# Orbital selective pairing in iron-based superconductors

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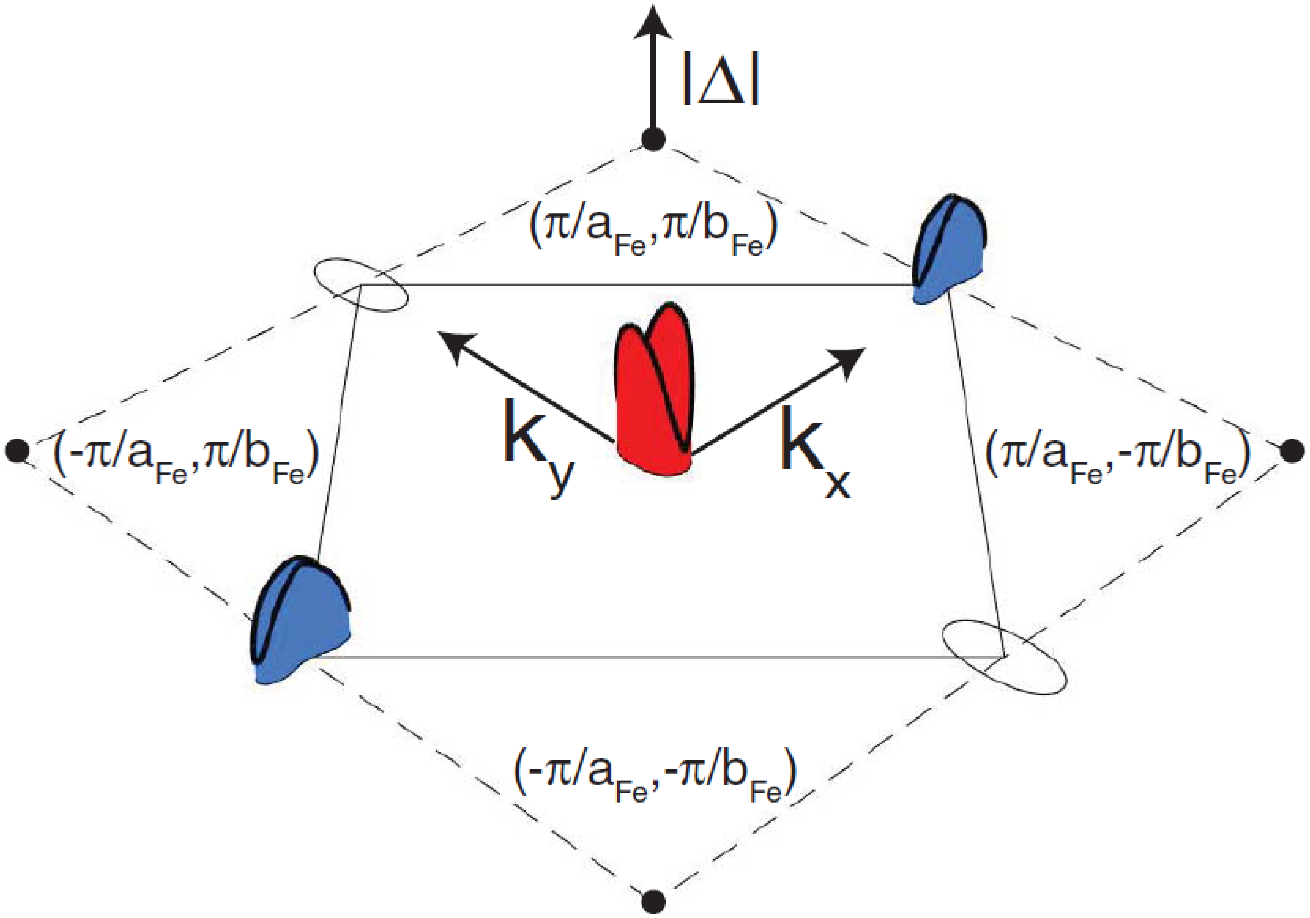
University of Florida



. ``Discovery of orbitally selective nematic Cooper pairing in FeSe", P.O. Sprau, A. Kostin, A. Kreisel, A. B\"ohmer, P.C. Canfield, P.J. Hirschfeld, B.M. Andersen, and J.C. Davis, Science 357, 75 (2017).

``Orbital selective spin-fluctuation pairing and gap structures of iron-based superconductors", A. Kreisel, P. O. Sprau, A. Kostin, J. C. Davis, B. M. Andersen, P. J. Hirschfeld, Phys. Rev. B 95, 174504 (2017).

“Robust determination of the superconducting gap sign structure via quasiparticle interference",
P. J. Hirschfeld, D. Altenfeld, I. Eremin, and I.I. Mazin, Phys. Rev. B92, 184513 (2015)

Beijing, August 2018

# Thanks to:

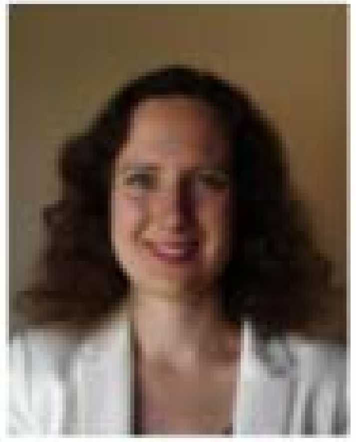
## Main collaborators

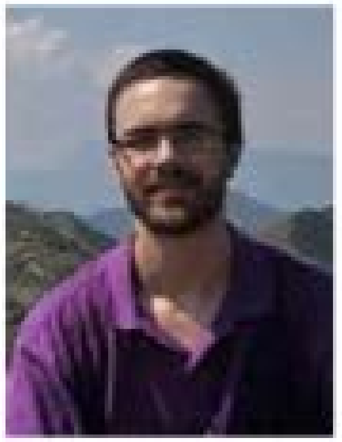
Cornell University Founded A.D. 1865

University of St Andrews

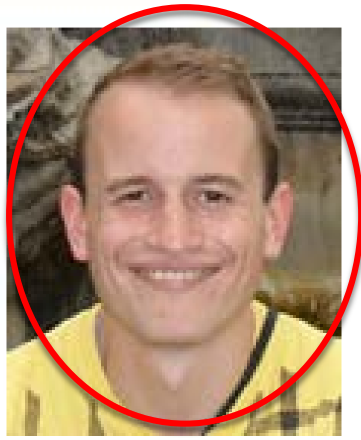

Andrey Kostin


Séamus Davis


Anna E. Böhmer


Valentin Taufour

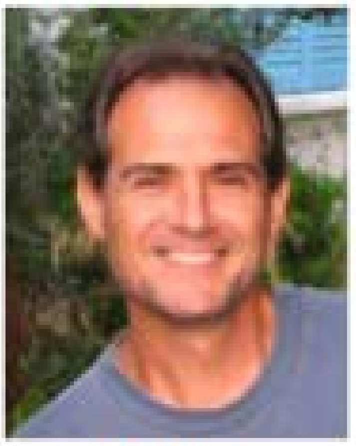

Paul C. Canfield


Peter Sprau


Andreas Kreisel


Shantanu Mukherjee


Brian M. Andersen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U.S. Department of Energy

