Nematic order and the superconducting gap in FeSe

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diamond

ARPES

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I05 @ diamond

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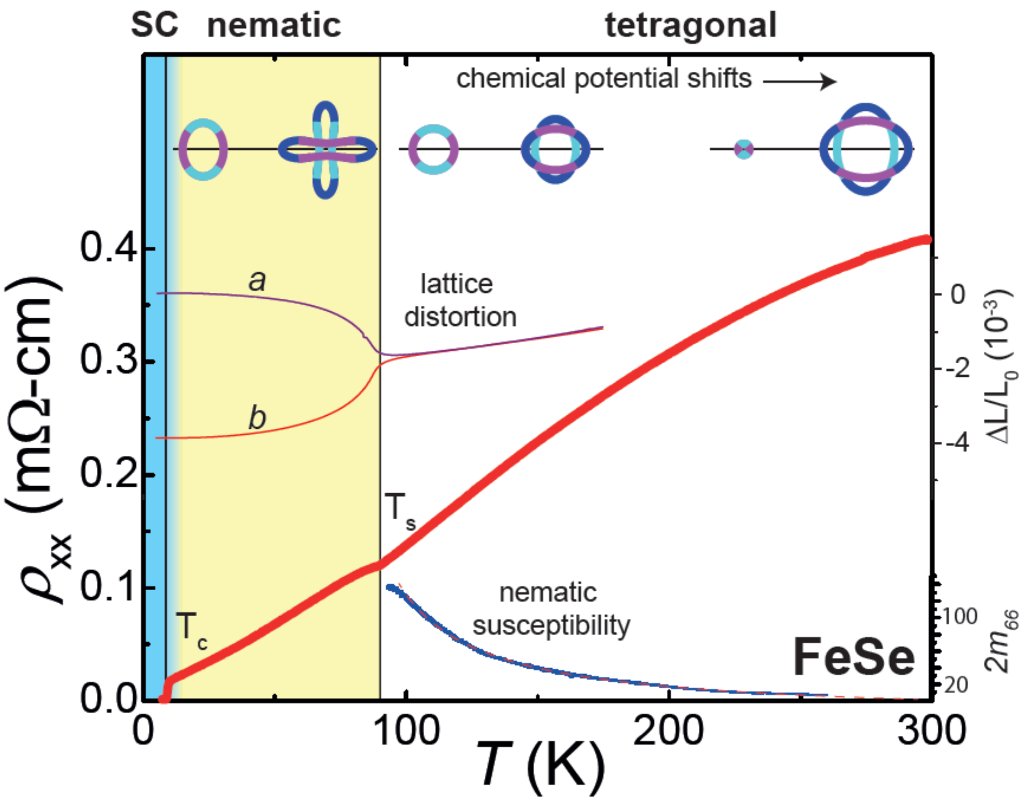
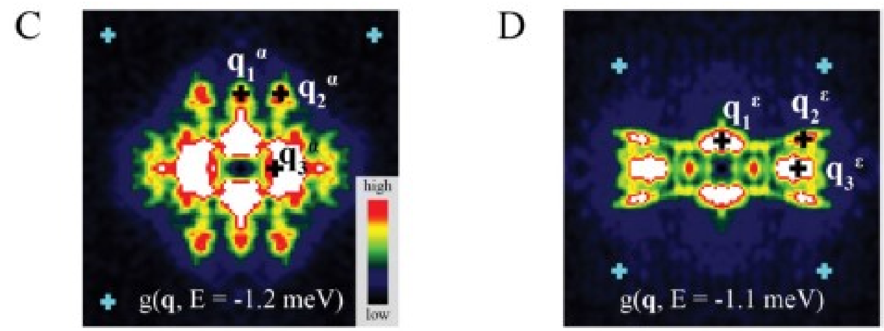
The nematic phase of FeSe

Small structural distortion, but large anisotropies in probes of *electronic* structure

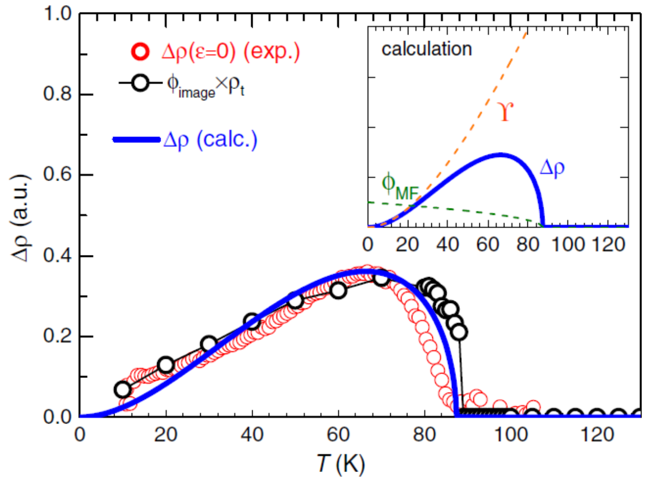


Bogoliubov quasiparticle interference



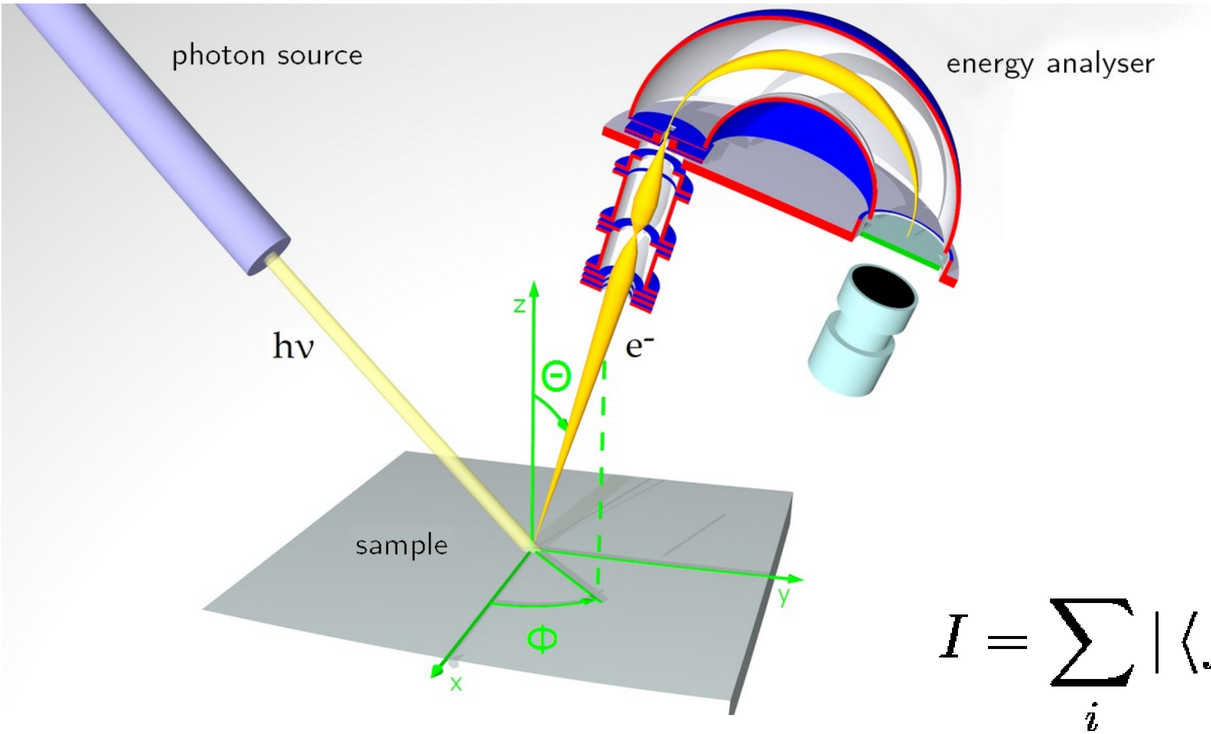
Sprau et al. Science **357**(6346) 75-80 (2017)

Resistivity anisotropy



Tanatar et al. PRL **117**, 127001 (2016)

Angle-resolved photo-emission spectroscopy



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

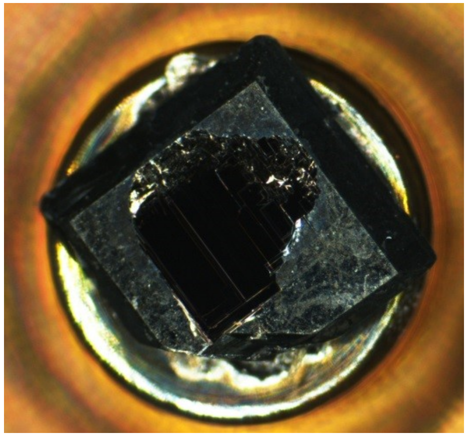
$$\vec{k}_{||} = \frac{1}{\hbar}\sqrt{2mE_{kin}}\sin\theta$$

$$I = \sum_i |\langle f|H_{el}|i\rangle|^2 A_i(\vec{k},\omega) f(\omega)$$

Matrix elements

Spectral function

Fermi-Dirac distribution



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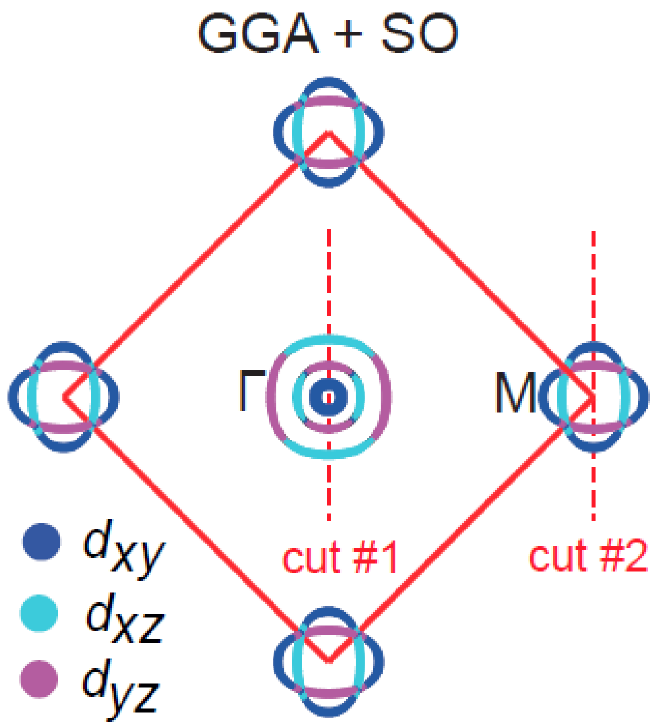
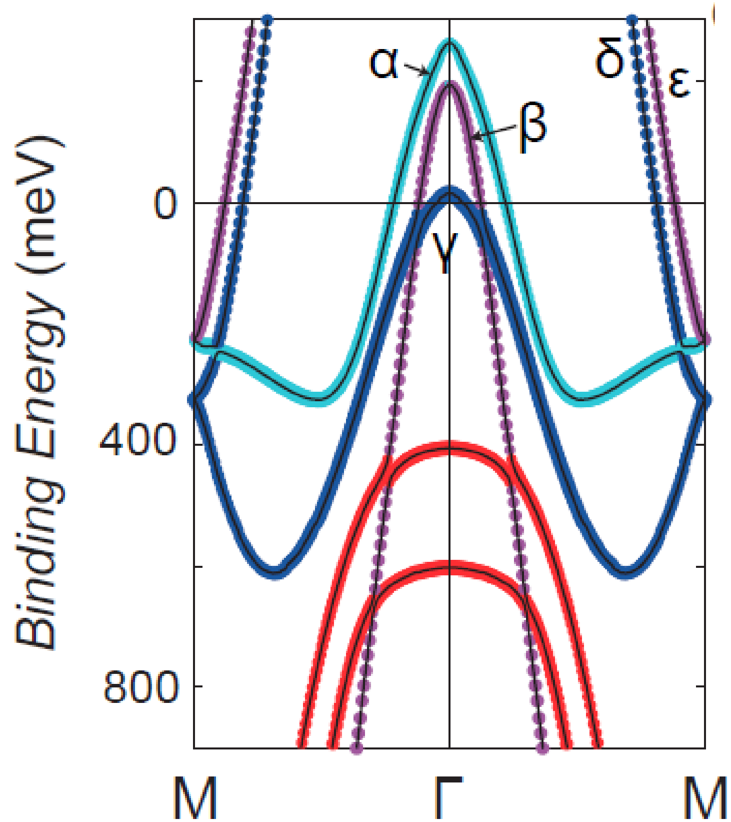
DFT: quasi-2D hole and electron pockets





