Direct observation of spin-orbit coupling in iron-based superconductors

S.V. Borisenko
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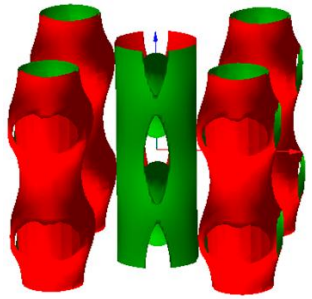
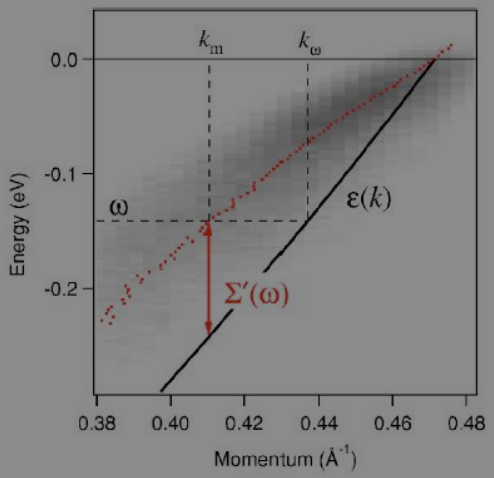


PHYSICAL REVIEW B 71, 214513 (2005)

Bare electron dispersion from experiment: Self-consistent self-energy analysis of photoemission data

A. A. Kordyuk,[1,2] S. V. Borisenko,[1] A. Koitzsch,[1] J. Fink,[1] M. Knupfer,[1] and H. Berger[3]



A. Well-defined quasiparticles

The linear behavior of $\Sigma'(\omega)$ over a wide energy range $|\omega|<|\omega_k|$ indicates, using the criterion $\lim_{\omega\to 0}\Sigma''(\omega)/\omega=0$, the existence of well-defined quasiparticles in the pseudogap state: for the underdoped Bi(Pb)-2212 at 130 K the coherence factor $Z=0.54\pm0.03$. The offset of $\Sigma''(\omega)$ not only

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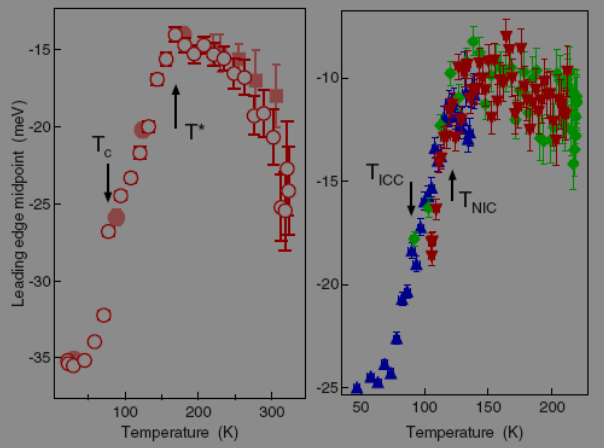
PHYSICAL REVIEW B 79, 020504(R) (2009)

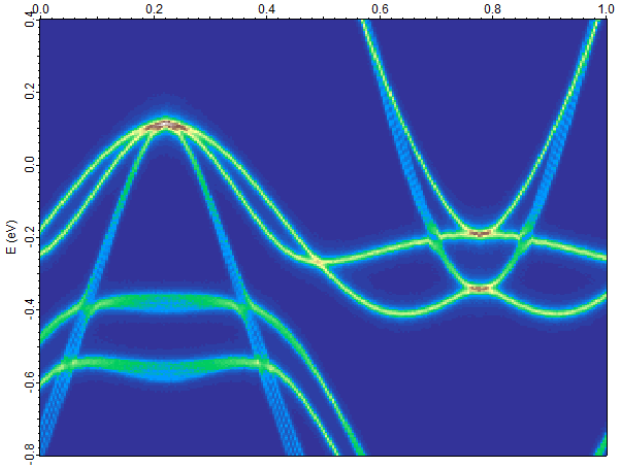
Nonmonotonic pseudogap in high-T_c cuprates

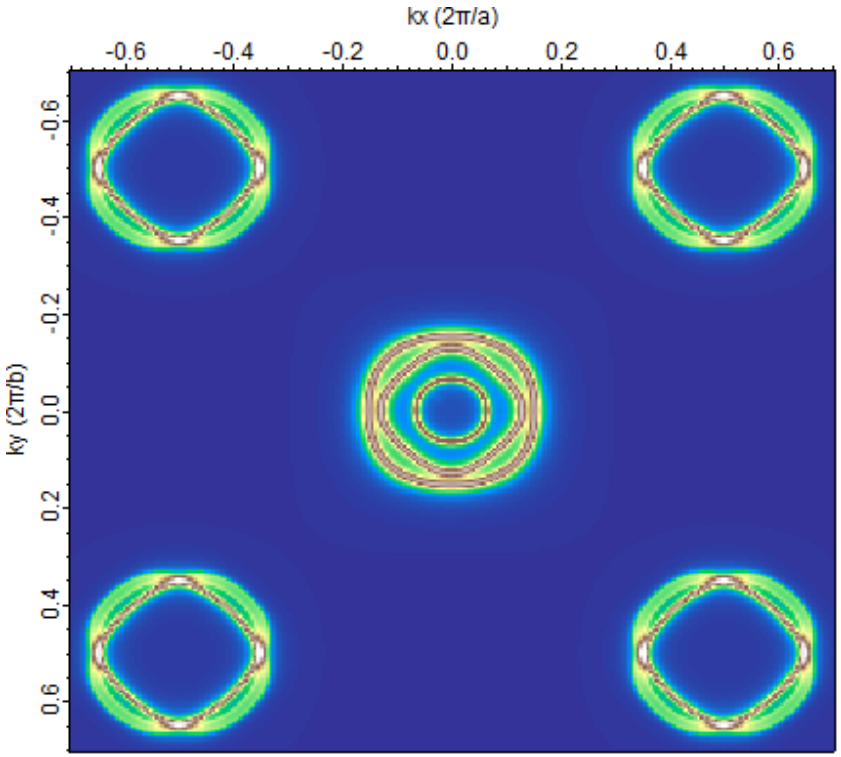
A. A. Kordyuk,[1,2] S. V. Borisenko,[1] V. B. Zabolotnyy,[1]



but does not vanish and starts to increase gradually again at higher temperature. The low-temperature behavior of the pseudogap is remarkably similar to one of the incommensurate charge ordering gap in the transition-metal dichalcogenides, while the reopening of the gap at room temperature fits the scenario of temperature-driven metal-insulator transition. This observation suggests that two phenomena, the electronic instability to density-wave formation and the entropy-driven metal-to-insulator crossover, may coexist in the normal state of cuprates.

LDA band structure and Fermi surface: 1111





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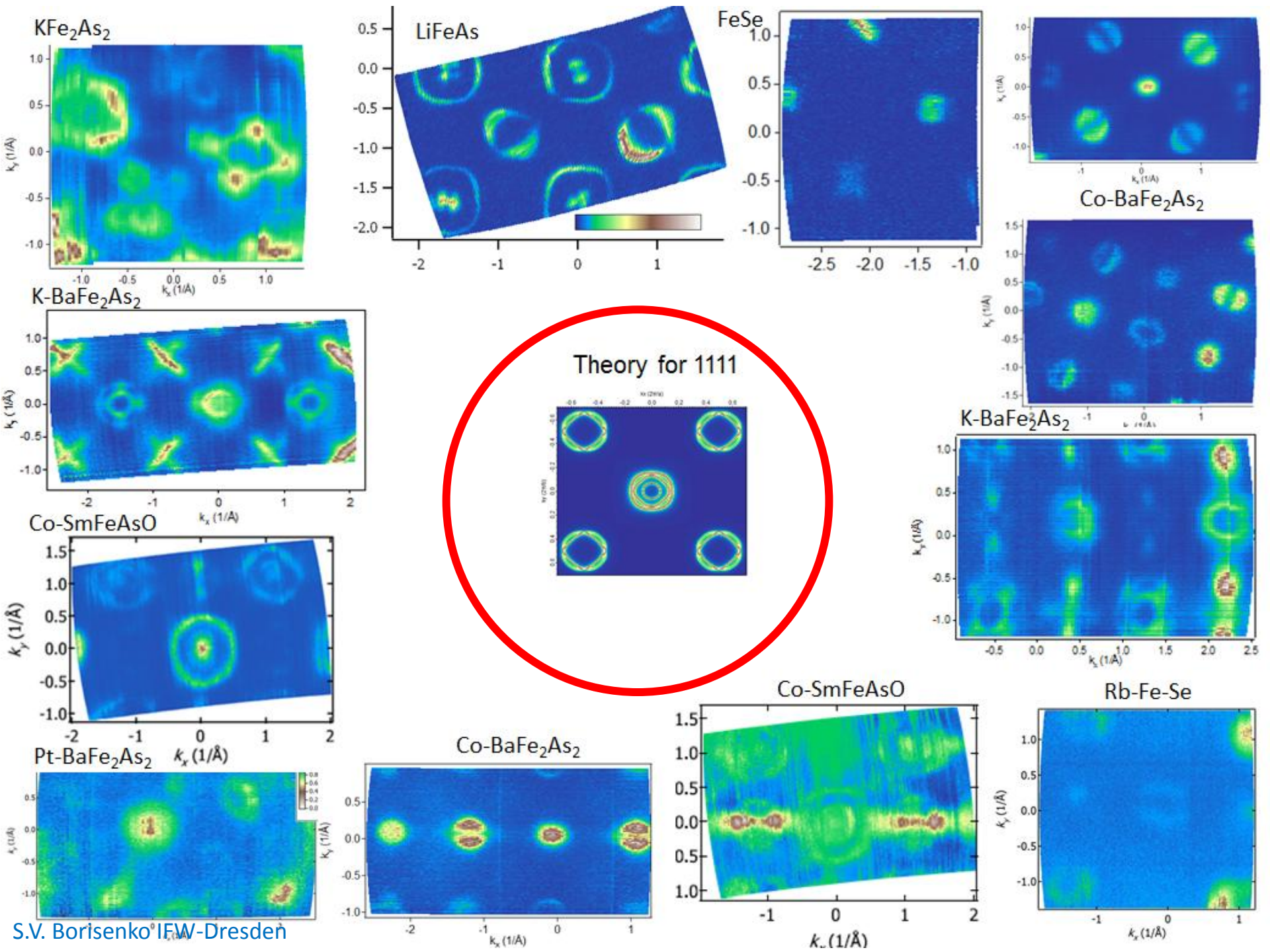
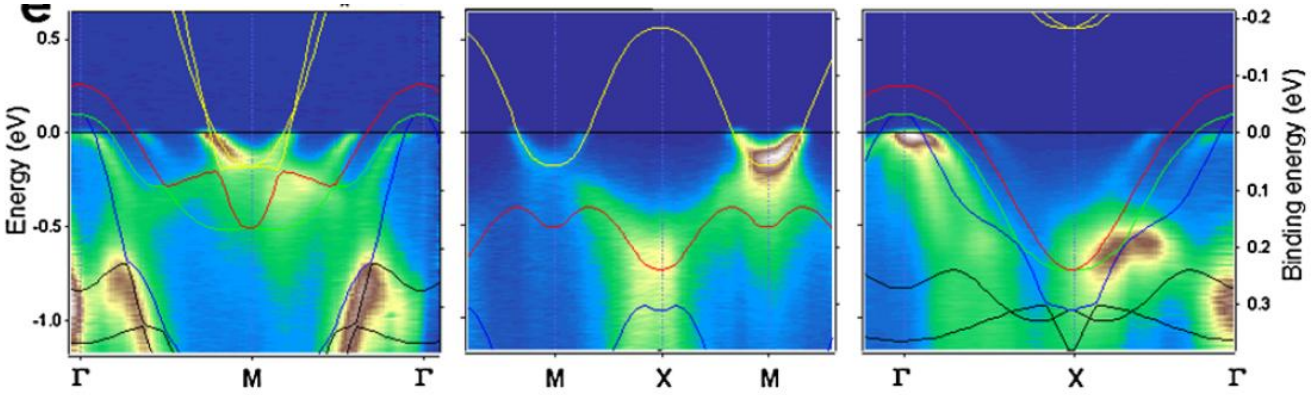
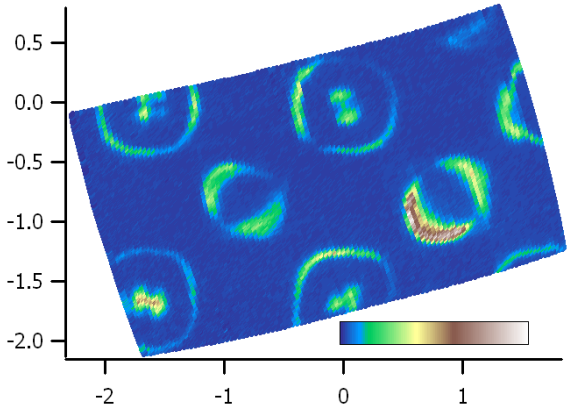

KFe2As2
LiFeAs
FeSe
Co-BaFe2As2
K-BaFe2As2
Theory for 1111
Co-SmFeAsO
K-BaFe2As2
Co-SmFeAsO
Rb-Fe-Se
Pt-BaFe2As2
Co-BaFe2As2
kx (1/Å)
ky (1/Å)

Energy scale of 1 eV

Superconducting material: LiFeAs

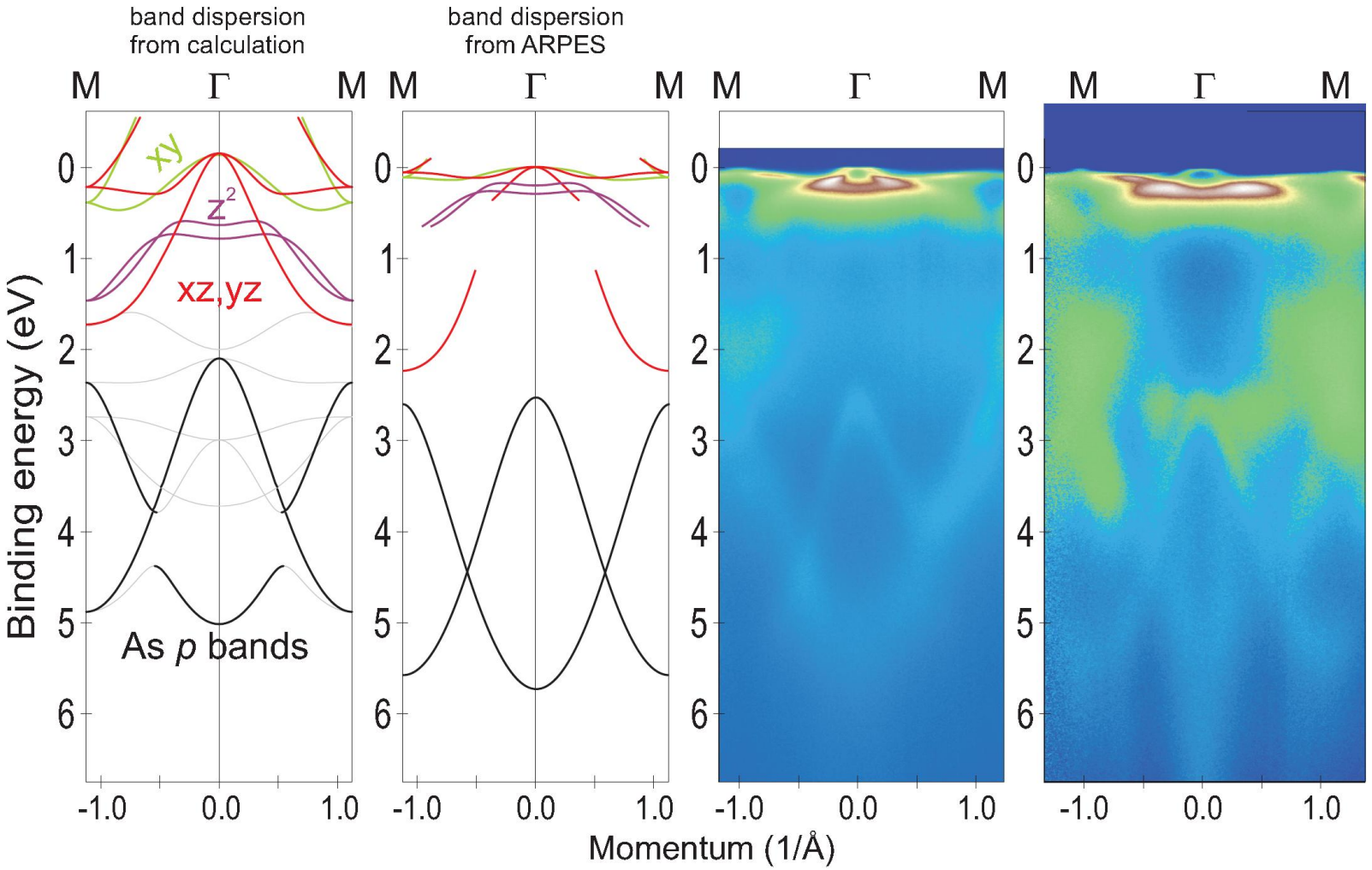




Renormalization ~ 3

SVB *et al.*, *PRL* (2010)