Brookhaven National Laboratory

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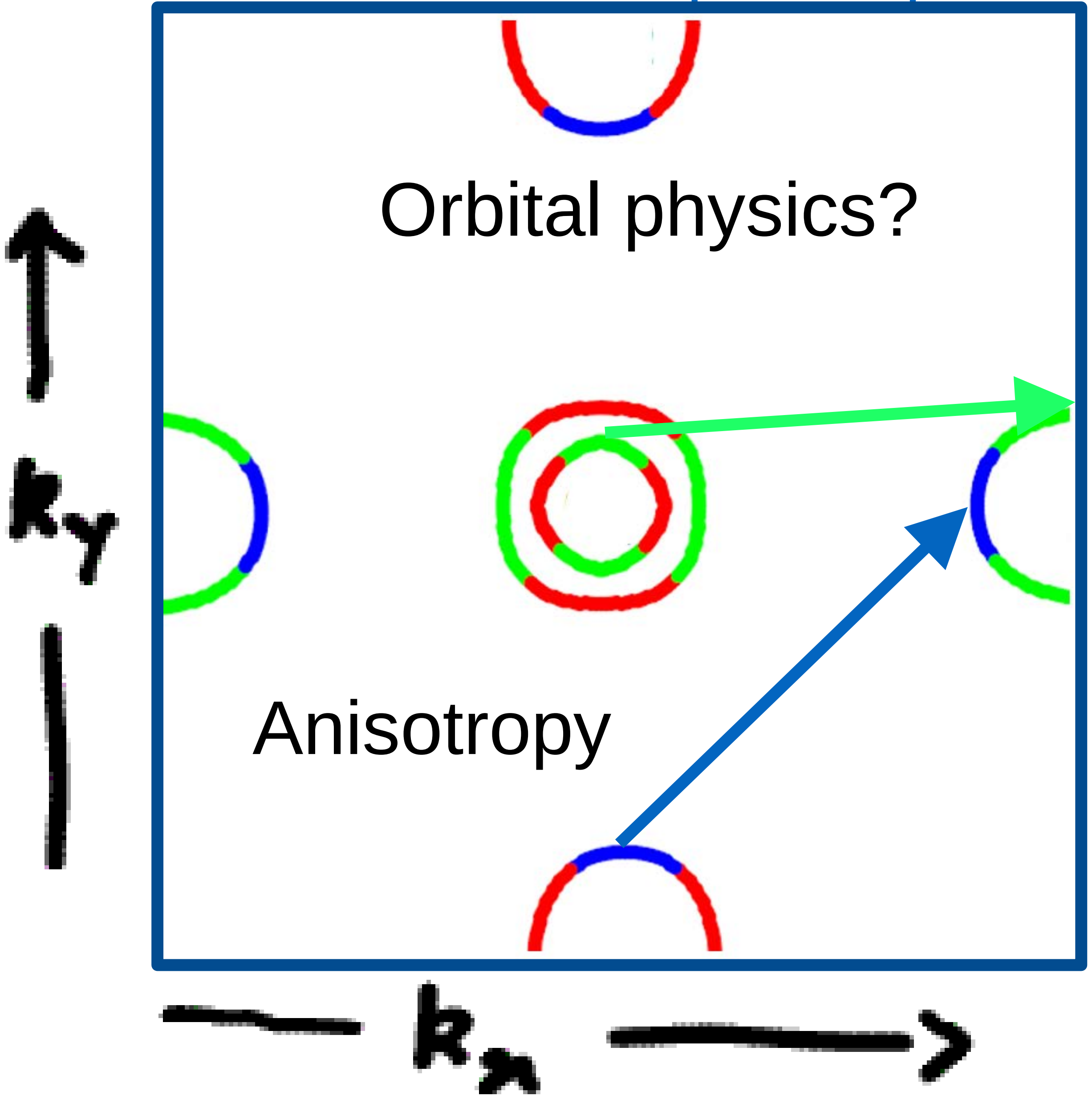
Creating Materials & Energy Solutions
U.S. Department of Energy

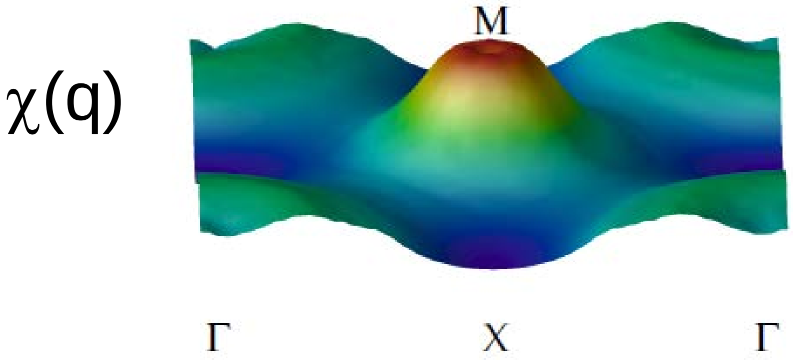
# $s_{+/-}$ pairing in Fe-pnictides Mazin et al PRL 2008

electron-hole pocket pair scattering dominates



Orbital physics?