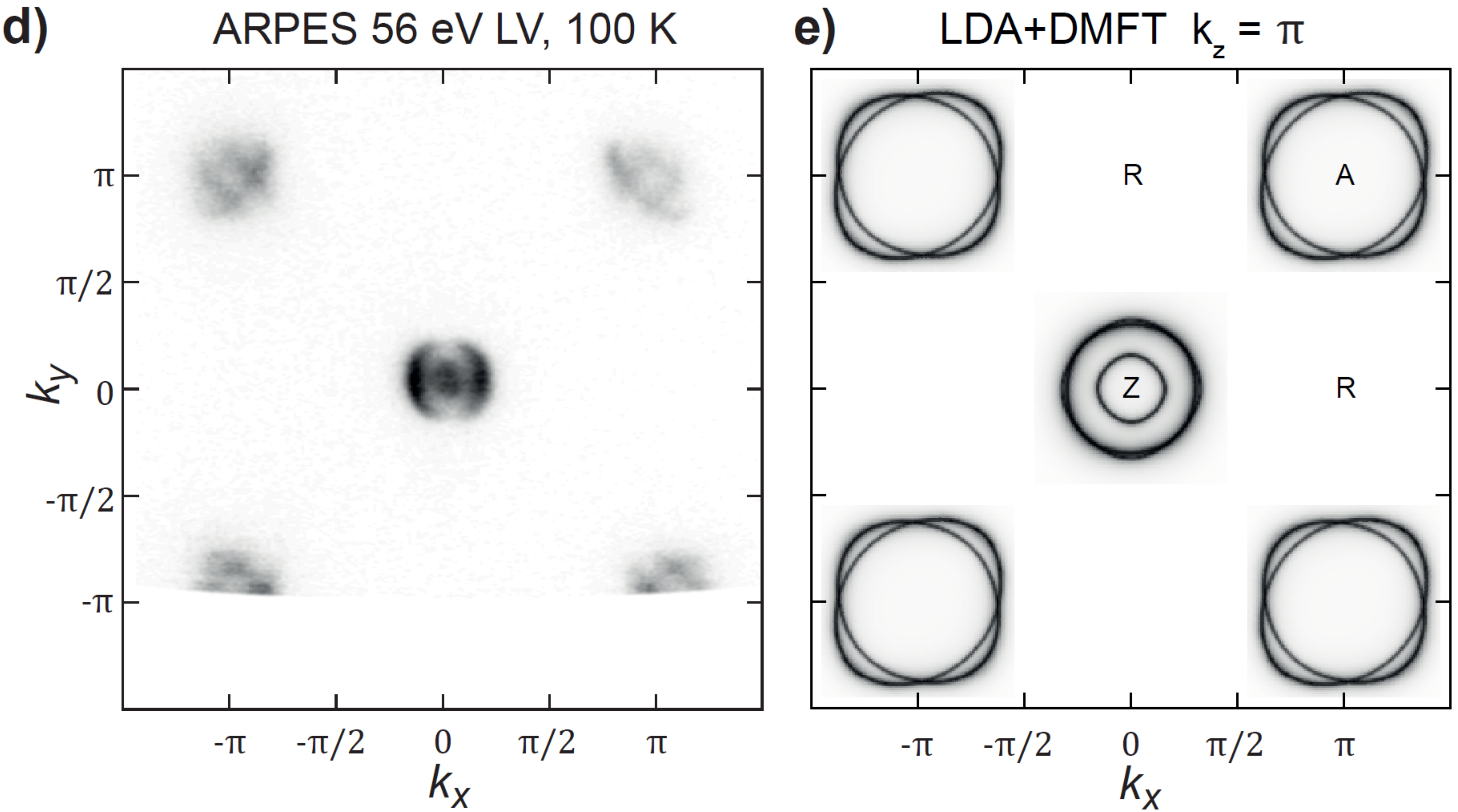
$$I = \sum_i |\langle f|H_{el}|i\rangle|^2 A_i(\vec{k},\omega) f(\omega)$$

Matrix elements

Spectral function

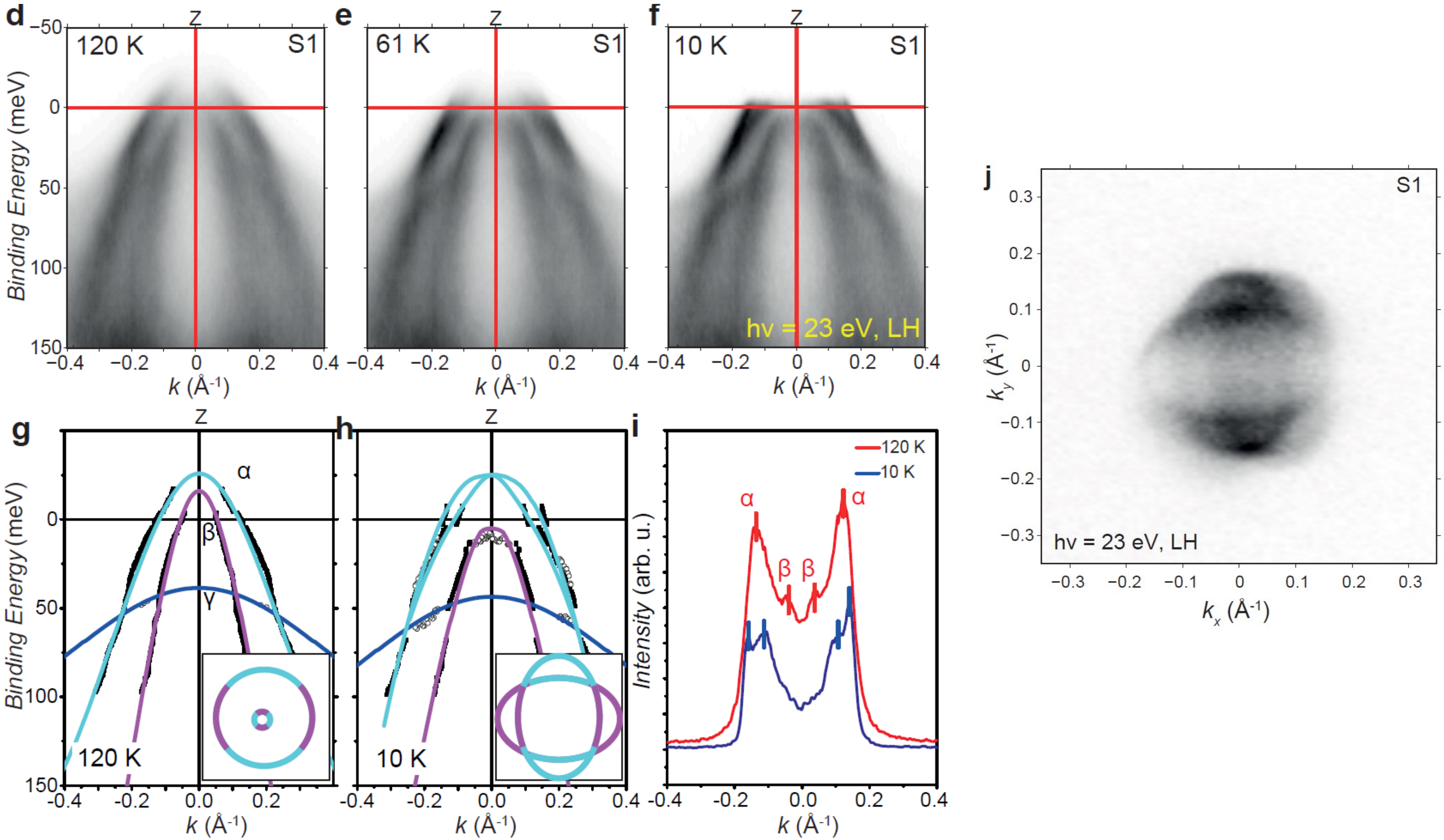
Fermi-Dirac distribution

Failures of DFT and DFT+DMFT at the Fermi level



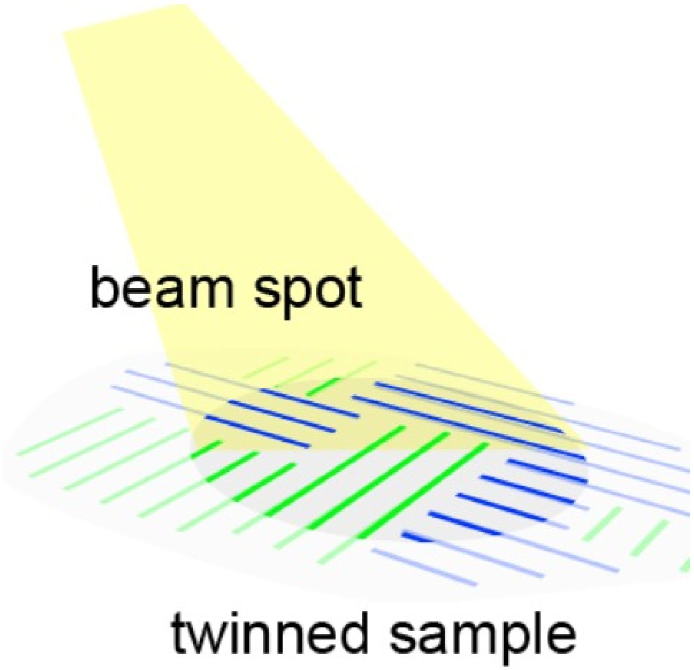
M. D. Watson, S. Backes et al. Phys. Rev. B 95, 081106(R) (2017)

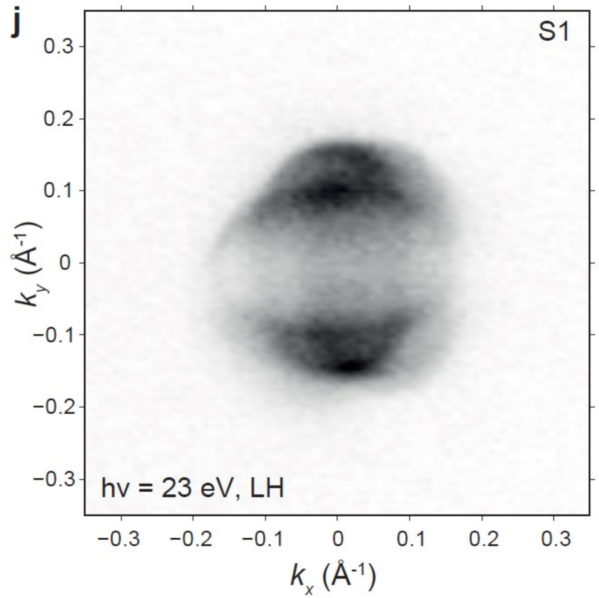
ARPES: one elliptical hole pocket at low temperature