Spectra of NaFeAs in a wide energy range



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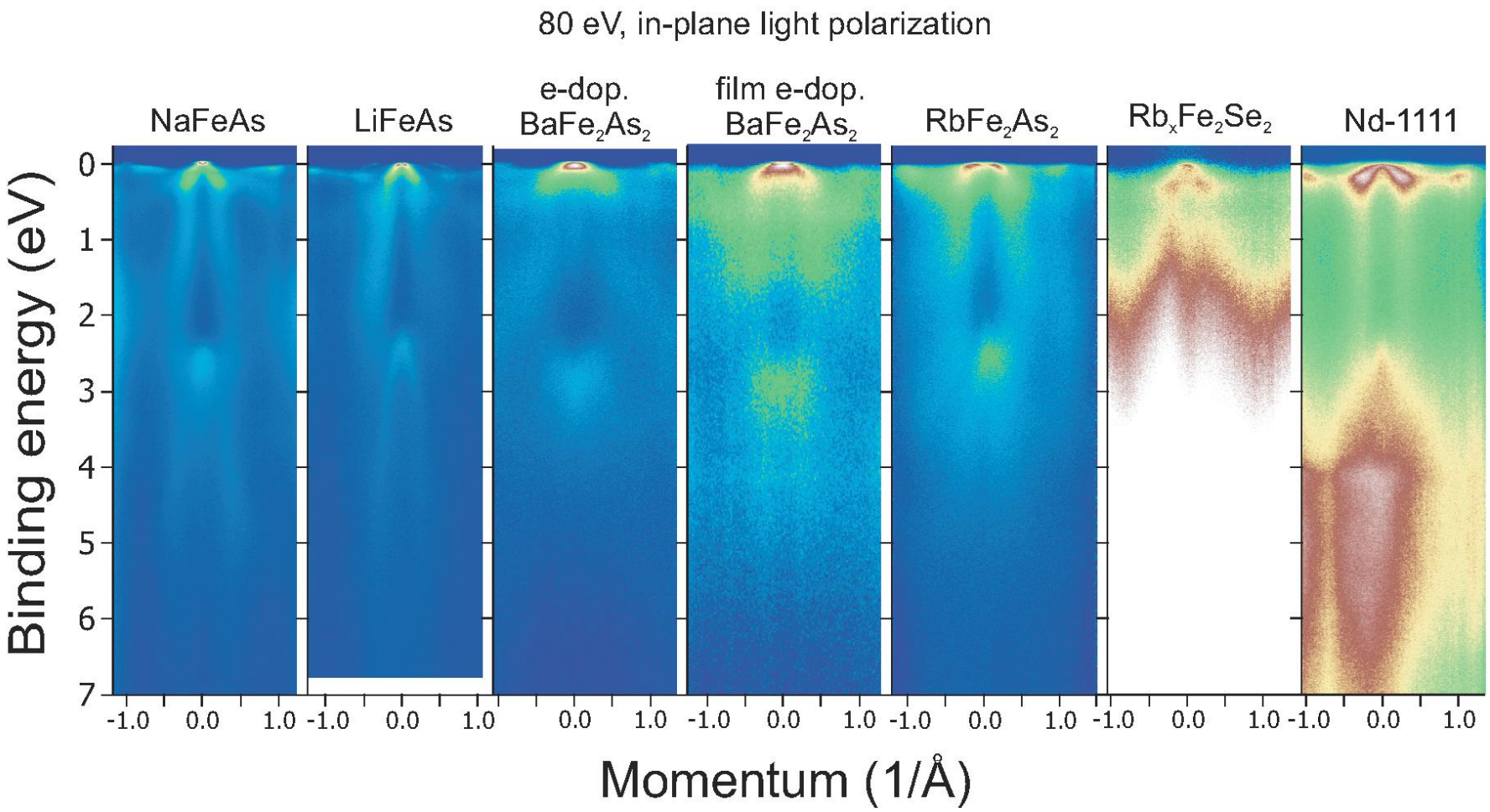
Evtushinsky *et al. arXiv*

High-energy anomaly in iron-based SC



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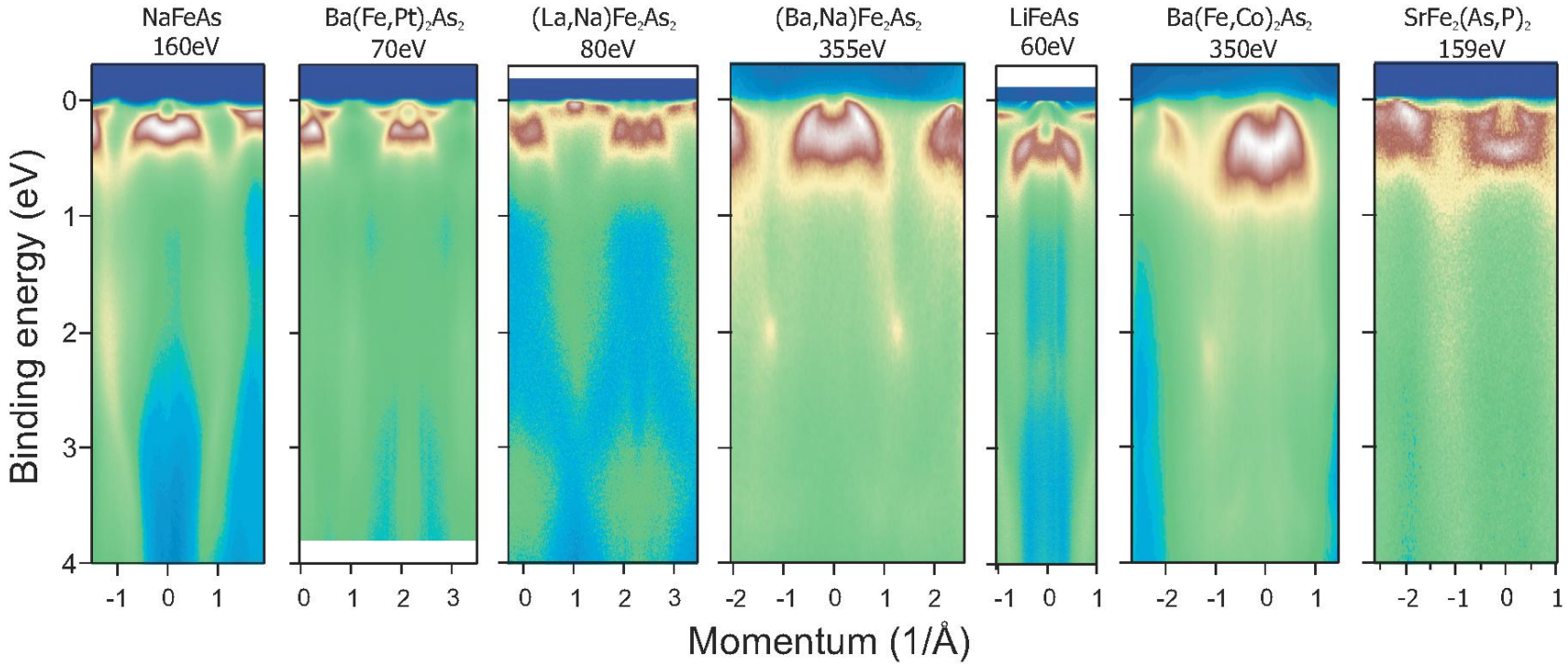
Evtushinsky *et al. arXiv*

High-energy anomaly in iron-based SC



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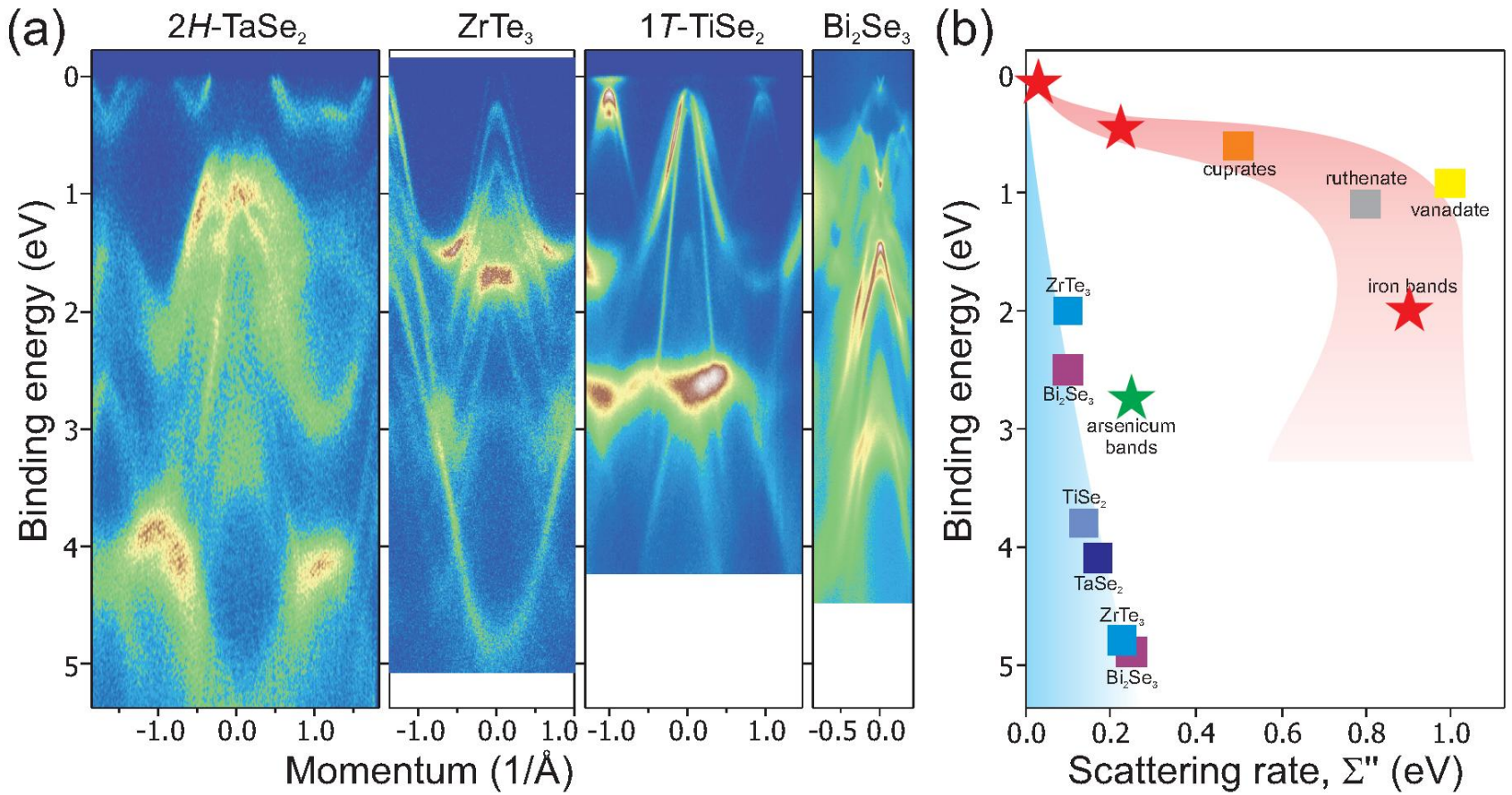
Electron scattering rate in ordinary and strongly interacting systems



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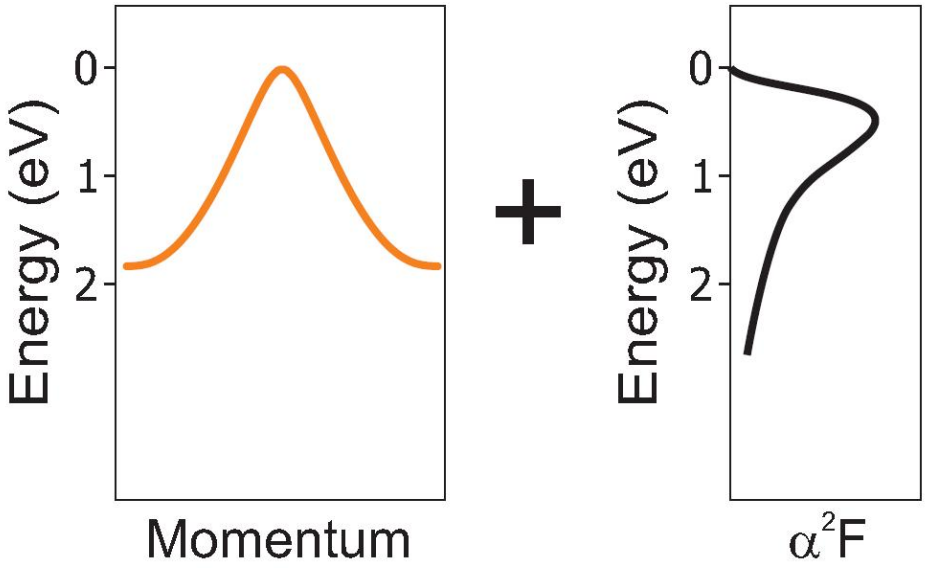
Model for high-energy spectral function



$$\Sigma'(\omega) = \int_0^{\infty} \alpha^2 F(\Omega) \cdot \ln\left|\frac{\omega + \Omega}{\omega - \Omega}\right| \cdot \mathrm{d}\Omega \qquad \Sigma''(\omega) = -\pi \int_0^{\omega} \alpha^2 F(\Omega) \cdot \mathrm{d}\Omega$$

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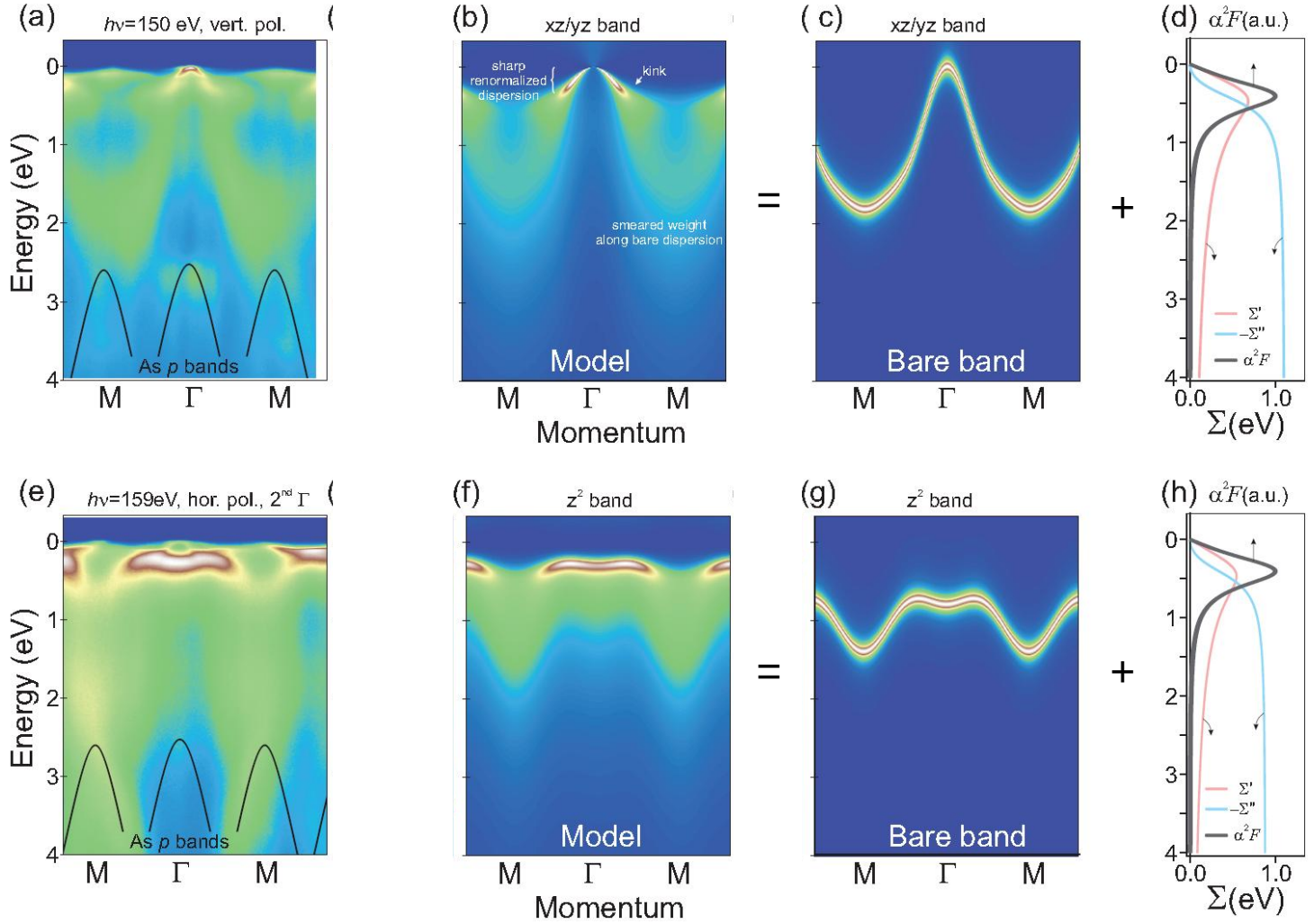
How to understand the electronic structure on 1 eV energy scale (alternative – DMFT)

Experiment Theory = bare band + α^2F



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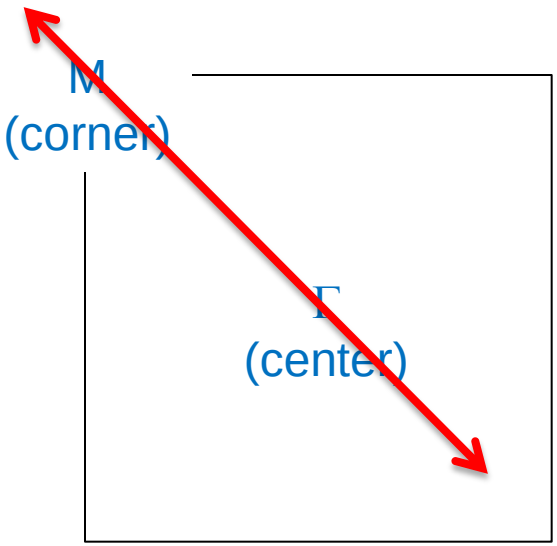
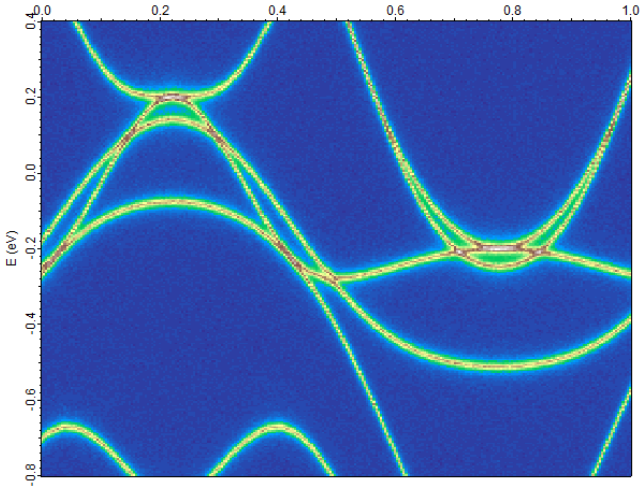
Energy scale of 0.1 eV