Anisotropy



also:

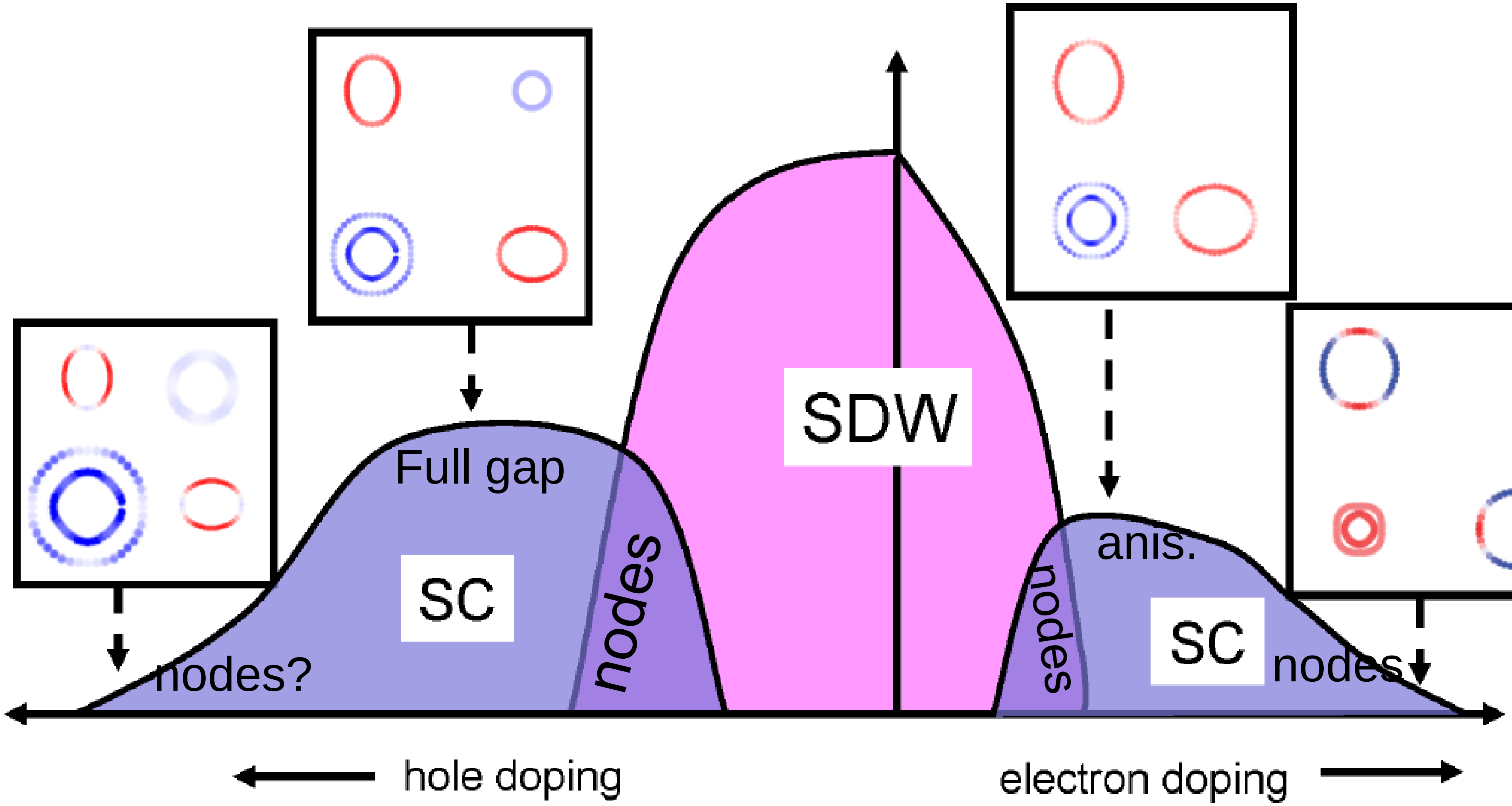
Graser et al 2009
Zhang et al 2009
Sknepnek et al 2009

$$\Delta_p = -\sum_{p'} \frac{V(p-p')\Delta_{p'}}{2E_{p'}}$$

- nesting peaks interaction $V(q)$ at $(\pi,0)$ in 1-Fe zone
- interaction is ~ constant over small pockets
- therefore sign-changing $s_{+/-}$ state solves gap eqn

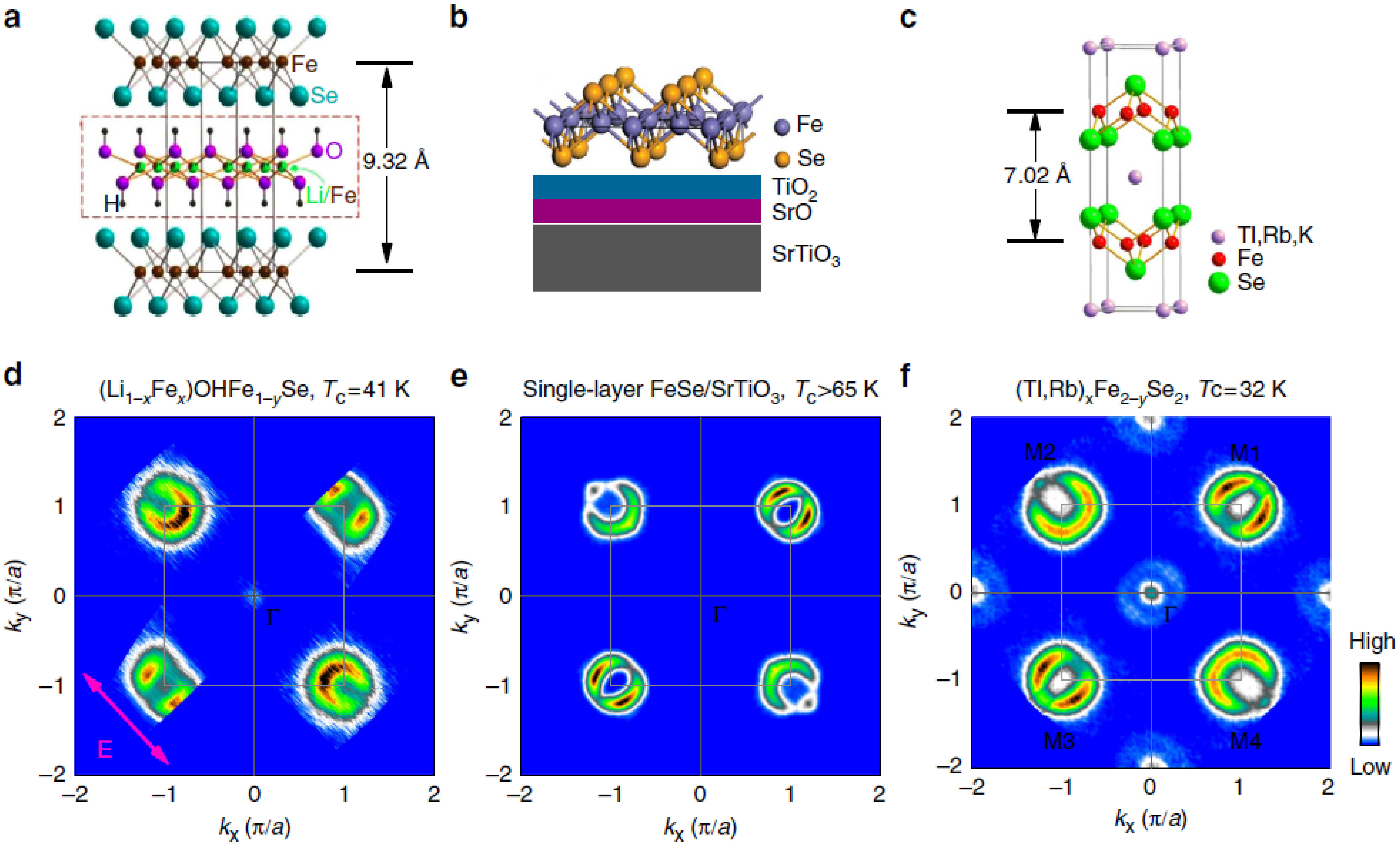
# Fe-pnictides: evolution of gap with doping from spin fluct. thy

