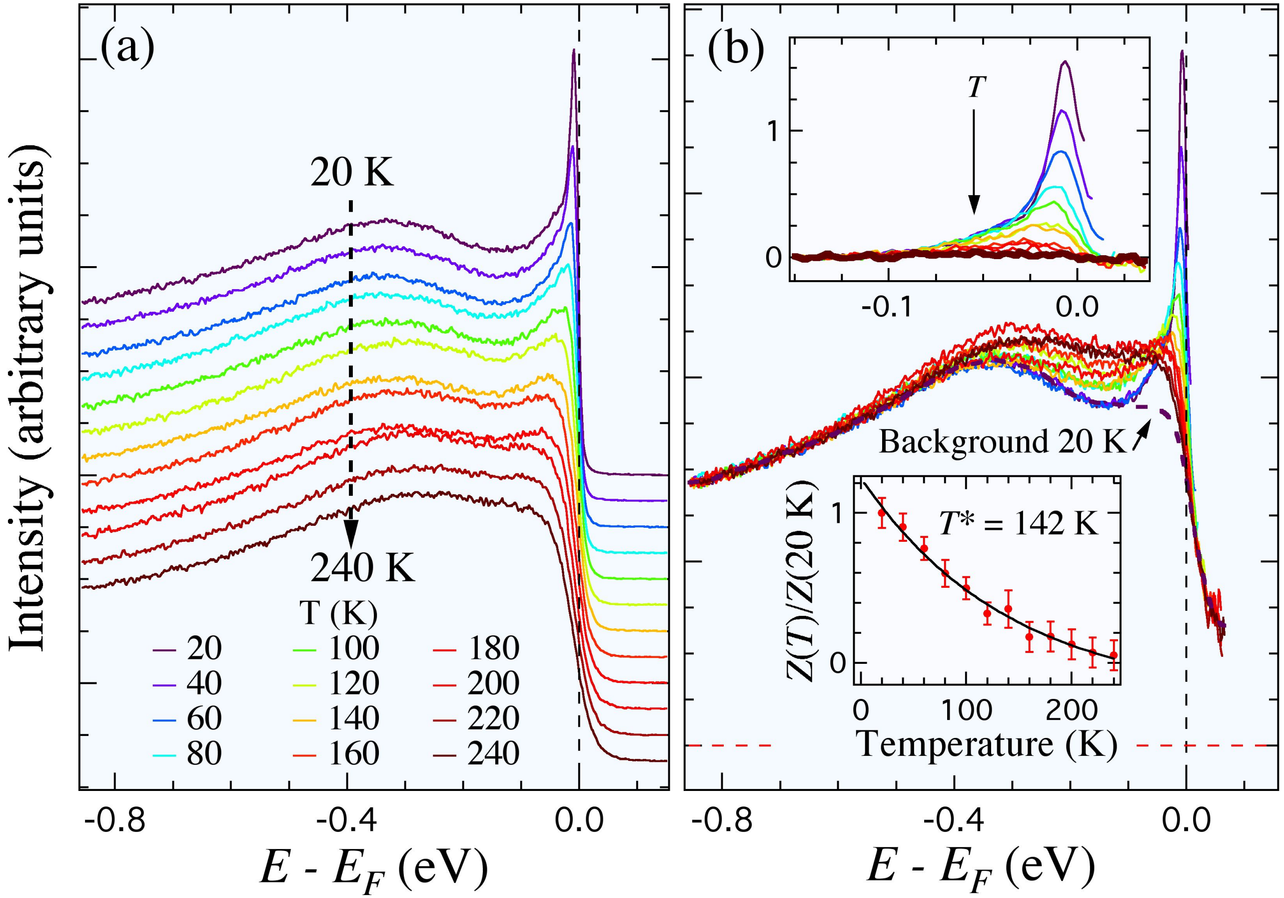
“Lifshitz transition” above 120 K?

N. Xu *et al.*, PRB **88**, 220508(R) (2013)

T evolution

The spectral weight intensity decreases exponentially with a characteristic temperature scale T* = 142 K





P. Richard *et al.*, Unpublished.

What is the cause for this behavior? The Hund's coupling or the low-energy excitations?

Summary

1. Electronic correlations come out naturally from "local physics" and they are tuned by the filling of the 3*d* shell.
2. SC does not come from a Fermi surface instability. The pairing glue is better described in the real space.
3. *k*-physics remains and is responsible for interesting phenomena such as non-Fermi liquid behavior.
4. The coherent to incoherent crossover in KFe_2As_2 *may not be* due to local electronic correlations?
5. PHYSICS is not *k* or *r*. It is *k* AND *r*. PHYSICS is not local or non-local. It is BOTH. Calls for more sophisticated calculation methods.

谢谢大家！