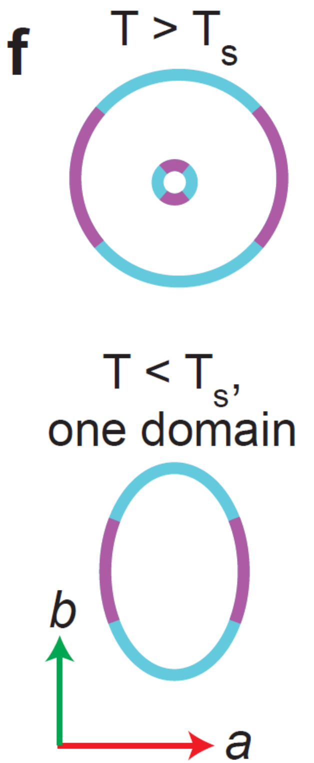


M. D. Watson et al. Phys. Rev. B 91, 155106 (2015)

The problem of twins

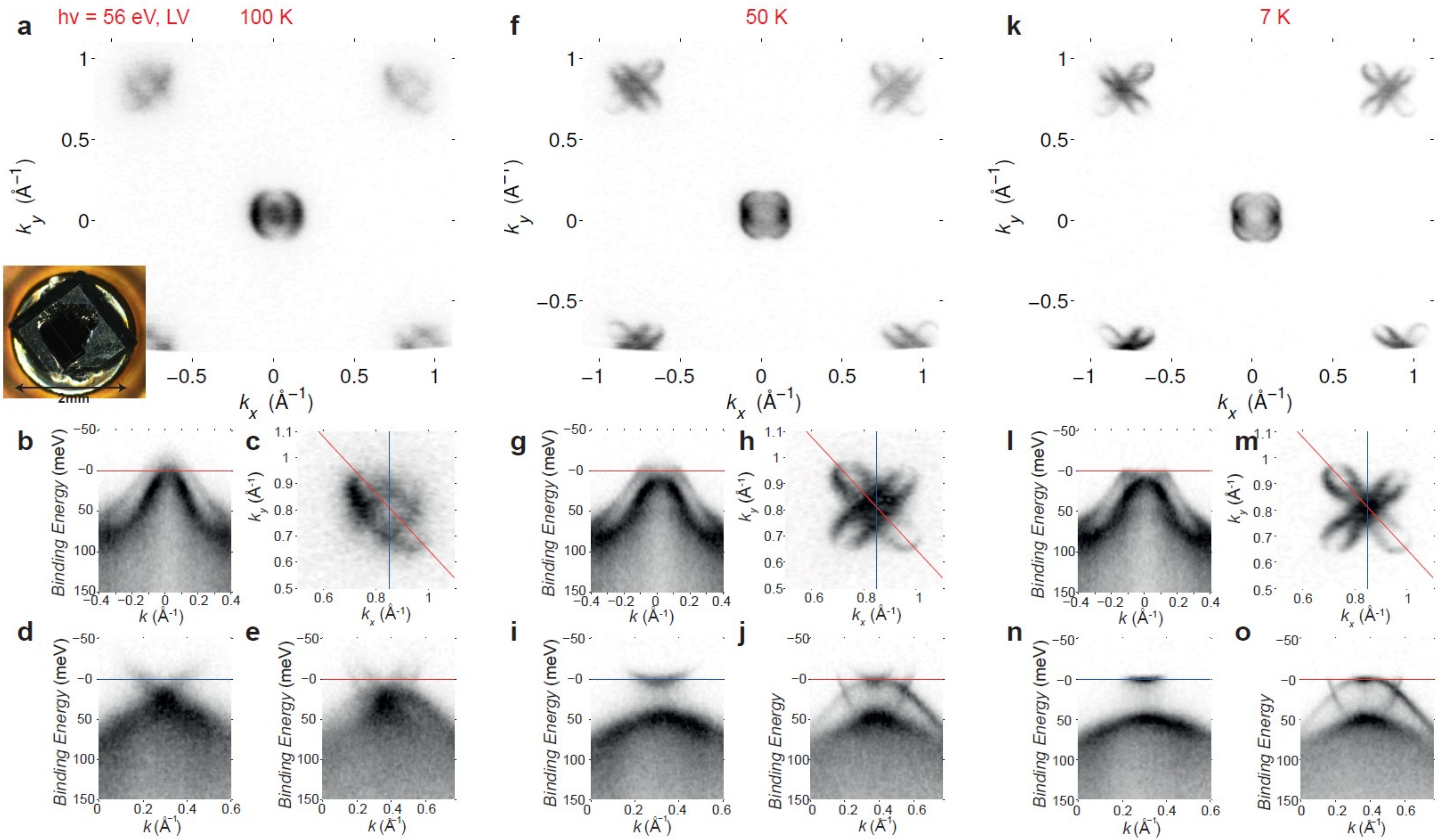






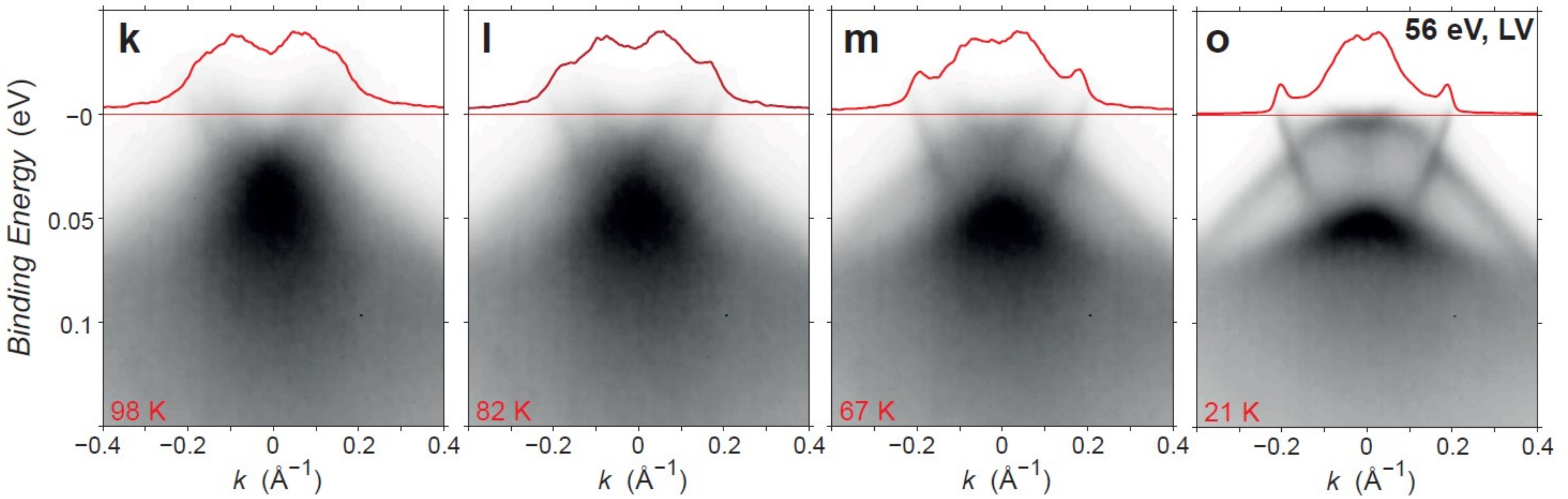
graphic: Yi et al. arXiv 1703.08622 (2017)

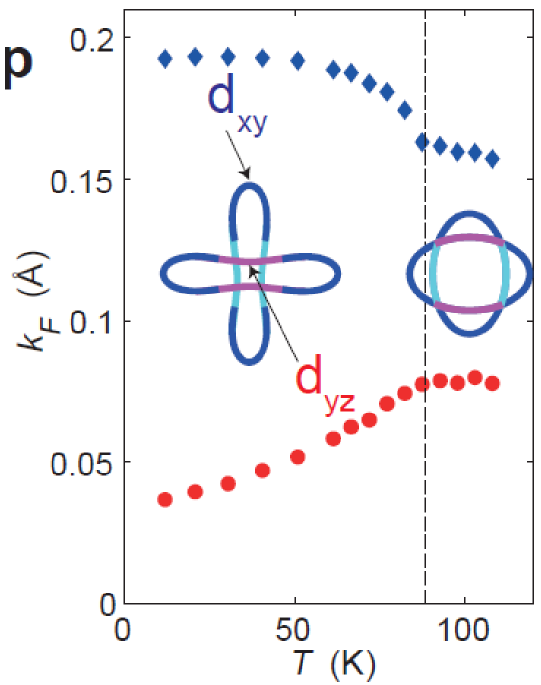
The whole Fermi surface is observed at T > T_s



M. D. Watson et al. Phys. Rev. B 94, 201107(R) (2016)

Interpreting ARPES at M: k_F

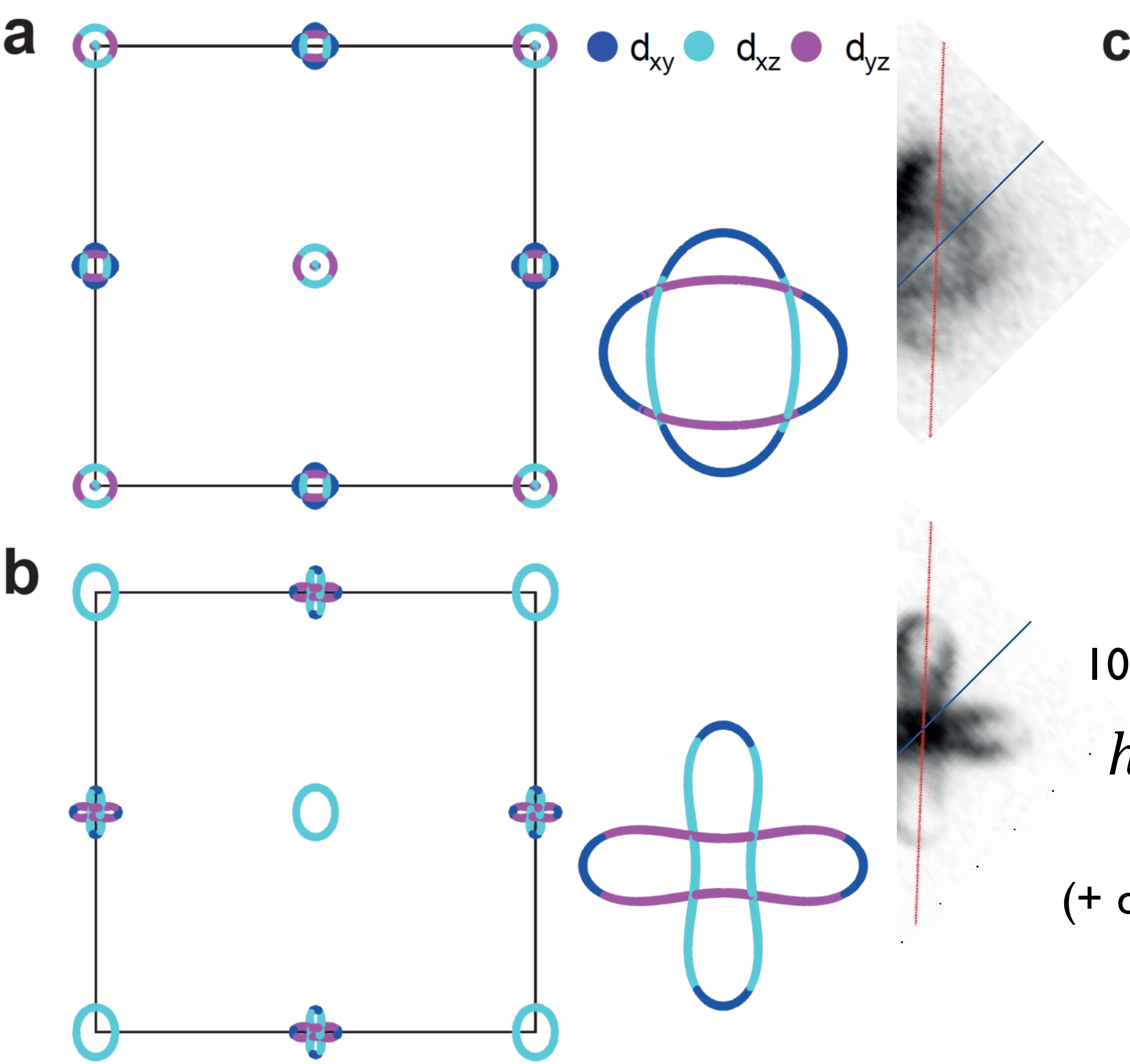


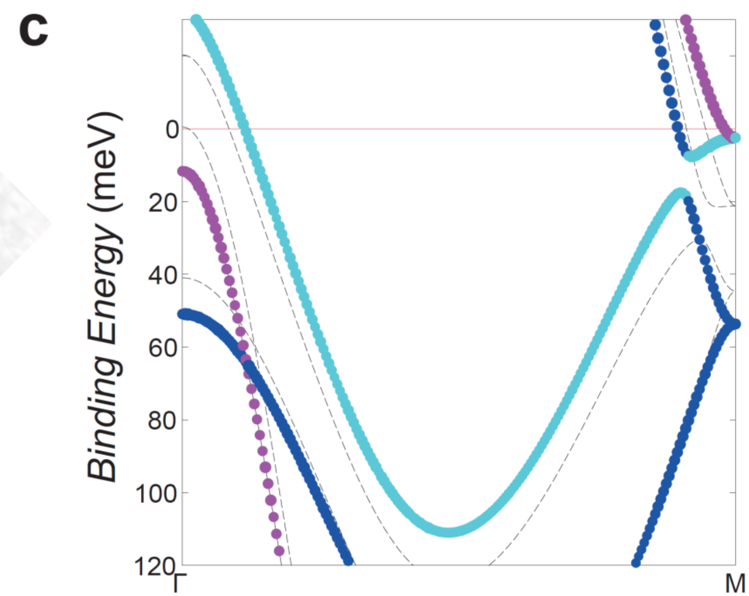


- 56 eV data: Outer electron pocket clearly visible even without curvature analysis above Ts.
- MDC analysis: k_F values separate below 90 K but distinct above T_s.

Proposed solution : nematic bond ordering

Elliptical distortions of the hole pocket + symmetric shifts at M = strong constraints for possible order parameters, but "unidirectional bond ordering" is compatible.





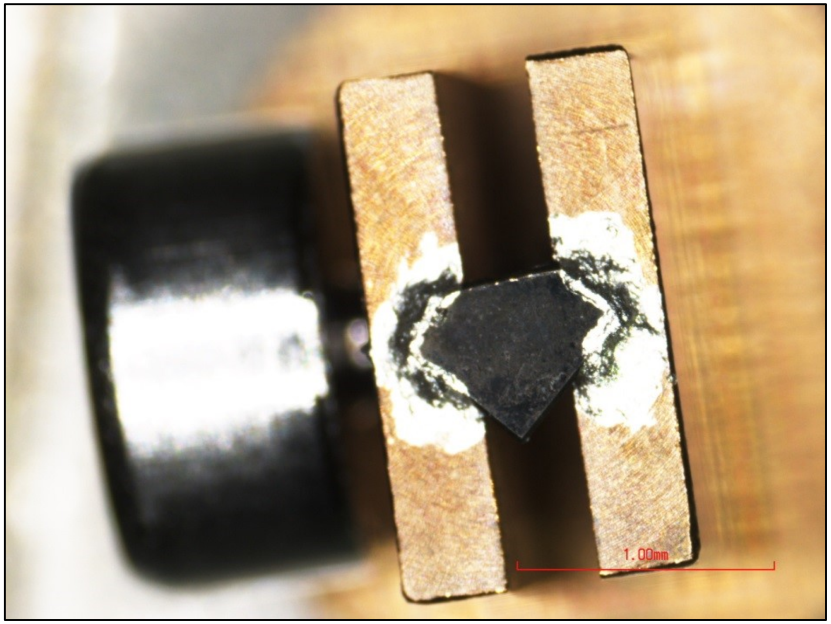
10 – orbital model + SO coupling.

