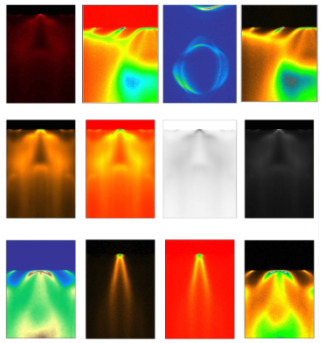
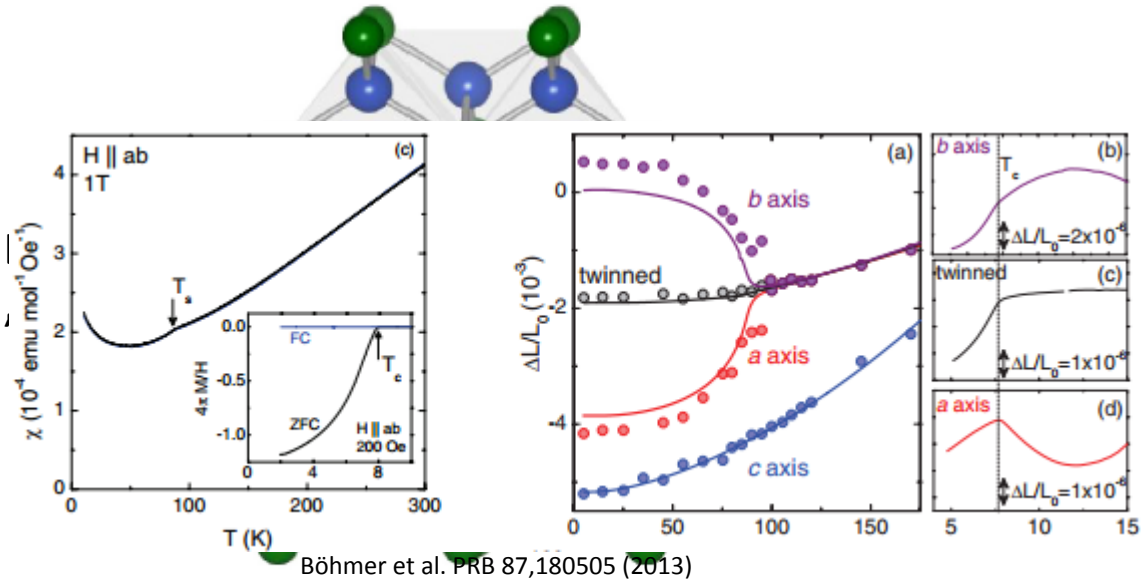
Spin-Orbit Coupling and Nematicity in Iron-Based Superconductors

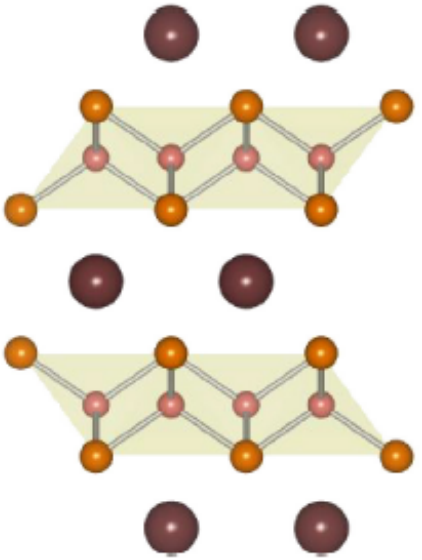
Sergey Borisenko
IFW-Dresden



Iron-based superconductors

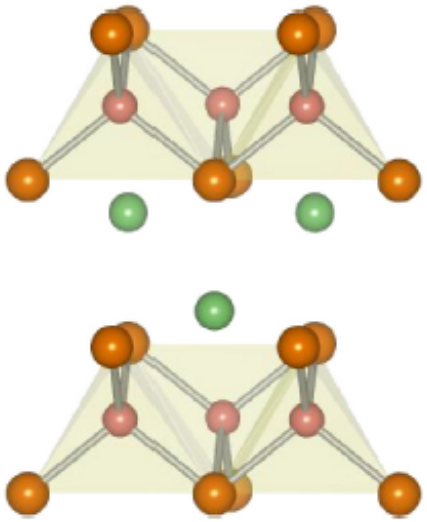


Böhmer et al. PRB 87,180505 (2013)

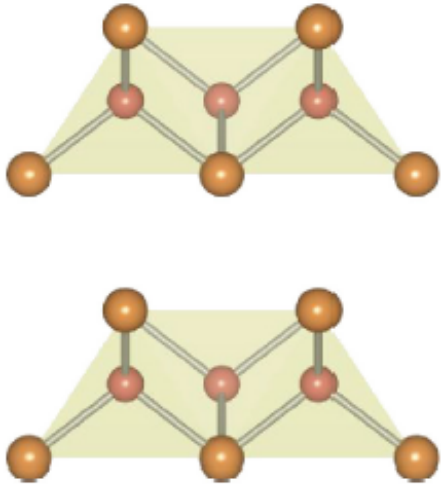


Ishida et al. JPSJ 78, 062001 (2009)

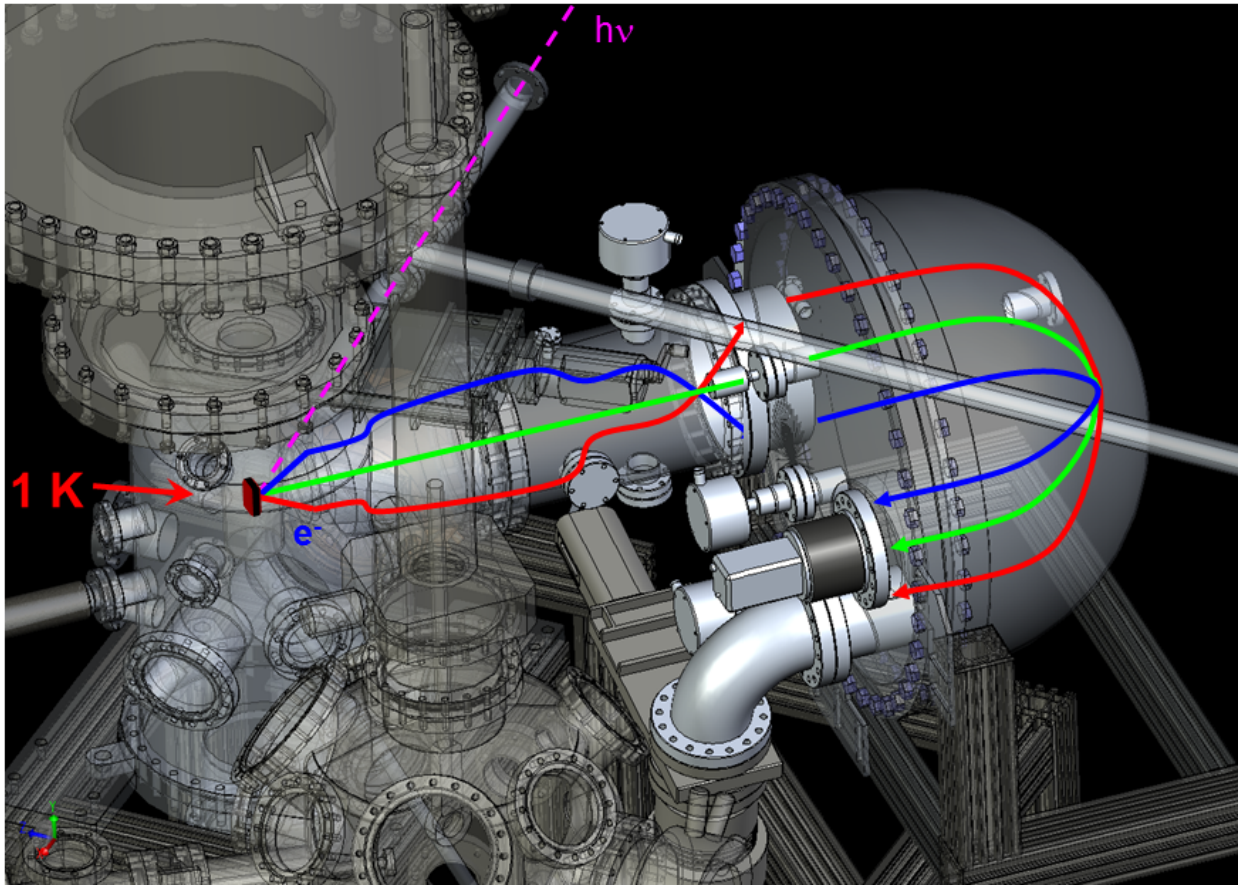
LiFeAs
„111“



FeSe
„11“



Synchrotron-based 3D-ARPES



$\delta E \sim$ meV

$\delta k_x \sim BZ/1000$

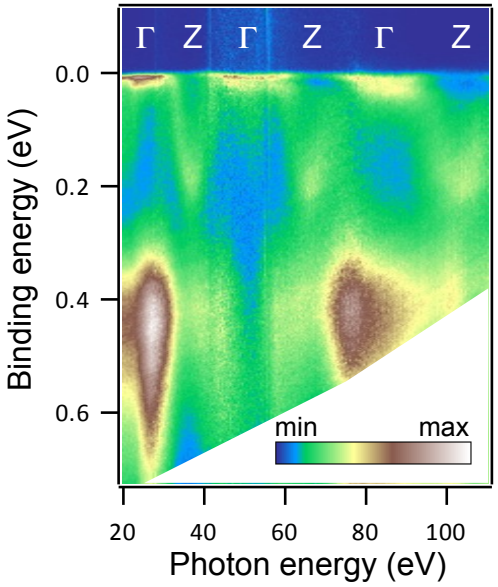
$\delta k_y \sim BZ/1000$

$\delta k_z \sim BZ/10$

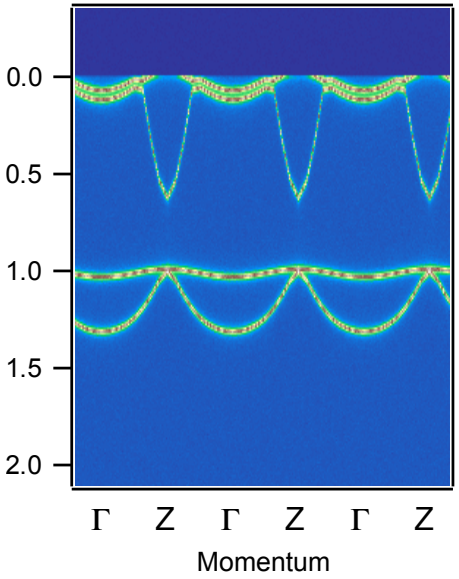
Synchrotron-based 3D-ARPES

LiFeAs

experiment



calculations



SVB et al. Nature Phys. 2016

δE ~ meV

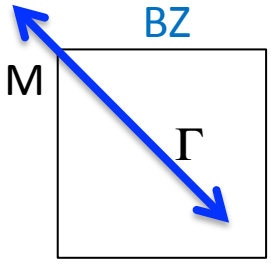
δk_x ~ BZ/1000

δk_y ~ BZ/1000

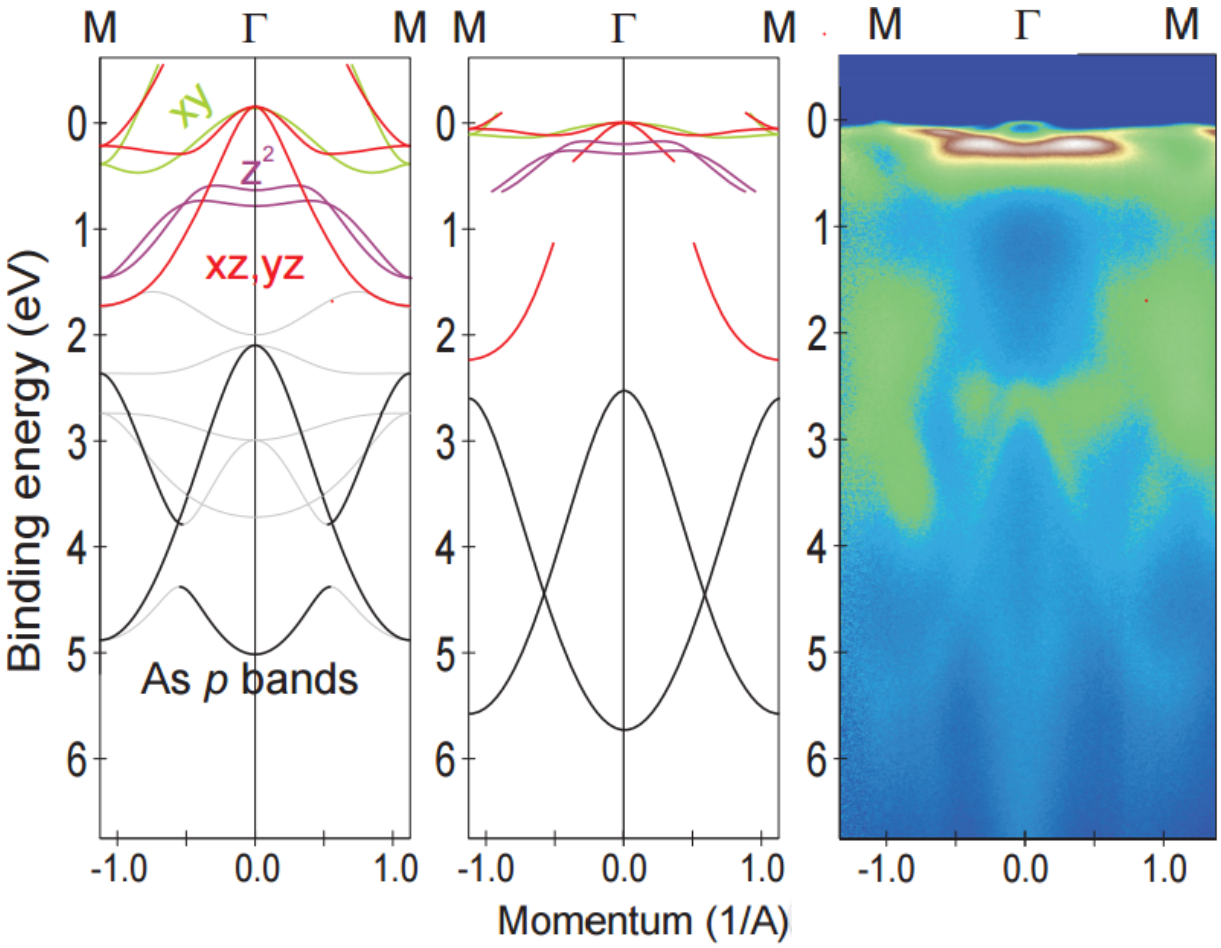
δk_z ~ BZ/10

first DFT, then exotic …

Electronic structure of IBS (~10 eV scale)



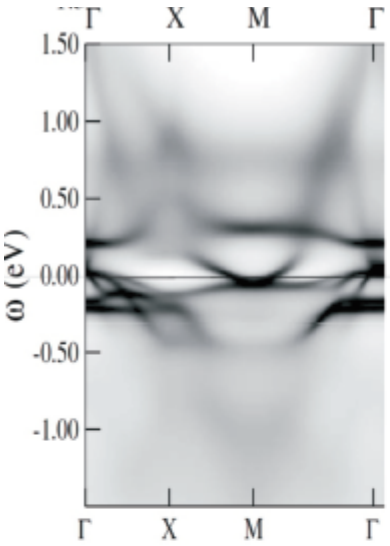
Theory Experiment Experiment



Evtushinsky et al. arXiv:1409.1537

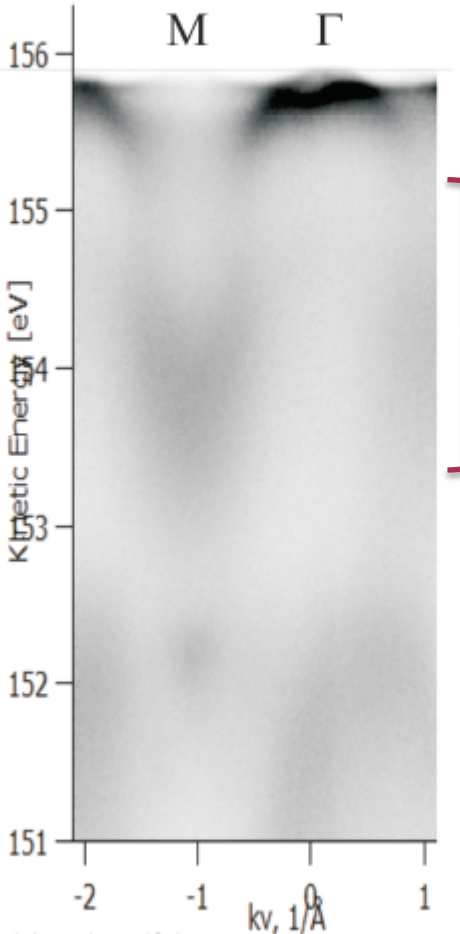
Iron pnictides – strongly correlated systems

FeSe

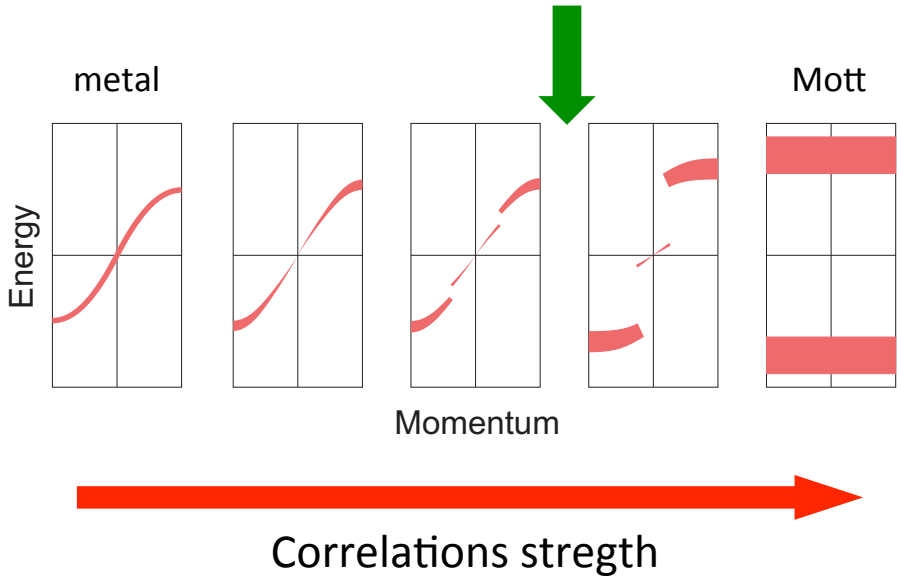


DMFT
(S. Biermann et al.)