PH, Korshunov and Mazin Rep. Prog. Phys. 2011



“trivial” (but important) *orbitally selective pairing*

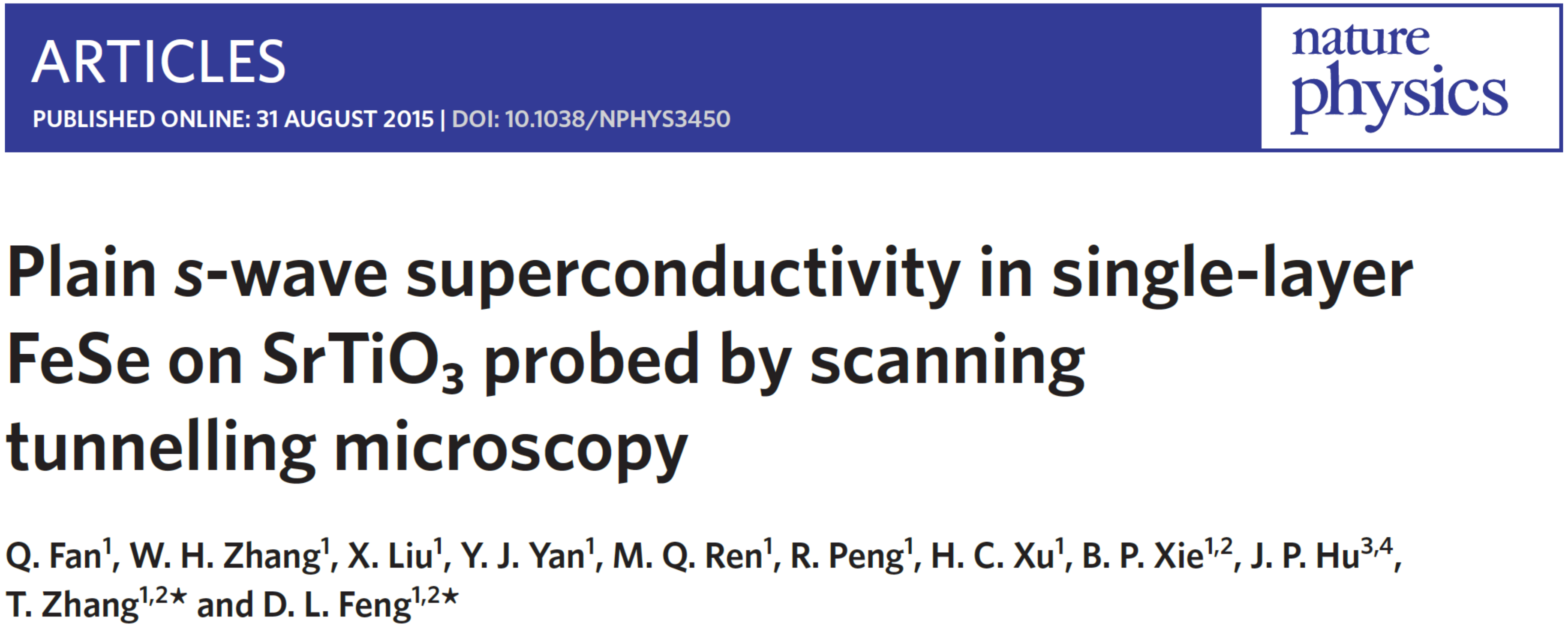
# High $T_c$ in Fe-chalcogenides



Zhao et al Nat. Comm 2016: “Common electronic origin of superconductivity…”