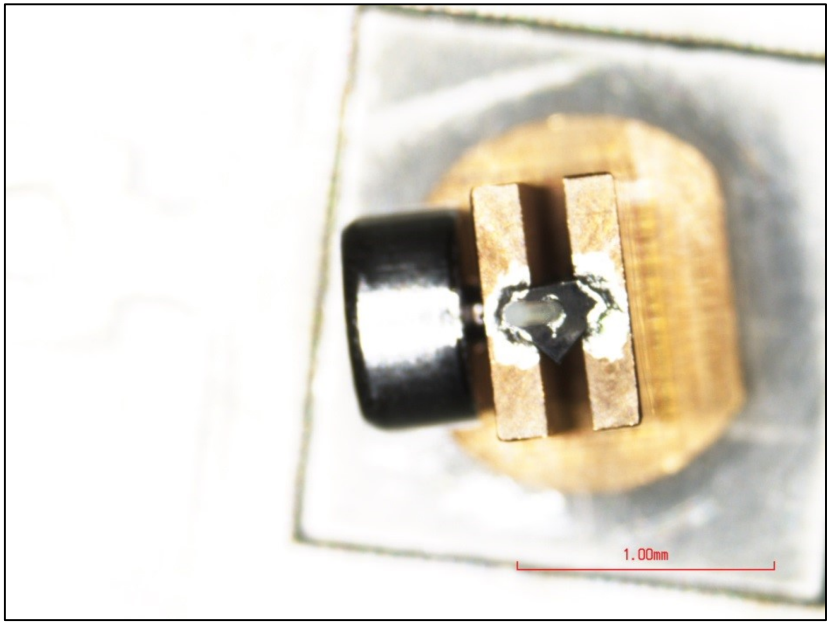
$$h = \Delta(n'_{xz} - n'_{yz}) \cos k_x$$

$$\Delta = 20\ meV$$

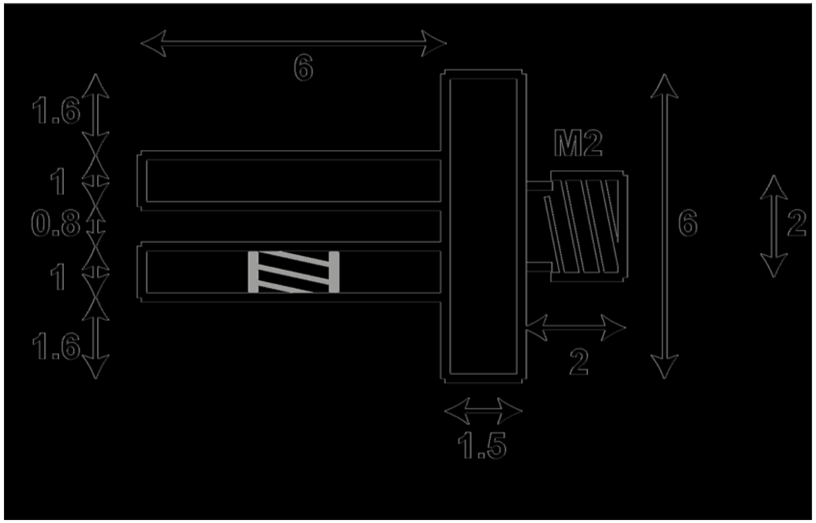
(+ dxy adjustment for compensation)

Detwinning device for I05-ARPES

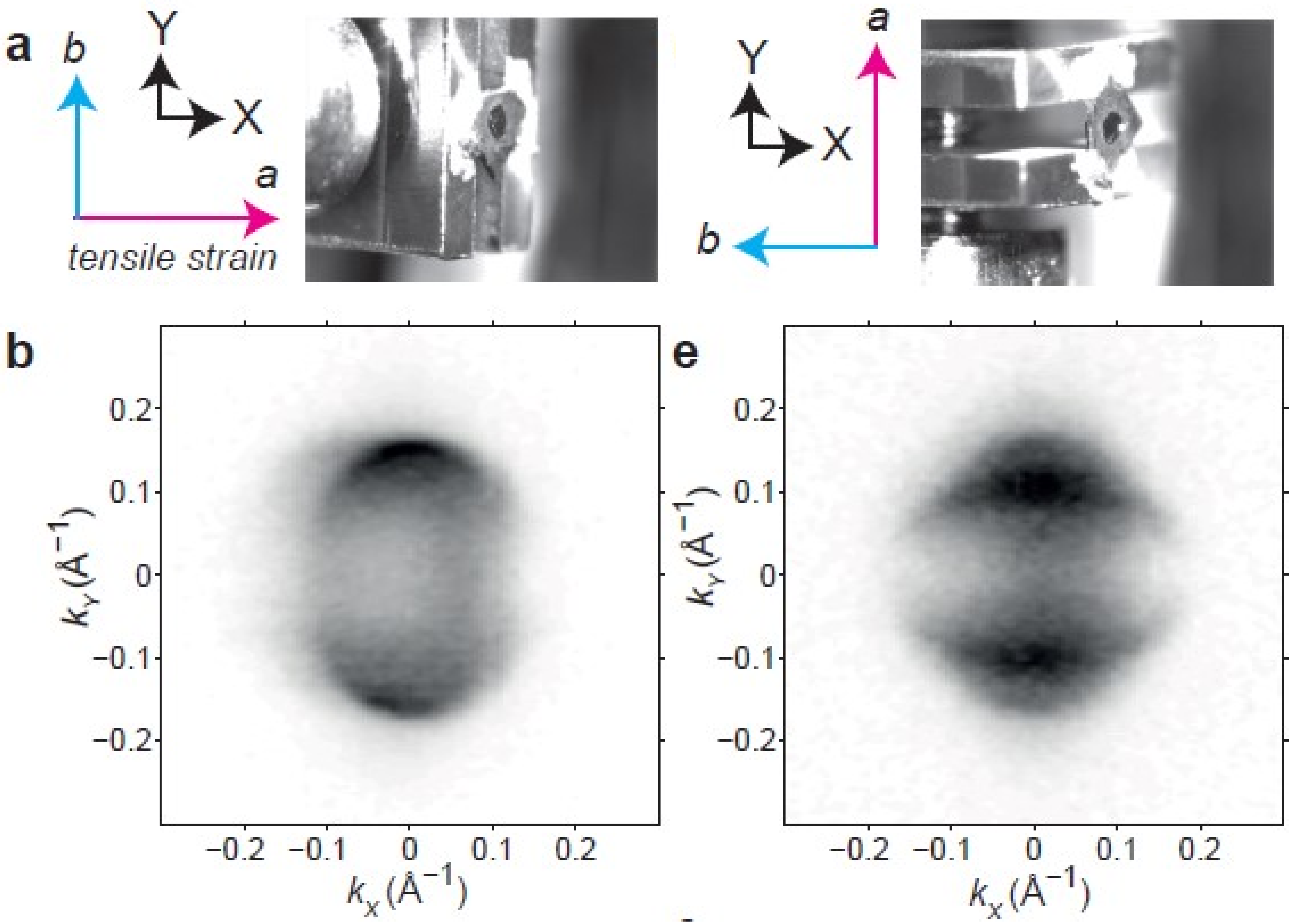




- Simple design to measure samples under tensile strain
- Degree of strain can be adjusted *in-situ*