ARPES

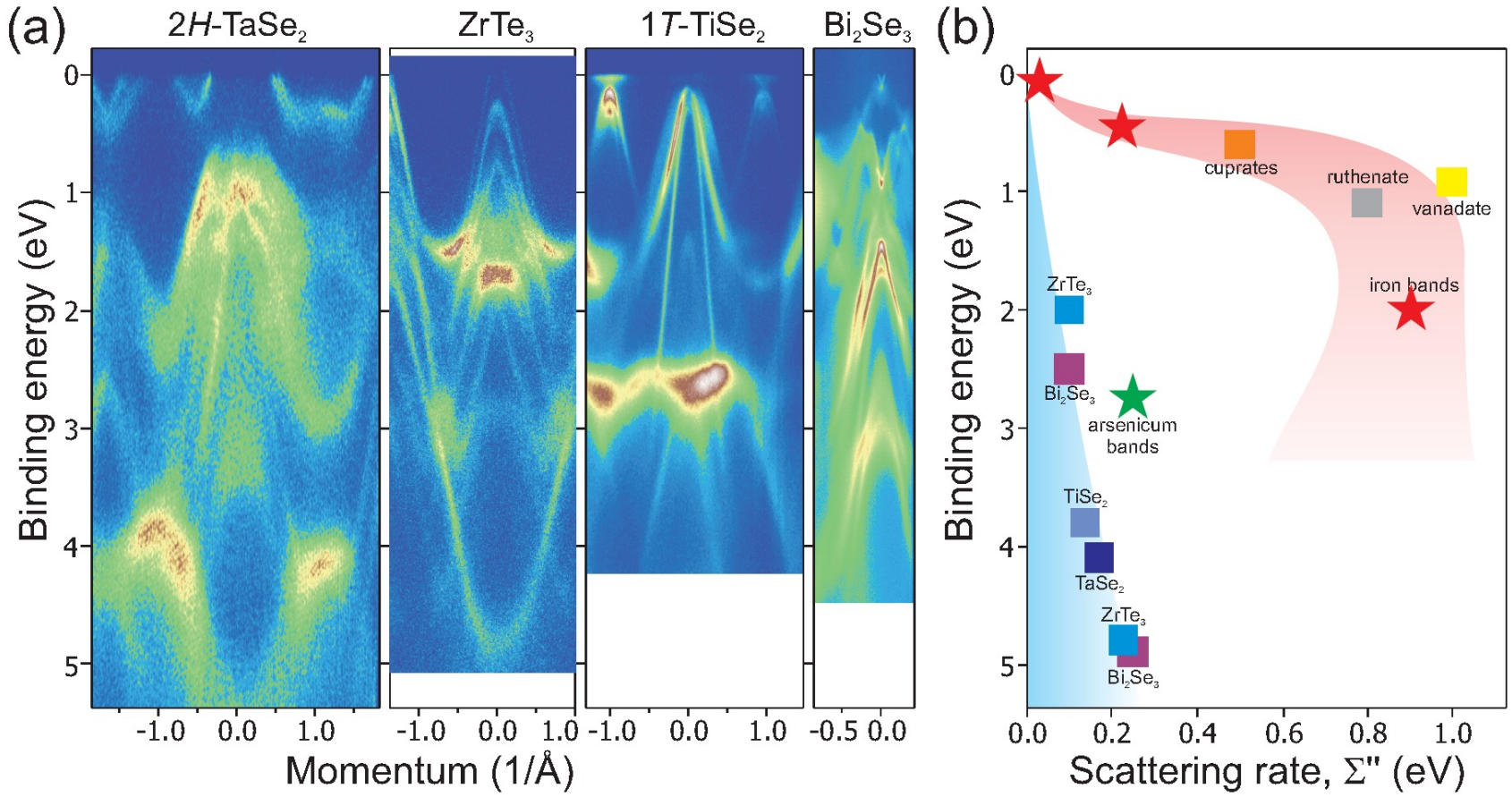


Lower
Hubbard
Band !



Evtushinsky et al.

Electron scattering rate in ordinary and strongly interacting systems



Evtushinsky *et al.* submitted

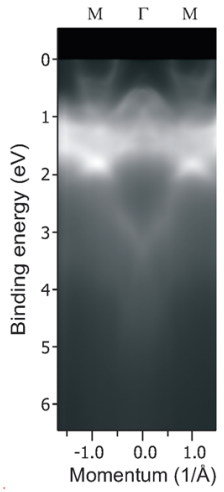
Is this important for high T_c?

Renormalization

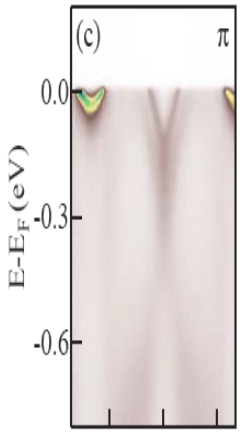
1 | 1.6 | 1.7 | 2 | ≈1 | 3

$KFeCoAs_2$

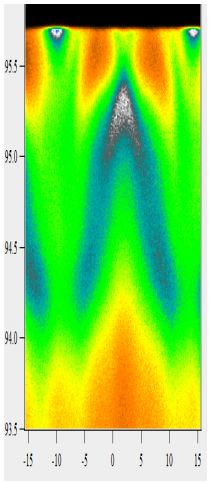
$BaNi_2As_2$ | KCo_2Se_2 | $Ba(Fe_{1/3}Co_{1/3}Ni_{1/3})_2As_2$ | $BaFeCoAs_2$ | $BaFe_2As_2$ | KFe_2As_2



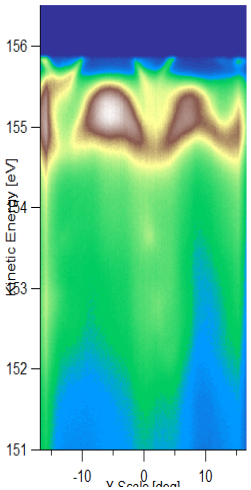
Kim, *et. al.*



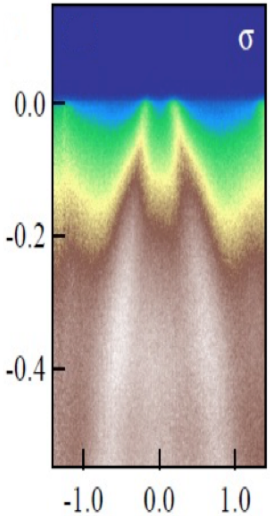
Liu et al., NJP 15



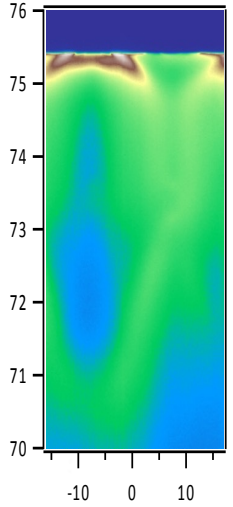
Liu et al.



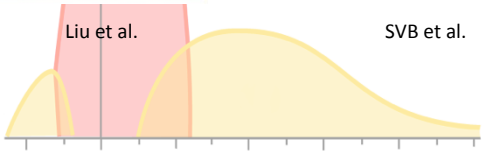
Liu et al.



Liu et al.

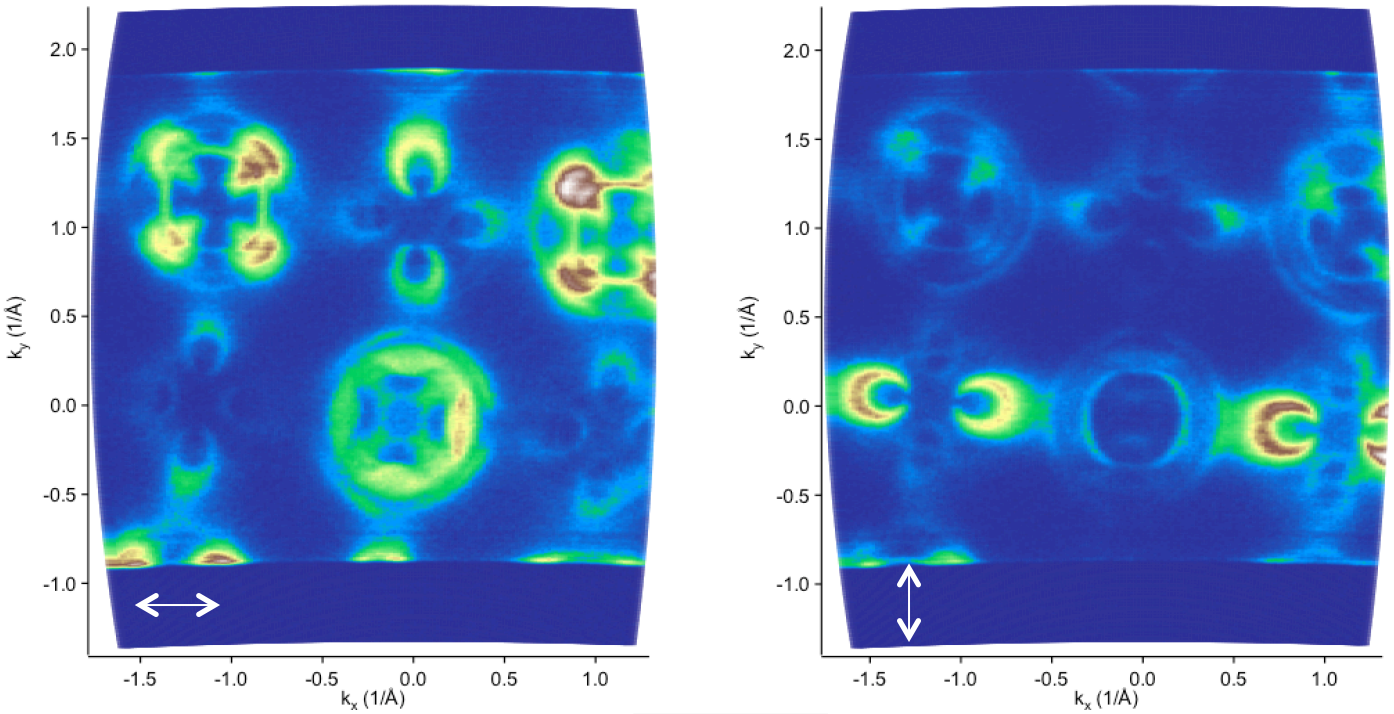


SVB et al.

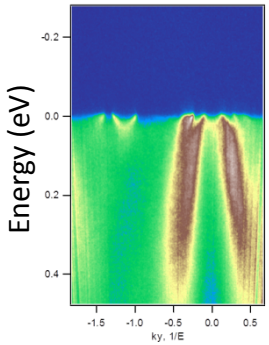


d^8 | $d^{7.5}$ | d^7 | $d^{6.5}$ | d^6 | $d^{5.5}$

KFe_2As_2- still far from „mottness”

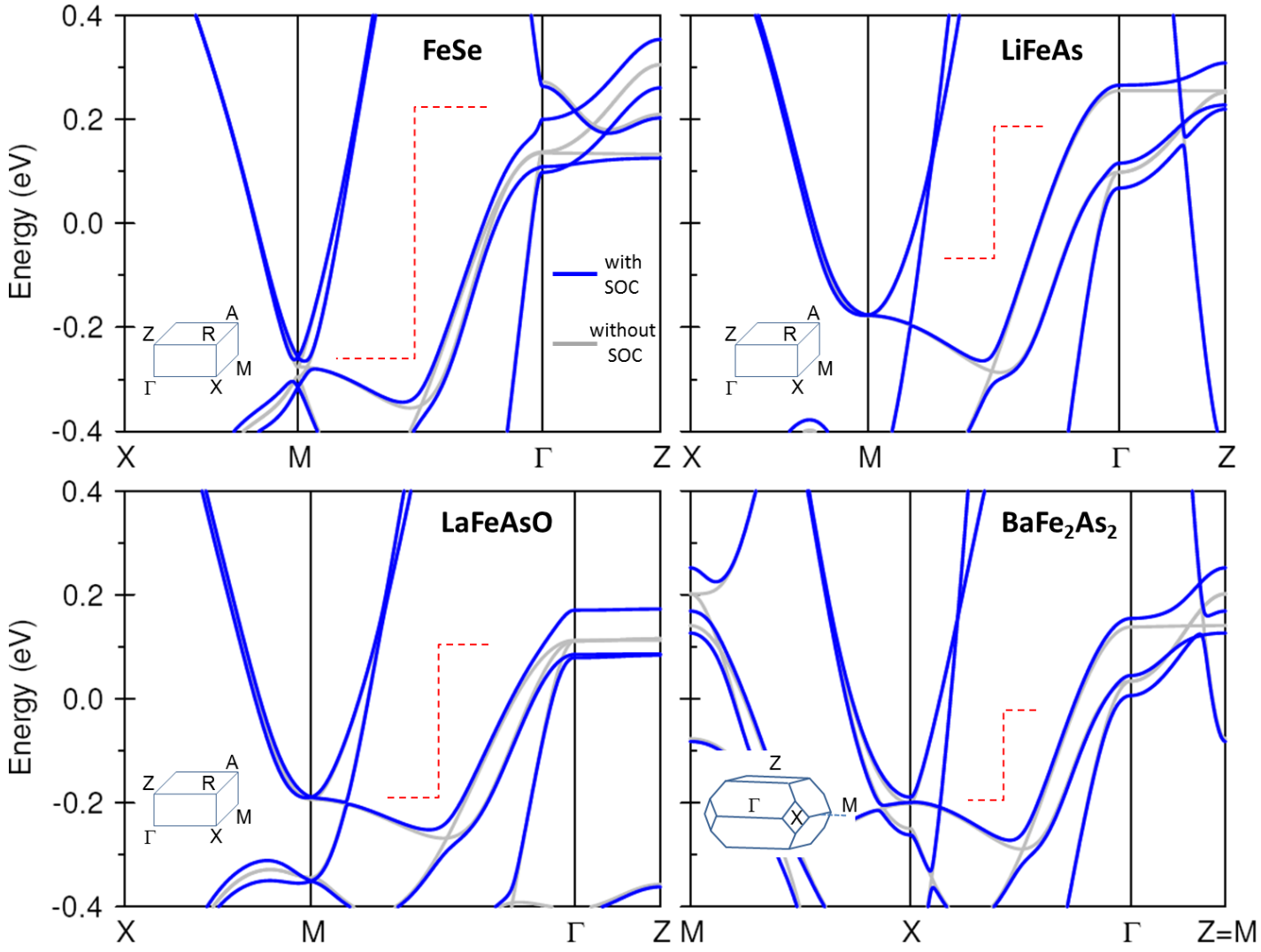


$d^{5.5}$



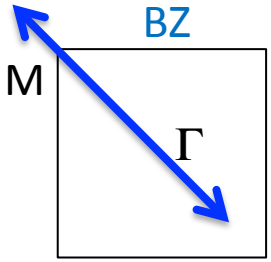
well-defined quasiparticles

SVB et al.