Is $T_c$ increased when you remove hole pocket? Disagrees with SF theory

# Are the Fe-chalcogenides fundamentally different?



ARTICLES

PUBLISHED ONLINE: 31 AUGUST 2015 | DOI: 10.1038/NPHYS3450

nature physics

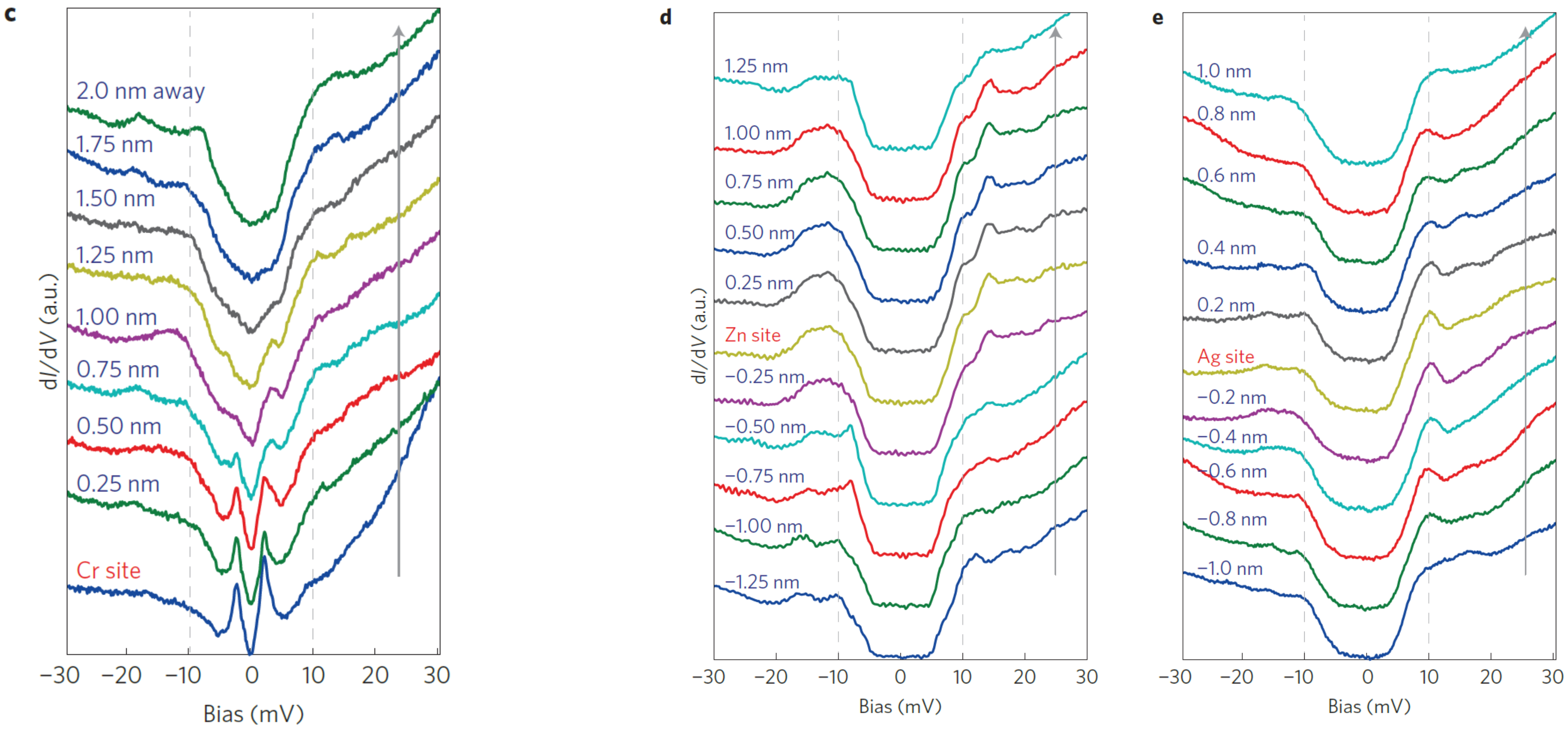
## Plain *s*-wave superconductivity in single-layer FeSe on $SrTiO_3$ probed by scanning tunnelling microscopy

Q. Fan[1], W. H. Zhang[1], X. Liu[1], Y. J. Yan[1], M. Q. Ren[1], R. Peng[1], H. C. Xu[1], B. P. Xie[1,2], J. P. Hu[3,4], T. Zhang[1,2]★ and D. L. Feng[1,2]★