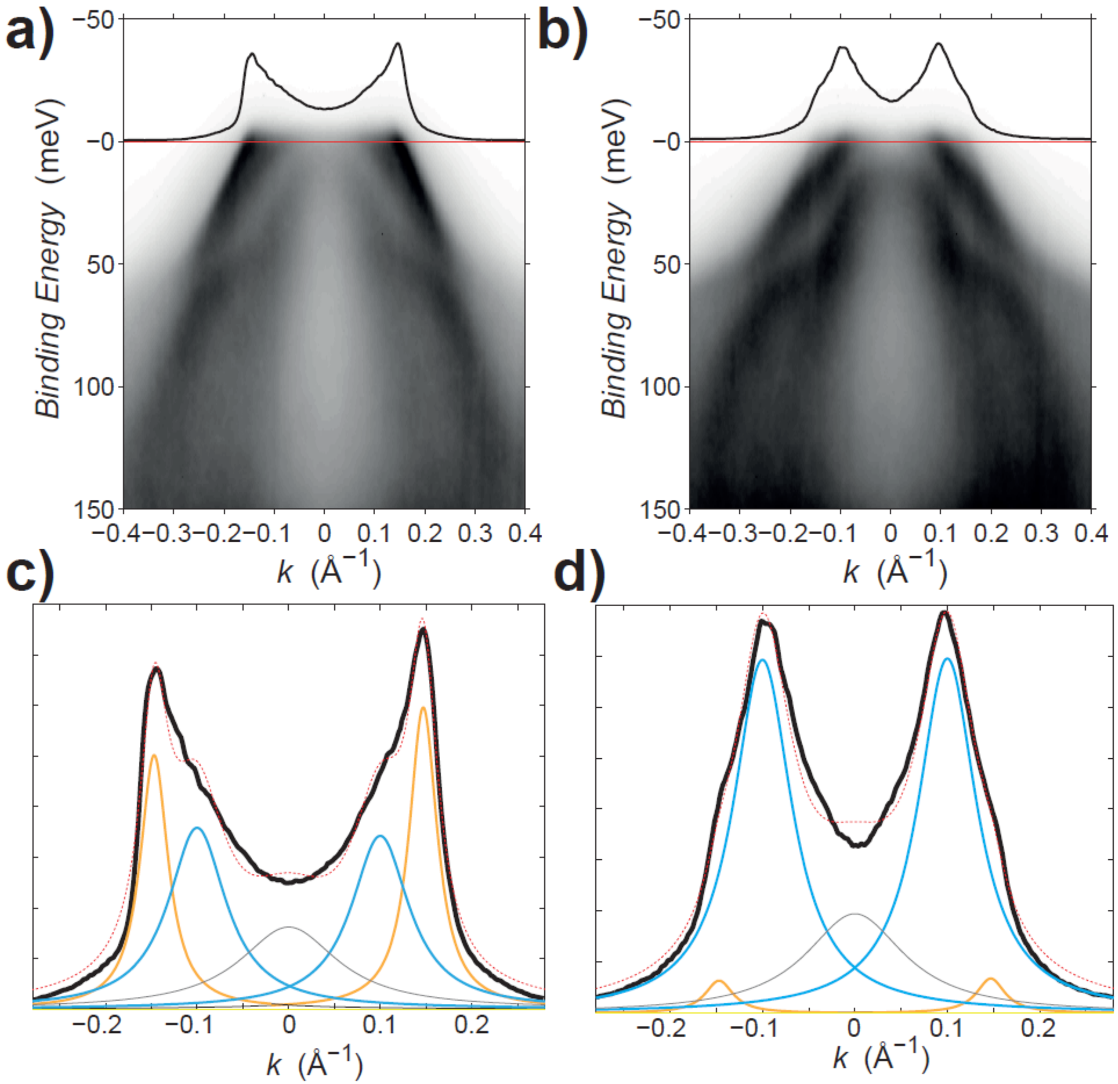


Detwinning: the hole pockets

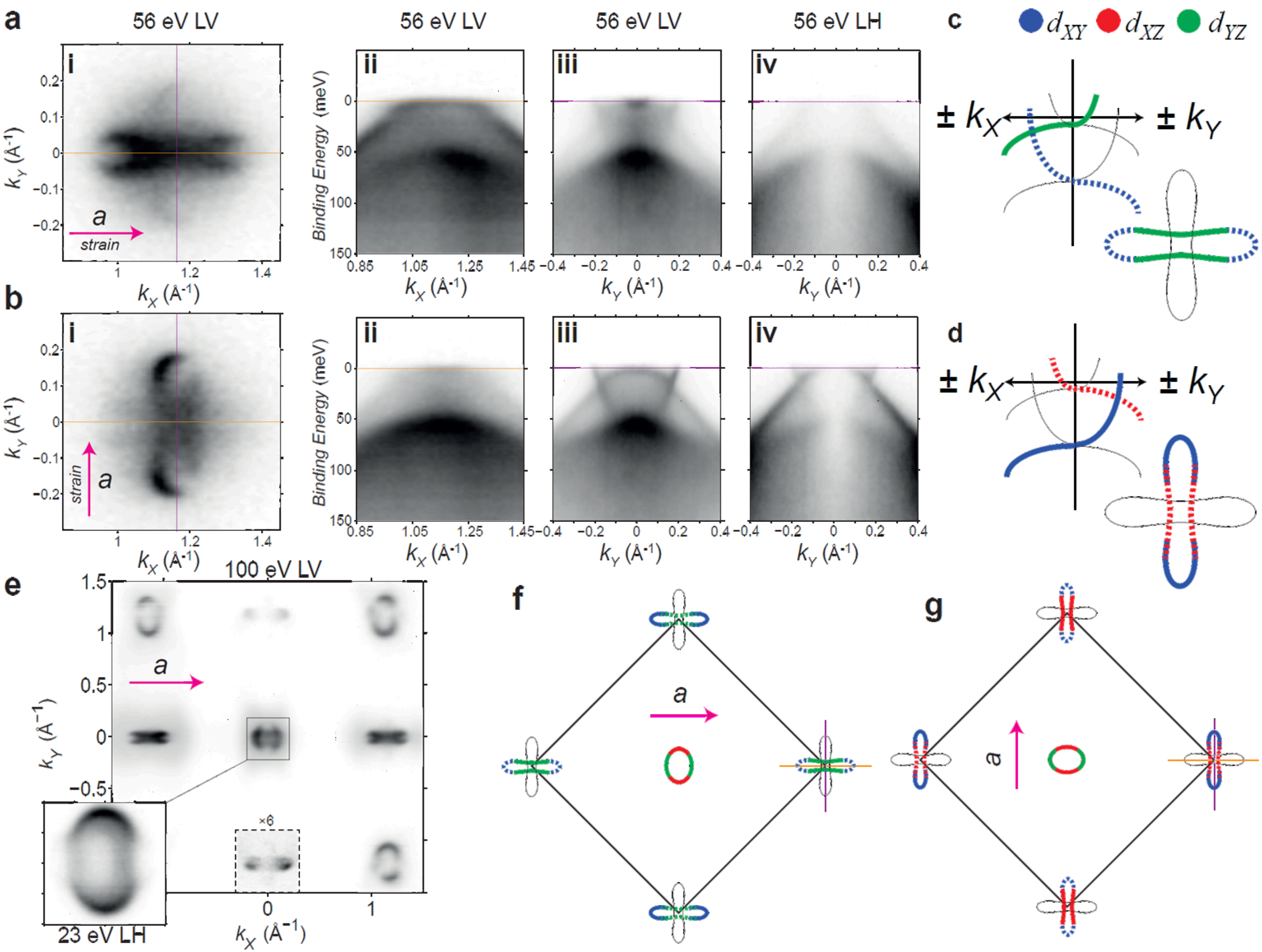


Calibrating the degree of detwinning

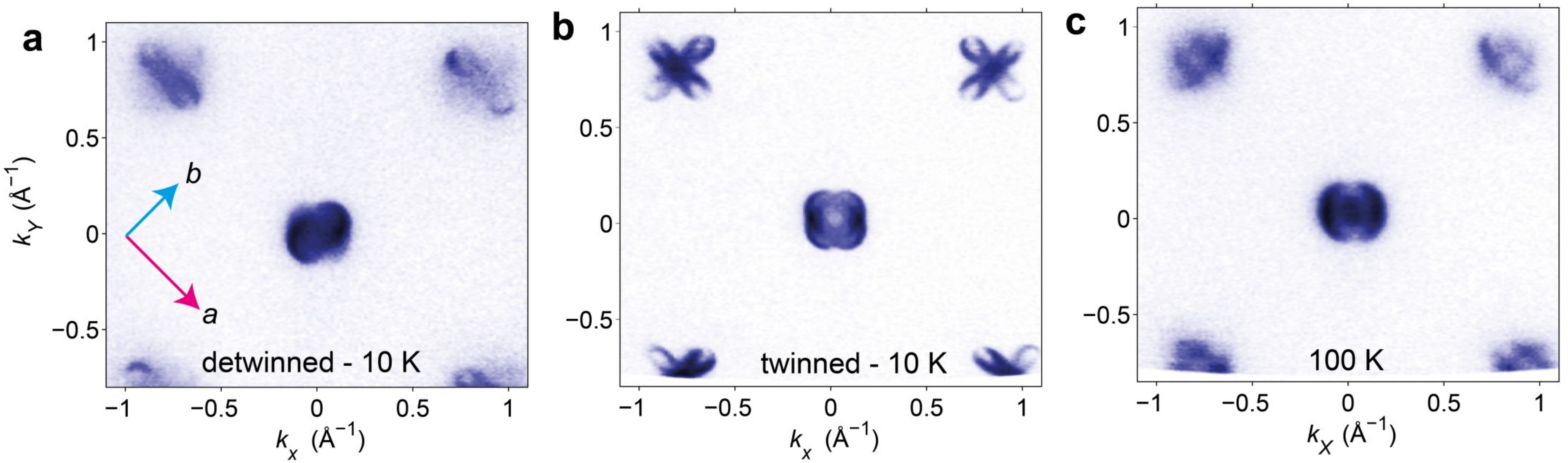
Estimated 80%-20% domain volume fractions

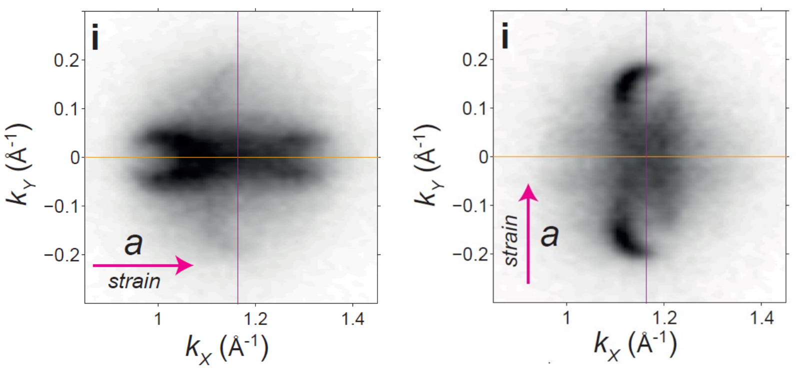


Detwinned FeSe: one "peanut" seen at the M point



Detwinned FeSe: whole Fermi surface

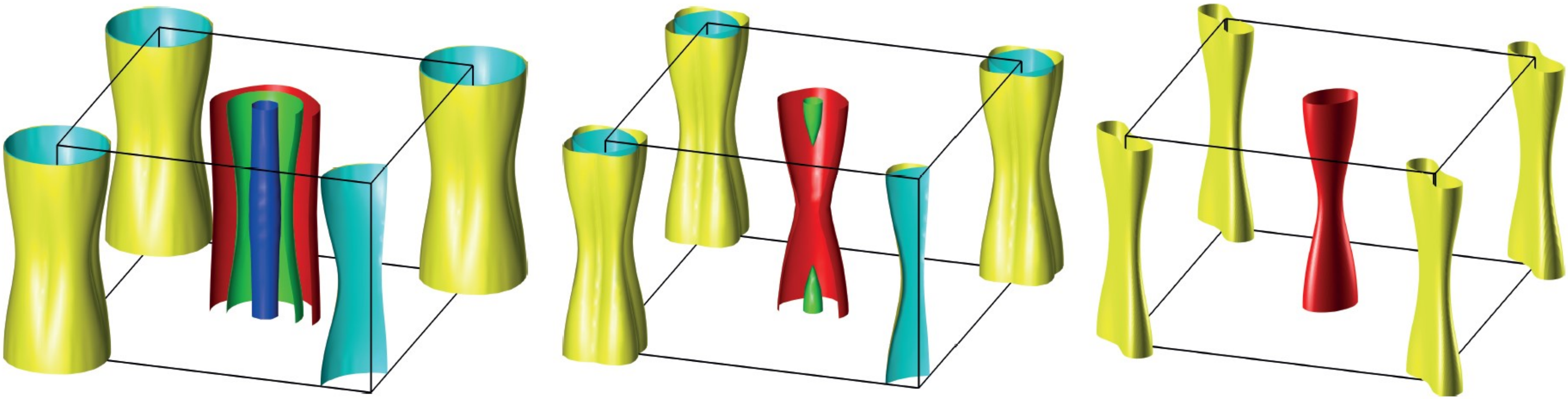




The one-peanut effect:

- **For the electron pockets, only the pocket which points along the longer orthorhombic axis *a* is observed.**

ARPES: schematic Fermi surfaces of FeSe – 3D

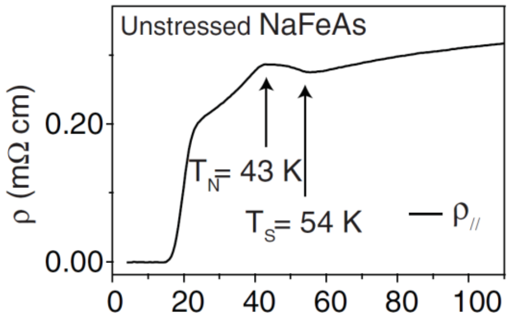


DFT calculation

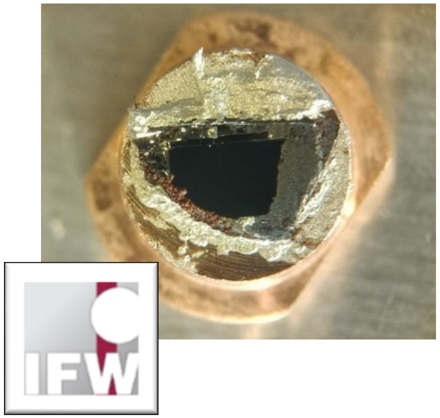
Tetragonal phase: smaller pockets and band renormalisations.

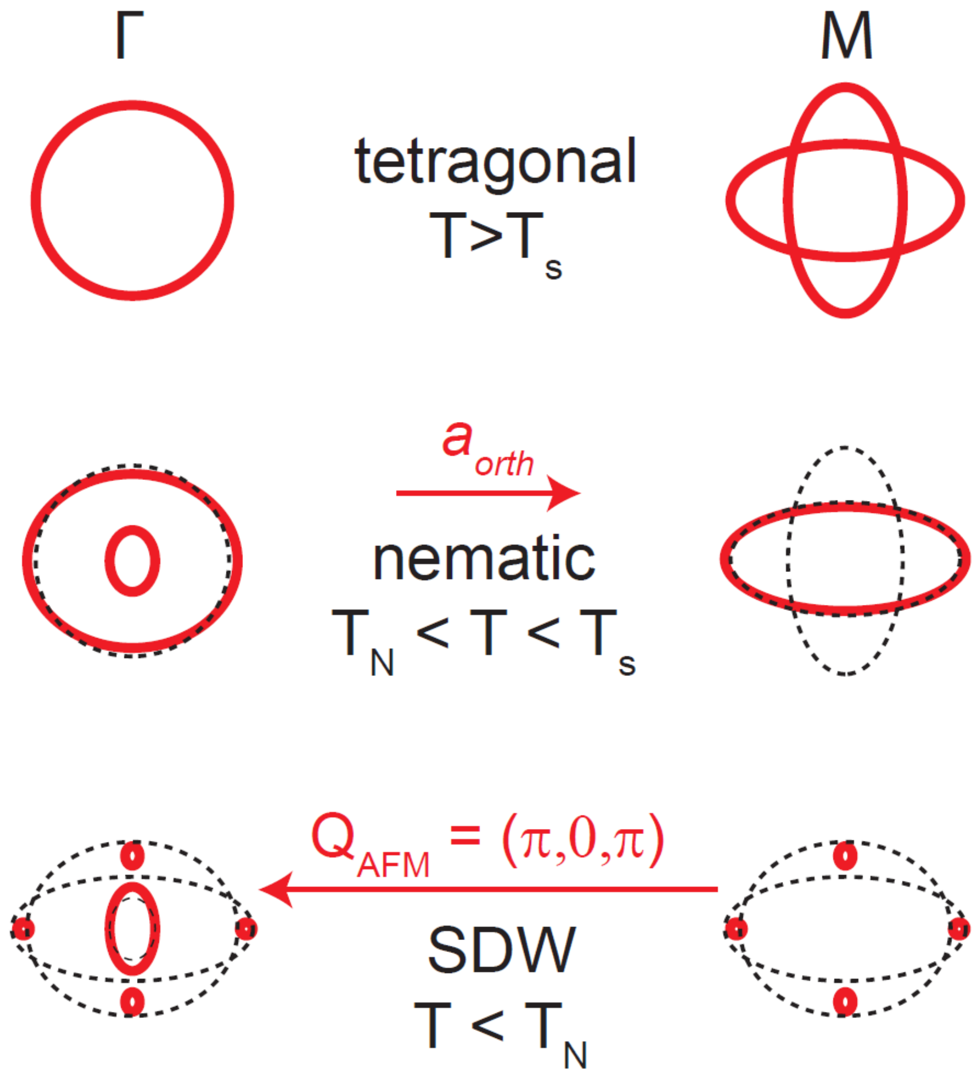
Nematic phase: the hole pocket distorts, one elongated electron pocket seen by ARPES.