SVB et al. Nat.Phys. 2016

DFT results with k_z-dispersion



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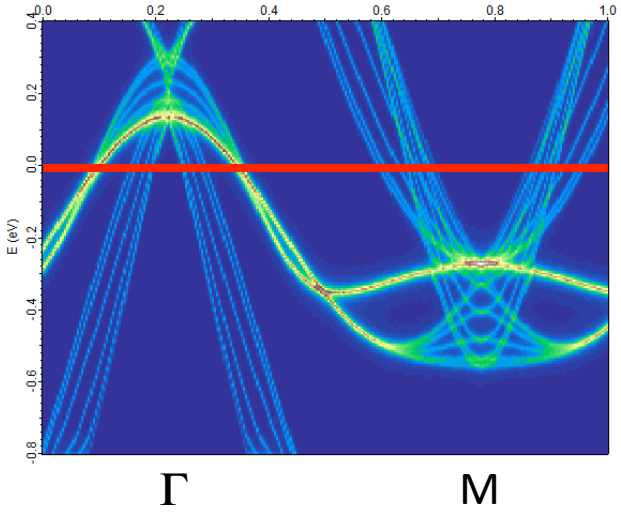

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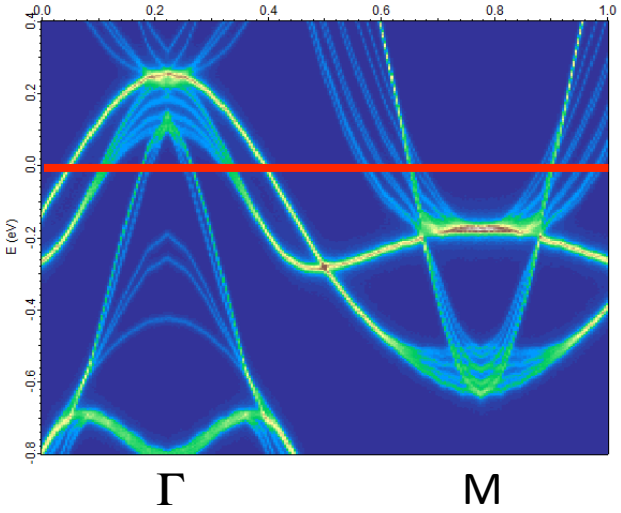

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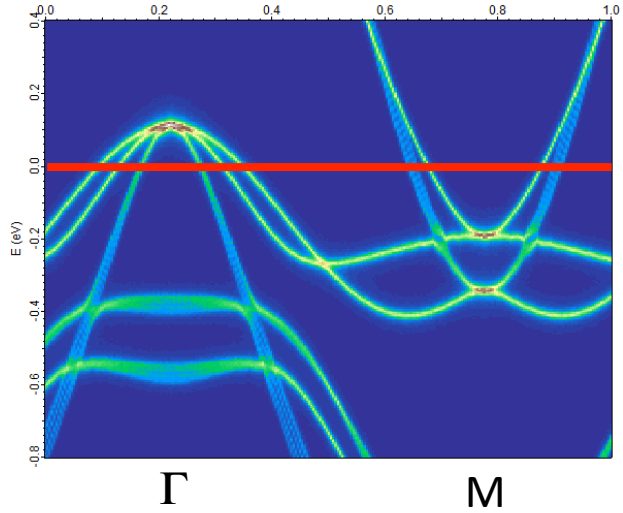

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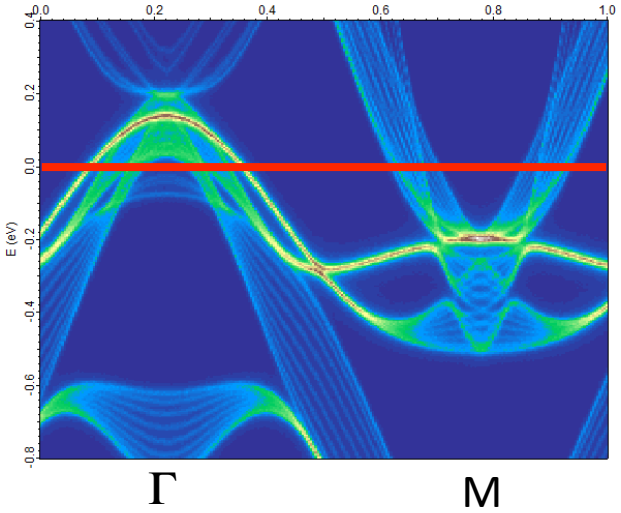
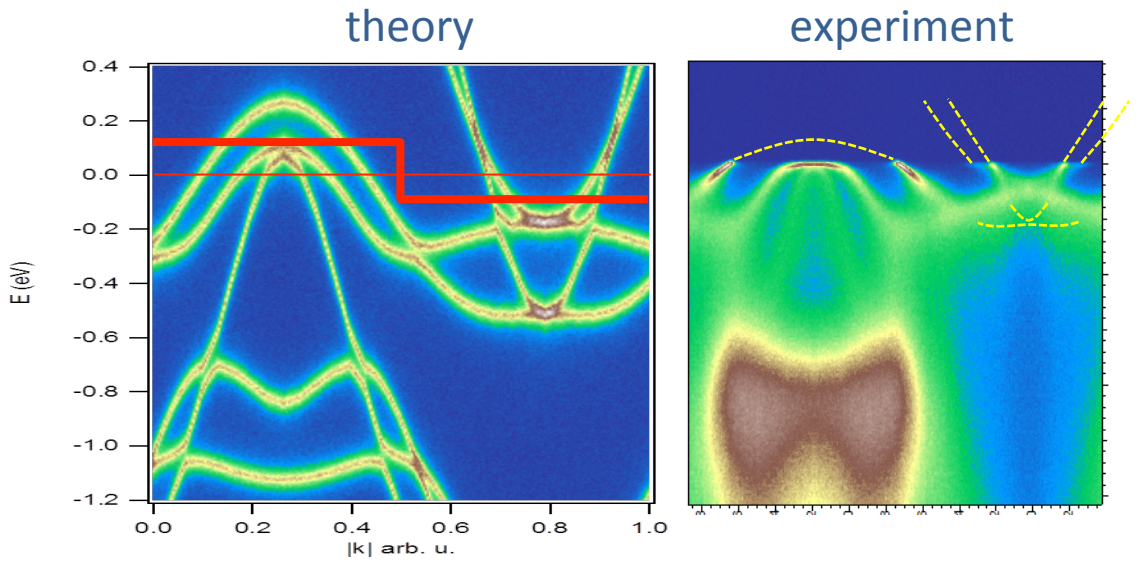
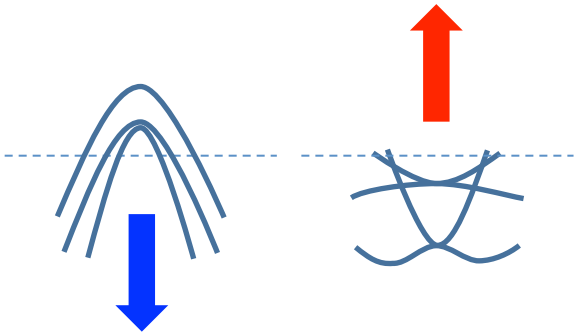
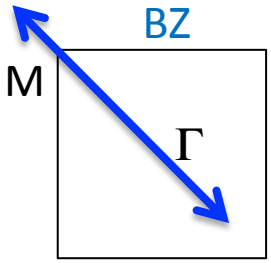


Blue/red shifts in LiFeAs







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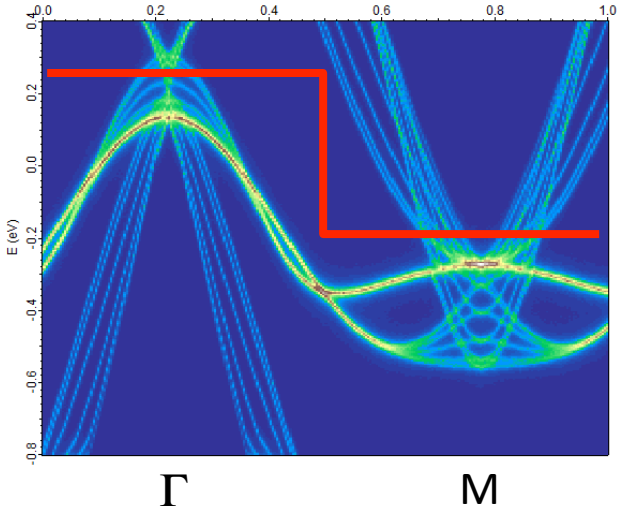

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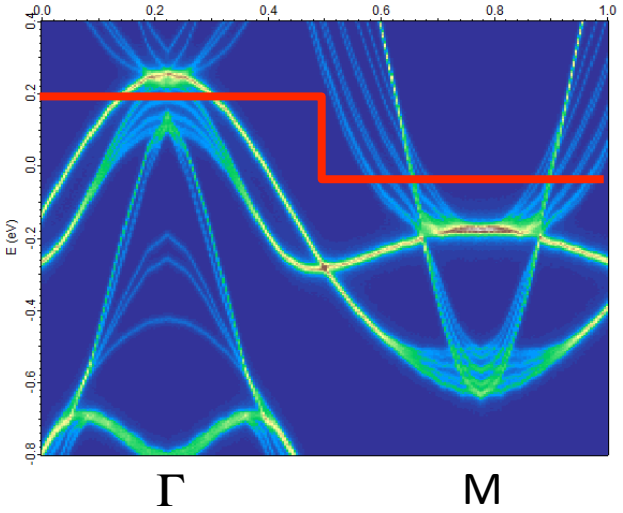

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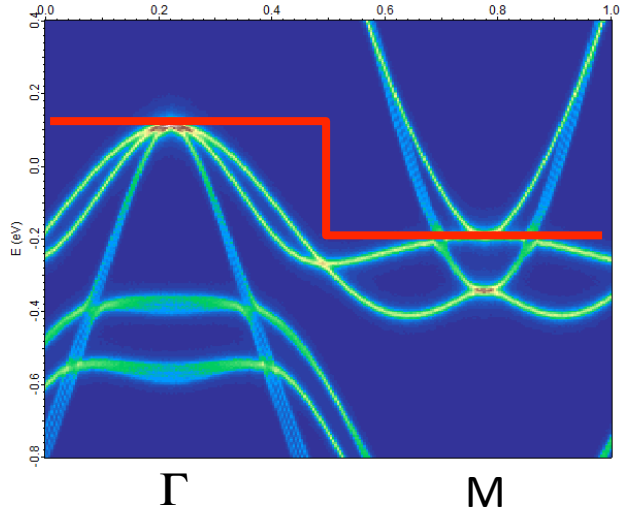

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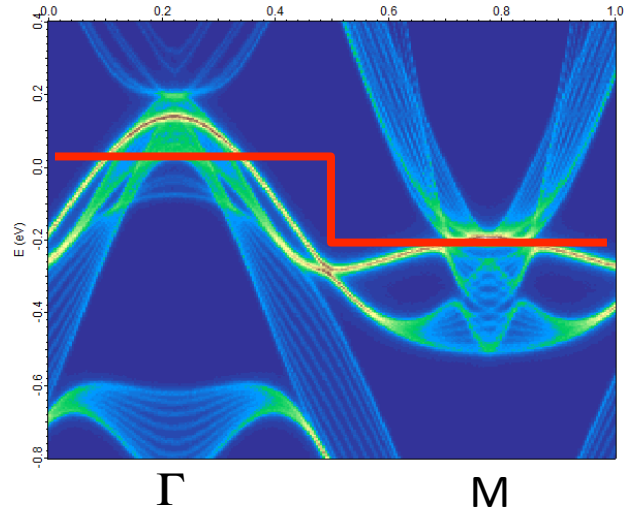
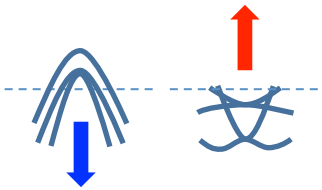
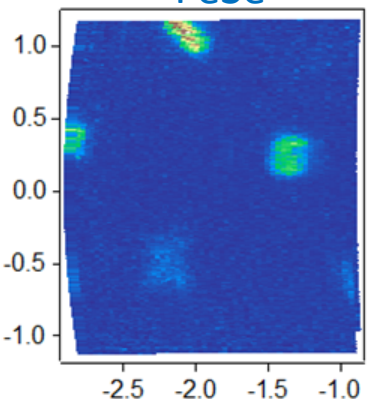
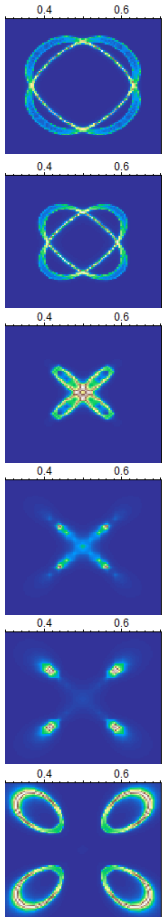


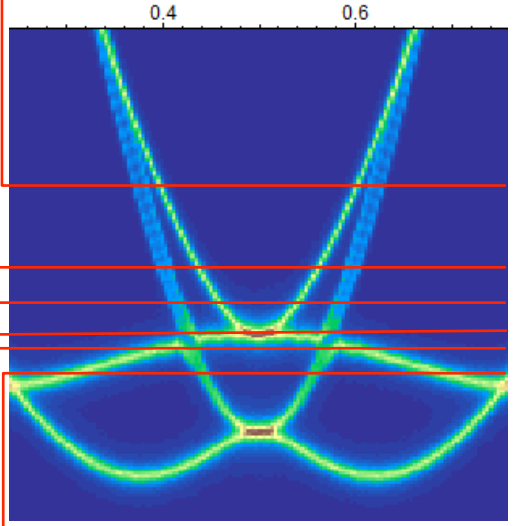
A zoo of Fermi surfaces



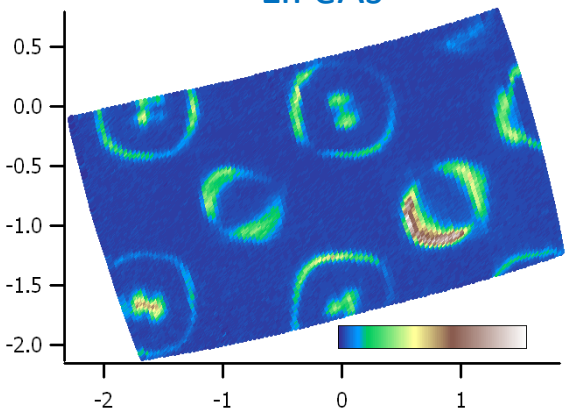
FeSe



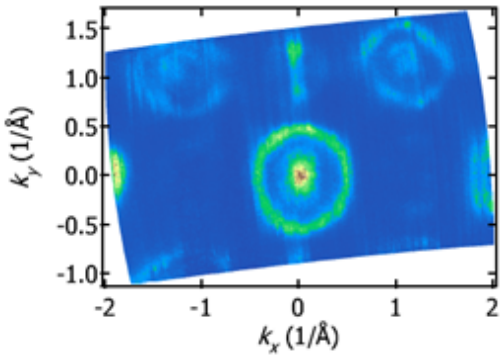




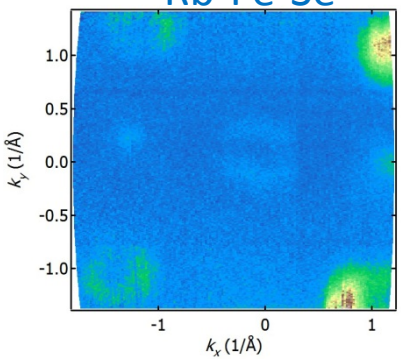
LiFeAs



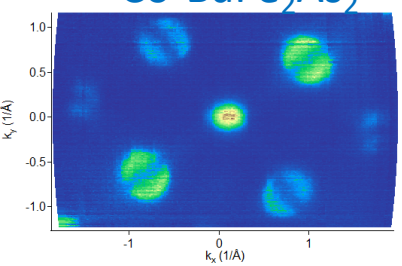
Co-SmFeAsO



Rb-Fe-Se



Co-$BaFe_2As_2$



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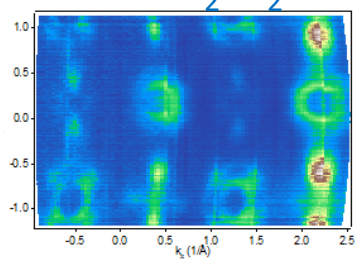

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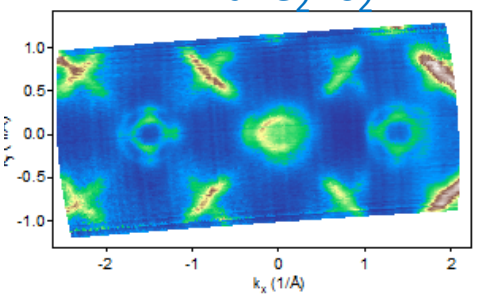
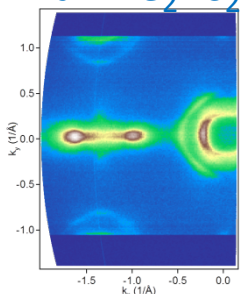
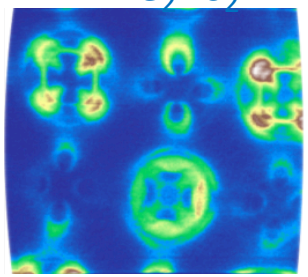