BZ

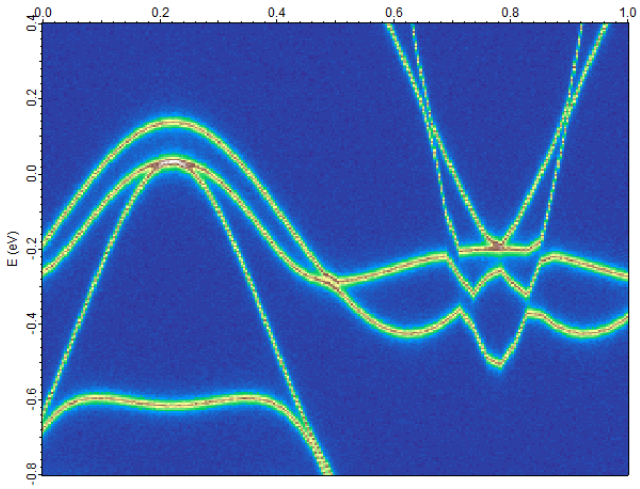


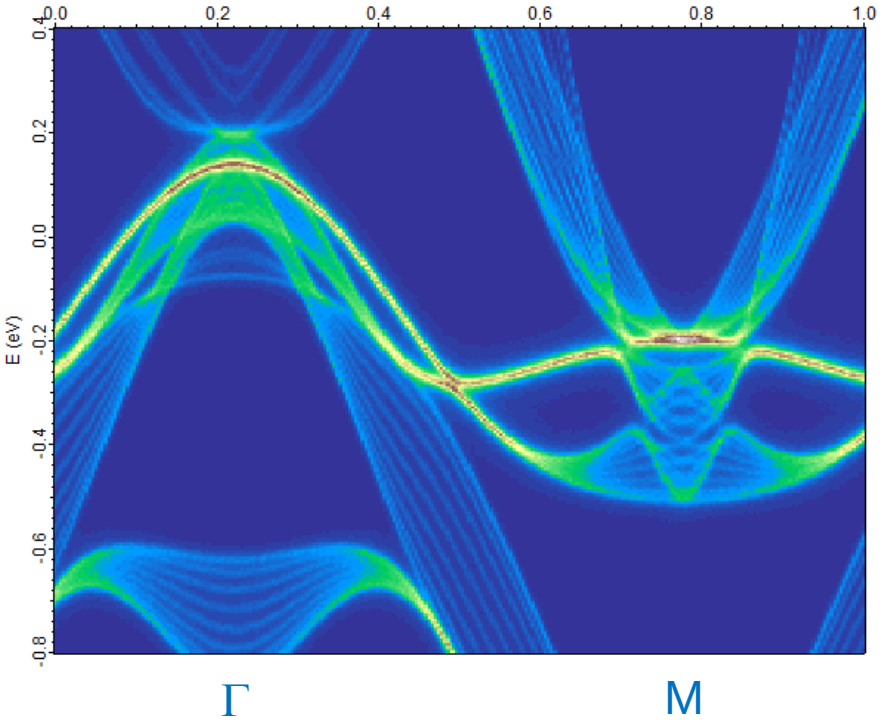
122

$k_z=\pi$



$k_z=0$





Calculations: A .Yaresko

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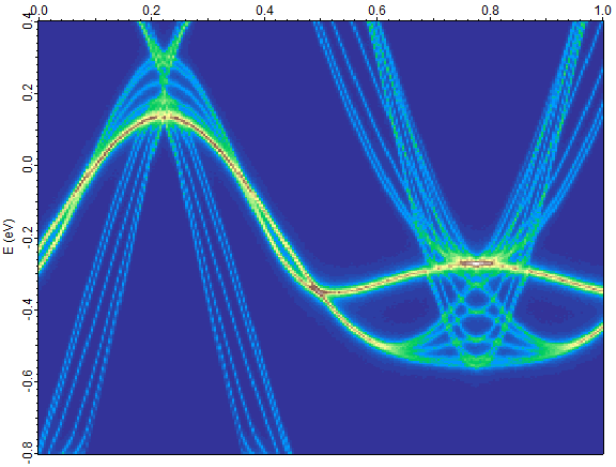

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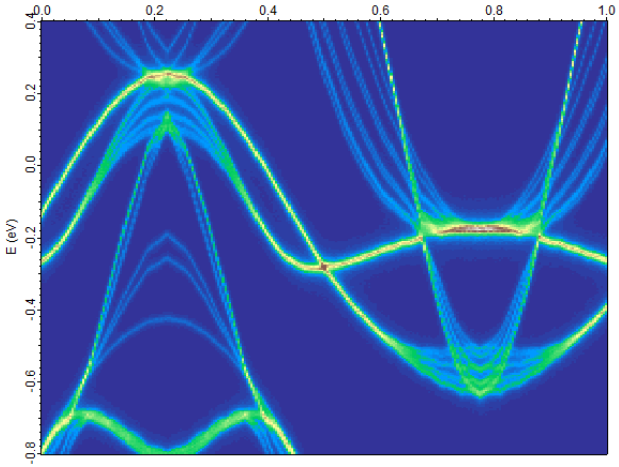

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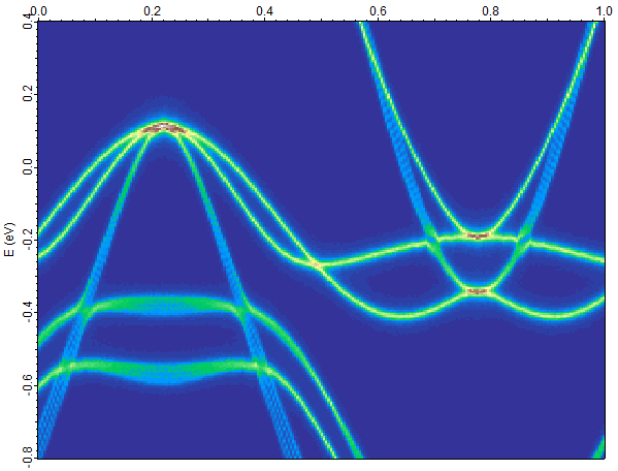

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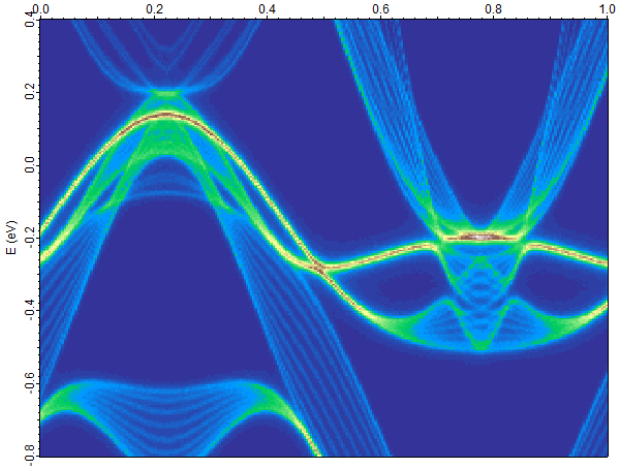

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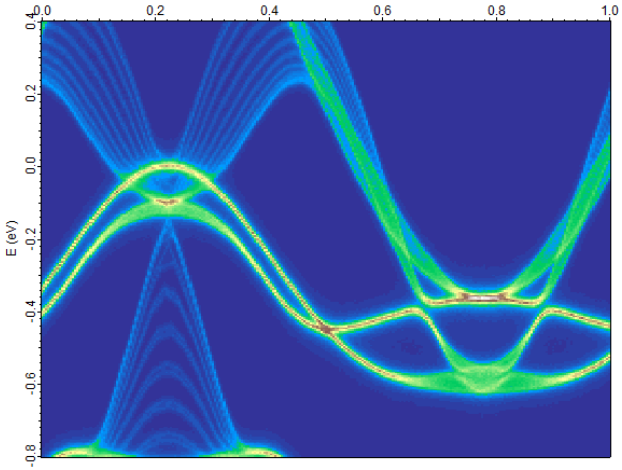

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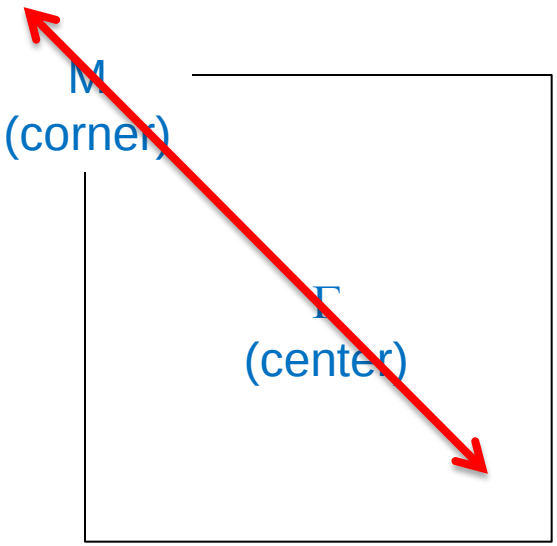
BZ



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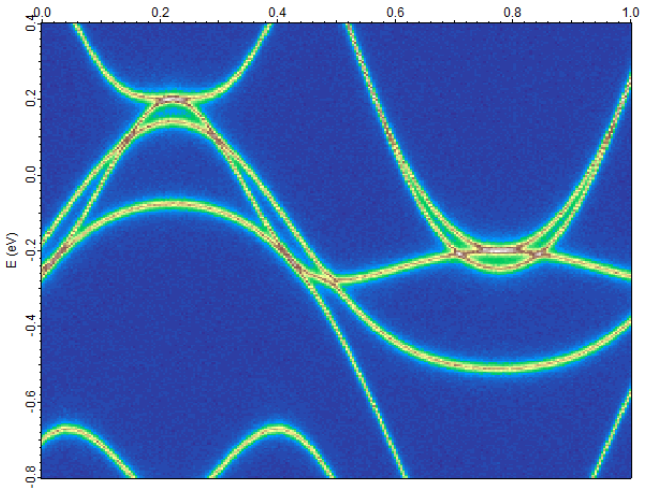

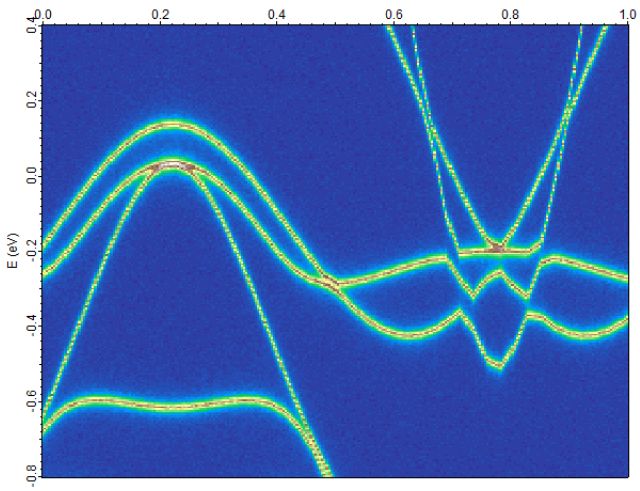

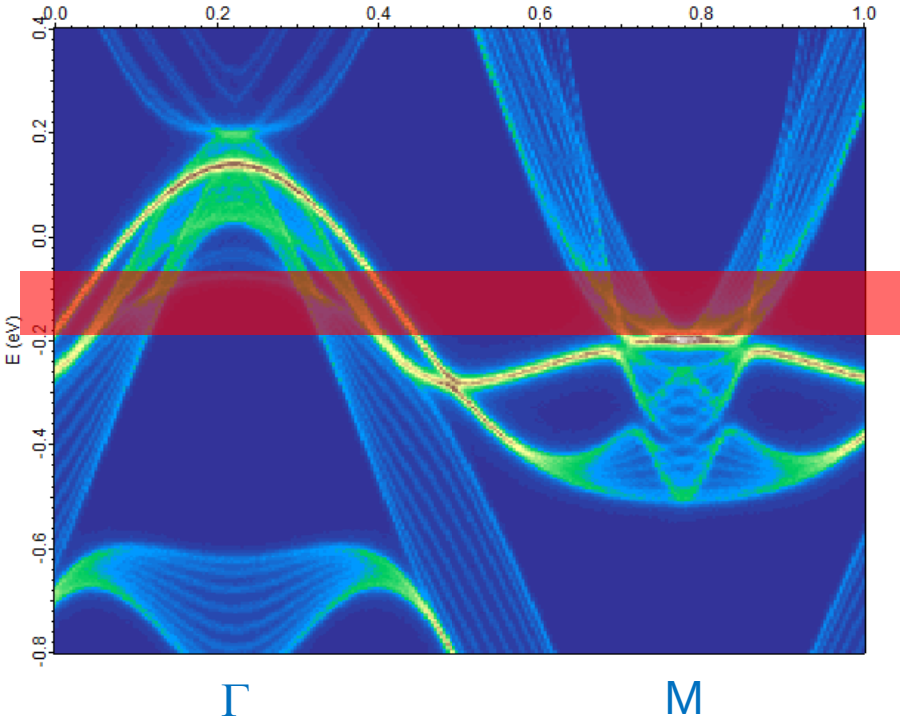

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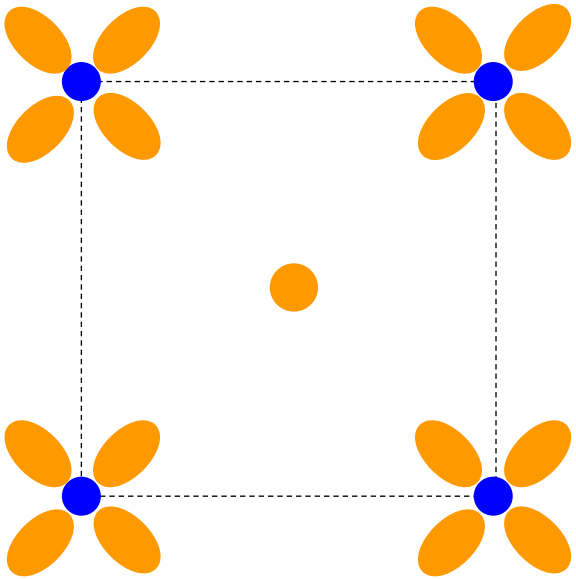
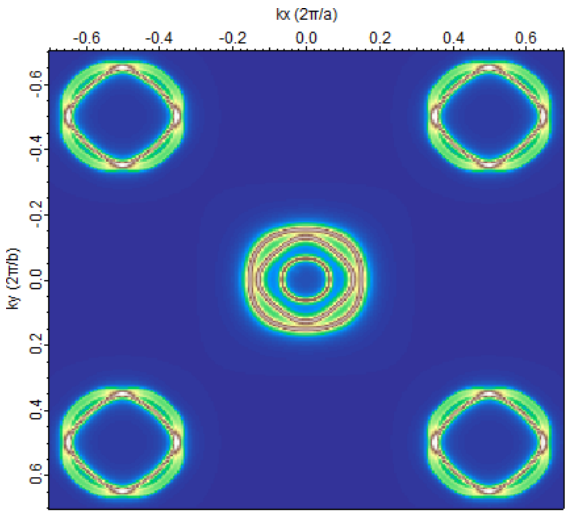
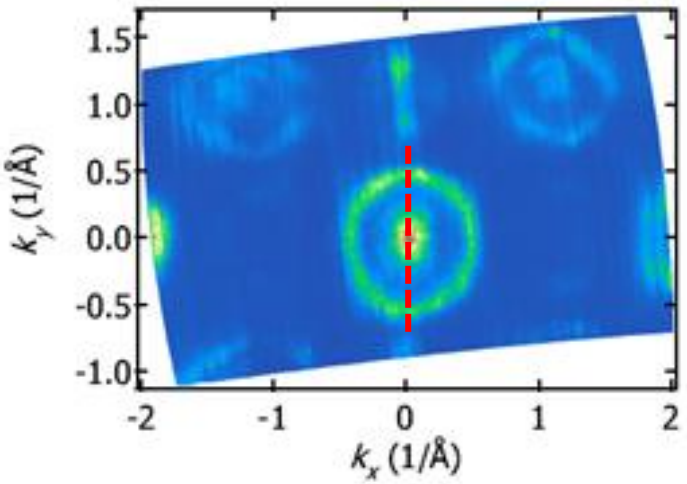
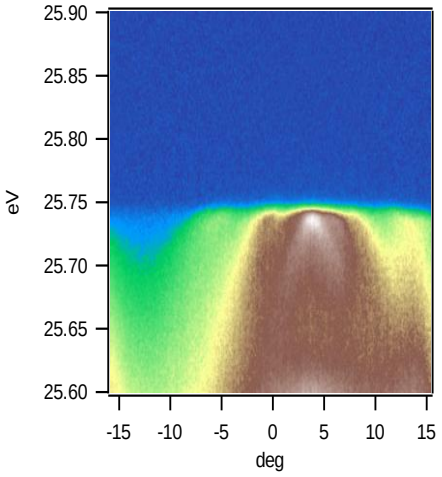
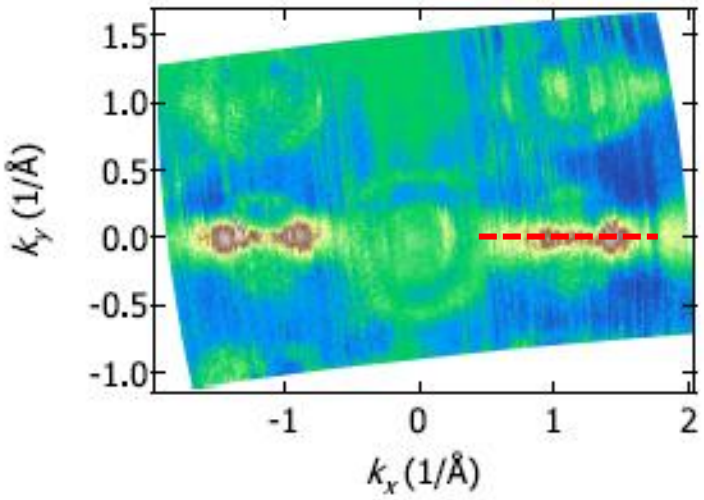
Co-SmFeAsO (T_c=16K)