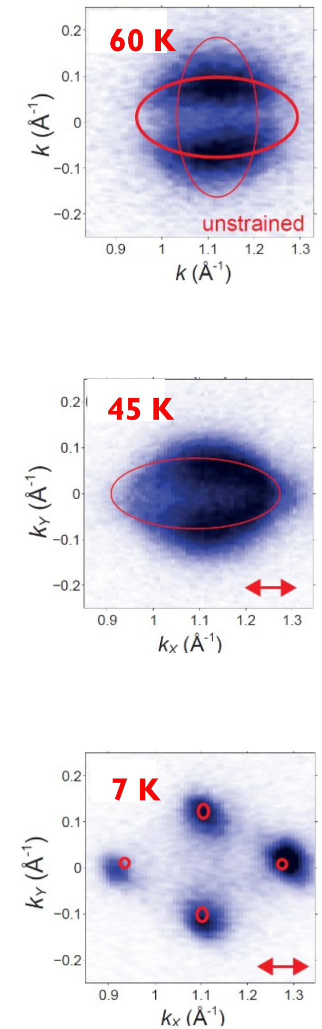
One-ellipse effect preceding SDW in NaFeAs



Zhang *et al.* PRB **85** 085121 (2012)





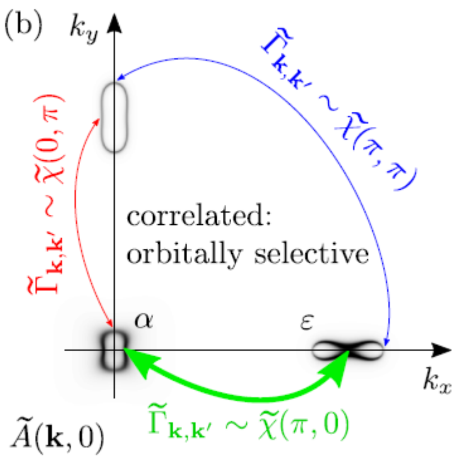


Watson et al. Phys. Rev. B **97**, 035134 (2018)

Interpretation of the one-peanut effect

- **ARPES-specific selection rule?**
  - But the whole FS observed above Ts?

- **Orbital-selective coherence? (Kreisel, Andersen, Hirschfeld, Davis)**



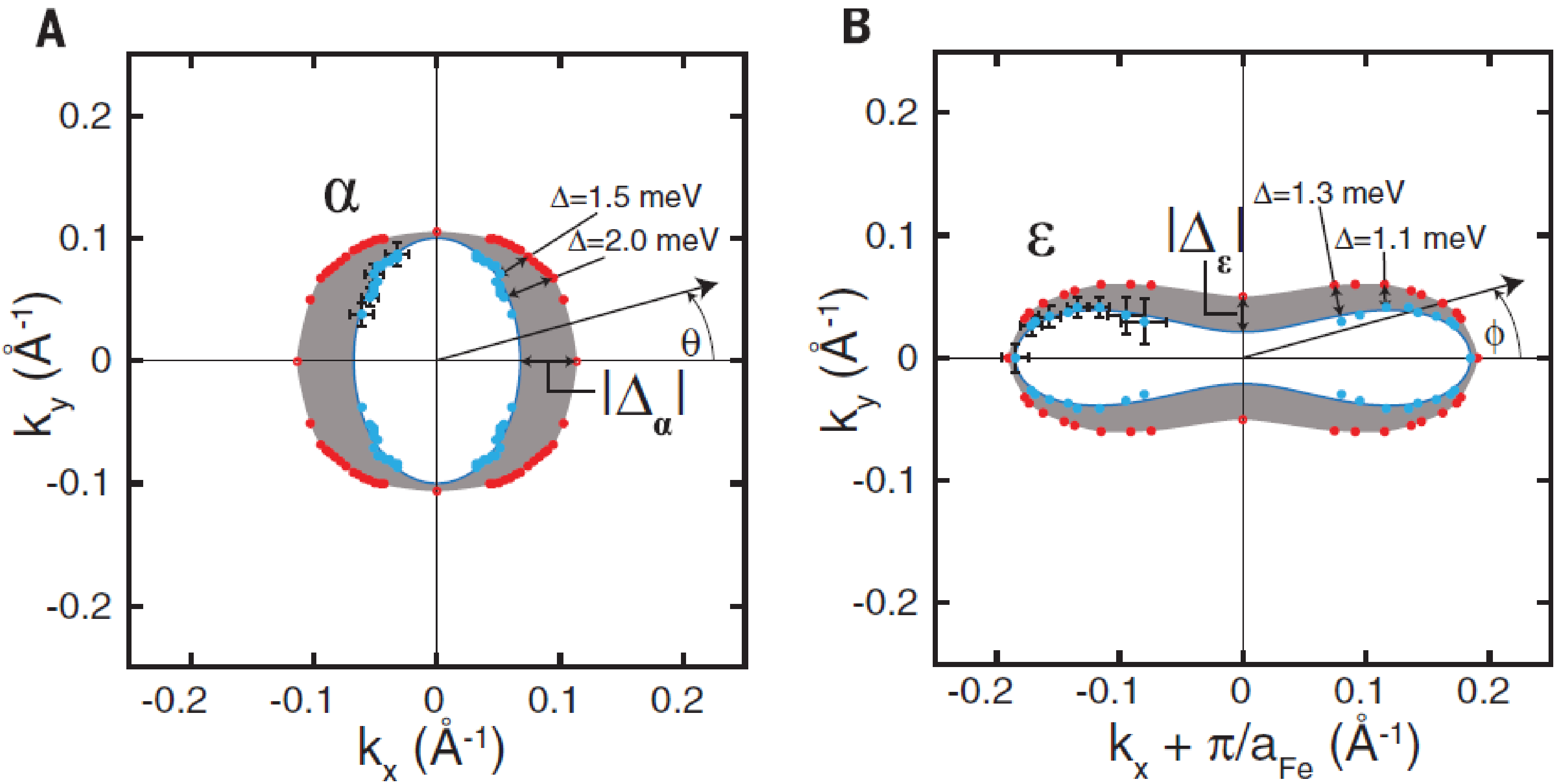
Kreisel et al. PRB (2017)

Sprau et al.
Science 357 75 (2017)

- **More precise:**
  - Our detwinned ARPES suggests that there is a pocket / momentum-selective loss of spectral weight on the electron pocket expected to exist along the b axis.

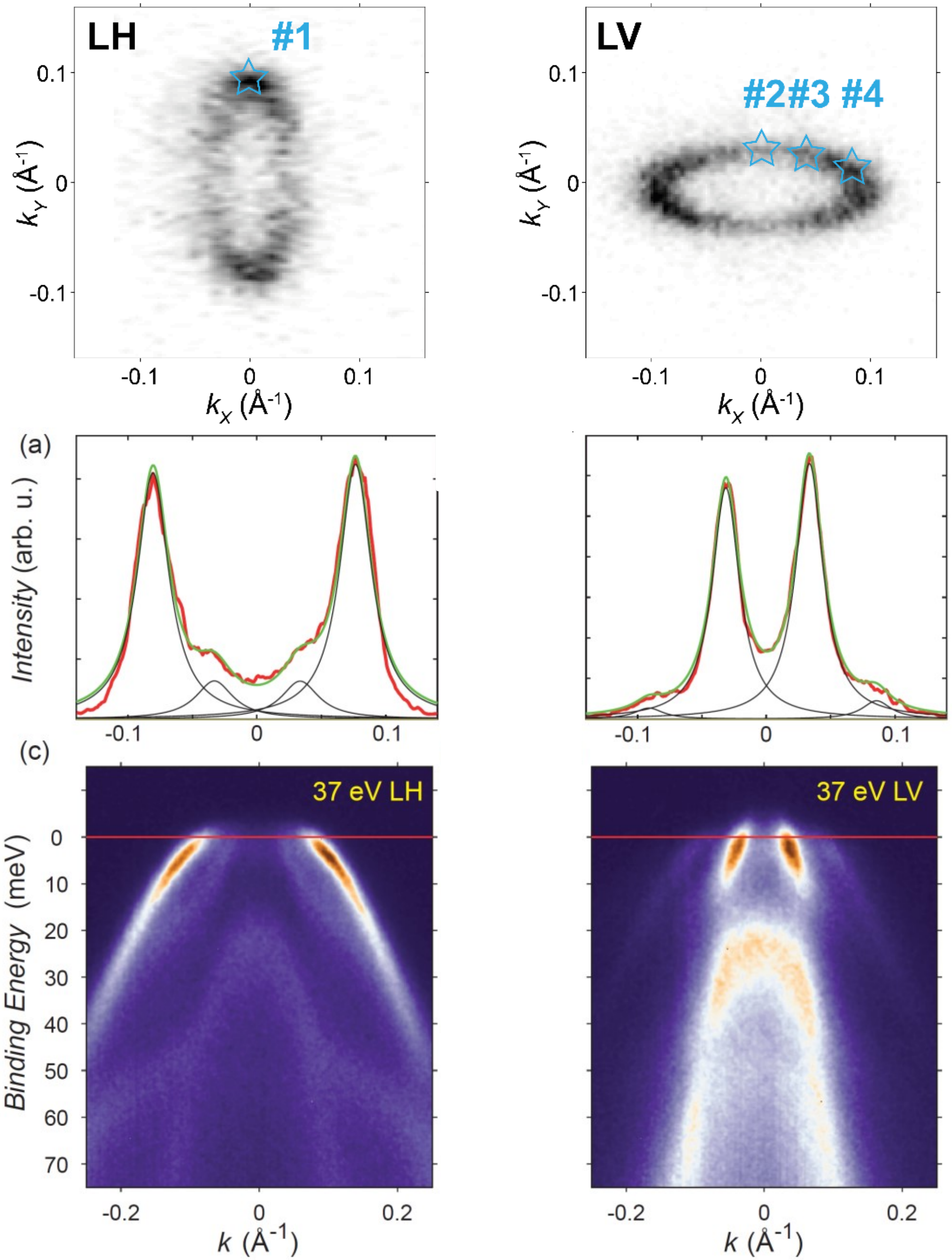
- **How does the one-peanut effect influence the SC pairing?**

The superconducting gap in FeSe



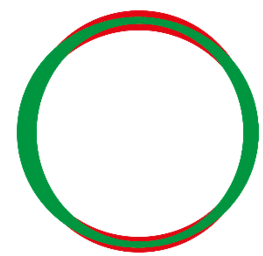
Sprau et al., Science 357 75 (2017)