Ba-KFe_2As_2

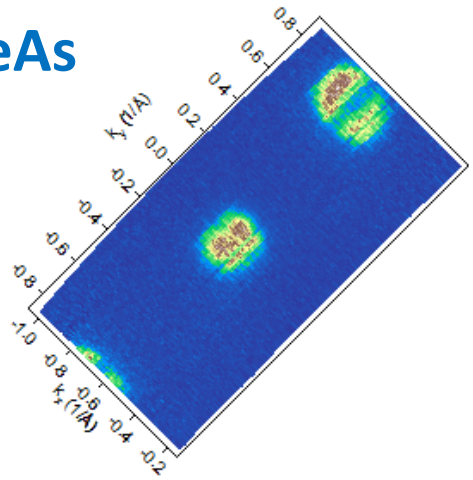


KFe_2As_2

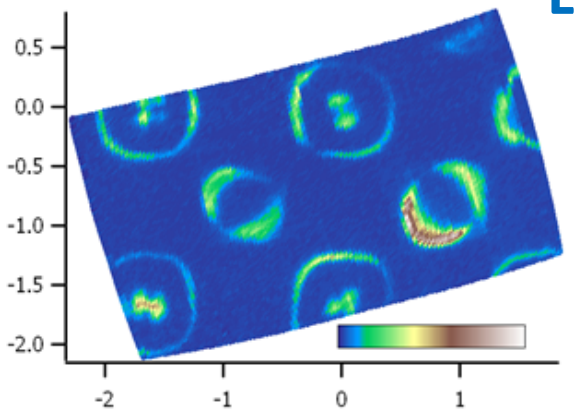


Center of the BZ (hole pockets)

Co-NaFeAs



LiFeAs



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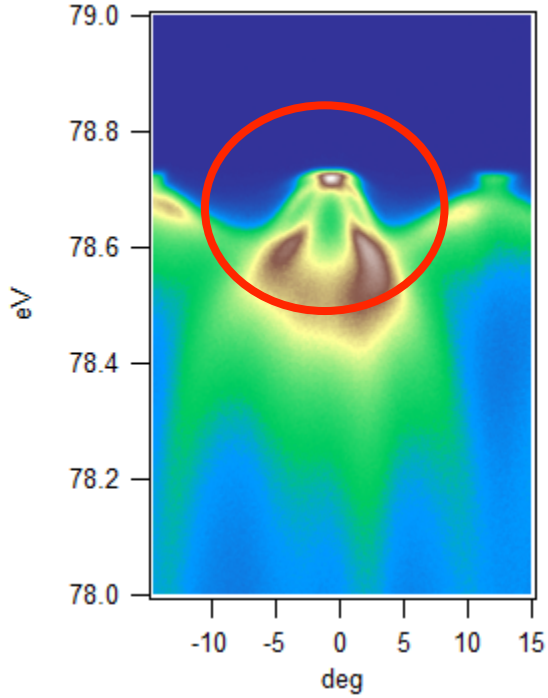

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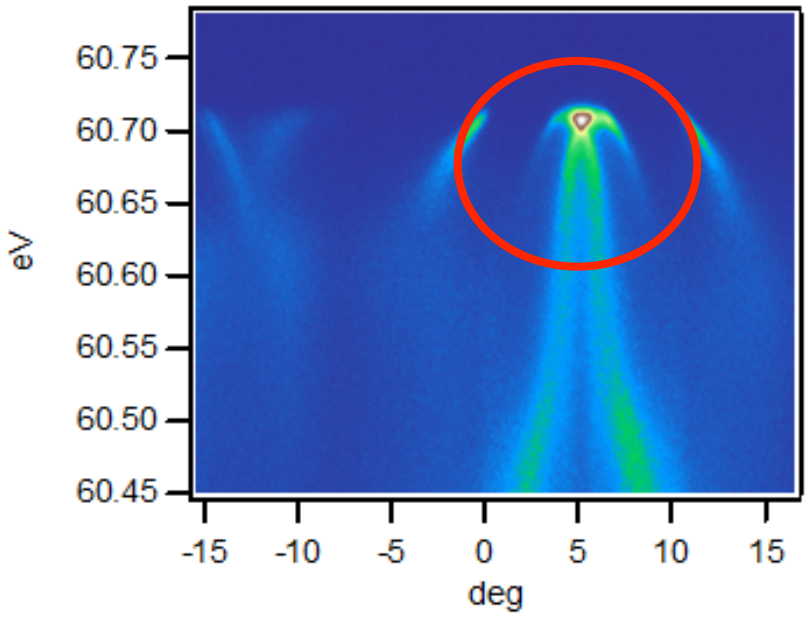

LiFeAs
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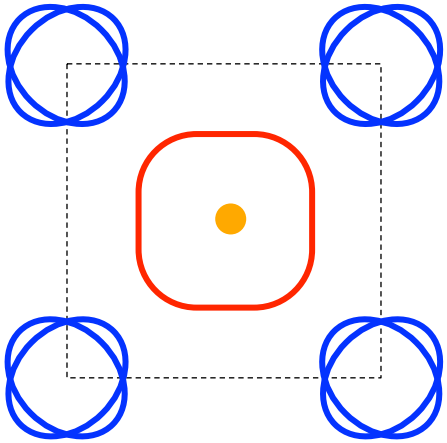
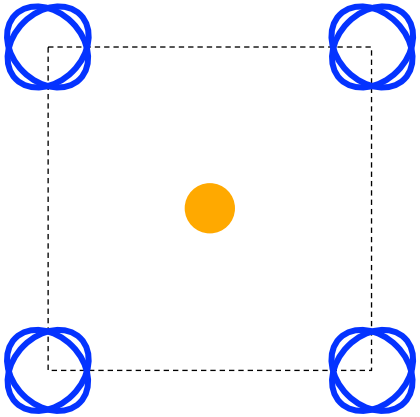
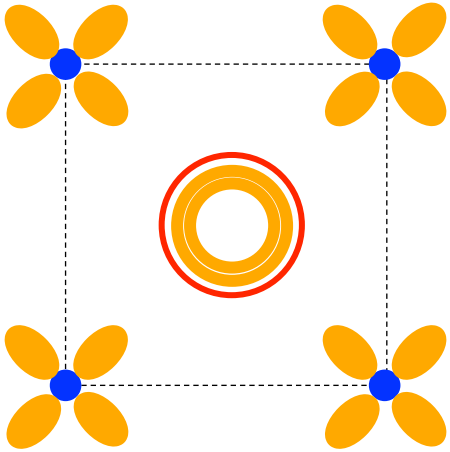


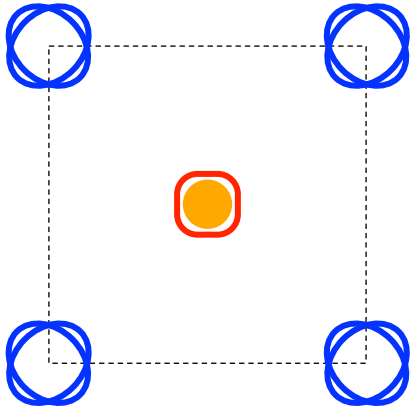
Pt-$BaFe_2As_2$
T_c=20K



K-$BaFe_2As_2$
T_c=38K



Co-$BaFe_2As_2$
T_c=25K



Pt-Ca-Fe-As
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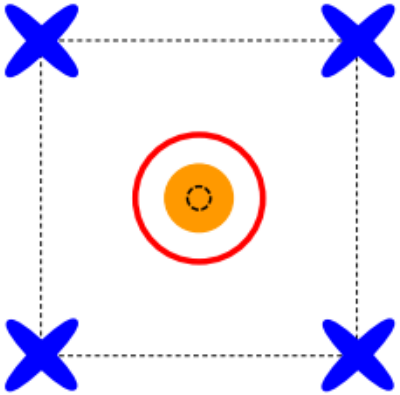
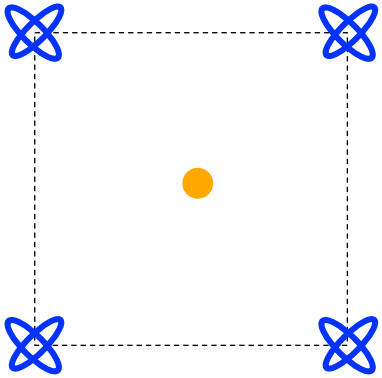
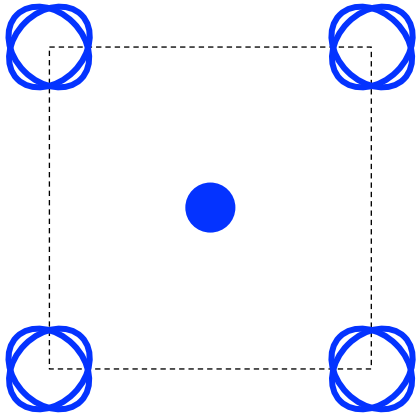


FeSe
T_c=8K



Rb-Fe-Se
T_c=33K



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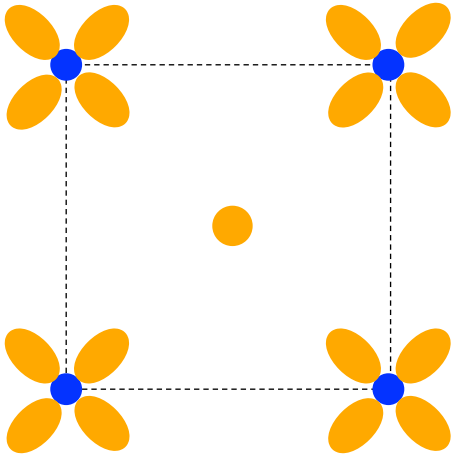
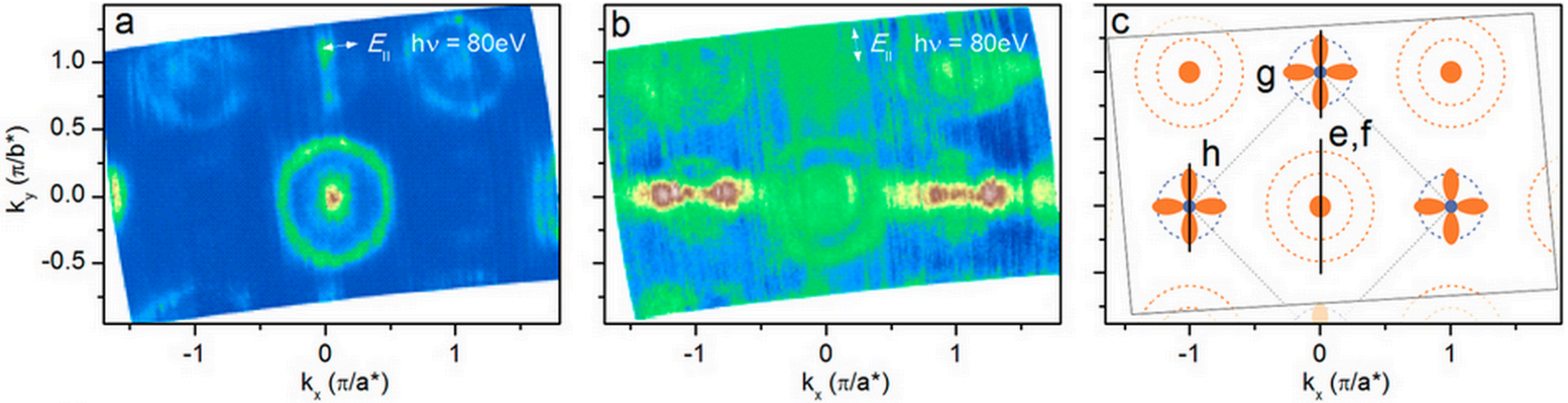
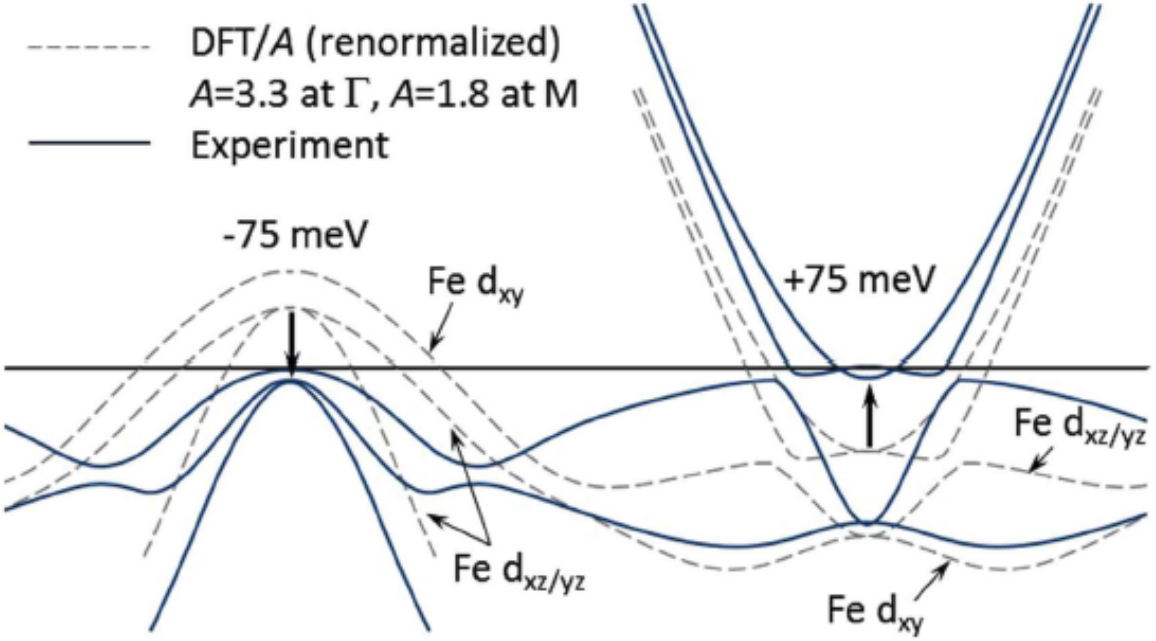