Zn adatom

Ag adatom

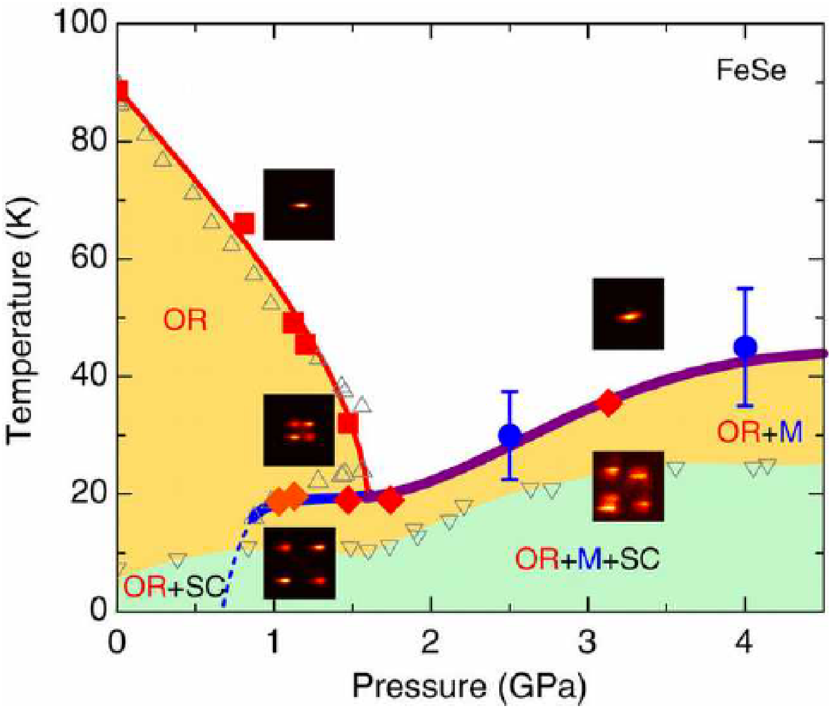
M adatom

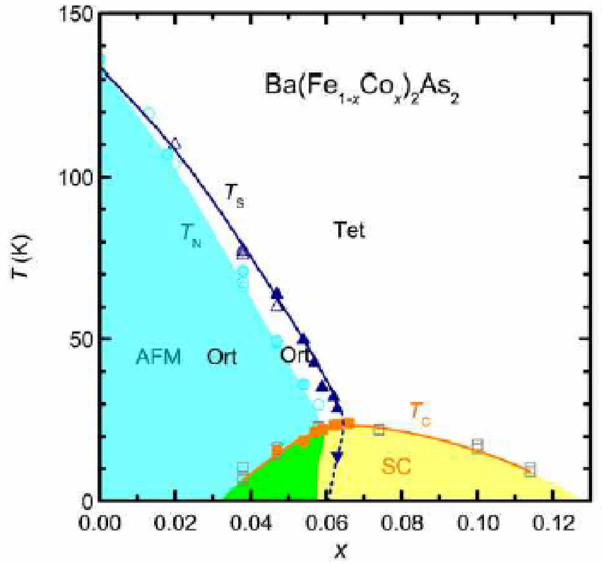


# FeSe: a proto-high $T_c$ superconductor

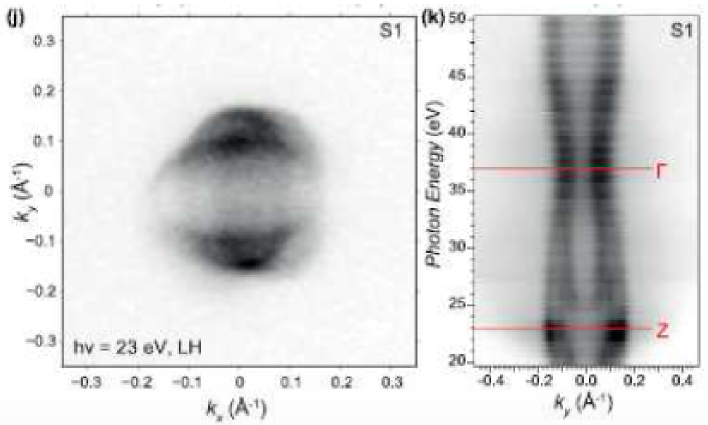
- nematic phase
  no magnetism
  (p=0)

K. Kothapalli, et al.,
Nat. Commun. **7**, 12728 (2016)

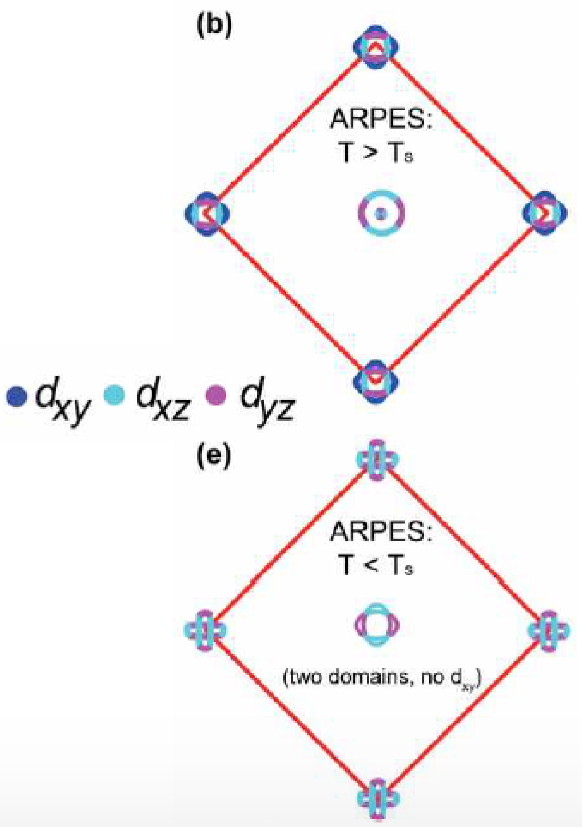




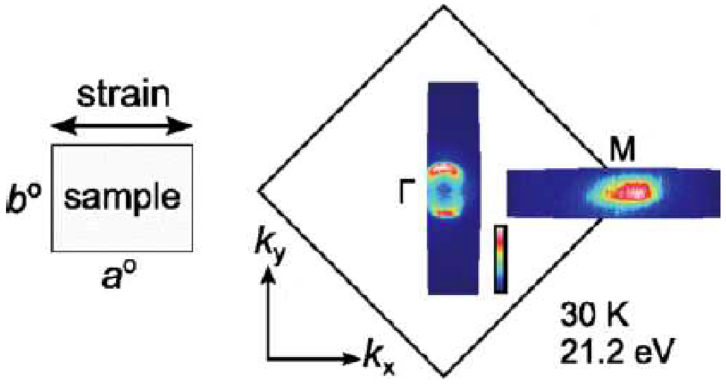
- ARPES
  measured band structure
  tiny Fermi surface
  (far from ab initio results)