Estimating orbital weights from polarisation analysis

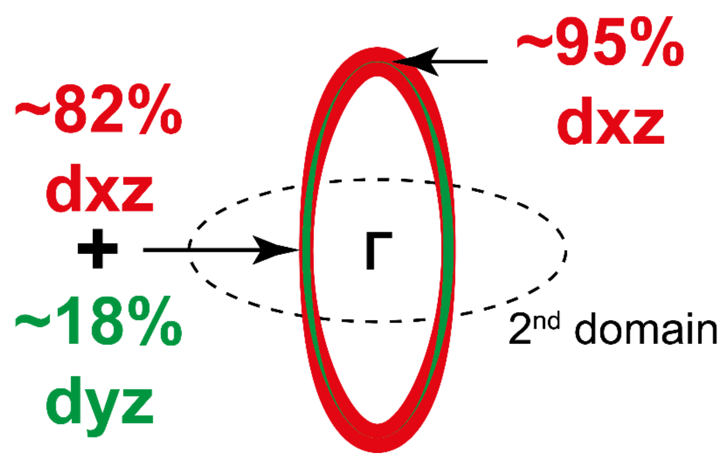


tetragonal phase

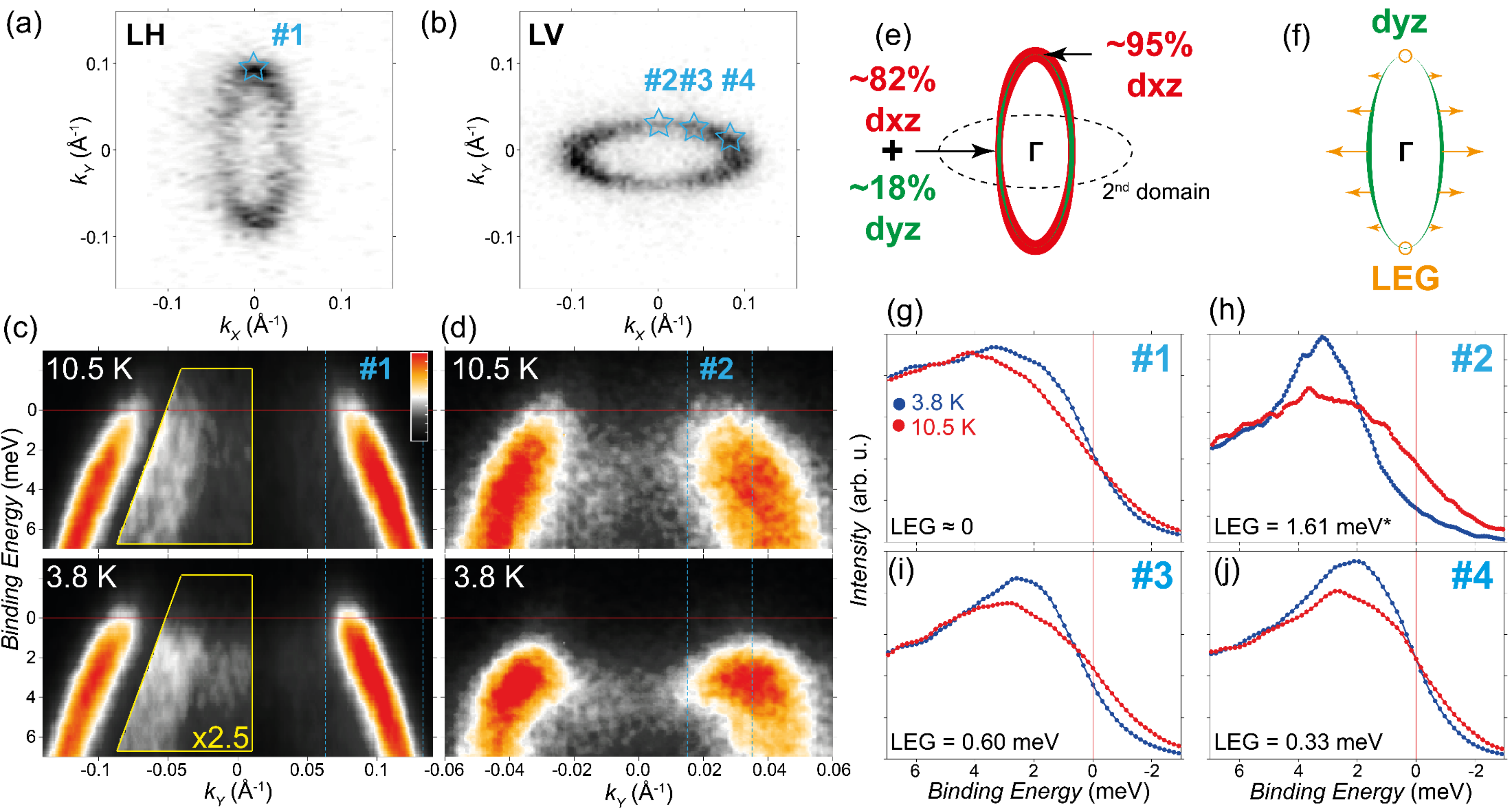
orbital characters are symmetric



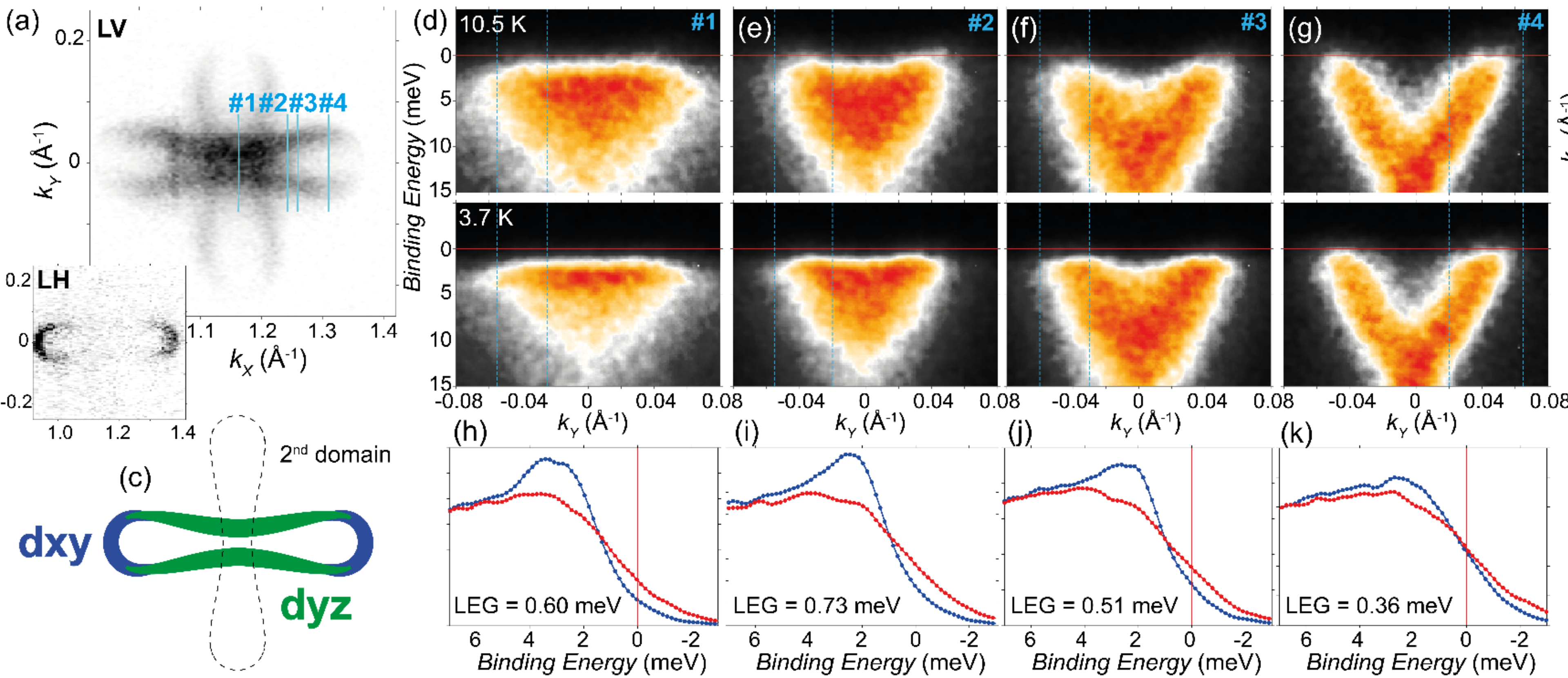
nematic phase



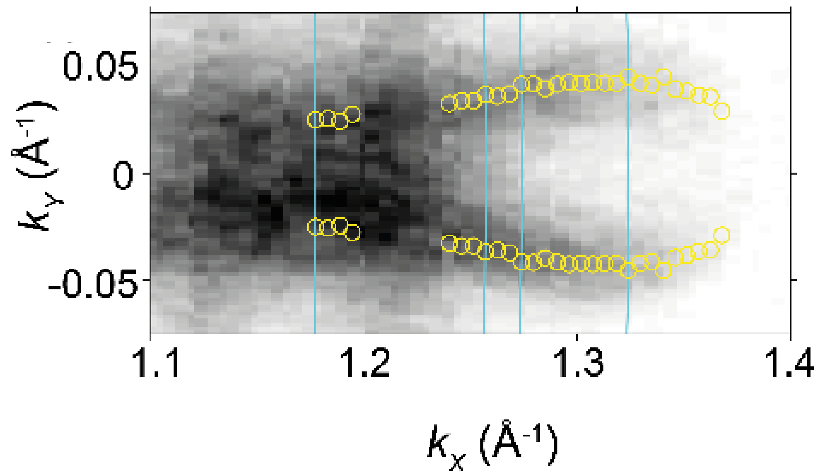
Hole pockets: gap follows minority dyz weight

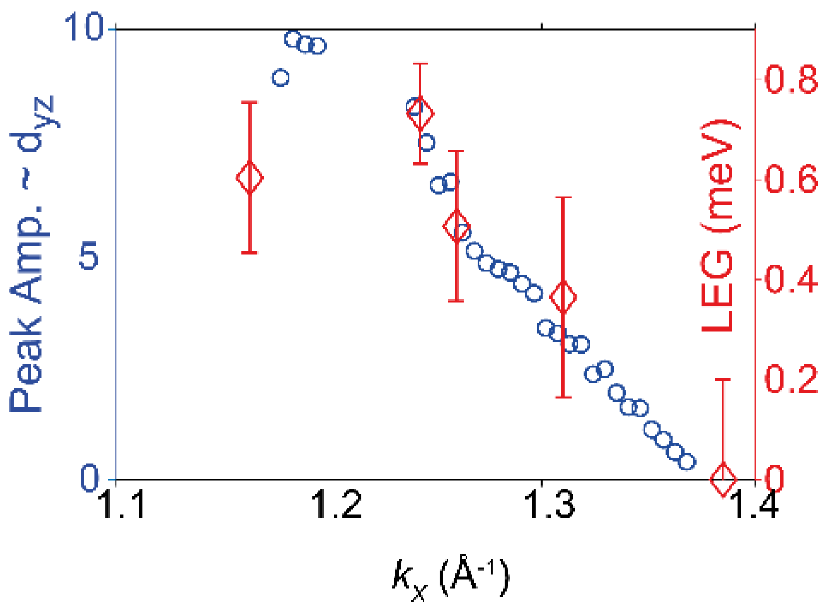


Electron pockets: gap follows dominant dyz weight



Scaling of leading edge shift with dyz orbital weight



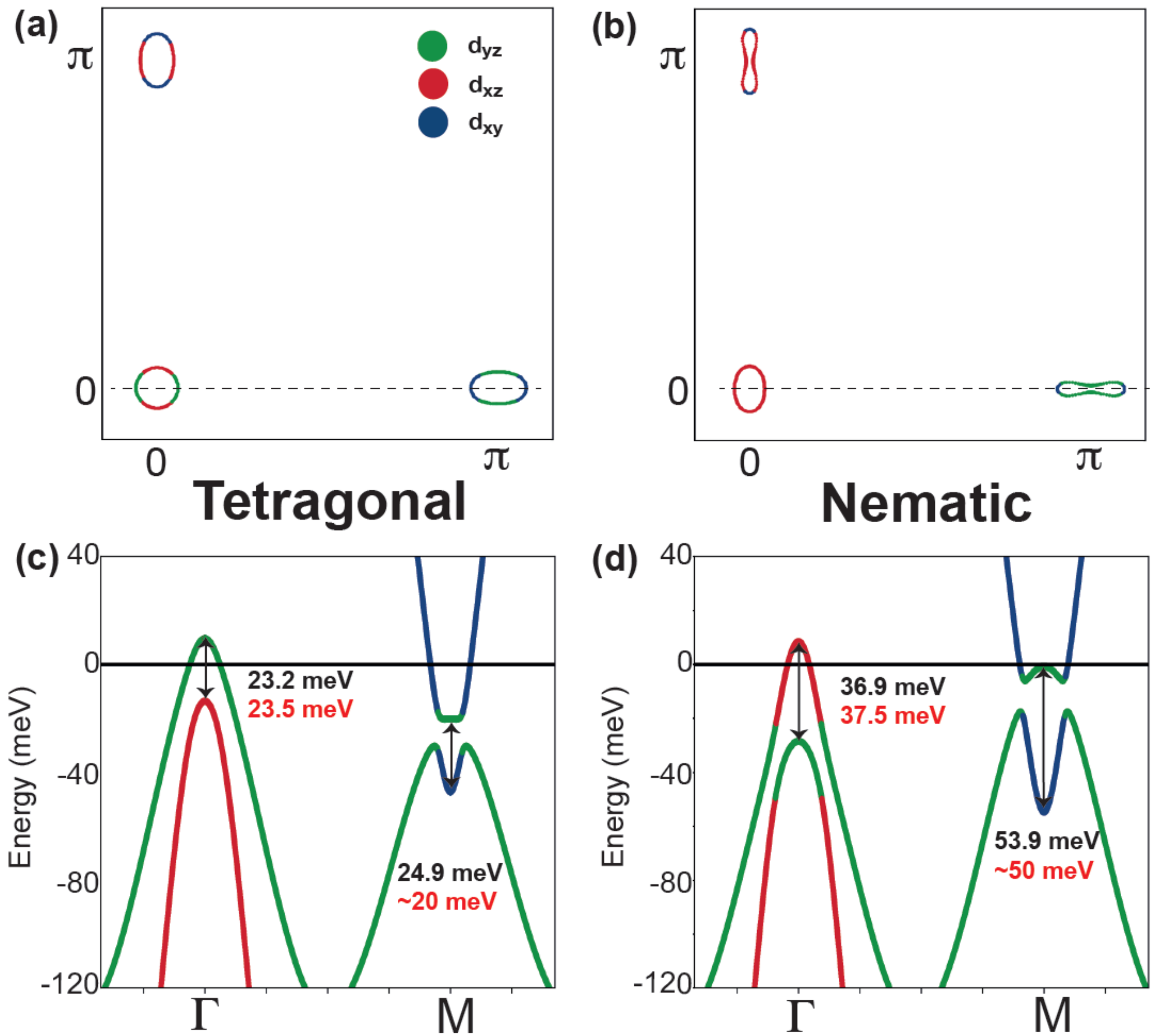


- Experimental evidence that the pairing interactions in FeSe are sensitive to the orbital character of the bands

- A hallmark of spin-fluctuation pairing

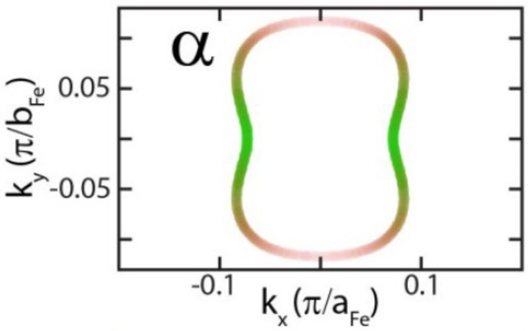
How one-peanut effect leads to the gap structure