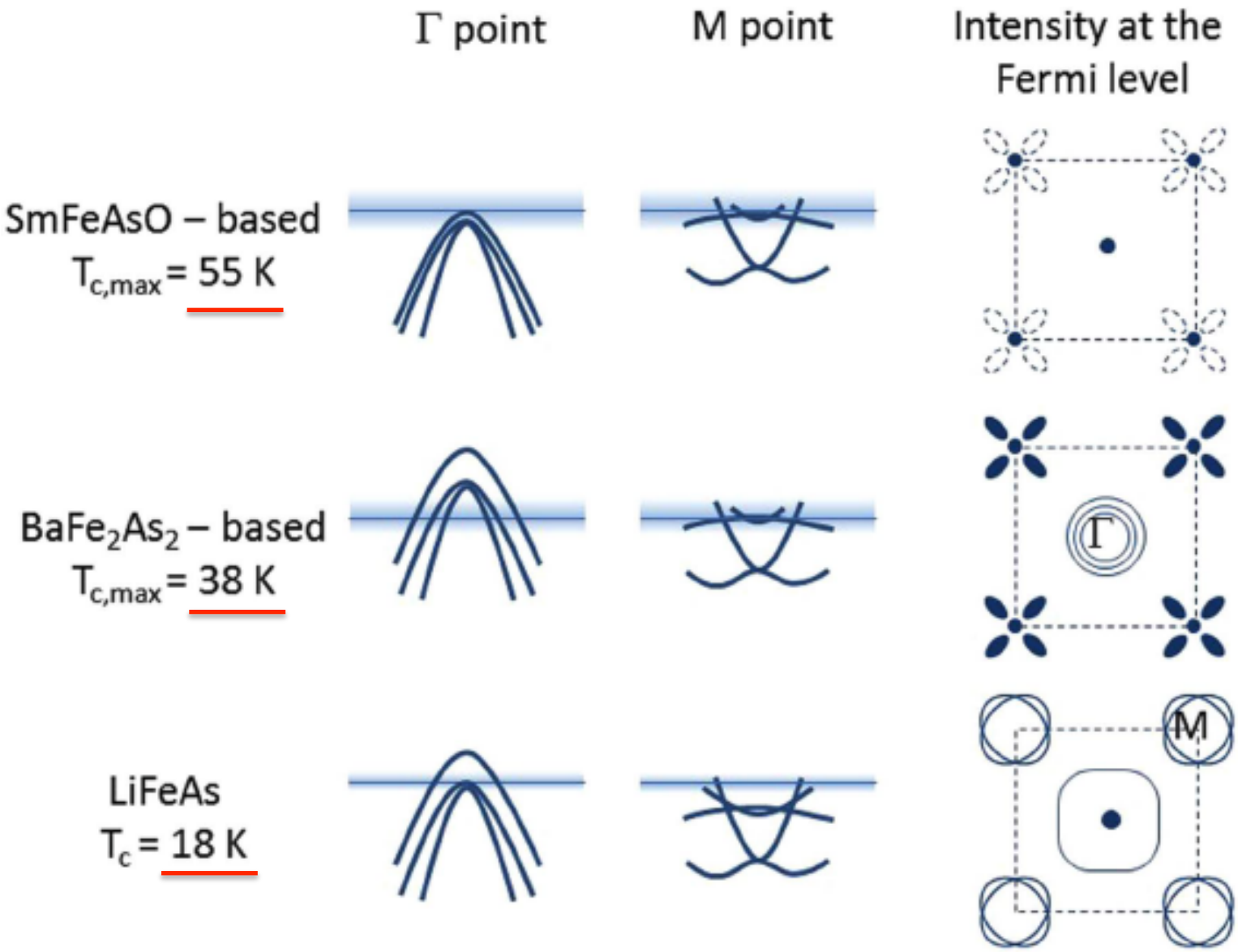
Co-SmFeAsO





Charnukha et al. Sci. Rep. 15

Importance of the singularities for high T_c



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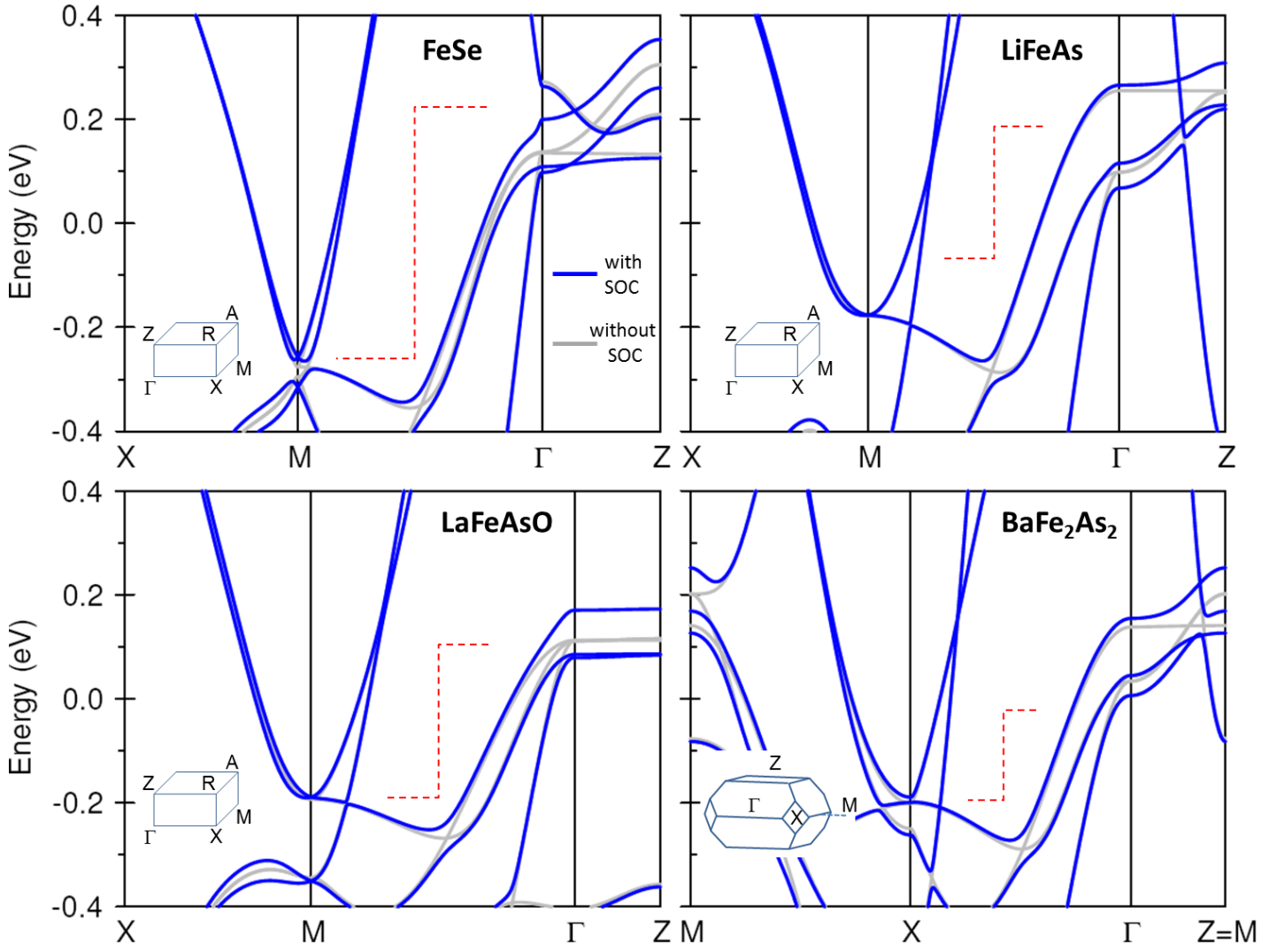
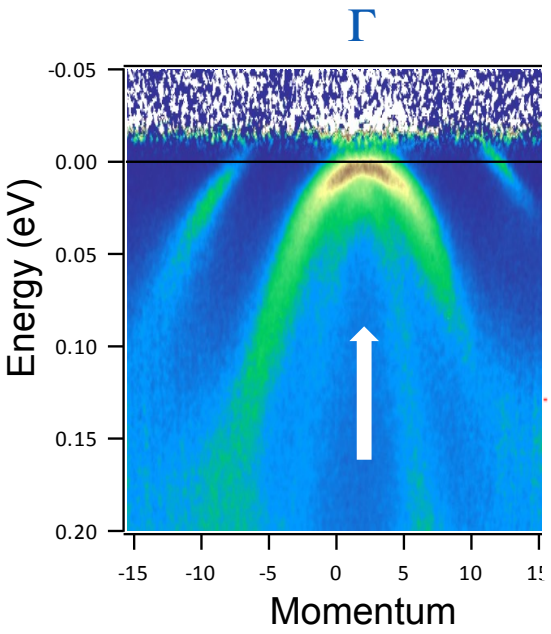
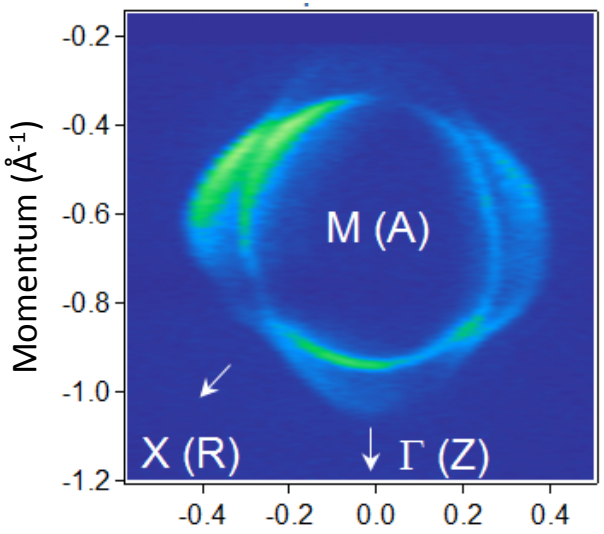
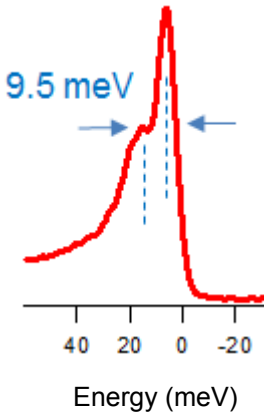


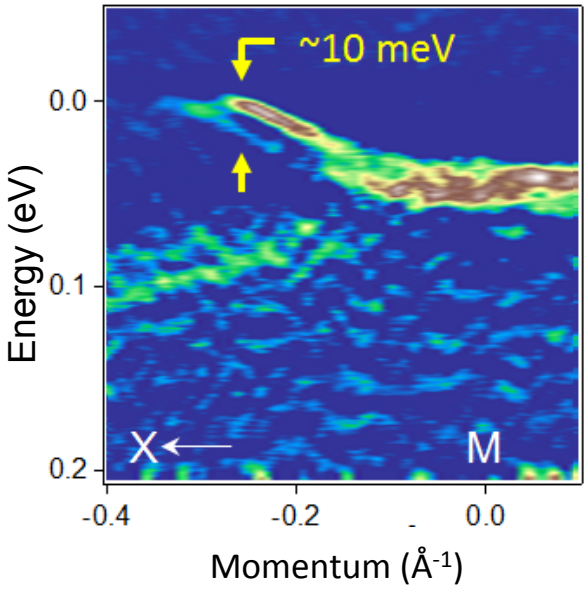
SVB et al. Nat.Phys. 2016

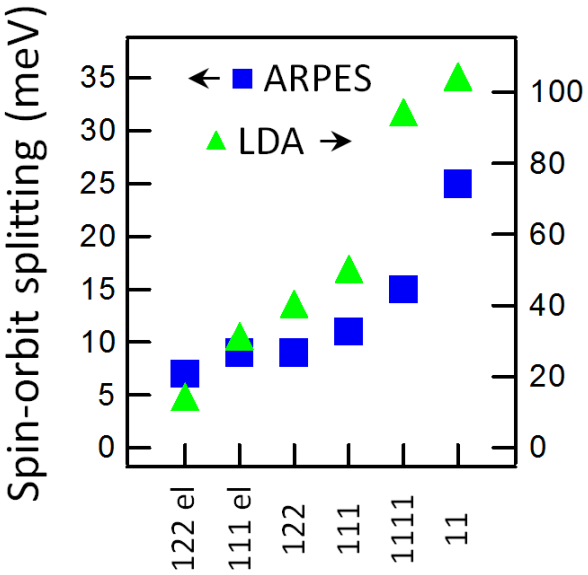
Spin-orbit splitting in LiFeAs and in all other IBS











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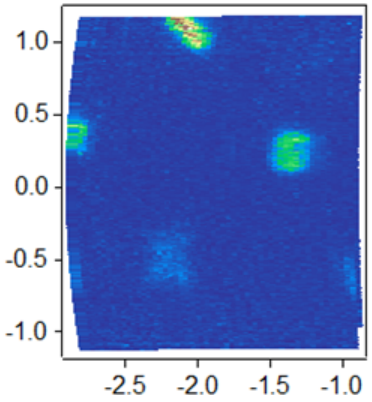
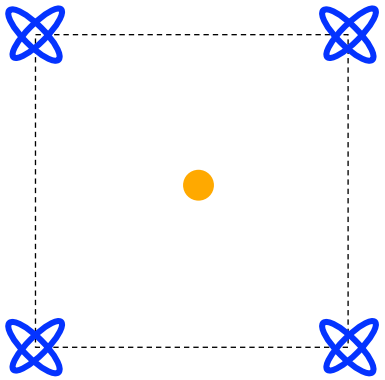
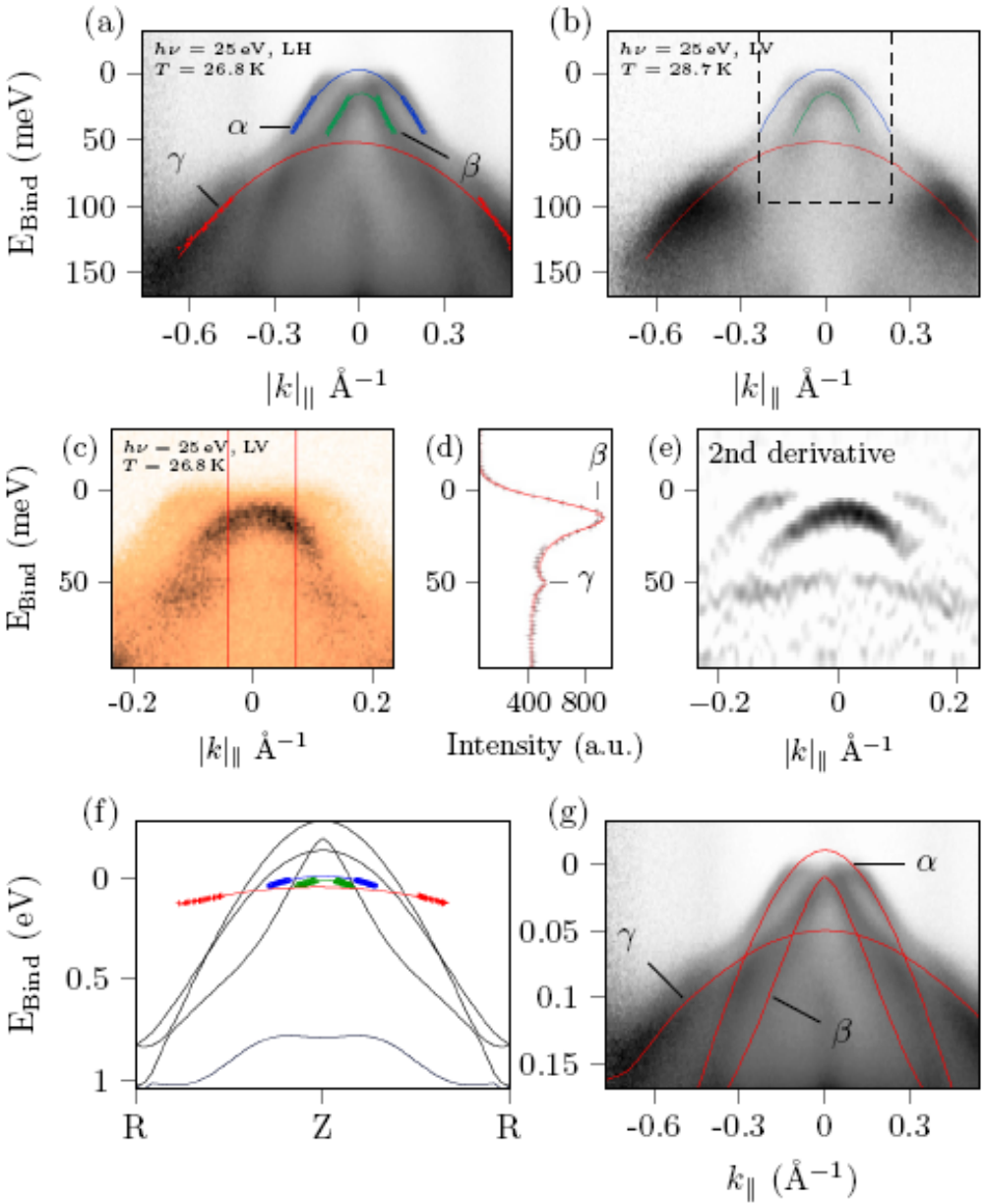
FeSe: orbital dependent renormalization







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Reconstruction of Band Structure Induced by Electronic Nematicity in an FeSe Superconductor

K. Nakayama,[1] Y. Miyata,[1] G. N. Phan,[1] T. Sato,[1] Y. Tanabe,[1] T. Urata,[1] K. Tanigaki,[1,2] and T. Takahashi[1,2]
[1]*Department of Physics, Tohoku University, Sendai 980-8578, Japan*
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(Received 4 April 2014; published 5 December 2014)

We have performed high-resolution angle-resolved photoemission spectroscopy on an FeSe superconductor ($T_c \sim 8$ K), which exhibits a tetragonal-to-orthorhombic structural transition at $T_s \sim 90$ K. At low temperature, we found splitting of the energy bands as large as 50 meV at the M point in the Brillouin zone, likely caused by the formation of electronically driven nematic states. This band splitting persists up

PHYSICAL REVIEW B 91, 155106 (2015)

Emergence of the nematic electronic state in FeSe

M. D. Watson,[1] T. K. Kim,[2] A. A. Haghighirad,[1] N. R. Davies,[1] A. McCollam,[3] A. Narayanan,[1] S. F. Blake,[1] Y. L. Chen,[1] S. Ghannadzadeh,[3] A. J. Schofield,[4] M. Hoesch,[2] C. Meingast,[5] T. Wolf,[5] and A. I. Coldea[1,*]
[1]*Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom*
[2]*Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, United Kingdom*
[3]*High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University, 6525 ED Nijmegen, The Netherlands*
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[5]*Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany*
(Received 11 February 2015; revised manuscript received 10 March 2015; published 7 April 2015; corrected 6 May 2015)

We present a comprehensive study of the evolution of the nematic electronic structure of FeSe using high-resolution angle-resolved photoemission spectroscopy (ARPES), quantum oscillations in the normal state, and elastoresistance measurements. Our high-resolution ARPES allows us to track the Fermi surface deformation from fourfold to twofold symmetry across the structural transition at ~87 K, which is stabilized as a result of the dramatic splitting of bands associated with d_{xz} and d_{yz} character in the presence of strong electronic interactions.

in the Fermi surface across the transition. The large band splitting of ~50 meV at the M point at 10 K [Fig. 2(e)] indicates the lifting of of d_{xz} and d_{yz} degeneracy in FeSe.

arXiv:1512.02526

Simultaneous emergence of superconductivity, inter-pocket scattering and nematic fluctuation in potassium-coated FeSe superconductor

Z. R. Ye[1, †], C. F. Zhang[2, 3, †], H. L. Ning[1], W. Li[2, 3], L. Chen[1], T. Jia[2, 3], M. Hashimoto[4], D. H. Lu[4], Z.-X. Shen[2, 3], and Y. Zhang[1, 5, *]

electron doping level by counting the Fermi surface volume. The nematic transition temperature (T_{nem}) is calculated from the energy splitting between the β_1 and β_2 bands (Δ_{nem}). The Δ_{nem}/k_BT_{nem} is 6.22 as determined by the Δ_{nem} and T_{nem} in undoped FeSe single crystal.