Measured
orbital
splitting

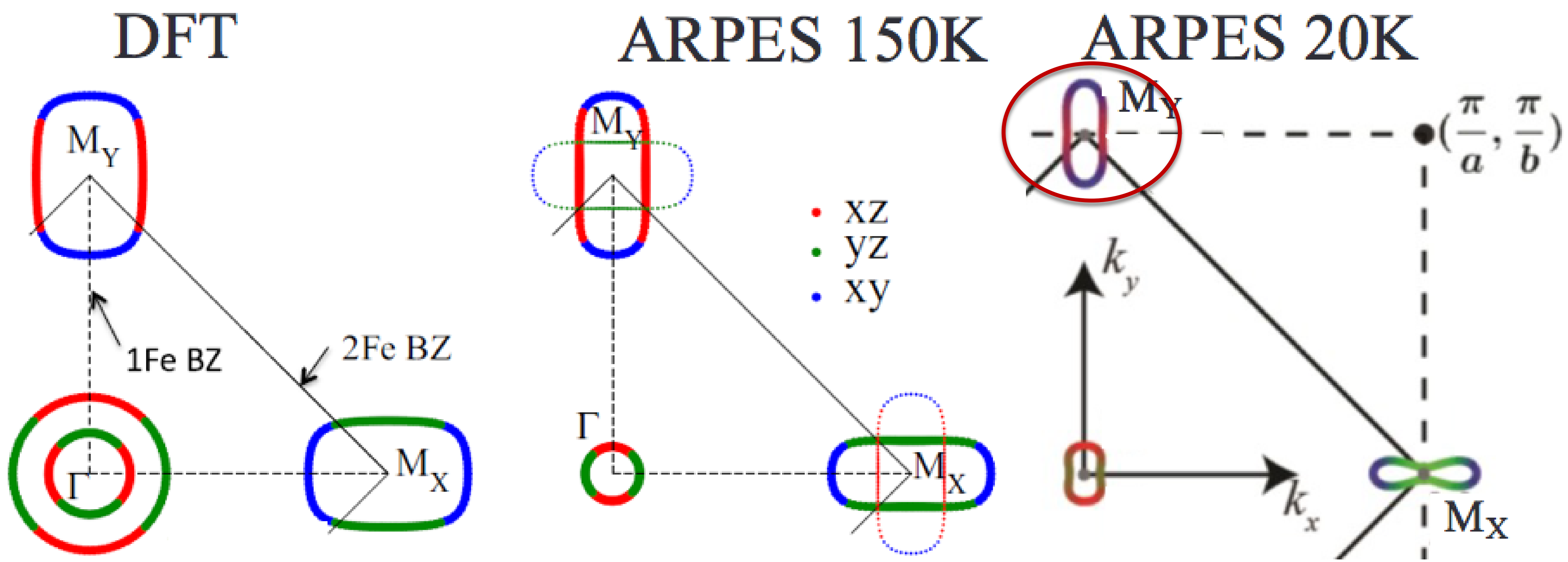


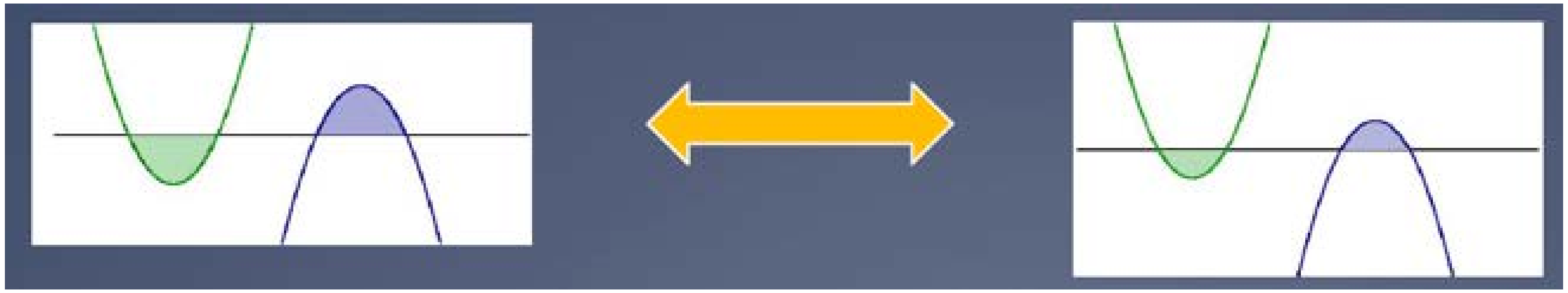
detwinned ARPES



Watson, et al., PRB 94, 201107(R) (2016)
Watson, et al., PRB 90, 121111(R) (2014)
Suzuki, et al., PRB 92, 205117 (2015)
Maletz, et al., PRB 89, 220506(R) (2014)
Fedorov, et al., Sci. Rep. 6, 36834 (2016)
Liu et al arXiv 2018
Kushnirenko et al arXiv 2018
Rhodes et al arXiv 2018

# Correlations in FeSe: expectations from twinned ARPES





Grazie a L. Benfatto

Yi et al PRB 2009, Ortenzi et al PRL 2009,
Borisenko et al Nat. Phys. 2016, Fanfarillo et al PRB 2016

# Questions/Outline

1) What is the superconducting gap structure in FeSe?

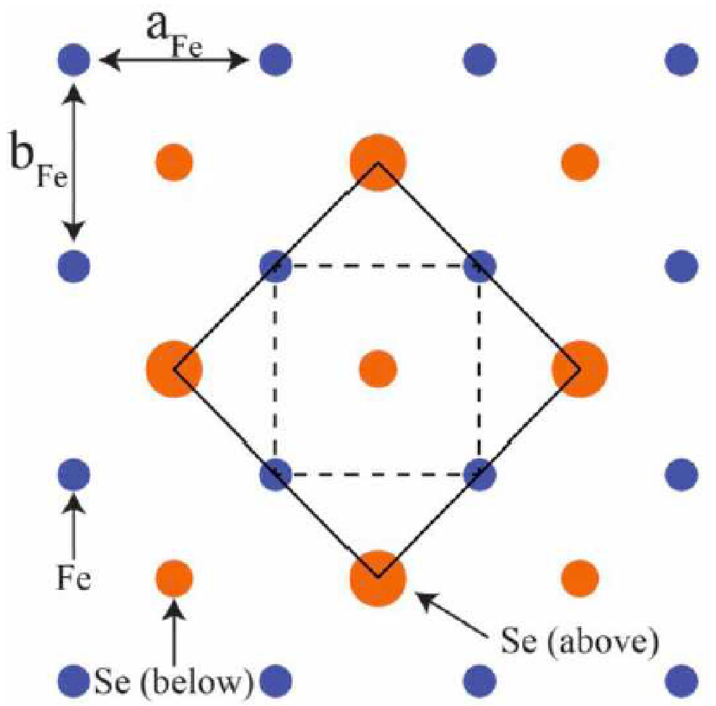
2) What is the origin of nematicity in FeSe?

3) How  do we understand the p-T-x phase diagram?

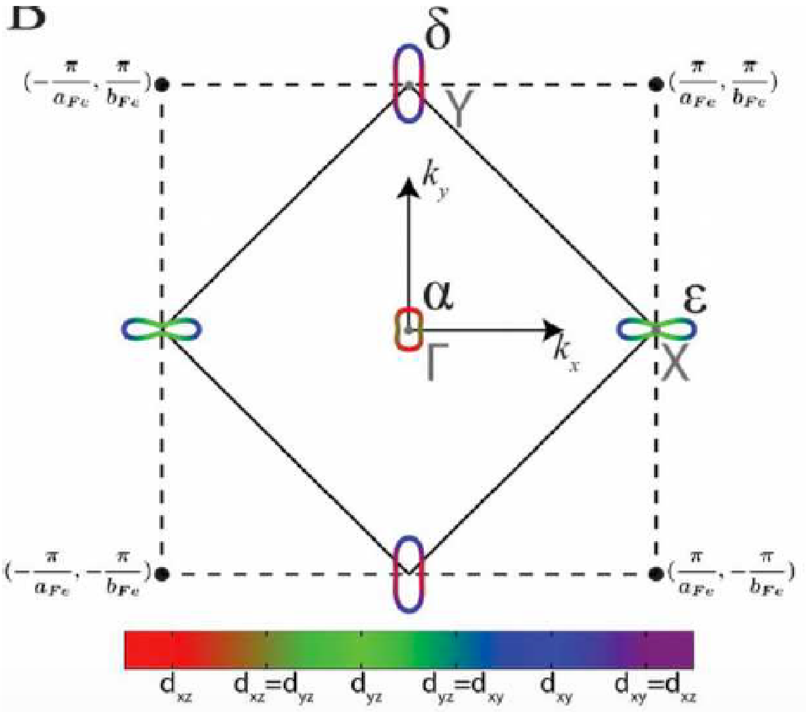
4) Is $T_c$ higher for systems with e-pockets only?  Why?