1. Construct a highly accurate tight-binding model including nematic order and SOC

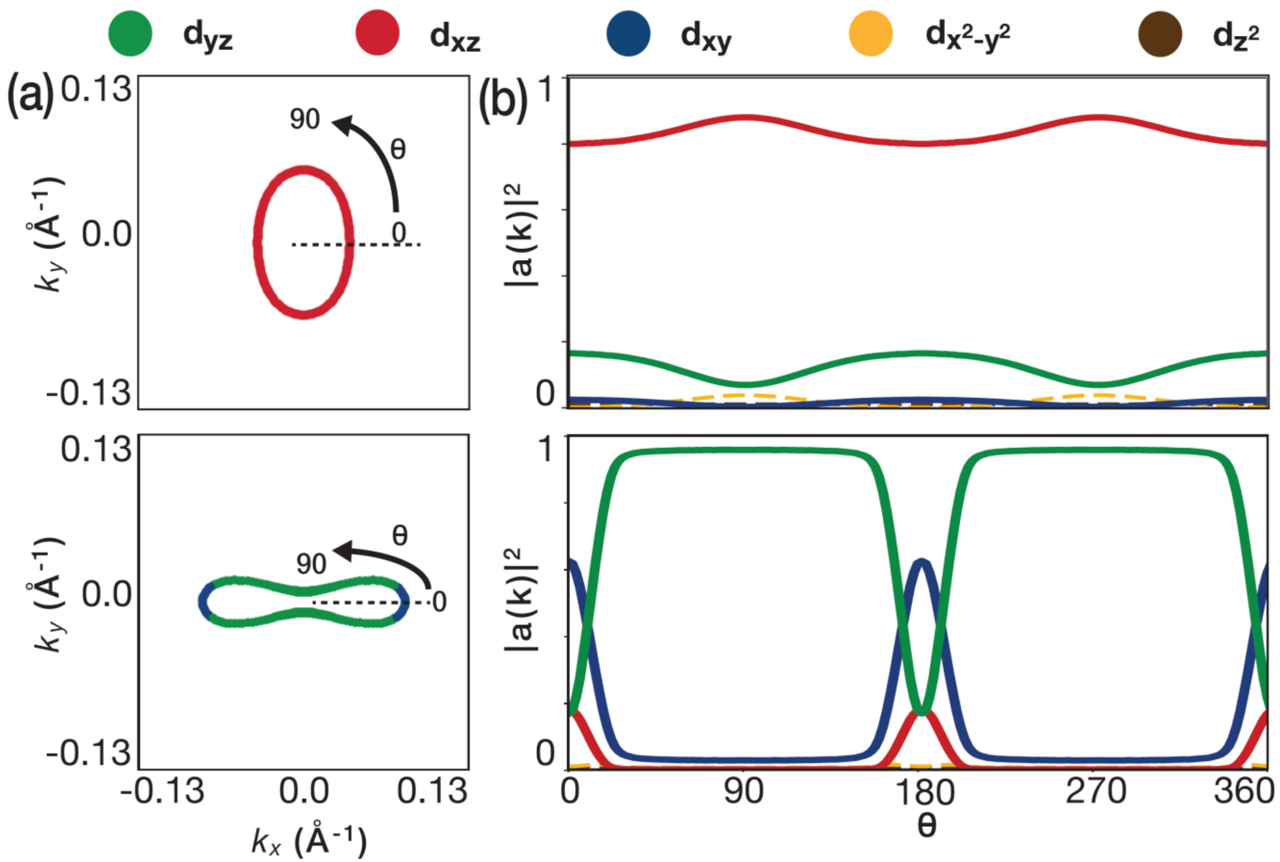


How one-peanut effect leads to the gap structure

2. Not only the bands, but also the orbital characters should match experiments

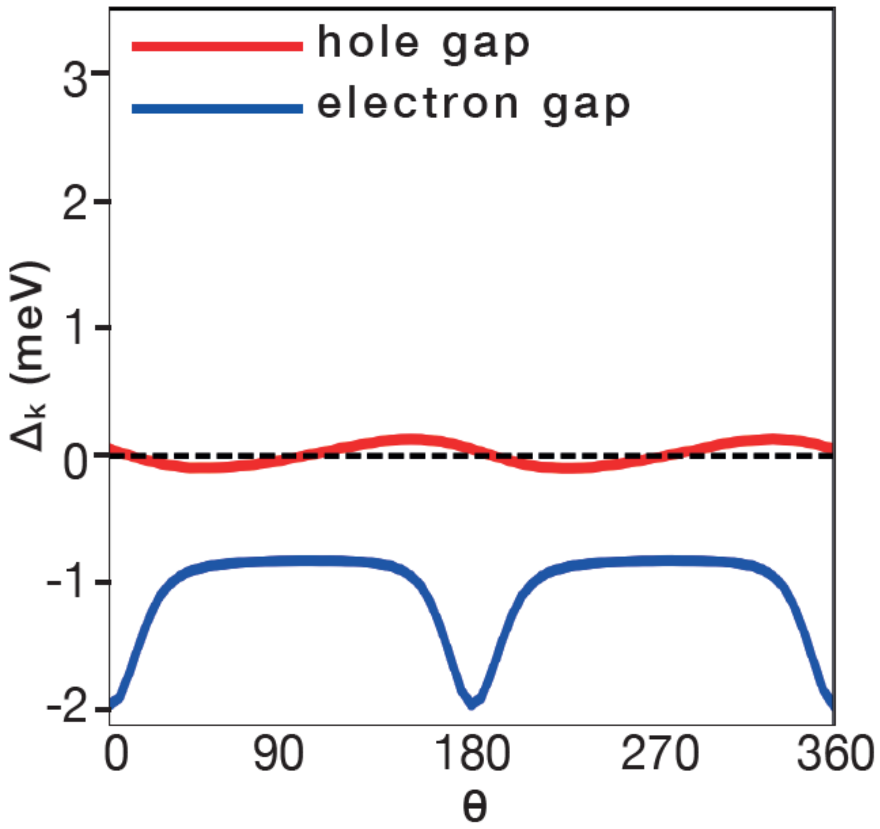


Kostin 2018



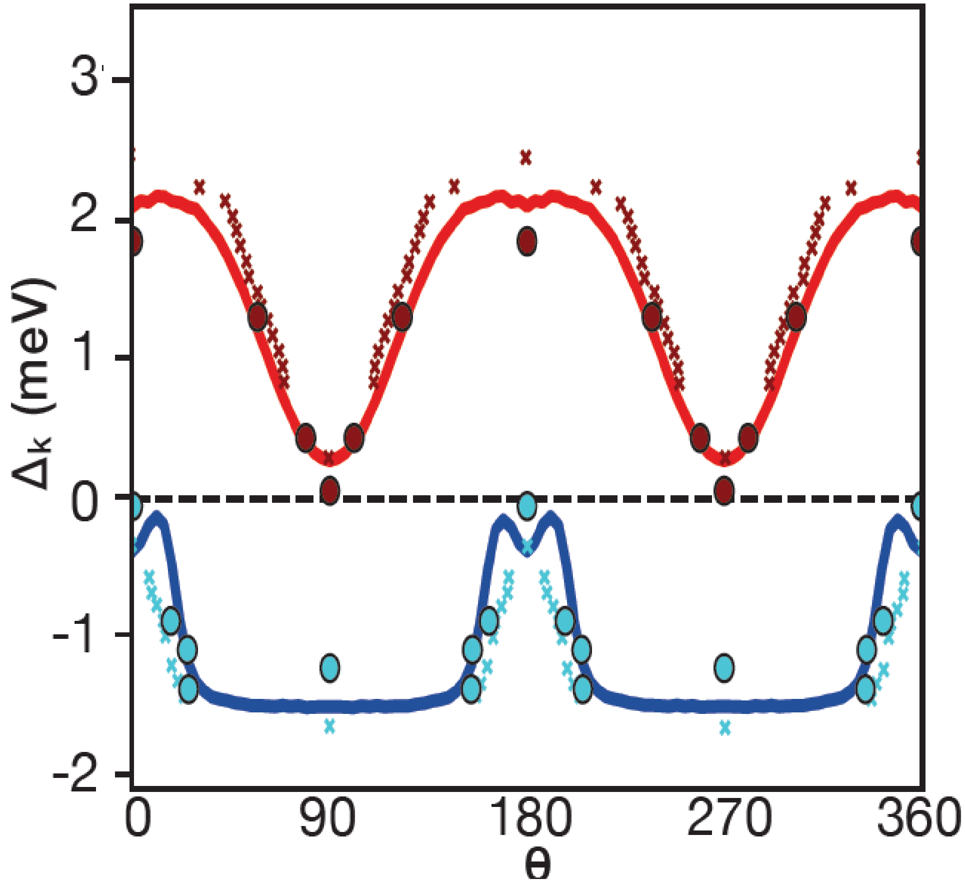
How one-peanut effect leads to the gap structure

3. Solve the linearized gap equation including both electron pockets – no agreement



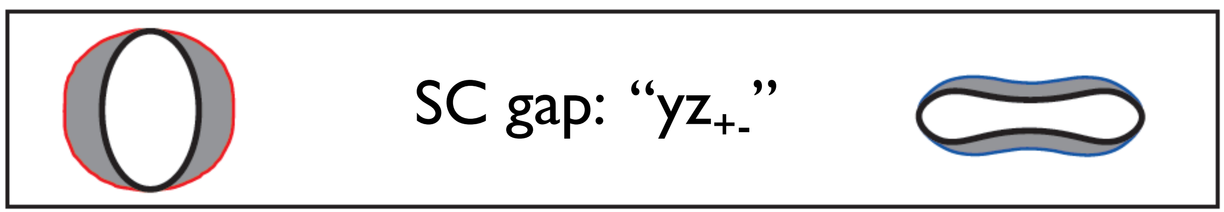
How one-peanut effect leads to the gap structure

4. Solve the linearized gap equation **including only one peanut** – excellent agreement!



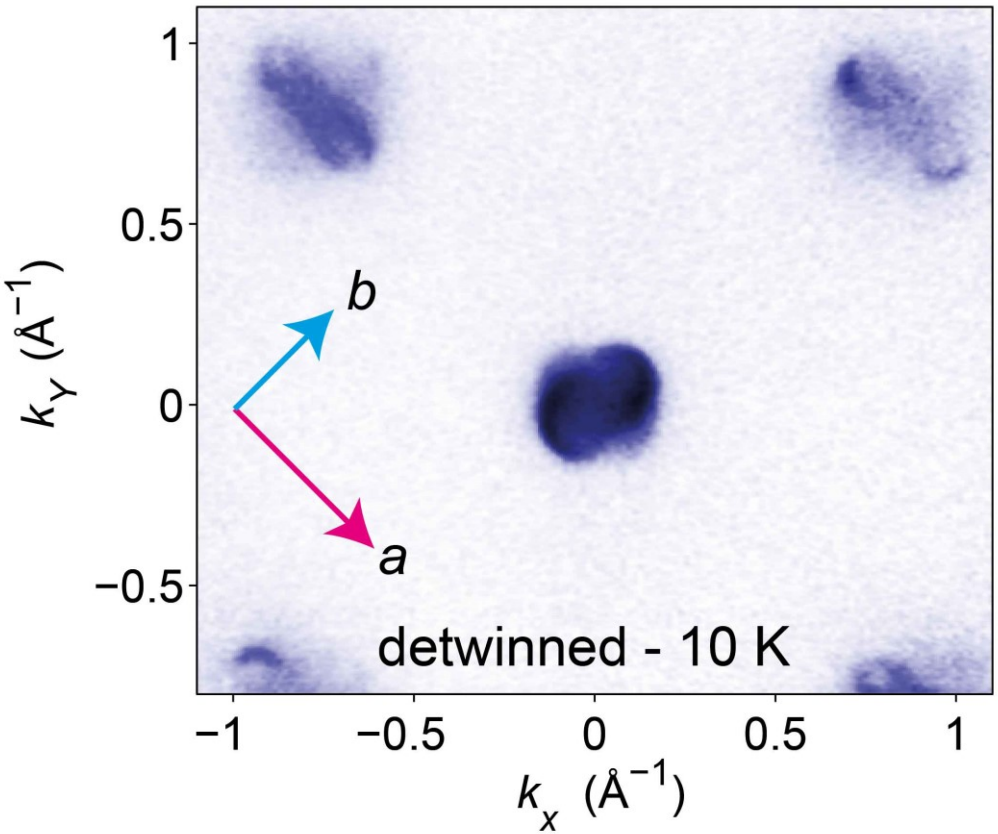
The intuitive picture

Given the one-peanut structure, for dominant interband pairing, the gap follows the dyz orbital character on both pockets as this is the only orbital present (in serious quantity) on both pockets



Conclusions

- In one domain, only the peanut-shaped electron pocket along the *a* axis is observed
- The highly anisotropic superconducting gap structure follows the dyz orbital weight on both pockets – direct evidence for spin-fluctuation pairing?
- By fully accounting for spin-orbit coupling, orbital characters, *and the one-electron pocket effect*, the gap structure can be fully reproduced.



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M. D. Watson *et al.* Phys. Rev. B **94**, 201107(R) (2016)

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