PHYSICAL REVIEW B 90, 121111(R) (2014)

Lifting of xz/yz orbital degeneracy at the structural transition in detwinned FeSe

T. Shimojima,[1,*] Y. Suzuki,[1] T. Sonobe,[1] A. Nakamura,[1] M. Sakano,[1] J. Omachi,[2] K. Yoshioka,[3] M. Kuwata-Gonokami,[2,3] K. Ono,[4] H. Kumigashira,[4] A. E. Böhmer,[5] F. Hardy,[5] T. Wolf,[5] C. Meingast,[5] H. v. Löhneysen,[5,6] H. Ikeda,[7] and K. Ishizaka[1]
[1]*Quantum-Phase Electronics Center (QPEC) and Department of Applied Physics, The University of Tokyo, Bunkyo, Tokyo 113-8656, Japan*
[2]*Photon Science Center, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan*
[3]*Department of Physics, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan*
[4]*KEK, Photon Factory, Tsukuba, Ibaraki 305-0801, Japan*
[5]*Institut für Festkörperphysik, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany*
[6]*Physikalisches Institut, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany*
[7]*Department of Physics, Kyoto University, Kyoto 606-8502, Japan*
(Received 4 July 2014; revised manuscript received 11 September 2014; published 29 September 2014)

We study superconducting FeSe ($T_c = 9$ K) exhibiting the tetragonal-orthorhombic structural transition ($T_s \sim 90$ K) without any antiferromagnetic ordering, by utilizing angle-resolved photoemission spectroscopy. In the detwinned orthorhombic state, the energy position of the d_{yz} orbital band at the Brillouin zone corner is 50 meV higher than that of d_{xz}, indicating the orbital order similar to the NaFeAs and $BaFe_2As_2$ families.

PHYSICAL REVIEW B 91, 214503 (2015)

Observation of two distinct d_{xz}/d_{yz} band splittings in FeSe

P. Zhang,[1] T. Qian,[1] P. Richard,[1,2,*] X. P. Wang,[3,2,1] H. Miao,[1] B. Q. Lv,[1] B. B. Fu,[1] T. Wolf,[4] C. Meingast,[4] X. X. Wu,[1] Z. Q. Wang,[5,1] J. P. Hu,[1,2,†] and H. Ding[1,2,‡]
[1]*Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
[2]*Collaborative Innovation Center of Quantum Matter, Beijing, China*
[3]*State Key Laboratory for Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China*
[4]*Institut für Festkörperphysik, Karlsruhe Institute for Technology, Karlsruhe 76021, Germany*
[5]*Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA*
(Received 16 March 2015; revised manuscript received 17 May 2015; published 4 June 2015)

We report the temperature evolution of the detailed electronic band structure in FeSe single crystals measured by angle-resolved photoemission spectroscopy (ARPES), including the degeneracy removal of the d_{xz} and d_{yz} orbitals at the Γ/Z and M points, and the orbital-selective hybridization between the d_{xy} and $d_{xz/yz}$ orbitals. The temperature dependences of the splittings at the Γ/Z and M points are different, indicating that they are controlled by different order parameters. The splitting at the M point is closely related to the structural transition and is attributed to orbital ordering defined on Fe-Fe bonds with a d-wave form in the reciprocal space that breaks

The splitting at M is about 60 meV with temperature increasing and

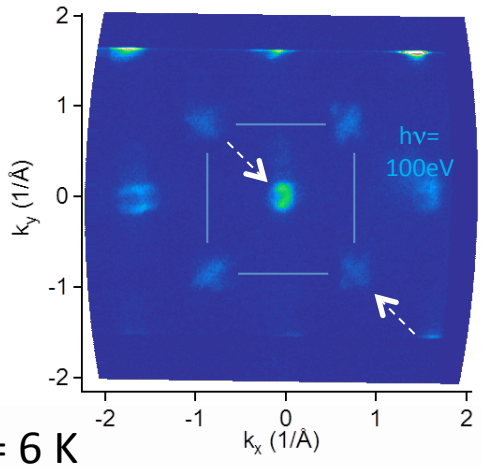
Highly anisotropic and two-fold symmetric superconducting gap in nematically ordered $FeSe_{0.93}$

H. C. Xu,[1] X. H. Niu,[1] D. F. Xu,[1] J. Jiang,[1] Q. Yao,[1] M. Abdel-Hafiez,[2,3] D. A. Chareev,[4] A. N. Vasiliev,[5] R. Peng,[1,*] and D. L. Feng[1,†]
[1]*State Key Laboratory of Surface Physics, Department of Physics, and Advanced Materials Laboratory, Fudan University, Shanghai 200433, People's Republic of China*
[2]*Center for High Pressure Science and Technology Advanced Research, Shanghai 201203, China*
[3]*Faculty of science, Physics department, Fayoum University, 63514-Fayoum, Egypt*

along Z-A_1, clearly indicating the splitting of 50 meV between bands ε and ε' due to the nematic order [14].