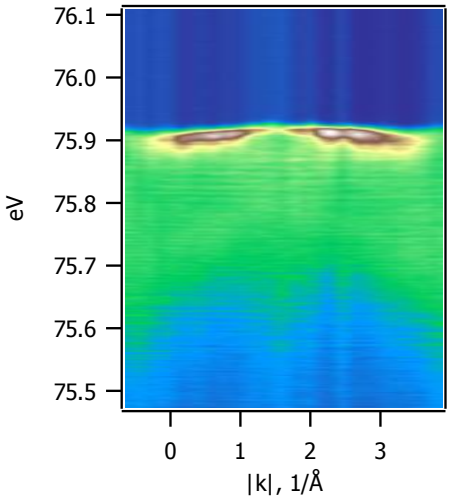












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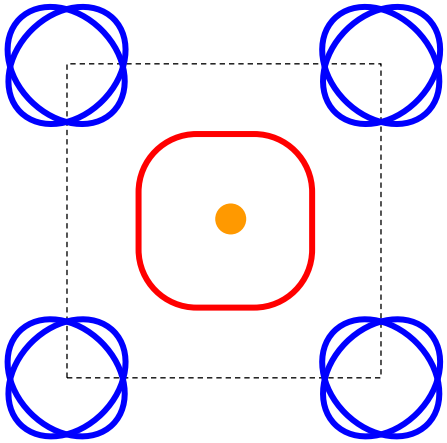
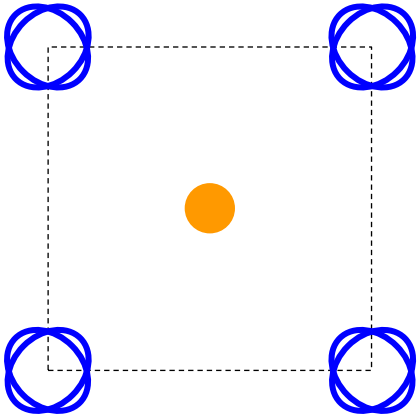
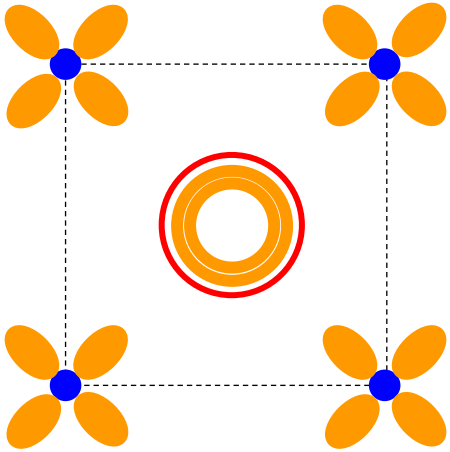
LiFeAs
T_c=18K



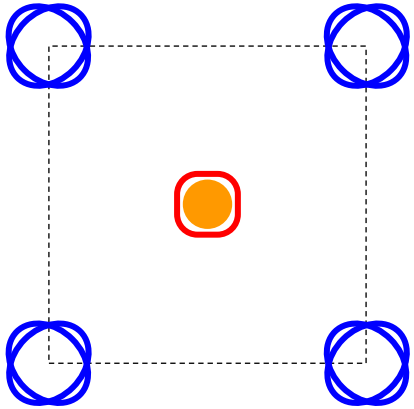
Pt-$BaFe_2As_2$
T_c=20K



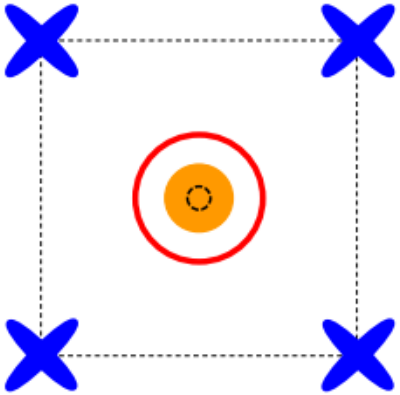
K-$BaFe_2As_2$
T_c=38K



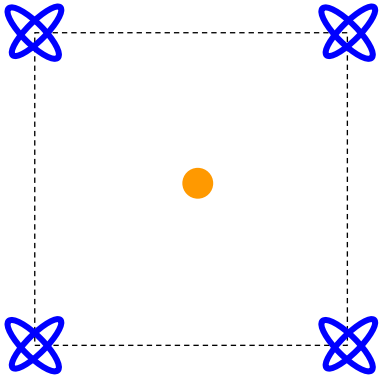
Co-$BaFe_2As_2$
T_c=25K



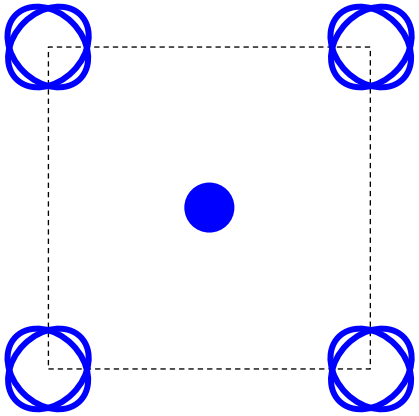
Pt-Ca-Fe-As
T_c=38K



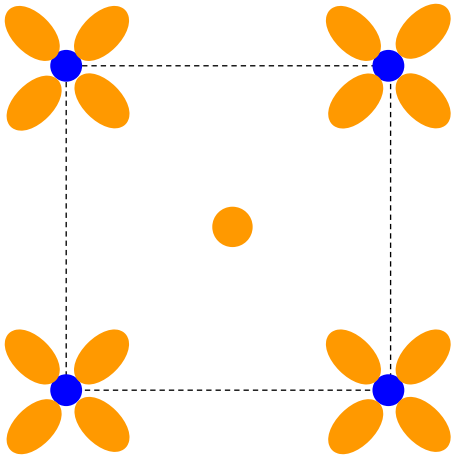
FeSe
T_c=8K



Rb-Fe-Se
T_c=33K



Co-SmFeAsO
T_c=16K



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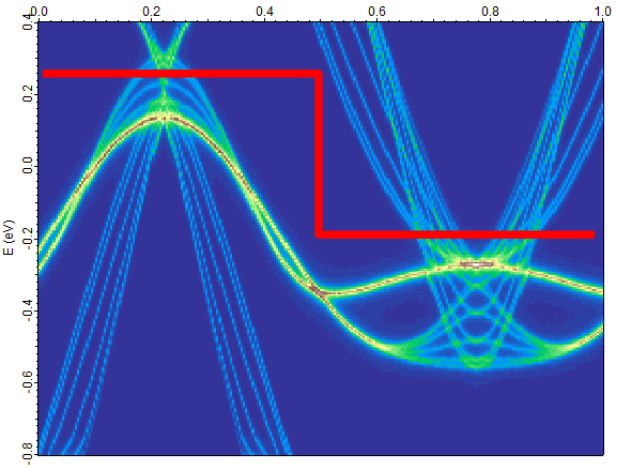
Simple way to understand the electronic structure on 0.1 eV scale

11



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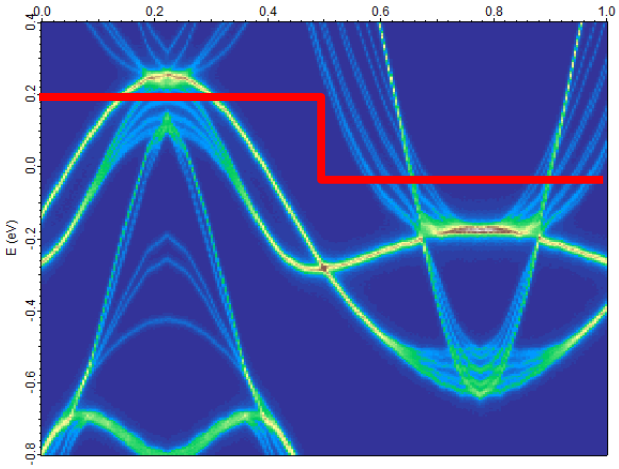

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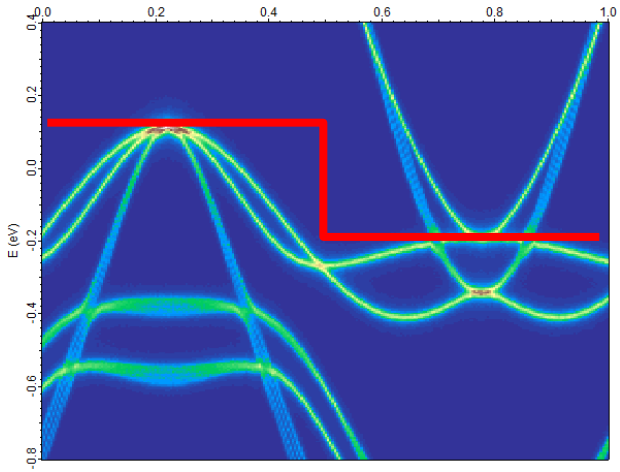

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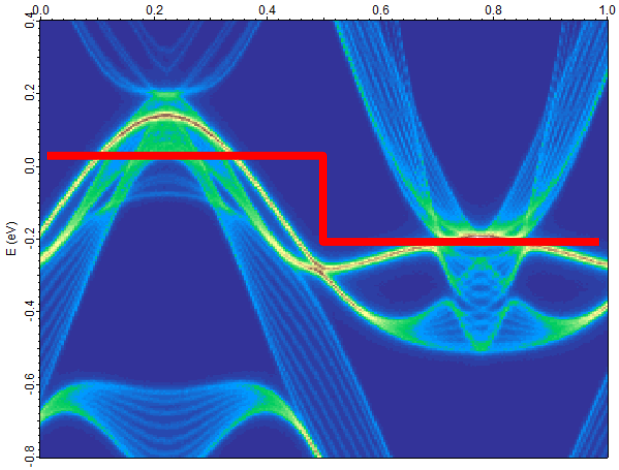

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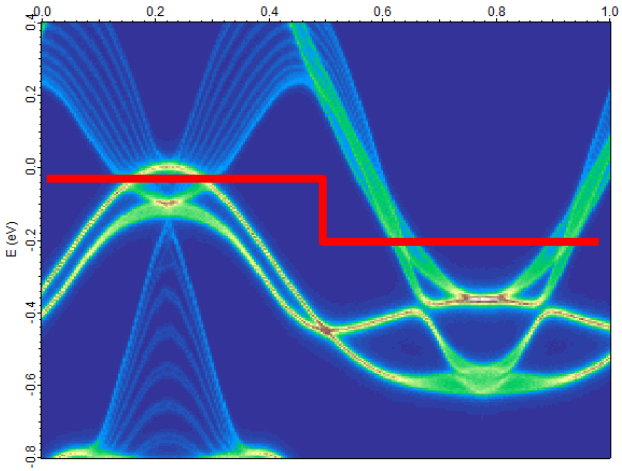

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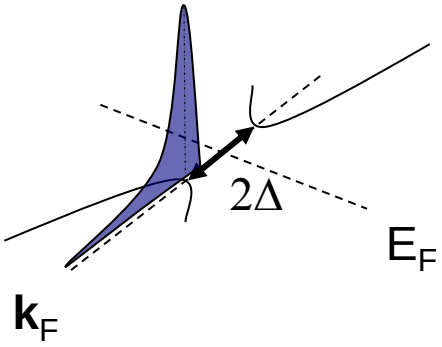
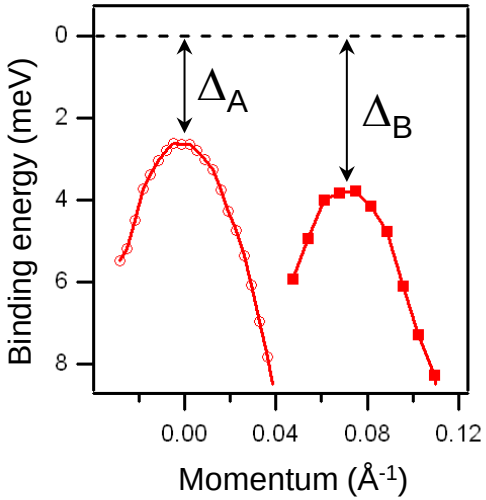
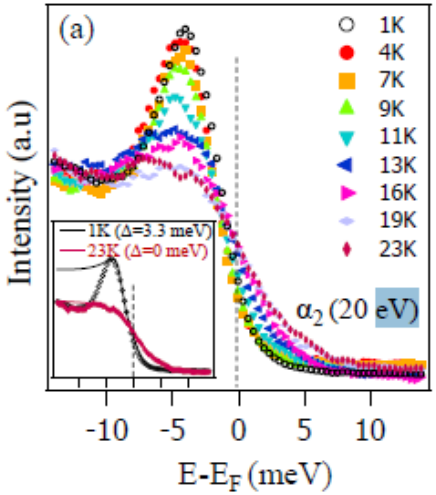
Energy scale of 0.001 eV (gaps)

Gaps







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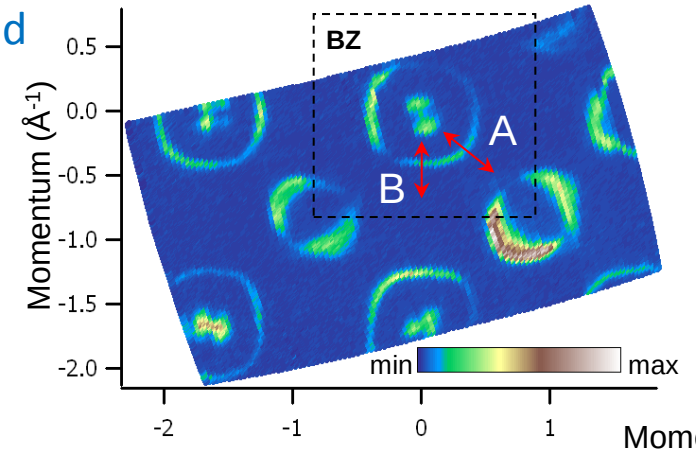
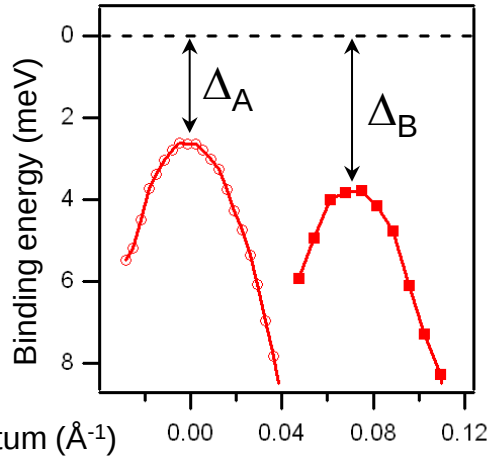
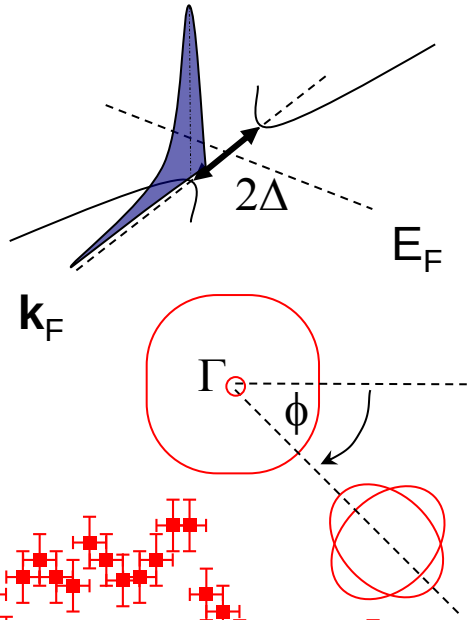
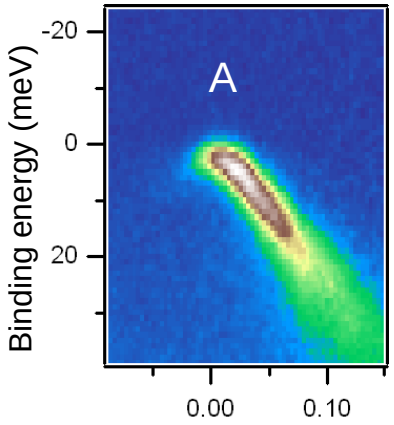
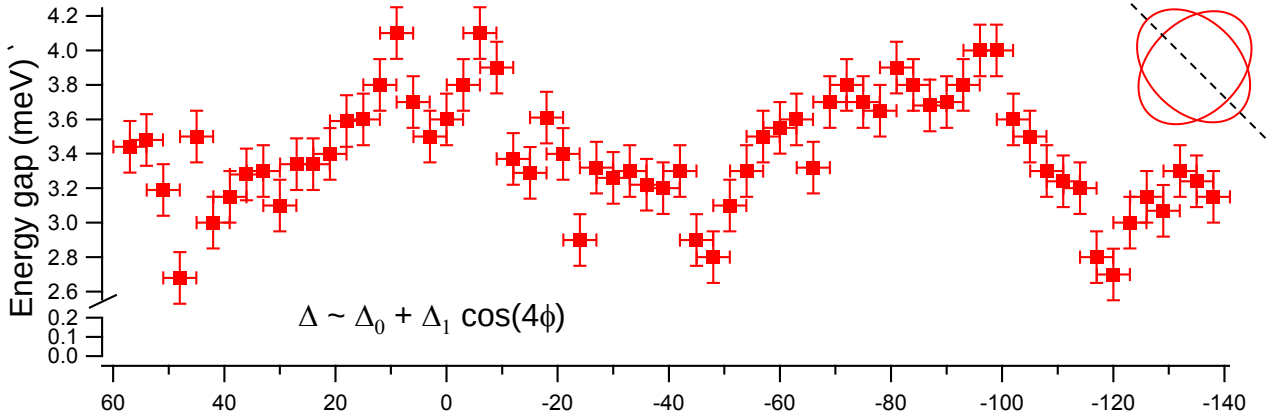
LiFeAs:
xy band

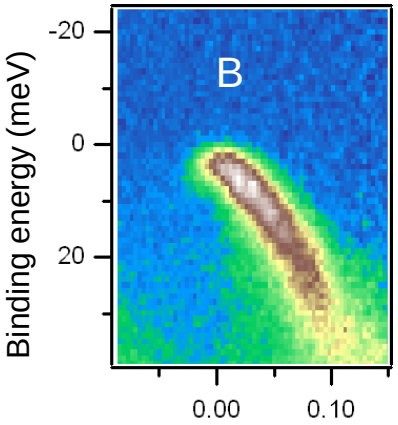


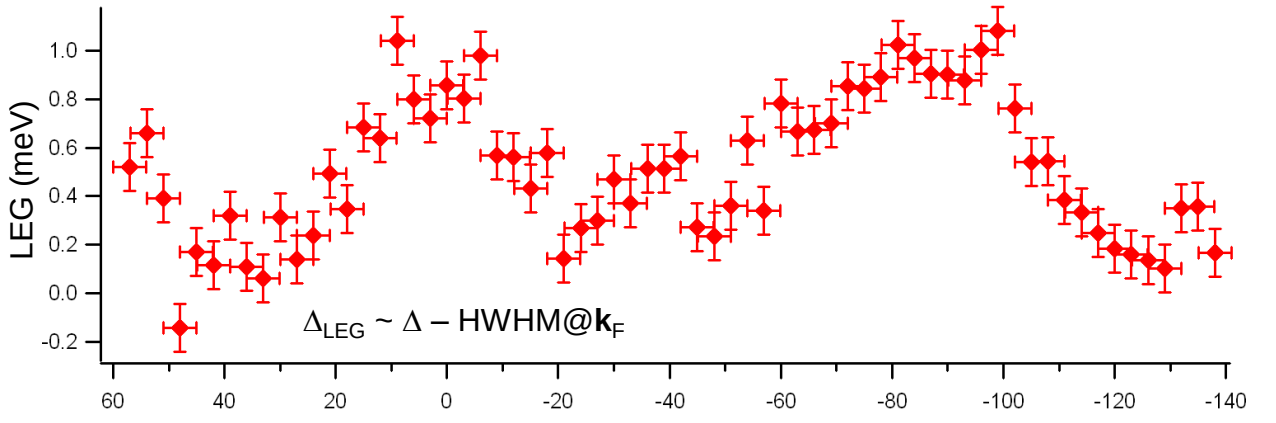






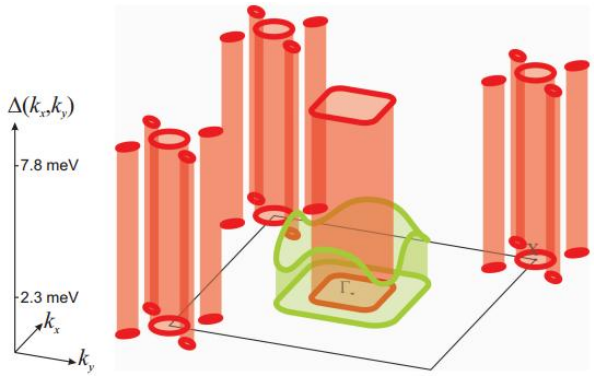






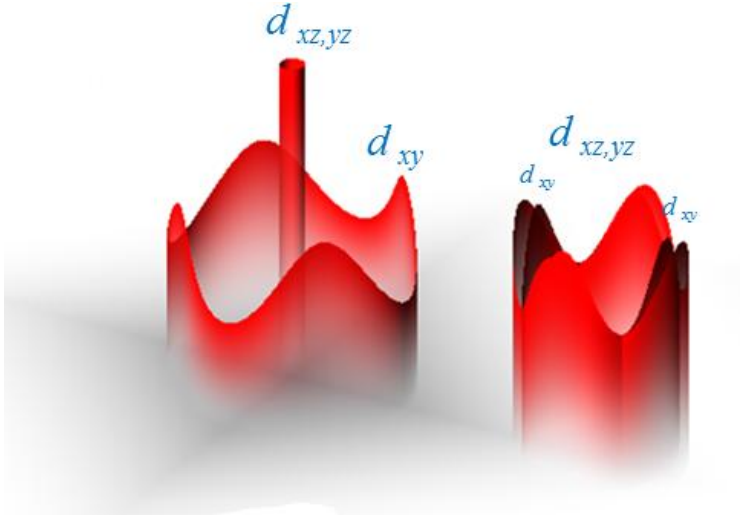
SVB et al.
Symmetry 12

Ca-$NaFe_2As_2$



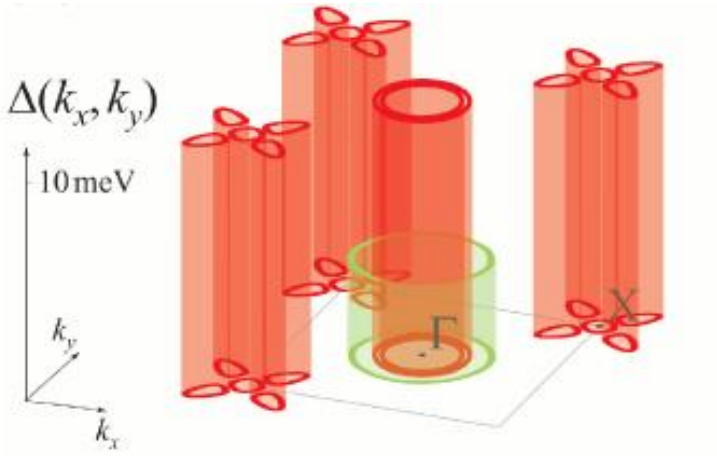
Evtushinsky et al. PRB 14

LiFeAs



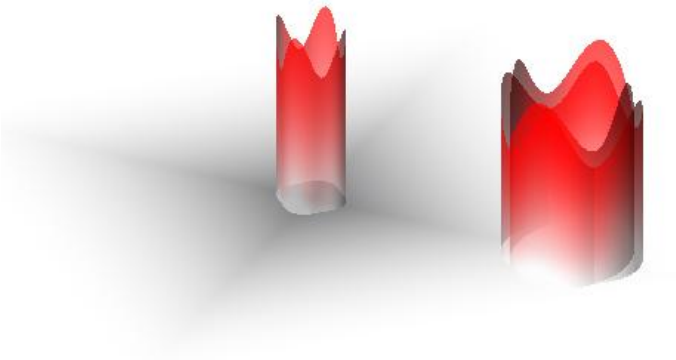
SVB et al. Symmetry 12

K-$BaFe_2As_2$

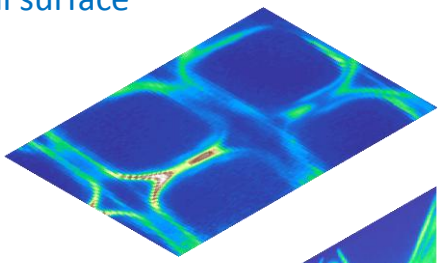


Evtushinsky et al. PRB 13

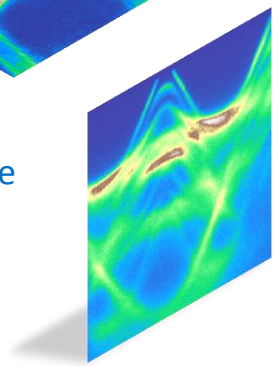
K-FeSe



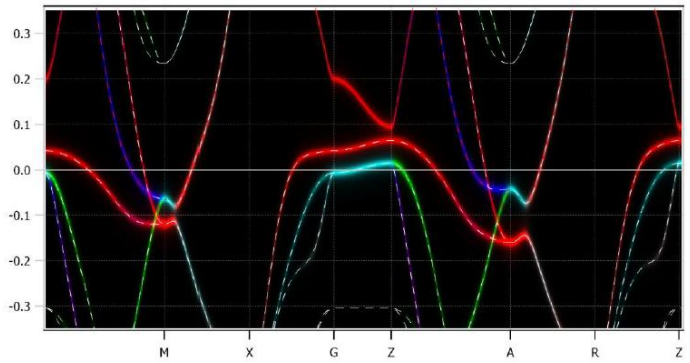
Fermi surface



Band structure



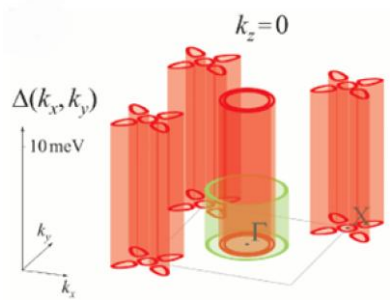
„Quasiparticle Tight-Binding Fit“



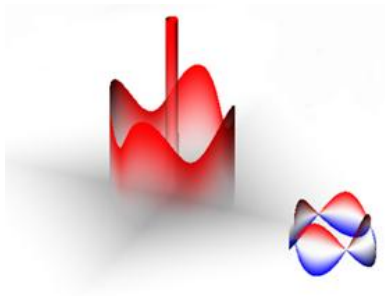
Orbitals: XY XZ YZ

Your Theory

Gap function from experiment



Gap function from theory



S.V. Borisenko
IFW-Dresden

Superconducting gap in LiFeAs from three-dimensional spin-fluctuation pairing calculations

Y. Wang,[1] A. Kreisel,[1] V. B. Zabolotnyy,[2,3] S. V. Borisenko,[2] B. Büchner,[2,4] T. A. Maier,[5] P. J. Hirschfeld,[1] and D. J. Scalapino[6]

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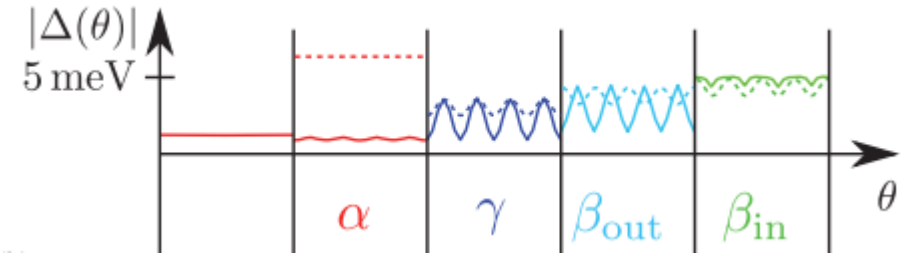
The lack of nesting of the electron and hole Fermi-surface sheets in the Fe-based superconductor LiFeAs, with a critical temperature of 18 K, has led to questions as to whether the origin of superconductivity in this material might be different from other Fe-based superconductors. Both angle-resolved photoemission and quasiparticle interference experiments have reported fully gapped superconducting order parameters with significant anisotropy. The system is also of interest because relatively strong correlations seem to be responsible for significant renormalization of the hole bands. Here we present calculations of the superconducting gap and pairing in the random-phase approximation using Fermi surfaces derived from measured photoemission spectra. The qualitative features of the gaps obtained in these calculations are shown to be different from previous two-dimensional theoretical works and in good agreement with experiment on the main Fermi-surface pockets. We analyze the contributions to the pairing vertex thus obtained and show that the scattering processes between electron and hole pockets that are believed to dominate the pairing in other Fe-based superconductors continue to do so in LiFeAs despite the lack of nesting, leading to gaps with anisotropic $s_{\pm}$ structure. Some interesting differences relating to the enhanced d_{xy} orbital content of the LiFeAs Fermi surface are noted.

DOI: 10.1103/PhysRevB.88.174516 PACS number(s): 74.70.Xa, 74.20.Rp, 74.20.Fg, 74.25.Jb



Reproduction of experimental gap structure in LiFeAs based on orbital-spin fluctuation theory: s_{++}-wave, $s_{\pm}$-wave, and hole-$s_{\pm}$-wave states

Tetsuro Saito,[1] Seiichiro Onari,[2] Youichi Yamakawa,[1] Hiroshi Kontani,[1] Sergey V. Borisenko,[3] and Volodymyr B. Zabolotnyy[3]

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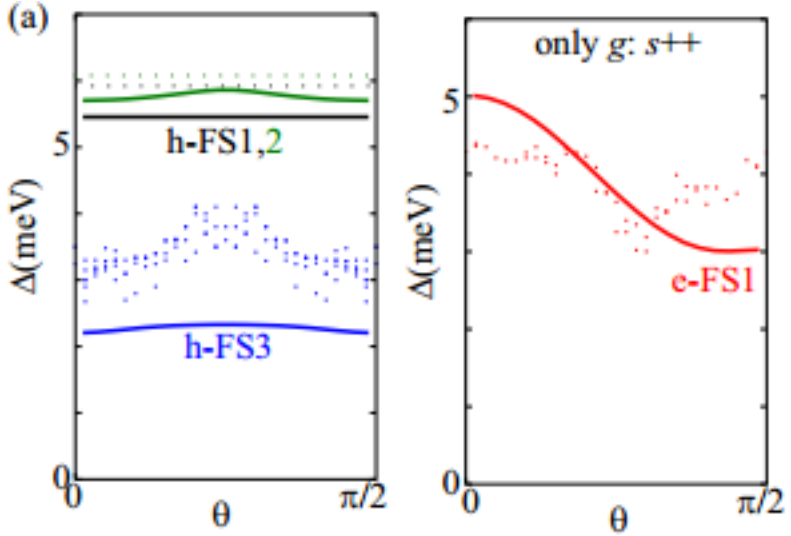
The absence of nesting between electron and hole pockets in LiFeAs with $T_c = 18$ K attracts great attention, as an important hint to understand the pairing mechanism of Fe-based superconductors. Here, we study the five-orbital model of LiFeAs based on the recently developed orbital-spin fluctuation theories. It is found that the experimentally observed gap structure of LiFeAs, which is a "fingerprint" of the pairing mechanism, is quantitatively reproduced in terms of the orbital-fluctuation-mediated s_{++}-wave state. Specifically, the largest gap observed on the two small hole pockets composed of (d_{xz}, d_{yz}) orbitals can be explained, and this is a hallmark of the orbital-fluctuation-mediated superconductivity. The s_{++}-wave gap structure becomes more anisotropic in the presence of weak spin fluctuations. As the spin fluctuations increase, we obtain the "hole-$s_{\pm}$-wave state," in which only the gap of the large hole pocket made of the d_{xy} orbital is sign reversed, due to the cooperation of orbital and spin fluctuations. This gap structure with "sign reversal between hole pockets" is similar to that recently reported in $(Ba,K)Fe_2As_2$.



PHYSICAL REVIEW B 89, 144513 (2014)

Superconductivity from repulsion in LiFeAs: Novel s-wave symmetry and potential time-reversal symmetry breaking

F. Ahn,[1] I. Eremin,[1,*] J. Knolle,[2] V. B. Zabolotnyy,[3] S. V. Borisenko,[3] B. Büchner,[3] and A. V. Chubukov[4]

[1]*Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany*

[2]*Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany*

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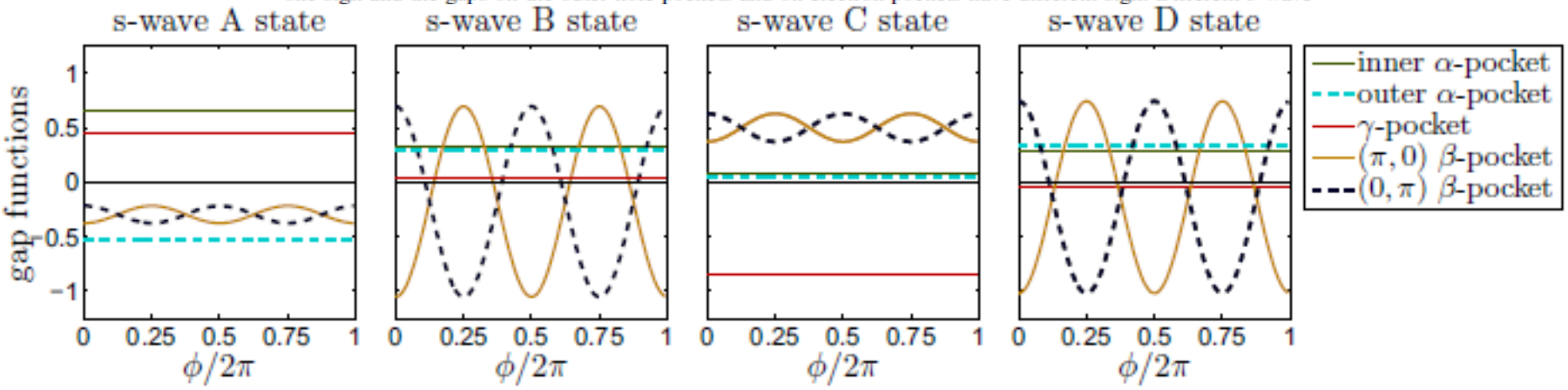
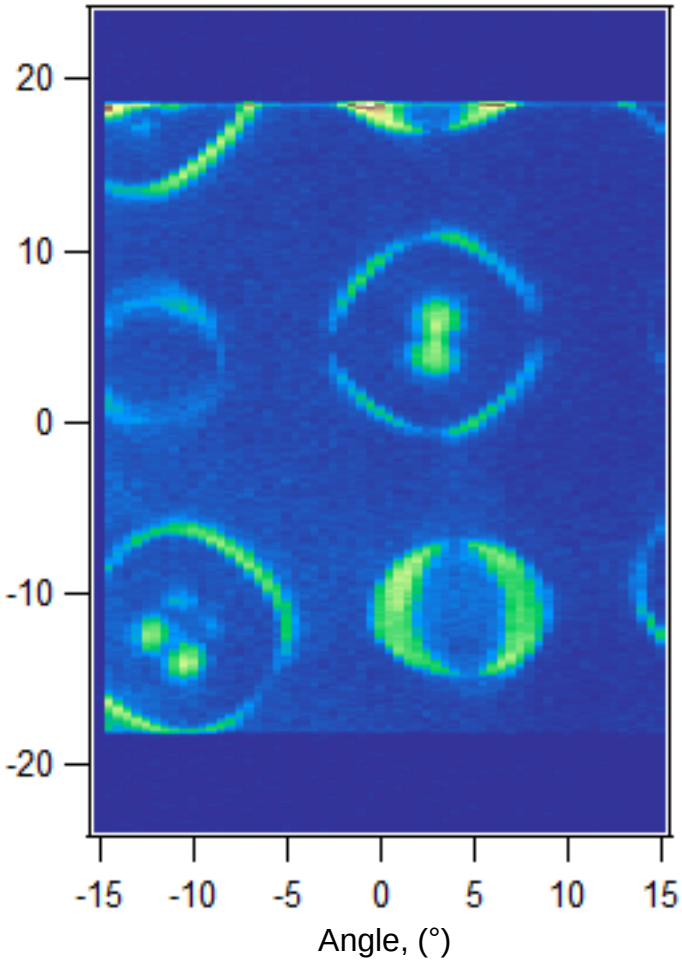
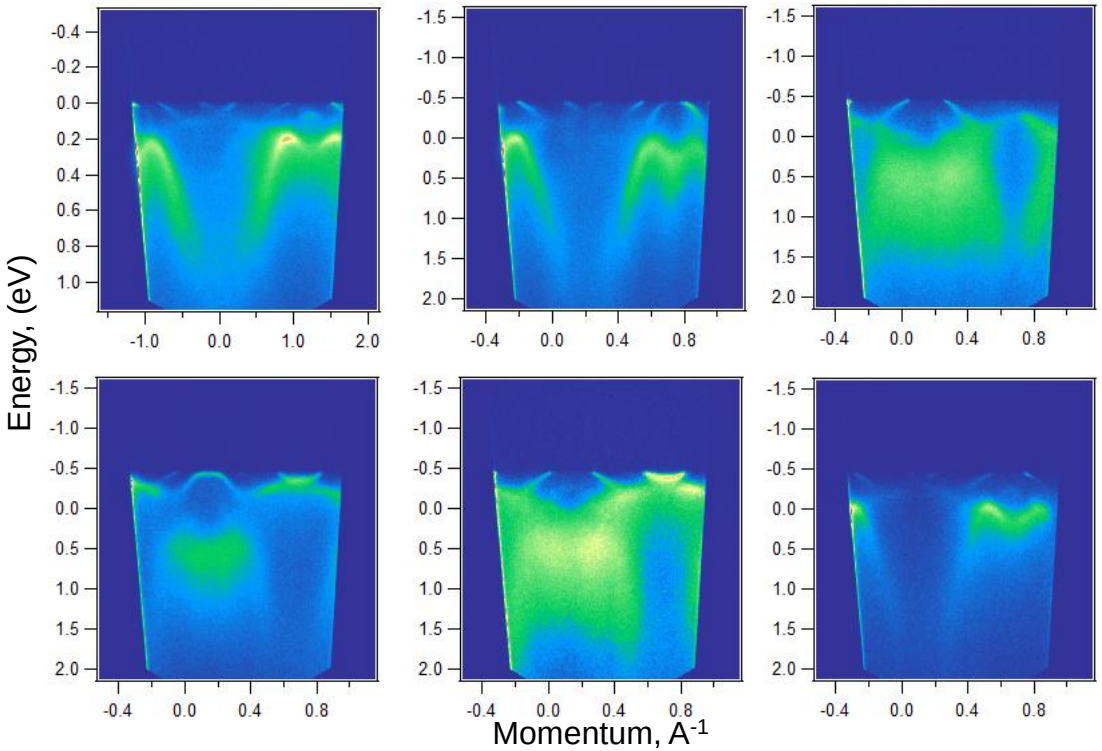
We analyze the structure of the pairing interaction and superconducting gap in LiFeAs by decomposing the pairing interaction for various k_z cuts into s- and d-wave components and by studying the leading superconducting instabilities. We use the ten-orbital tight-binding model, derived from *ab initio* LDA calculations with hopping parameters extracted from the fit to ARPES experiments. We find that the pairing interaction almost decouples between two subsets; one consists of the outer hole pocket and two electron pockets, which are quasi-2D and are made largely out of the d_{xy} orbital, and the other consists of the two inner hole pockets, which are quasi-3D and are made mostly out of d_{xz} and d_{yz} orbitals. Furthermore, the bare interpocket and intrapocket interactions within each subset are nearly equal. In this situation, small changes in the intrapocket and interpocket interactions due to renormalizations by high-energy fermions give rise to a variety of different gap structures. We focus on s-wave pairing which, as experiments show, is the most likely pairing symmetry in LiFeAs. We find four different configurations of the s-wave gap immediately below T_c: one in which the superconducting gap changes sign between two inner hole pockets and between the outer hole pocket and two electron pockets, one in which the gap changes sign between two electron pockets and three hole pockets, one in which the gap on the outer hole pocket differs in sign from the gaps on the other four pockets, and one in which the gaps on two inner hole pockets have one sign and the gaps on the outer hole pockets and on electron pockets have different sign. Different s-wave