arXiv:1603.05219

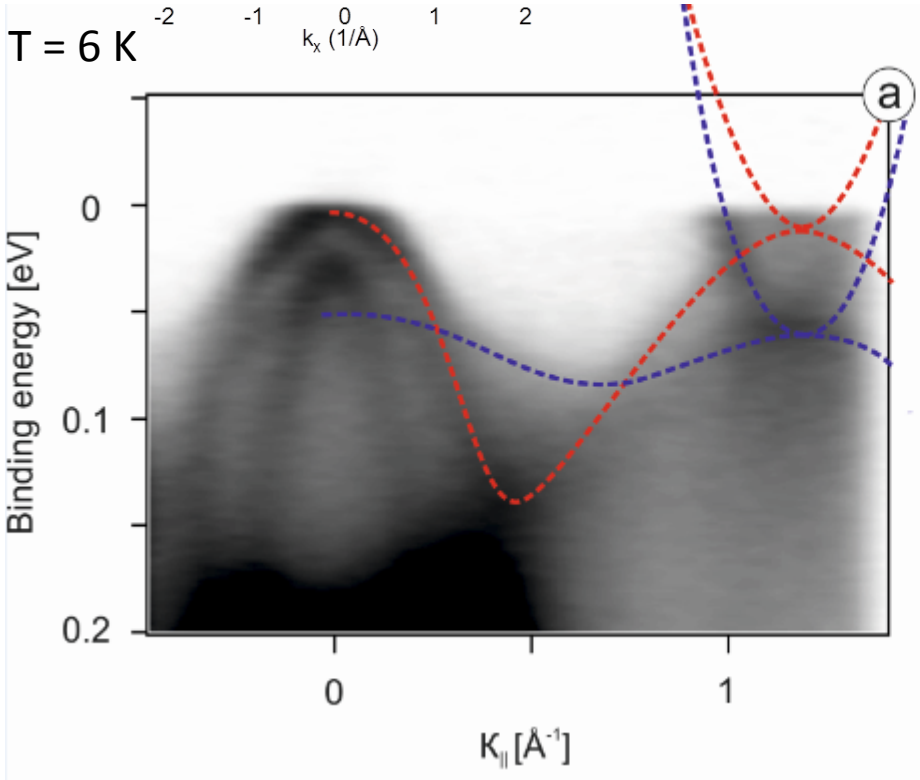
FeSe: comparison with a=b calculations

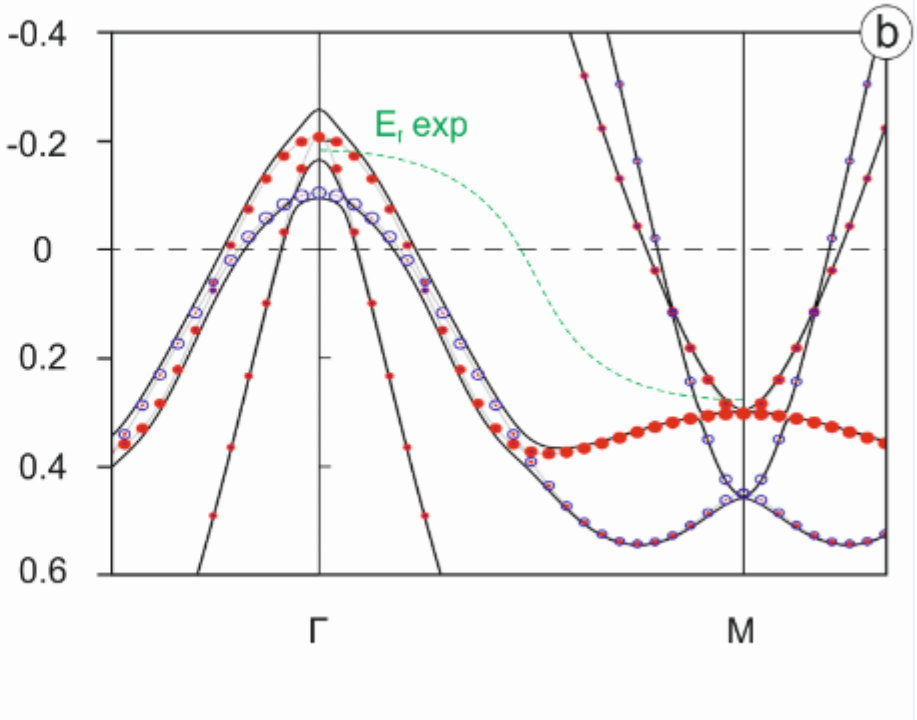


xy

xz/yz

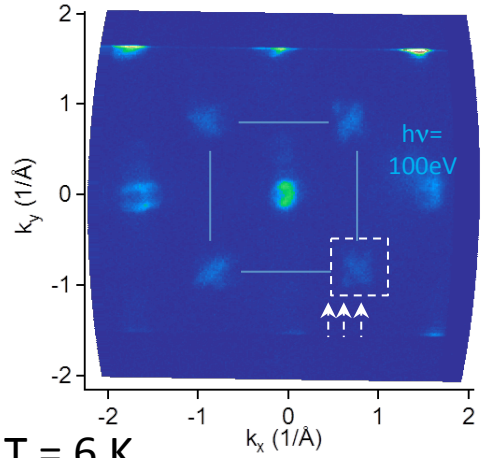
T = 6 K



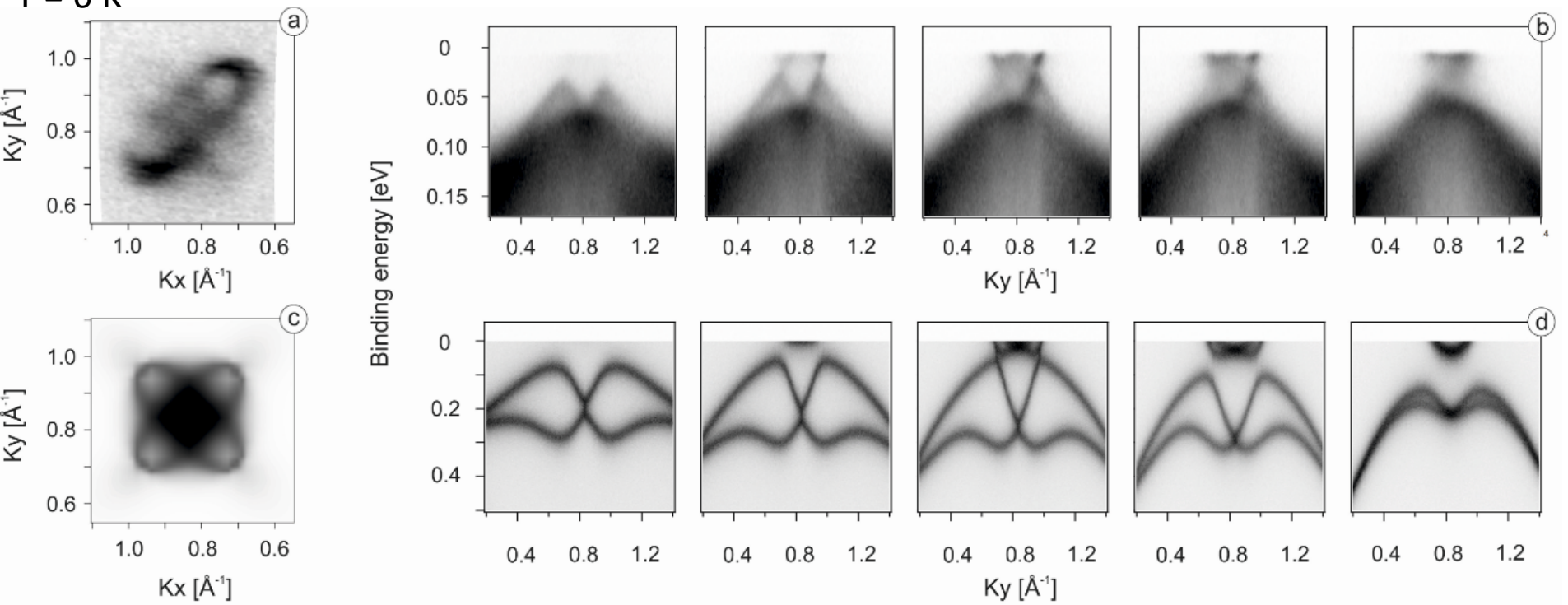


Fedorov et al. arXiv:1606.03022

FeSe: comparison with a=b calculations



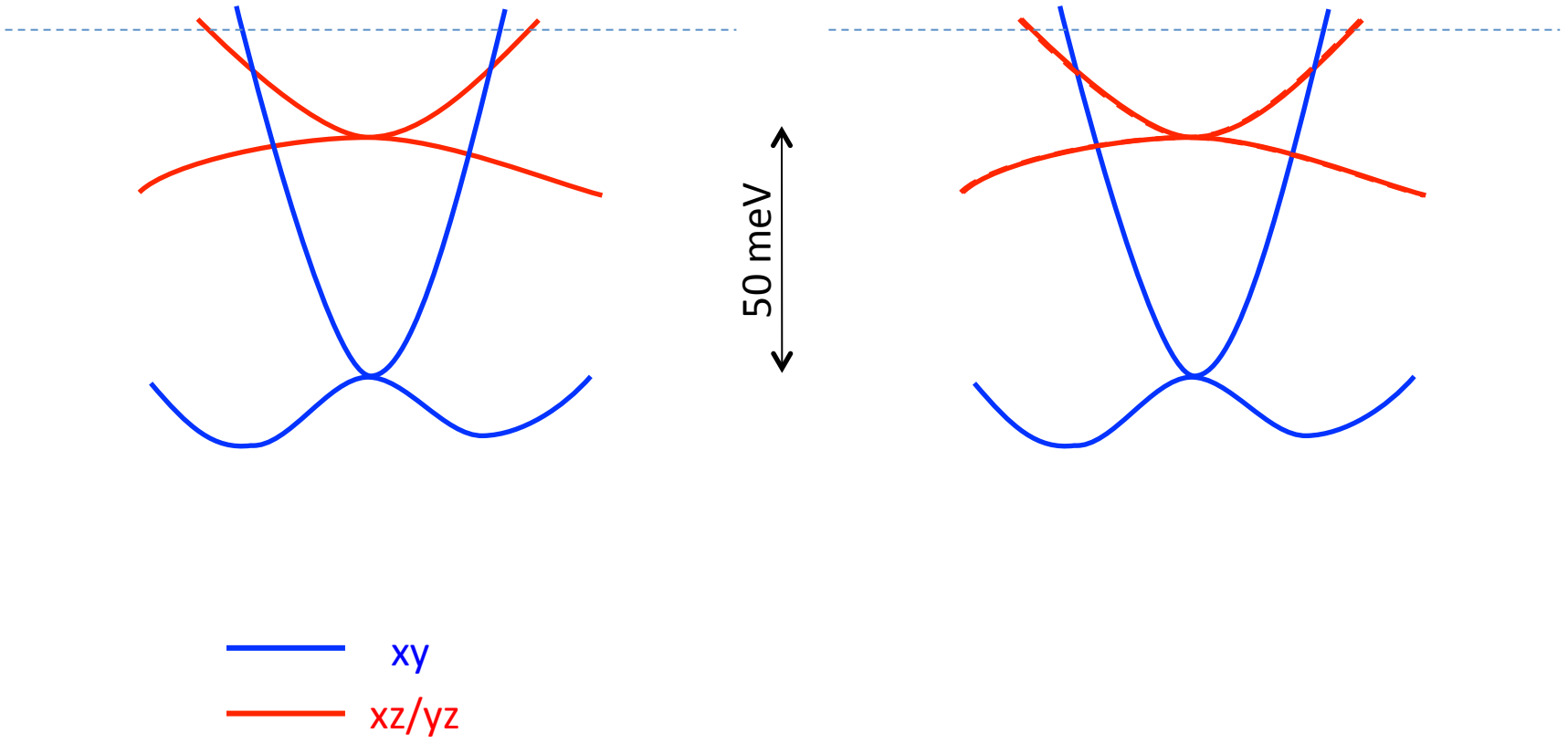
T = 6 K



Fedorov et al. arXiv:1606.03022

Our interpretation

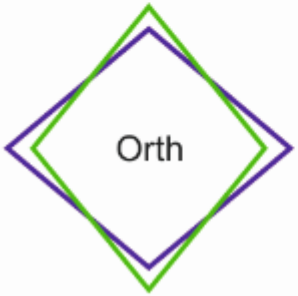
Their interpretation

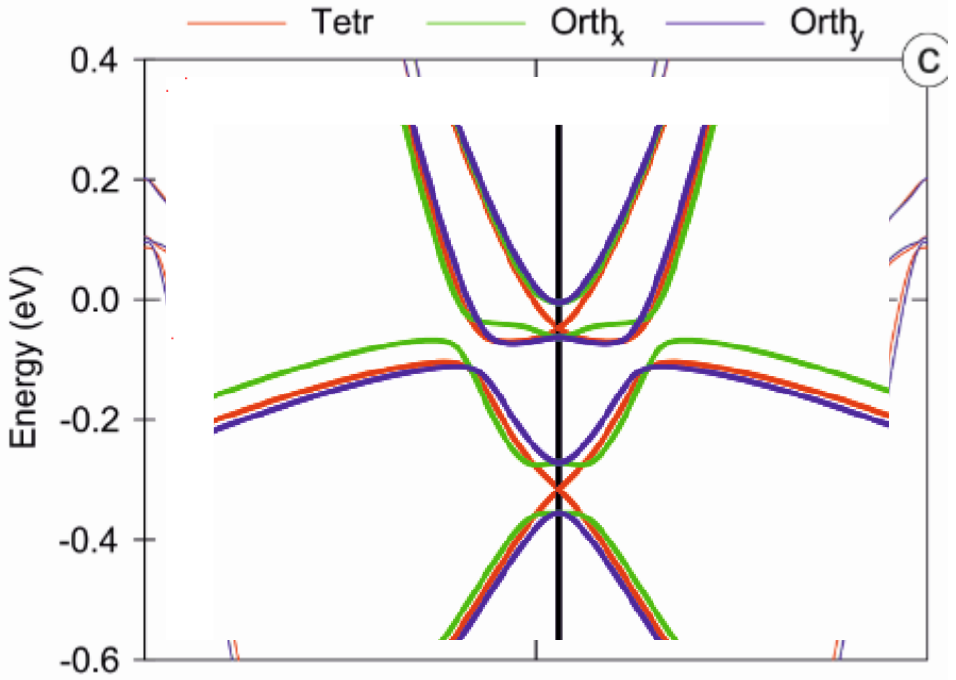


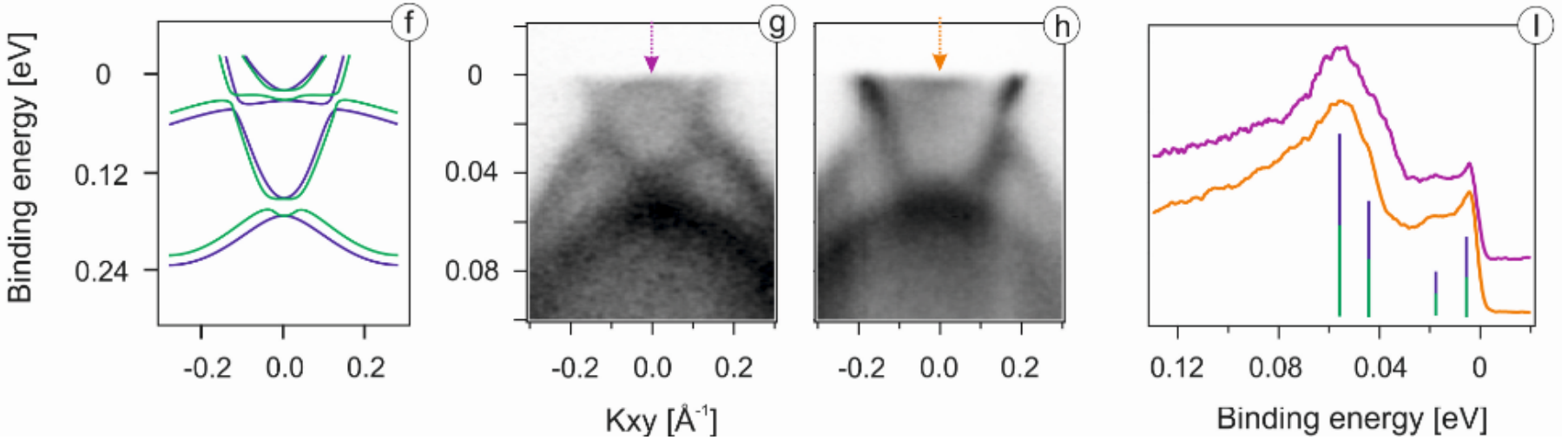
FeSe: comparison with a≠b calculations

T>T*

T<T*

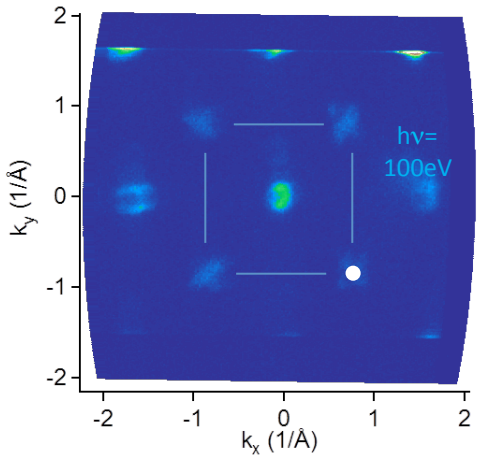


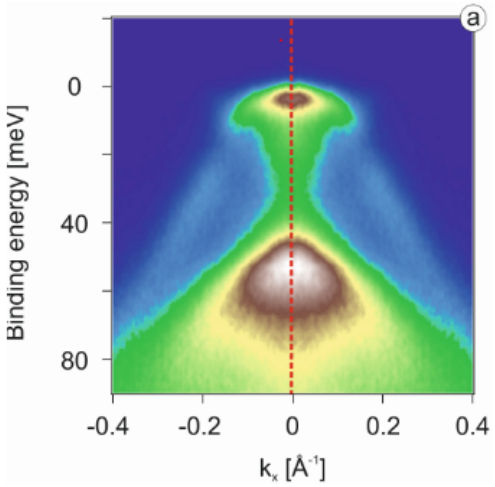


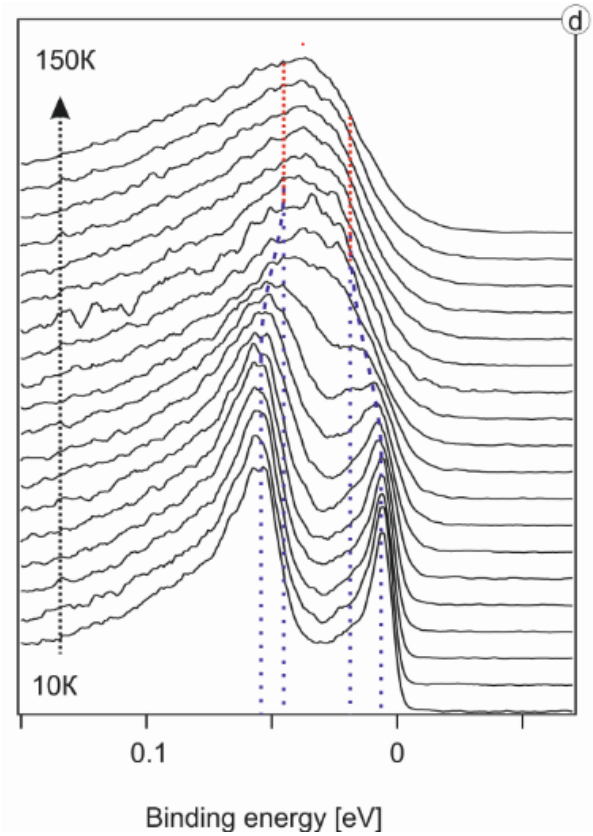


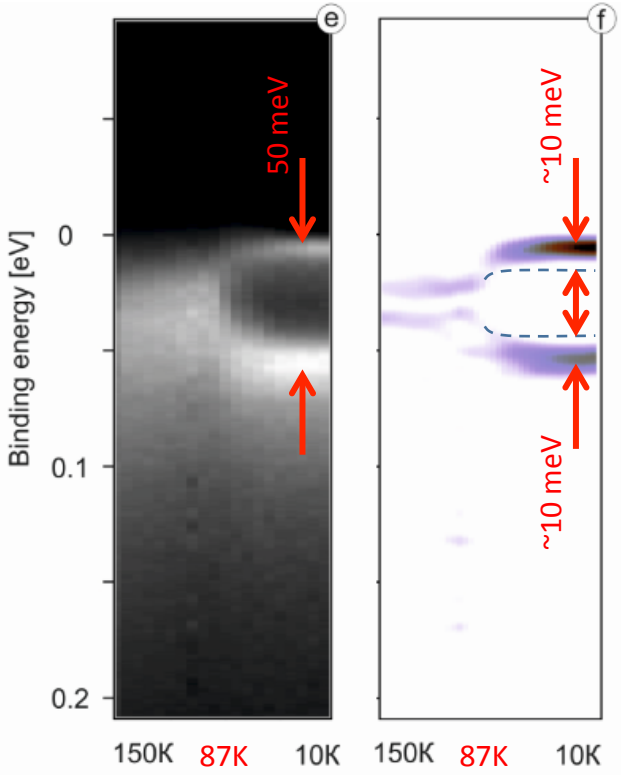
Fedorov et al. arXiv:1606.03022

FeSe: temperature dependence of M-point EDC



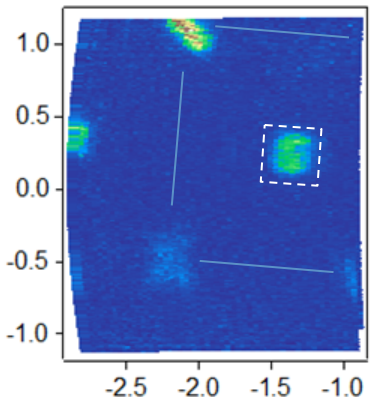


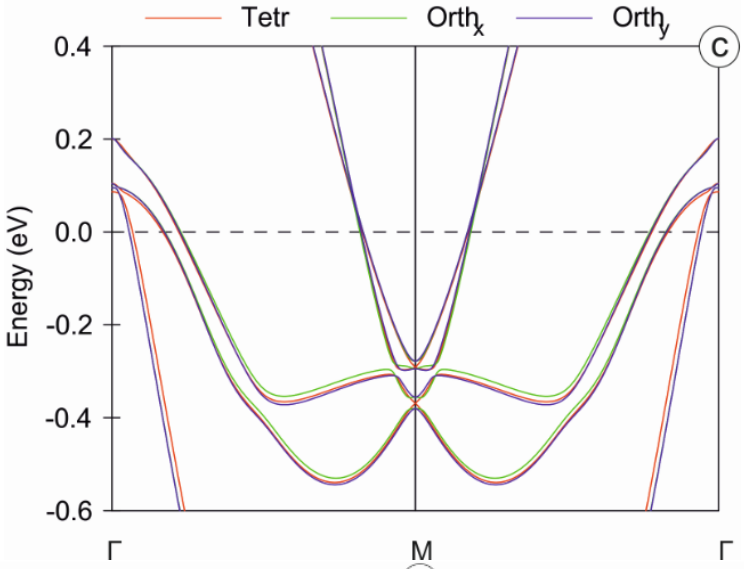


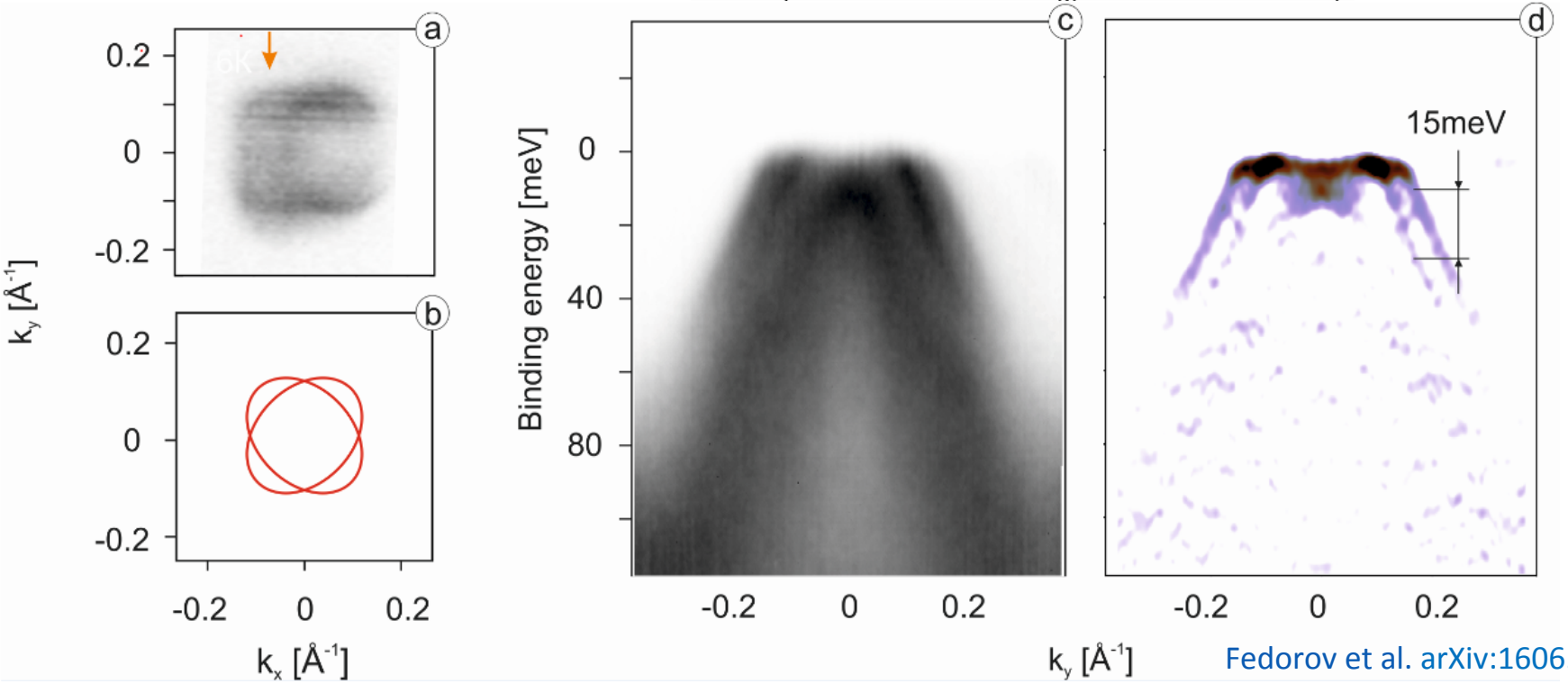


Fedorov et al. arXiv:1606.03022

FeSe: electronic structure in the center of BZ

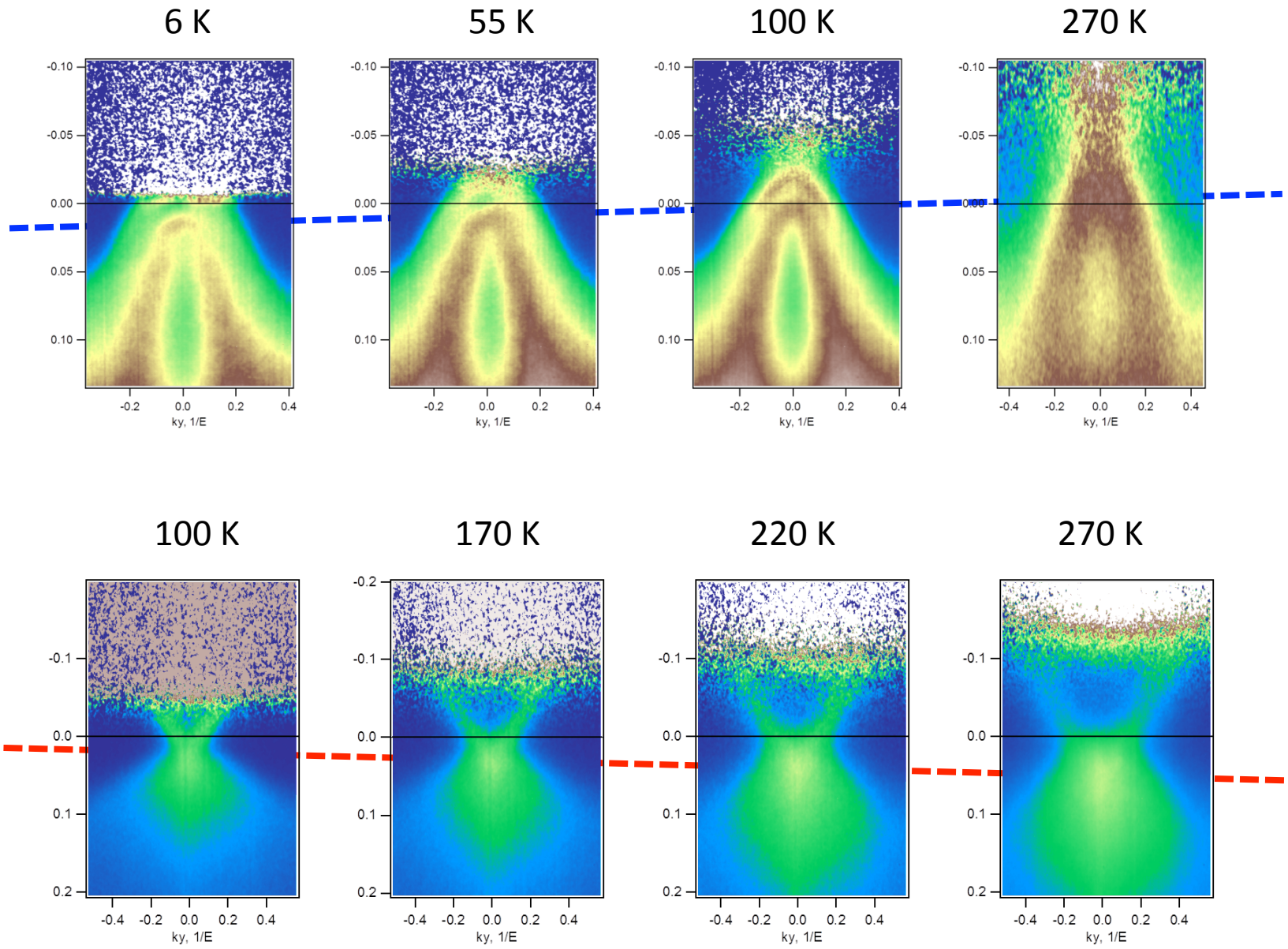






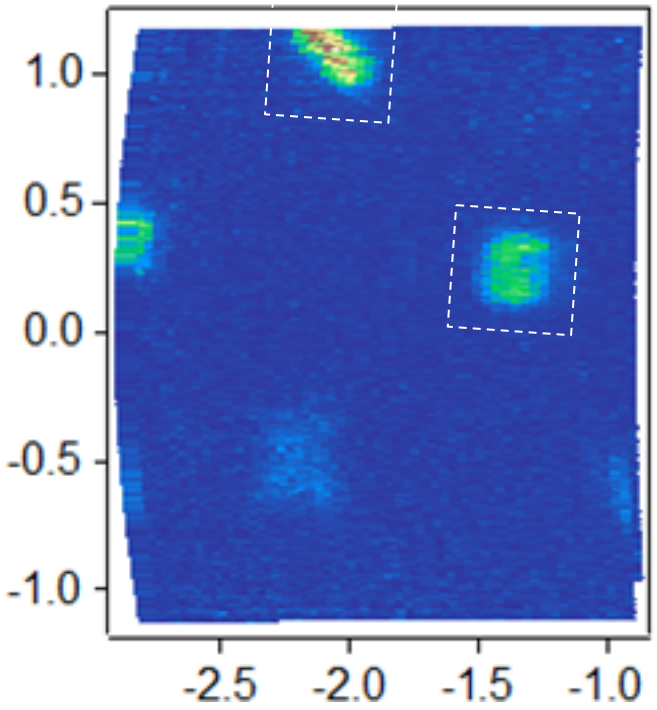
Fedorov et al. arXiv:1606.03022

FeSe: back to DFT Fermi surfaces with temperature

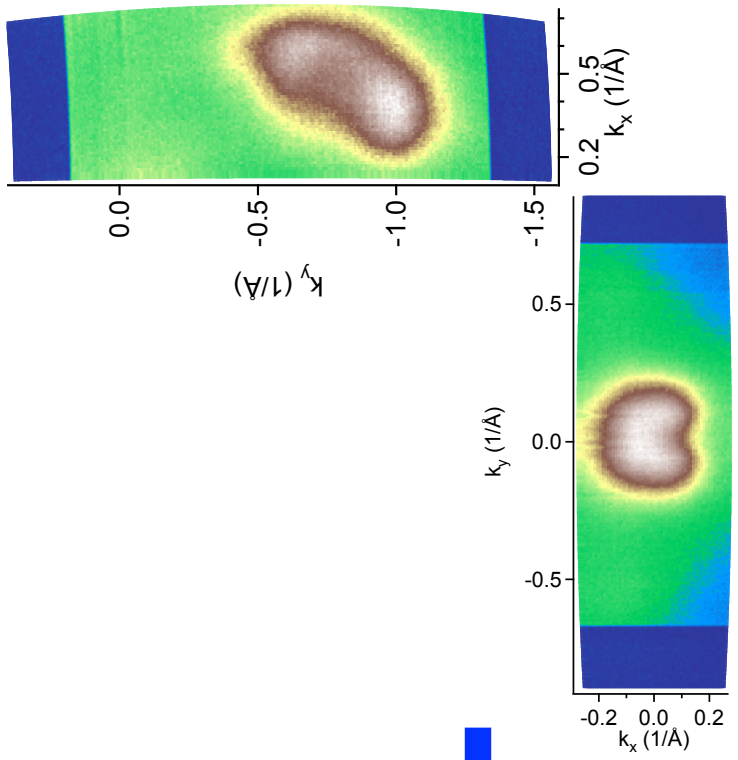


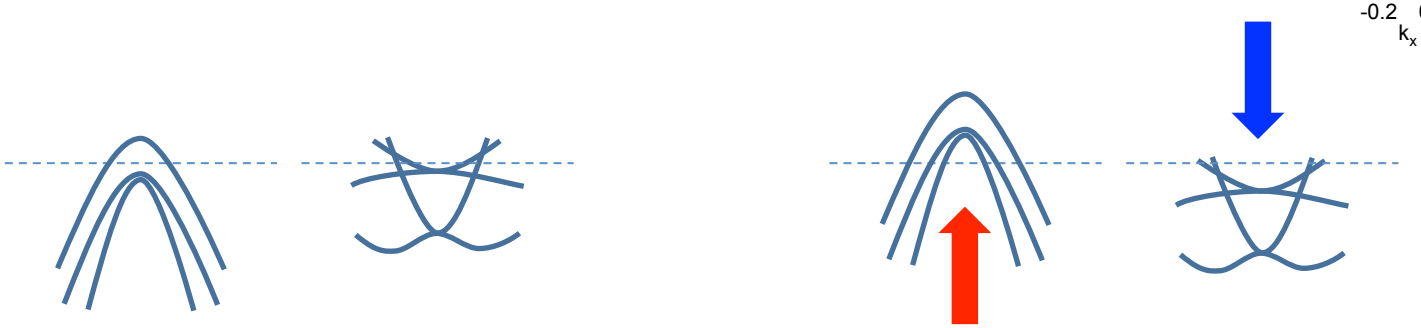
FeSe: back to DFT Fermi surfaces with temperature

1 K



270 K

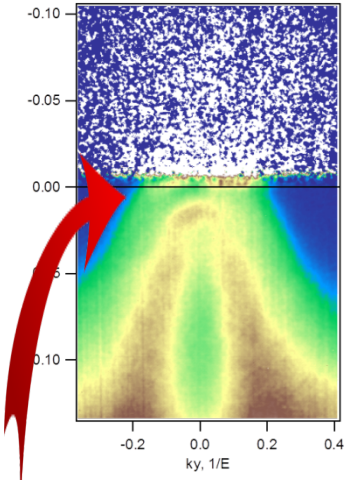




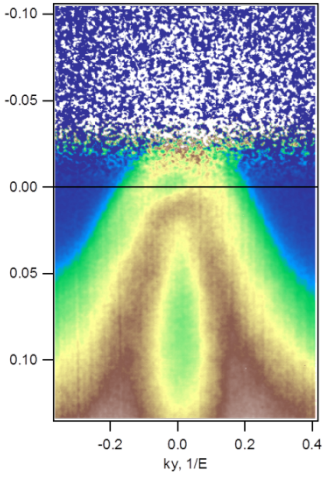
Pomeranchuk instability?

FeSe: spin-orbit splitting and nematicity quantitatively

6 K

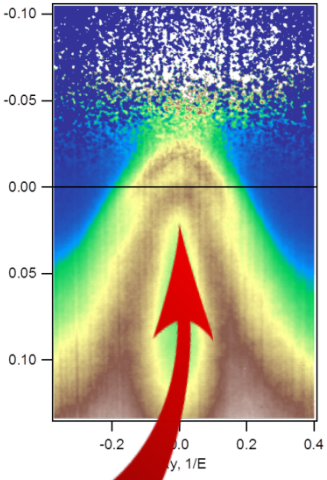


55 K