More precision is needed !

LiFeAs: more precision





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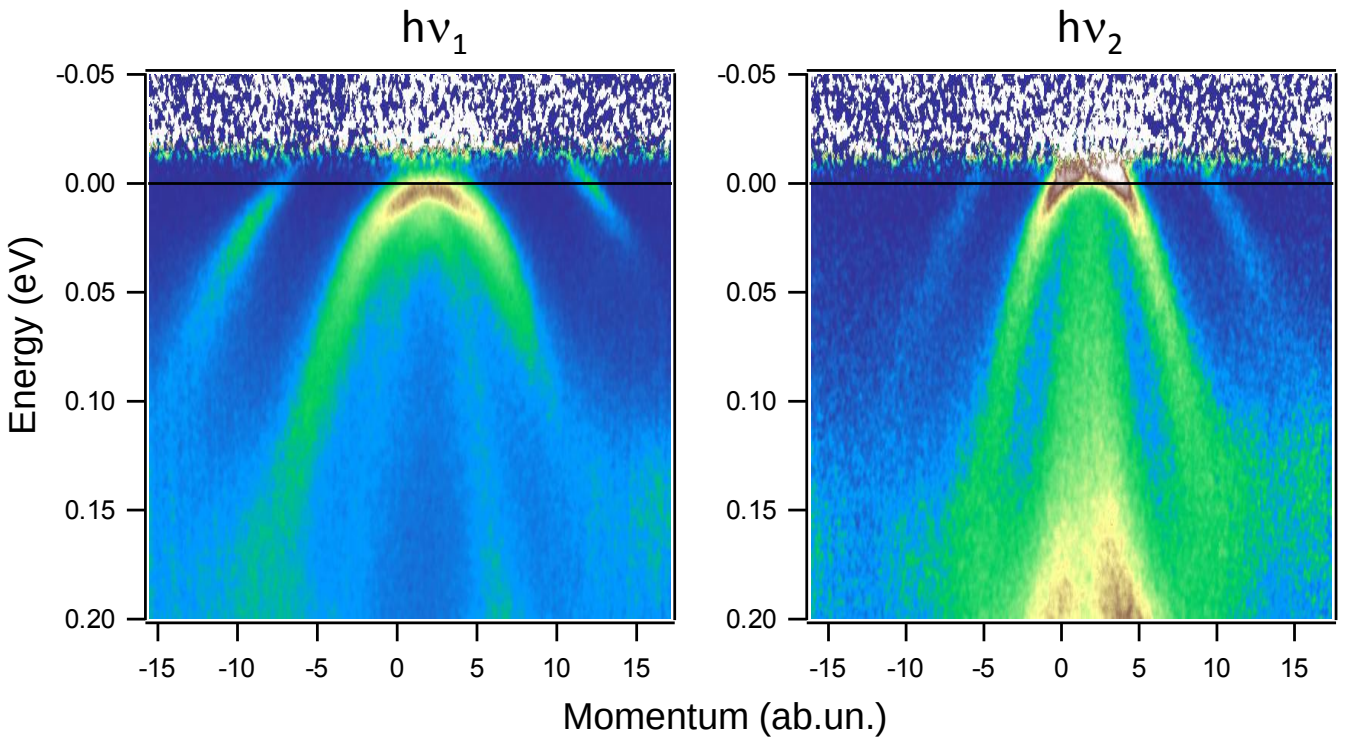
LiFeAs: structure near center of BZ



?

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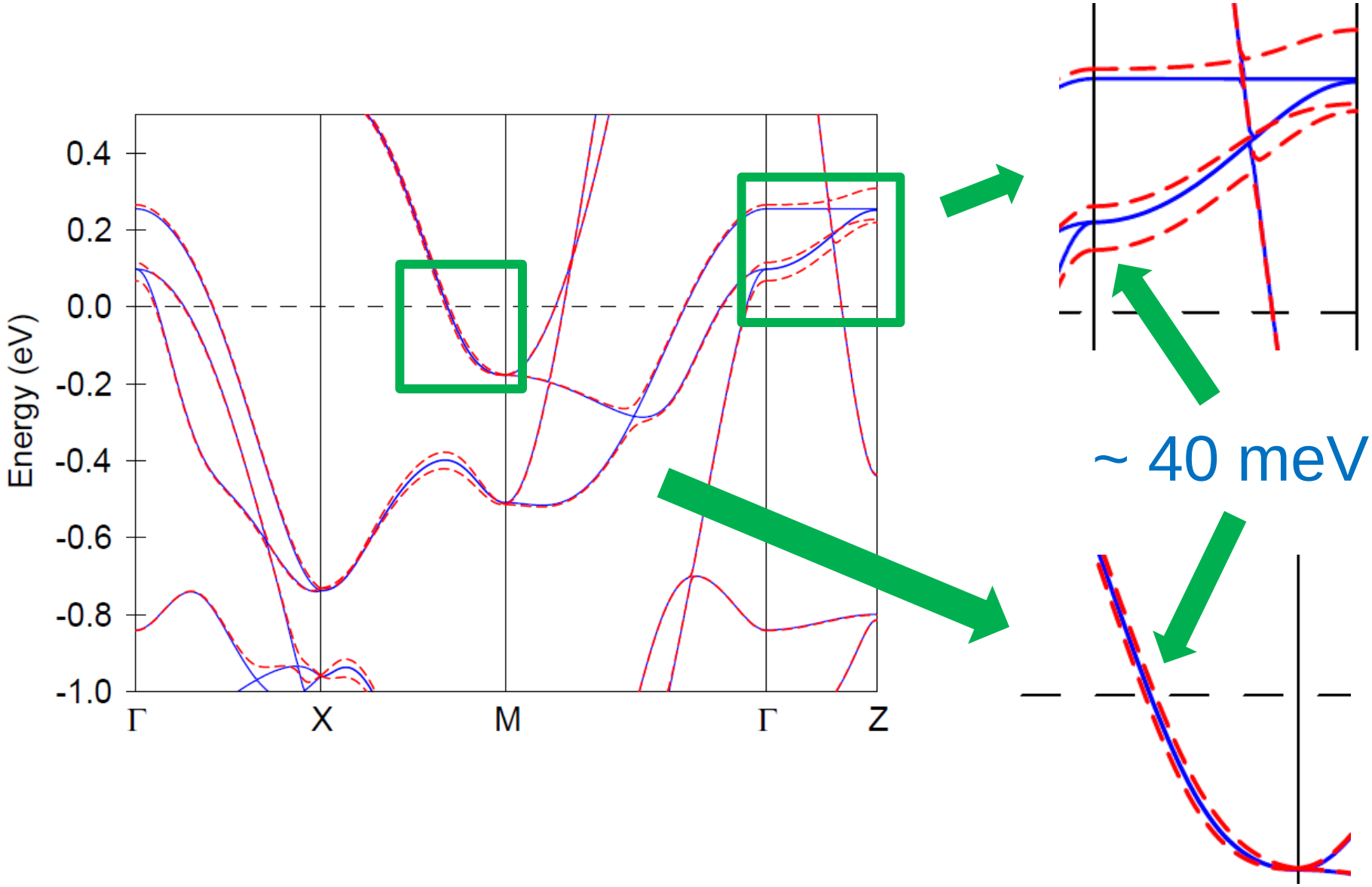
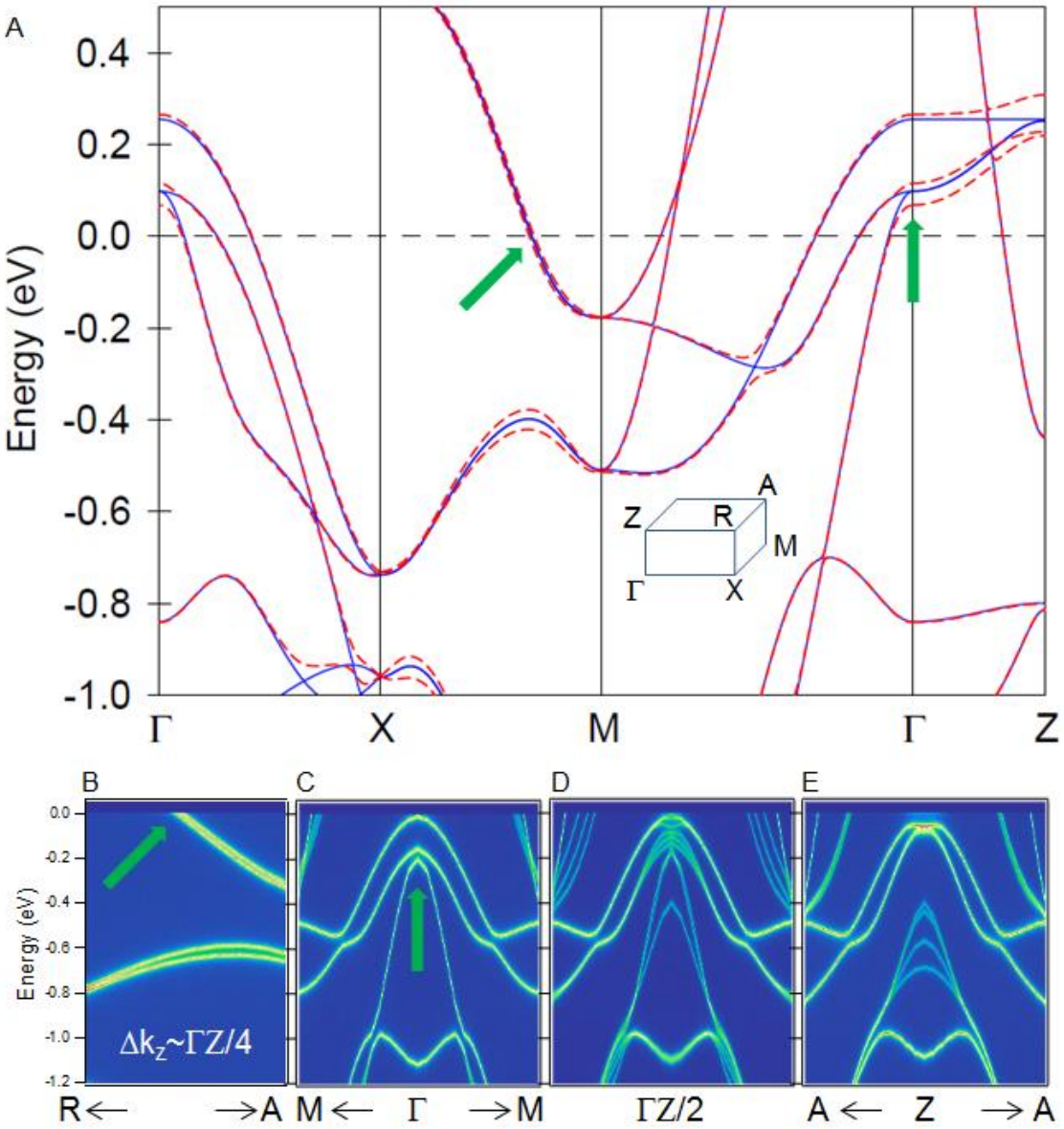
LiFeAs: spin-orbit coupling



Calculations: A. Yaresko

What to expect in ARPES spectra



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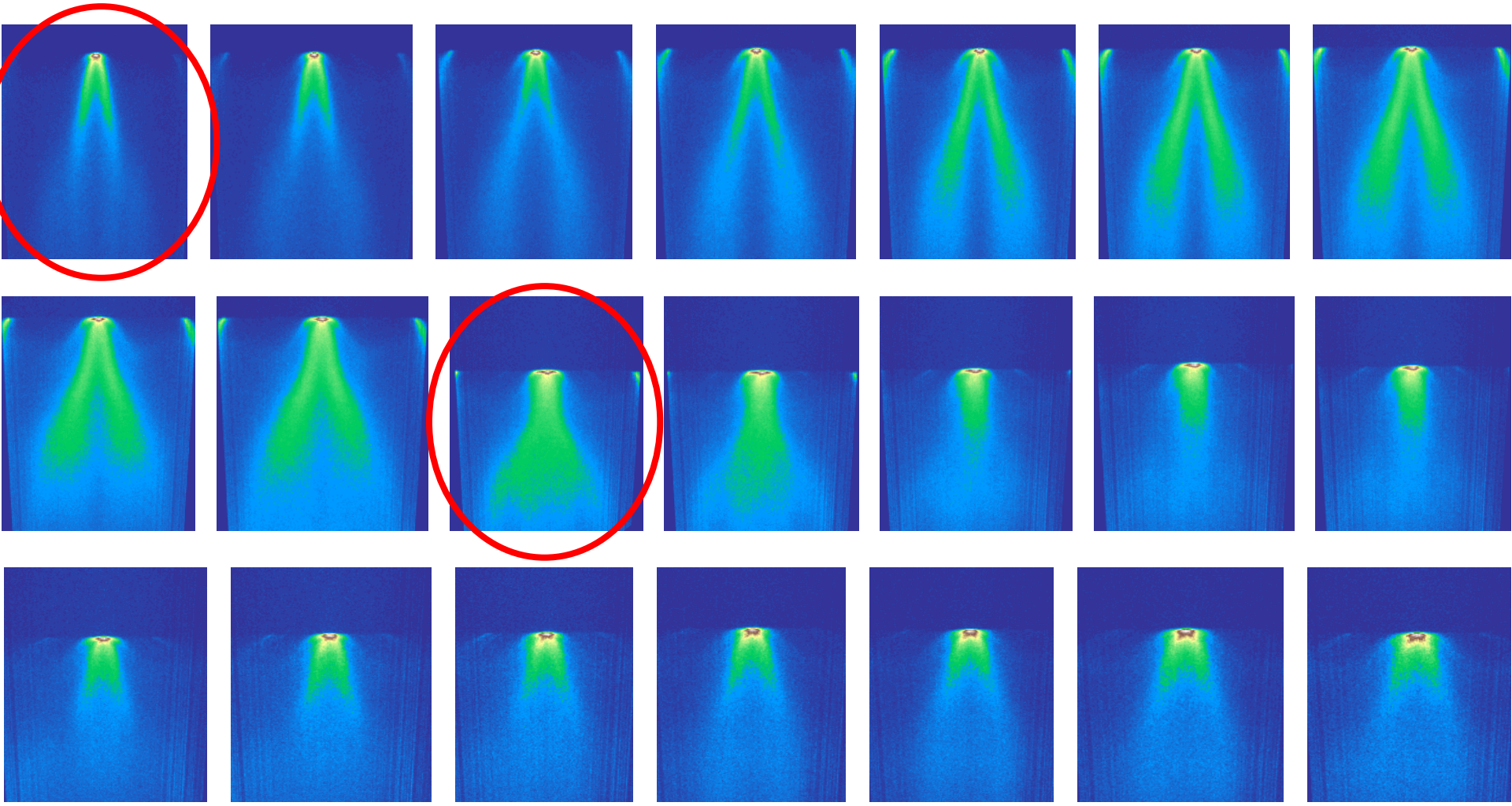
LiFeAs: k_z-dependence



hν – scan (from 80 to 30 eV)

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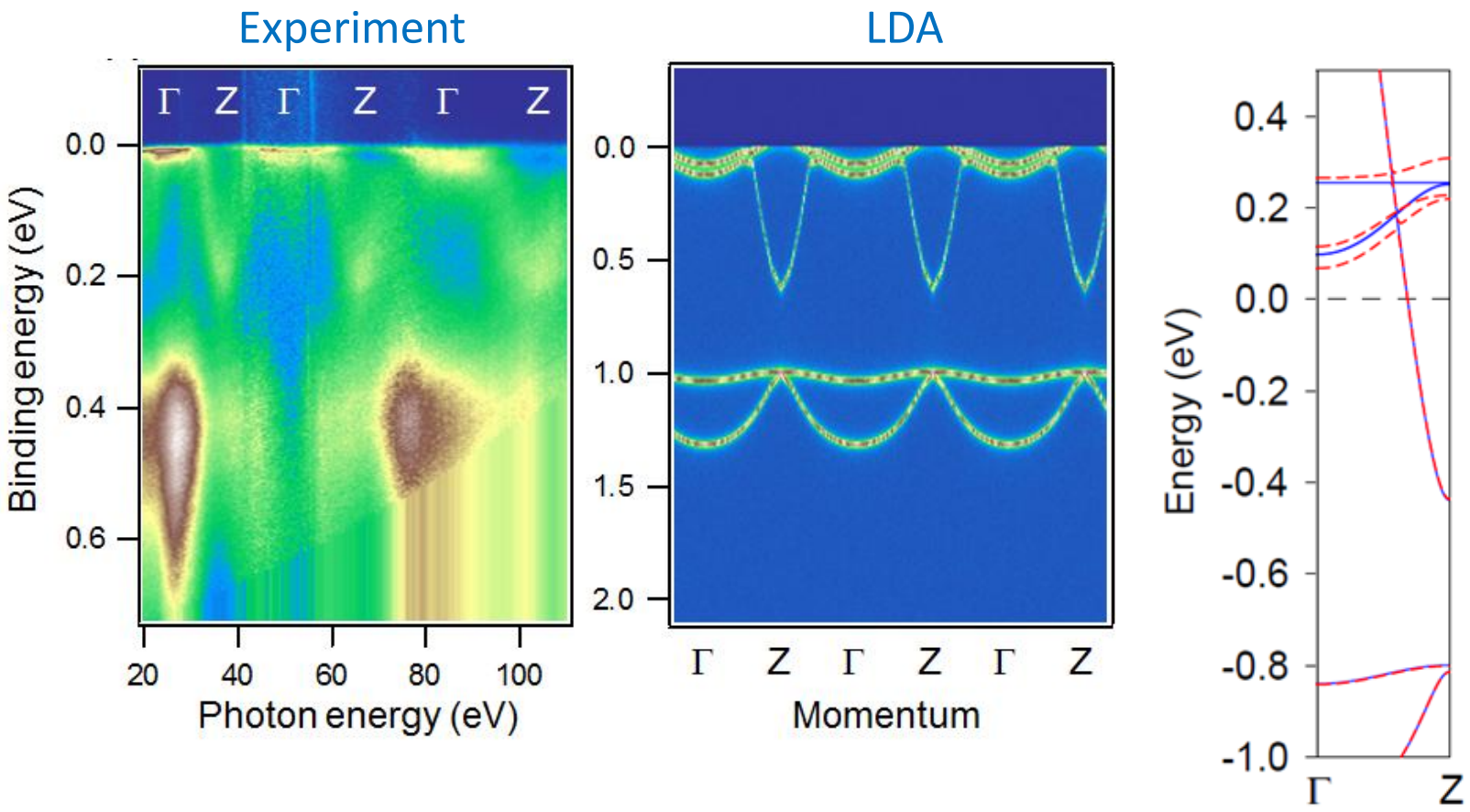
LiFeAs: photon energy dependence



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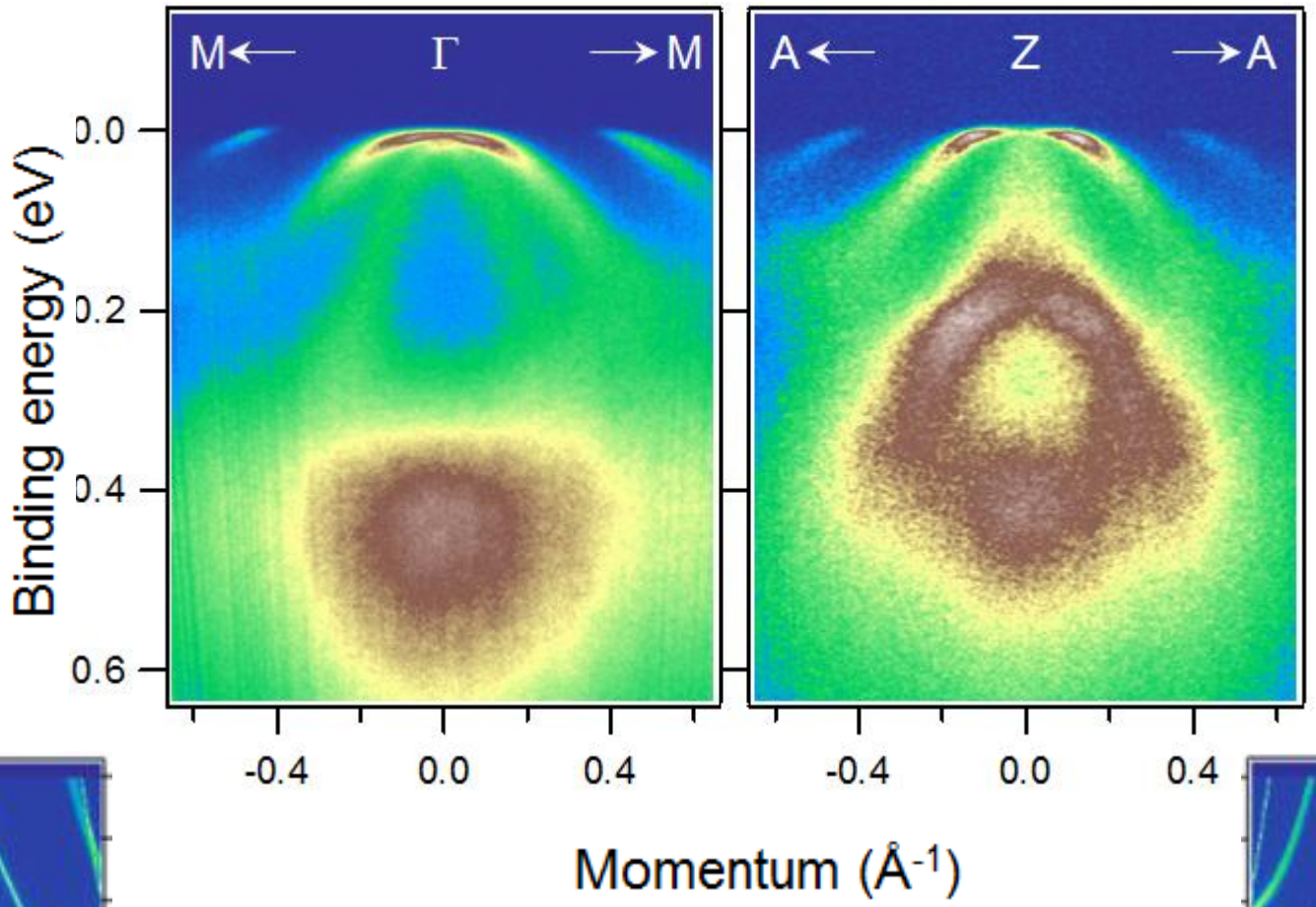
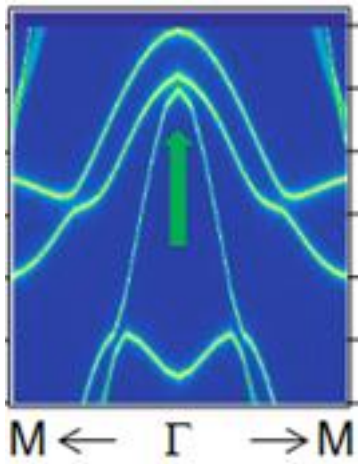
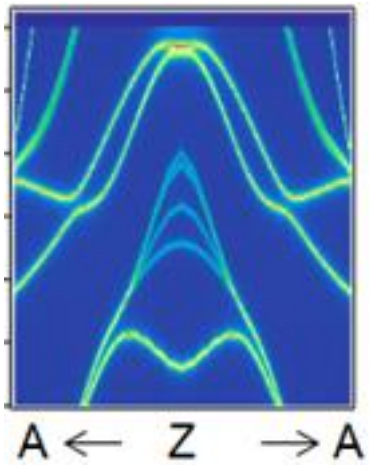
LiFeAs: k_z-resolved electronic structure







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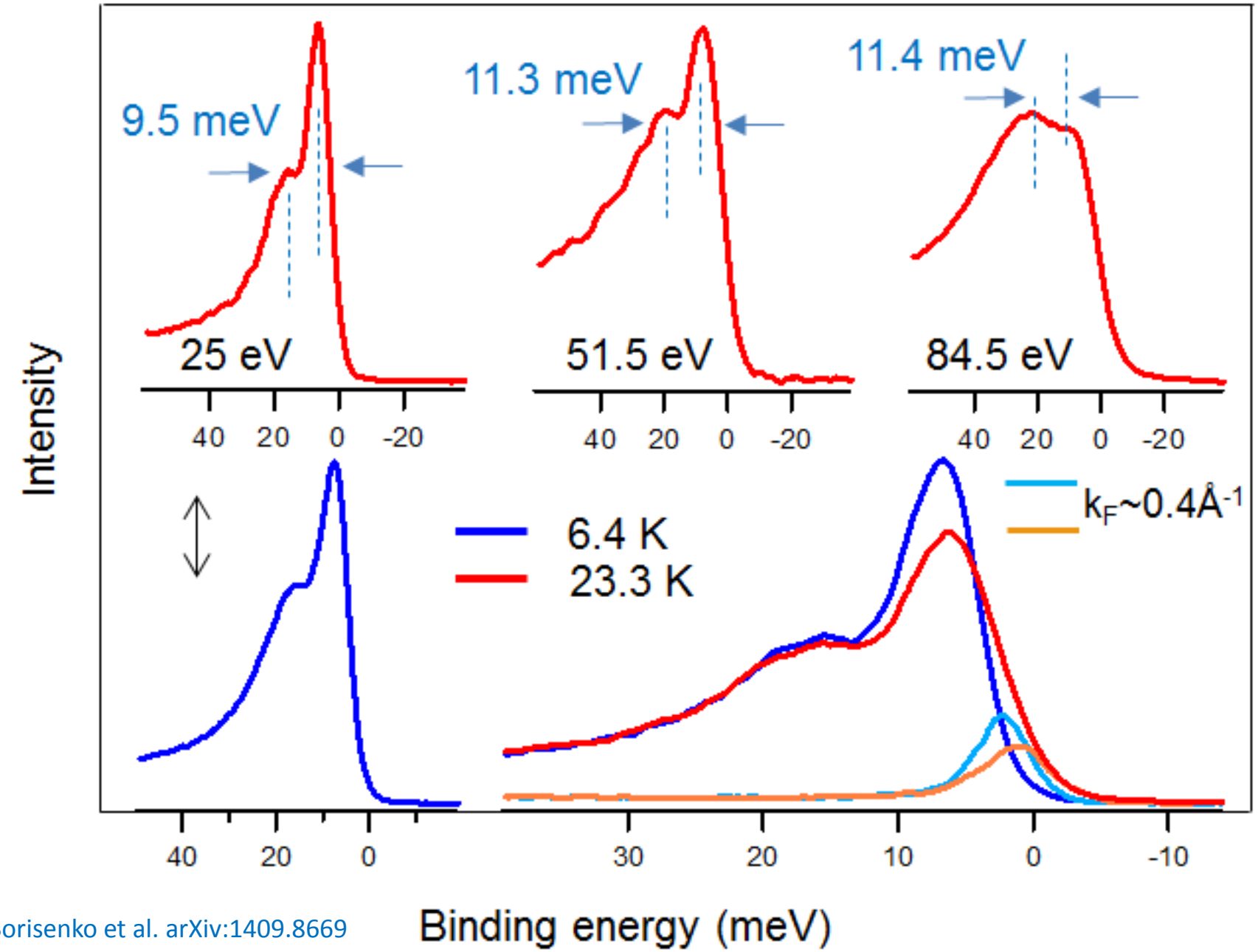
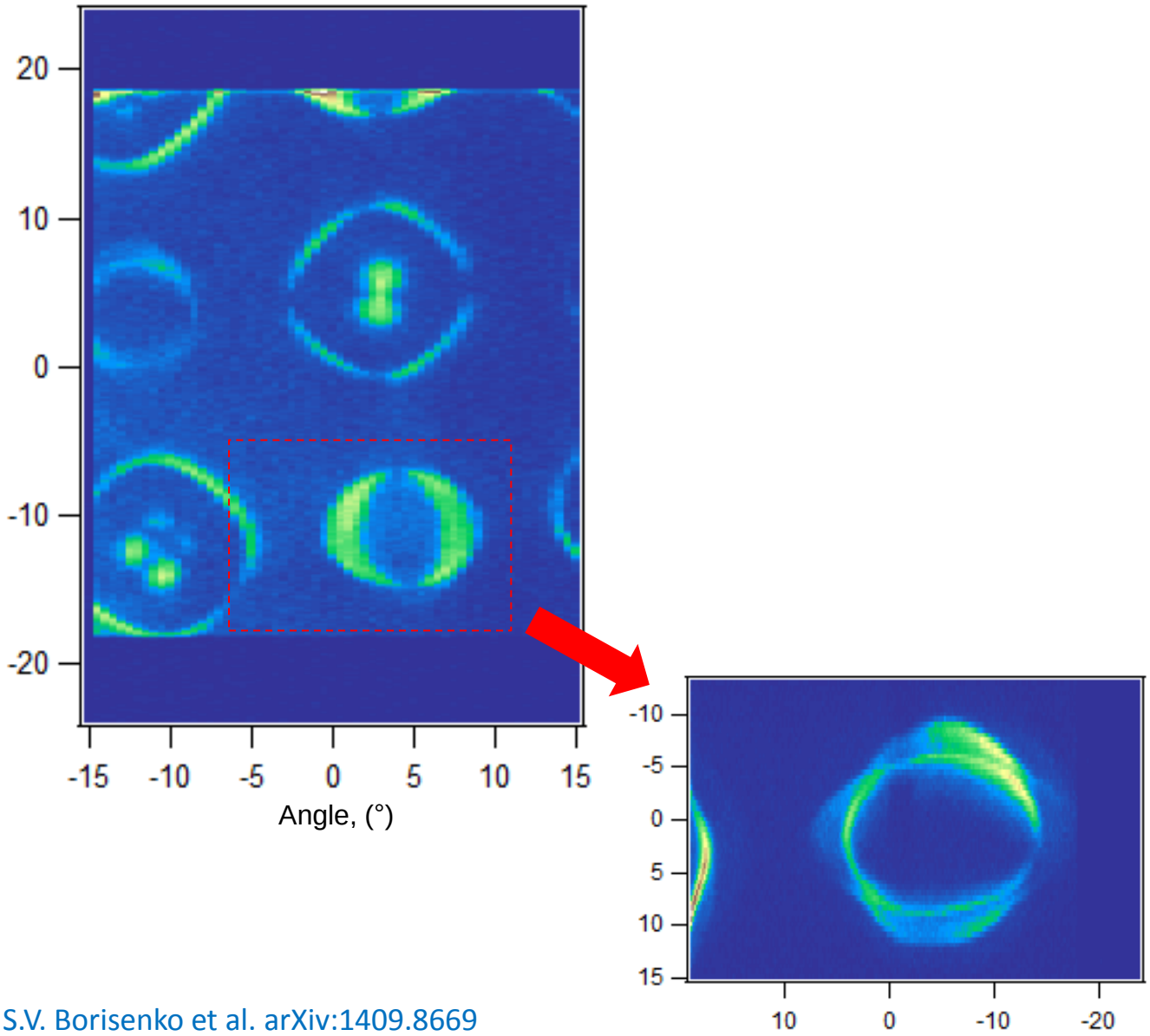
LiFeAs: magnitude of SOC at Γ

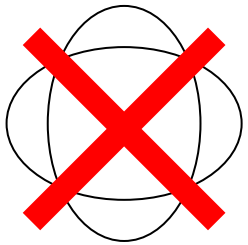


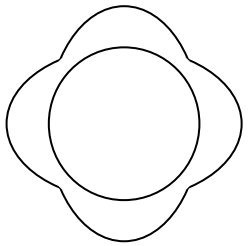
S.V. Borisenko et al. arXiv:1409.8669

LiFeAs – electron pockets



Electron pockets





Spin-orbit interaction !