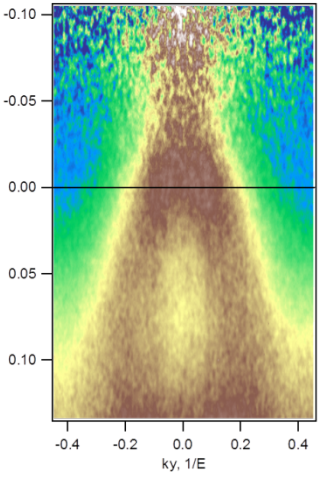


TET-ORTH transition

100 K

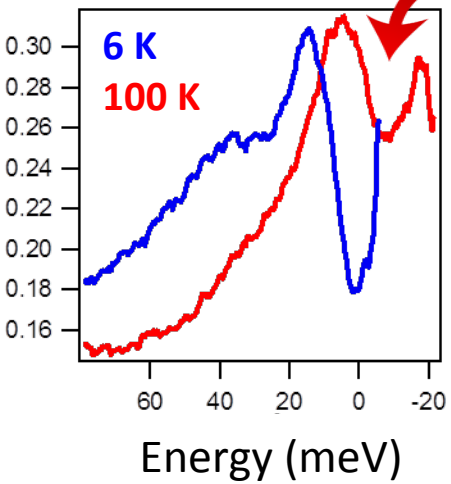


270 K



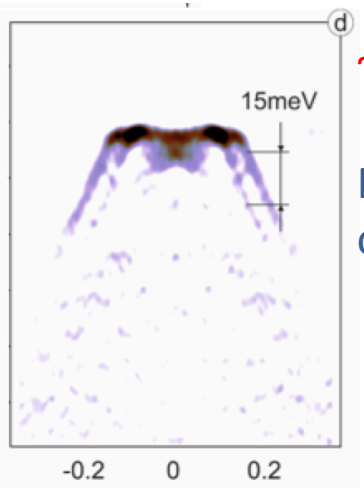
~25 meV

Spin-orbit splitting + Nematic splitting



~20 meV

Spin-orbit splitting only

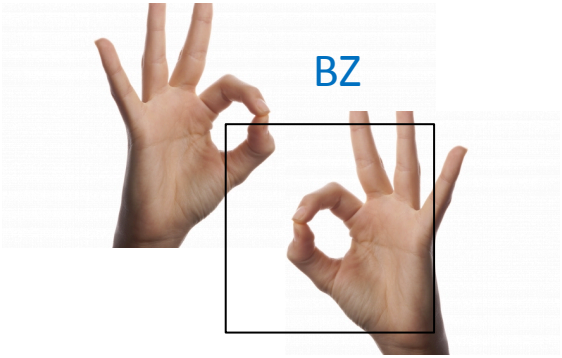


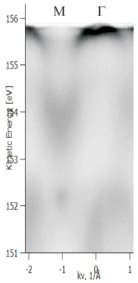
~15 meV

Nematicity only

$25^2 = 20^2 + 15^2$

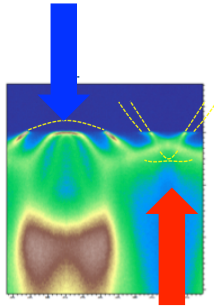
From „double-OK“ model to reality (conclusions)





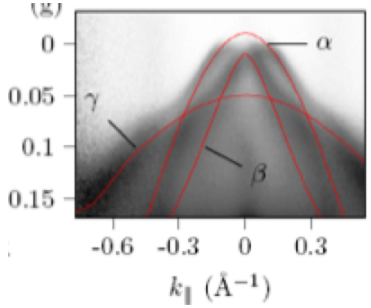
Renormalization
by a factor ~3 on
10 eV scale

Physics: J



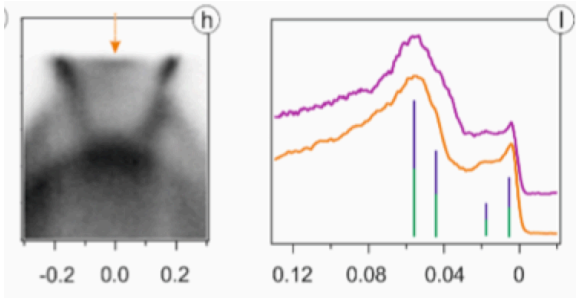
Blue/red shifts
scale of 0.1 eV

Physics: particle-hole asymmetry ?



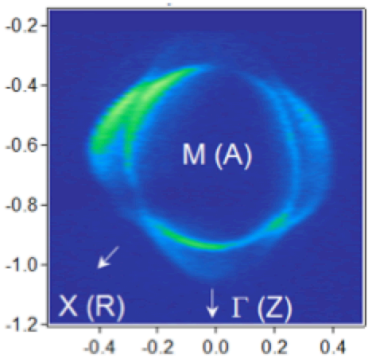
Oribital-dependent
renormalization
by up to another factor 3 on
the scale of 1 eV

Physics: ?



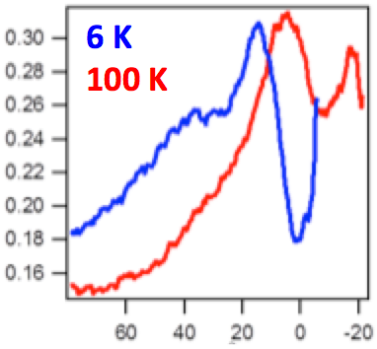
Orthorhombic distorsion
10-15 meV

Physics: electronic nematicity



Spin-orbit splitting
up to 20 meV

Physics: (l,s)

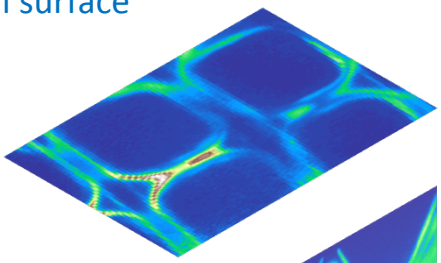


T-dependence
Scale 10 meV

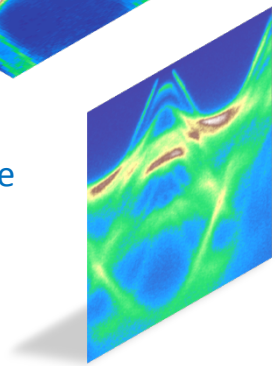
Physics: s+- Pomeranchuk ?

Theory test

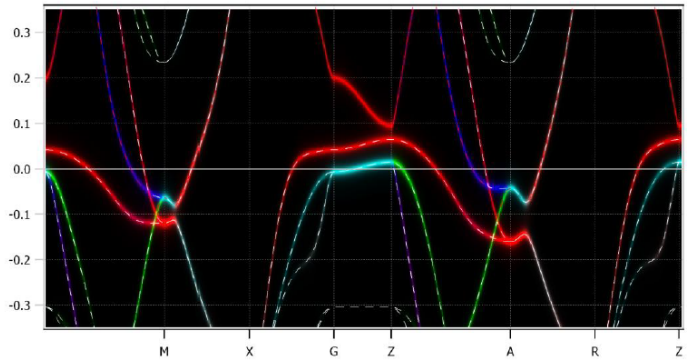
Fermi surface



Band structure



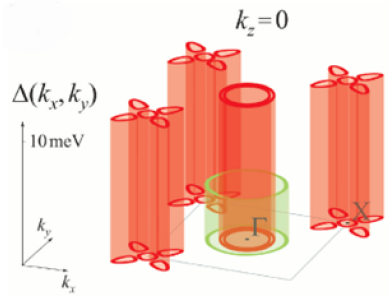
„Quasiparticle Tight-Binding Fit“



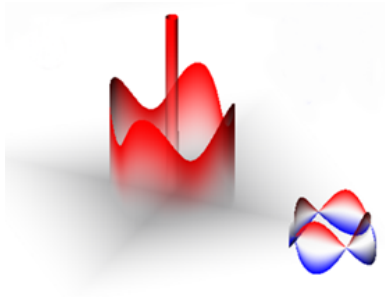
Orbitals: XY XZ YZ

Your Theory

Gap function from experiment



Gap function from theory



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Single crystals Thomas Wolf (KIT)

FeSe

Experiments Danil Evtushinsky, Zhonghao Liu, Alex Charnukha,
Setti Thirupathaiah (IFW-Dresden)

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