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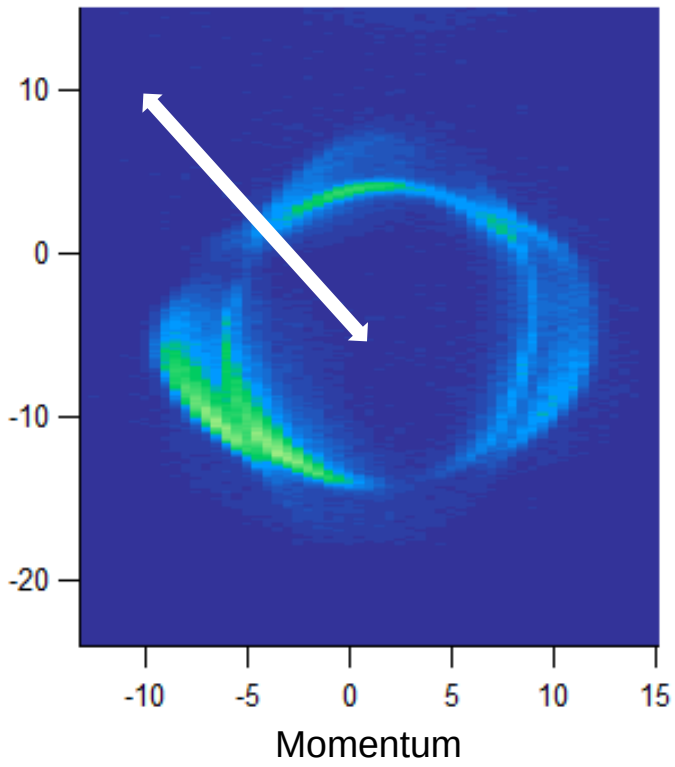
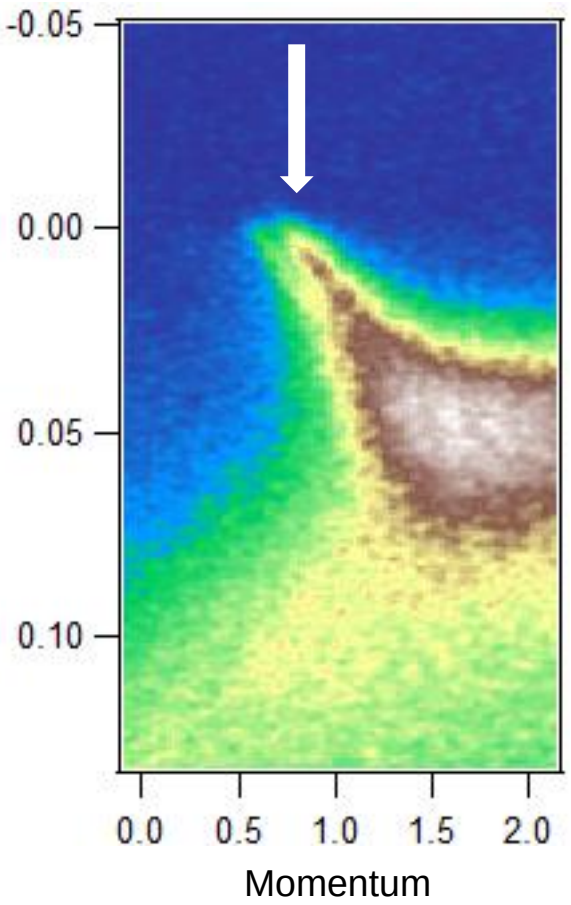
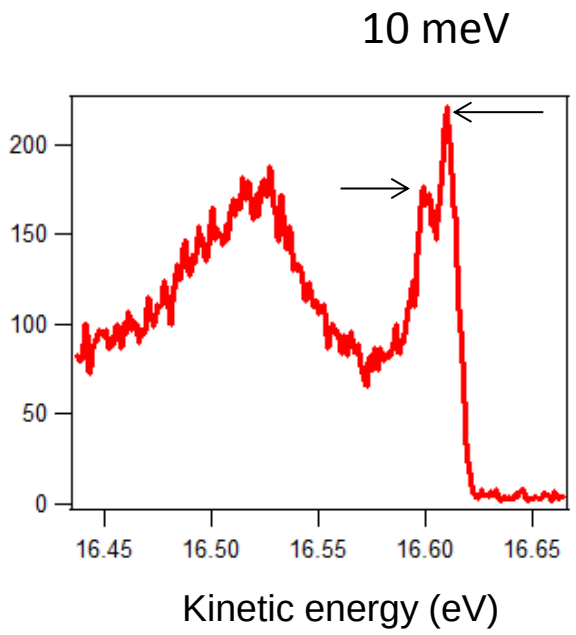
LiFeAs: magnitude of SOC along at MX







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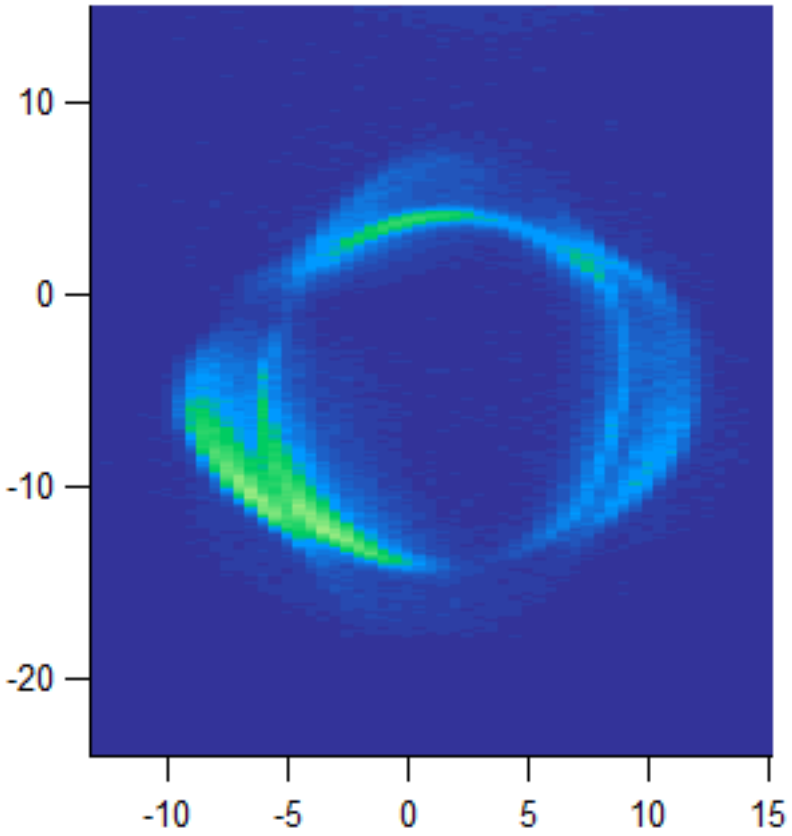
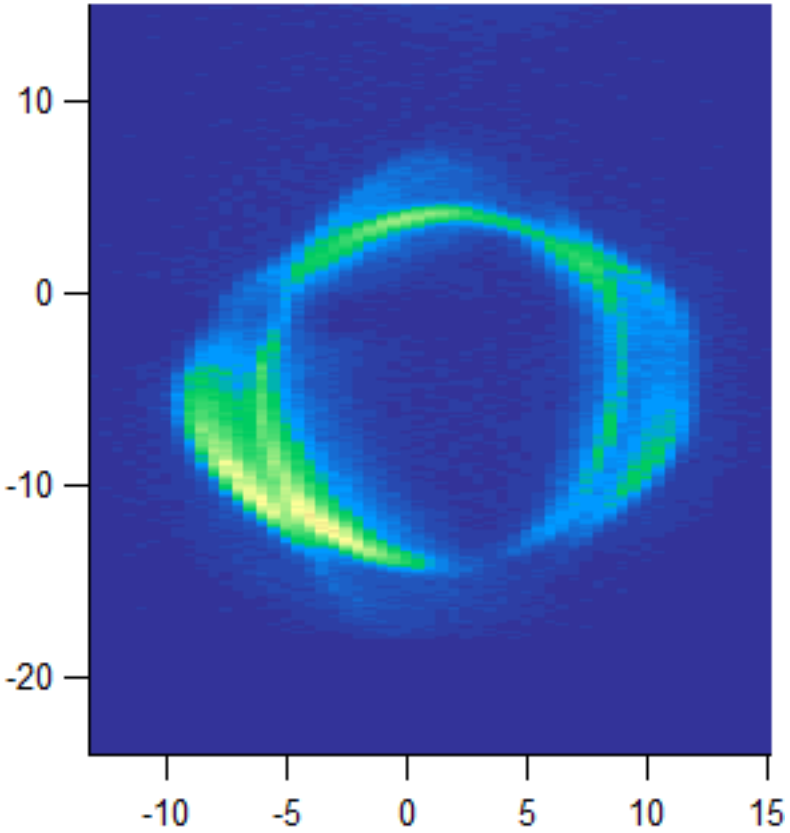
LiFeAs: SOC does not depend on T





$T<T_c$

$T>T_c$

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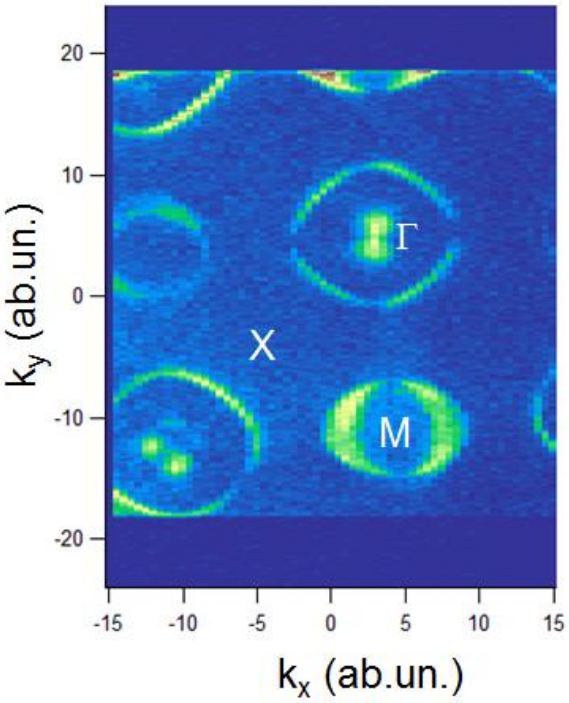
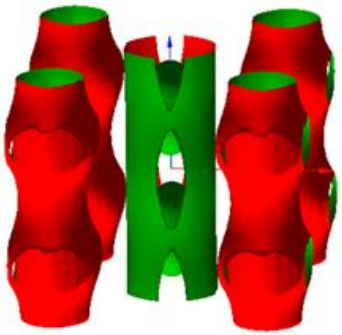
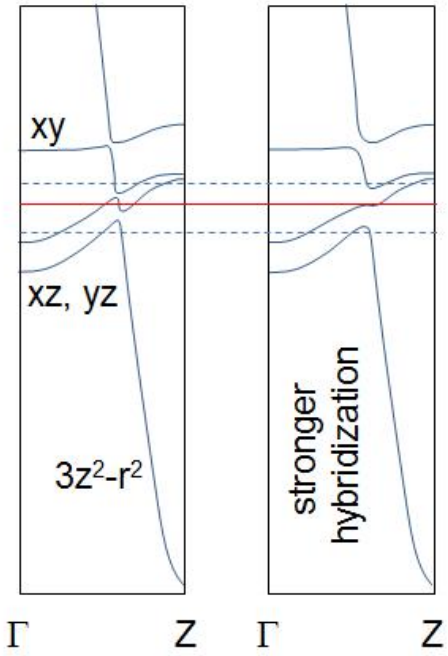
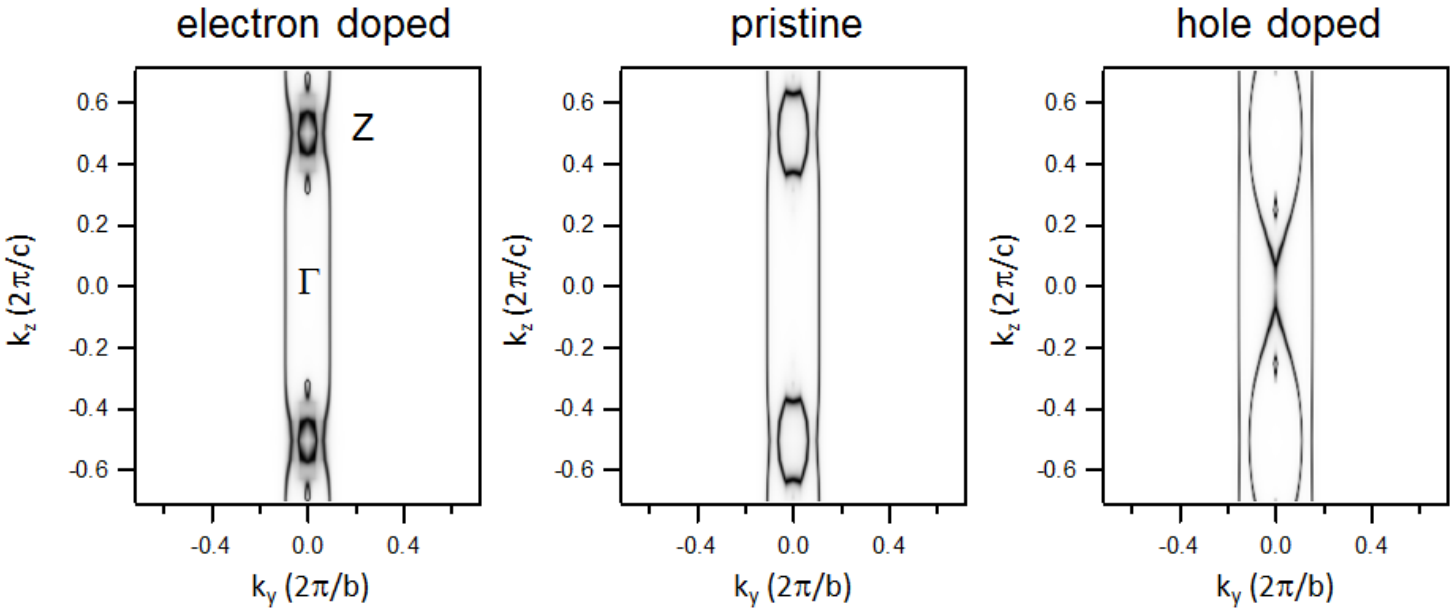
LiFeAs: Fermi surface in the center of BZ









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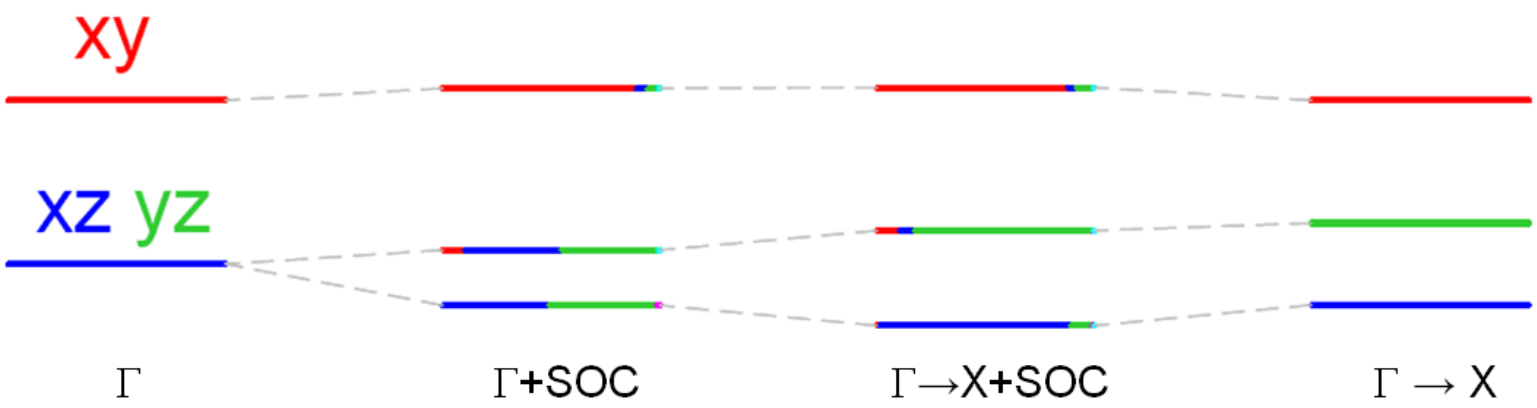
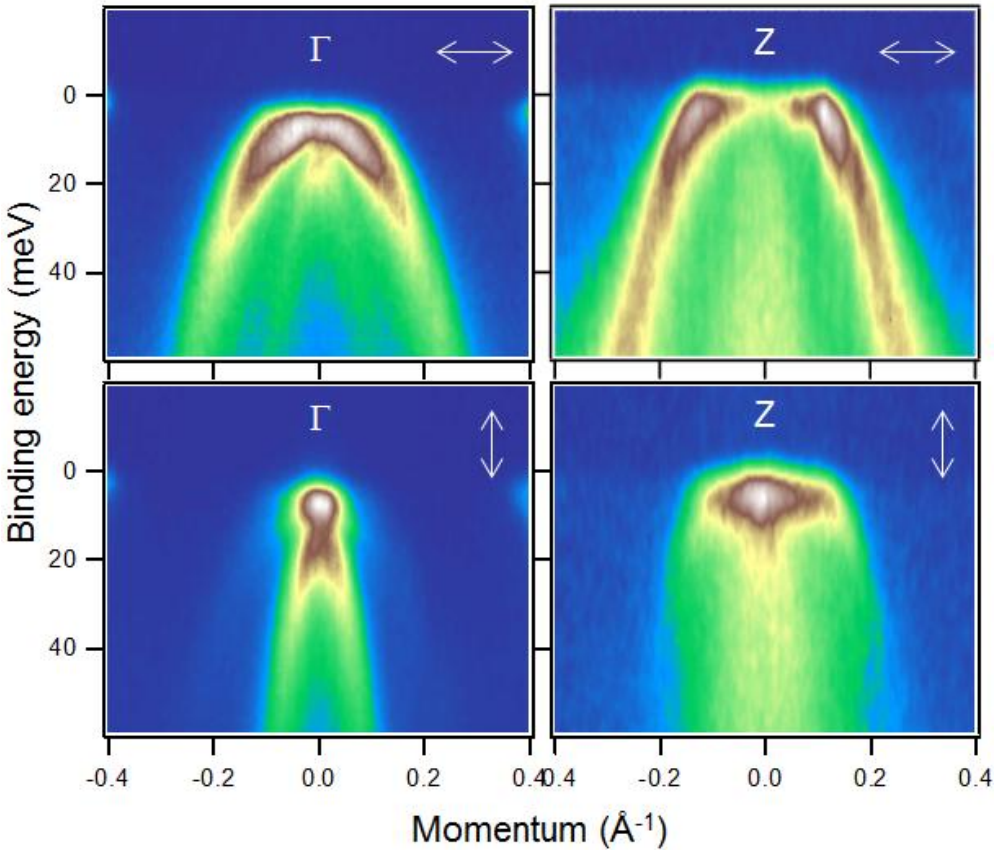
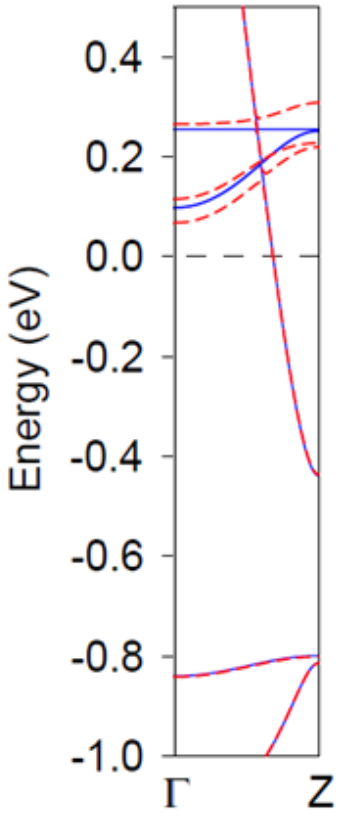
LiFeAs: orbital mixing







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Conclusions

- Iron-based superconductors are „moderately“ correlated systems: far from insulating state but Hubbard bands start to be formed.
- DMFT is a proper theoretical tool to describe electronic structure on 1 eV energy scale: U and J can be extracted from comparison with ARPES.
- Orbital-dependent renormalization strongly modifies the low-energy electronic structure and Fermi surface given by 3D relativistic LDA band-structure, but all features/dispersions are present.
- Significant spin-orbit interaction defines the Fermi surfaces bearing the largest gaps in optimally doped materials.
- Important details of the electronic structure of iron-based superconductors are not yet understood.