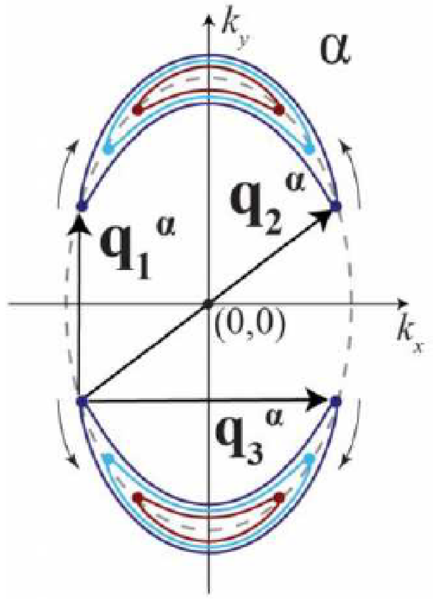
5) Are Fe-chalcogenides fundamentally different from Fe-pnictides due to stronger correlations?

# FeSe BQPI



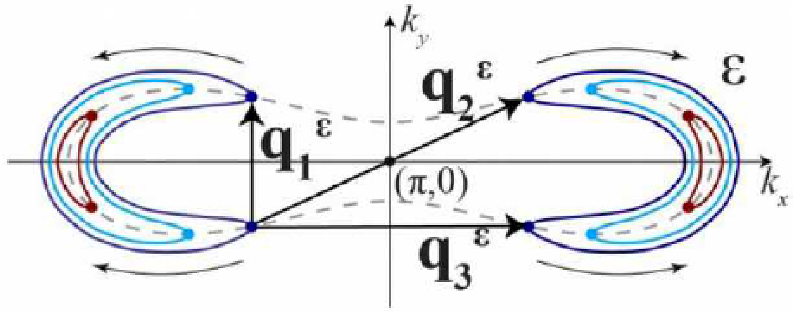
Coordinate system, expected Fermi surface

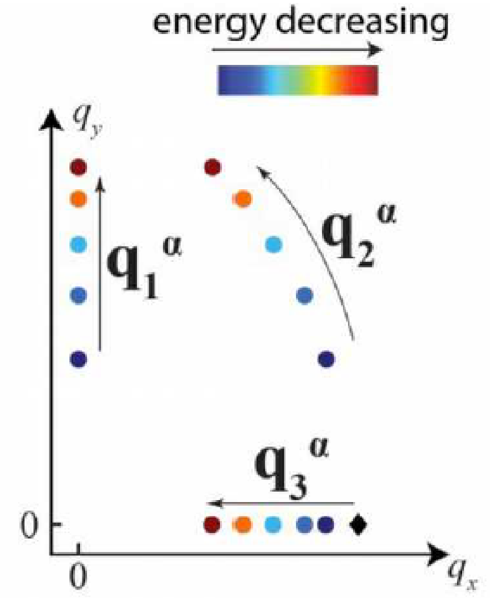




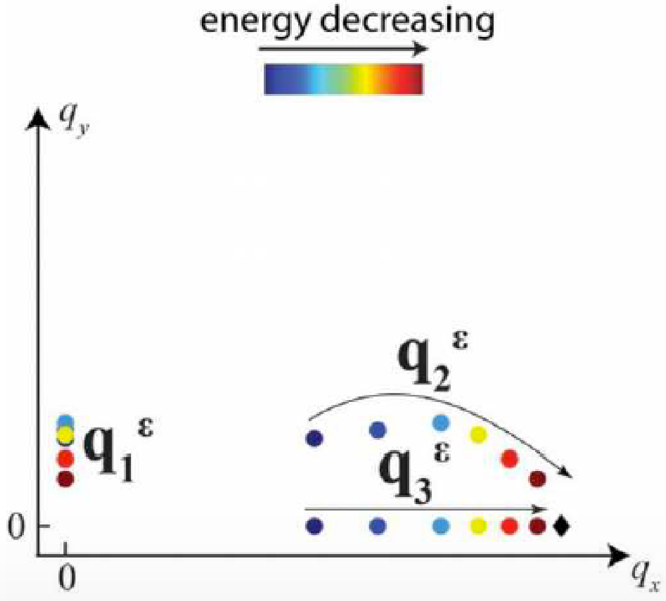
CEC: constant energy contour
Expected scattering vectors

$$E_{\mathbf{k}} = \pm\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$$



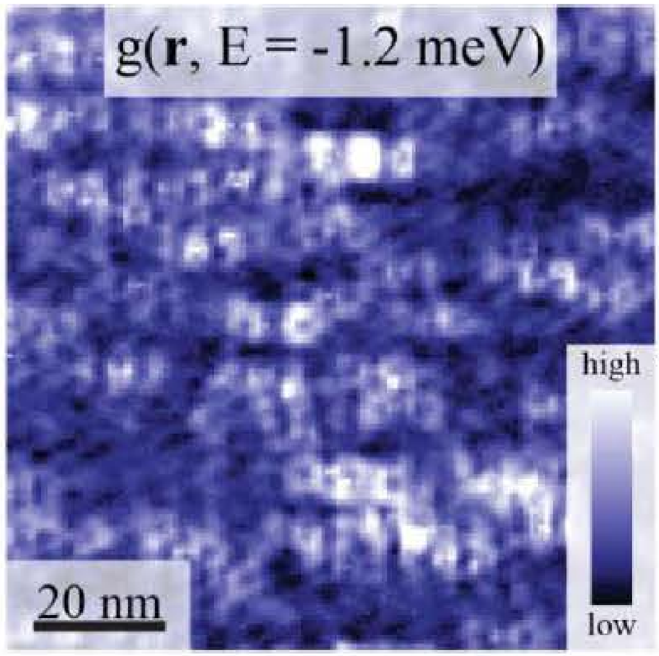


Dispersion of QPI peaks
q(E) → k(E) → E(k)



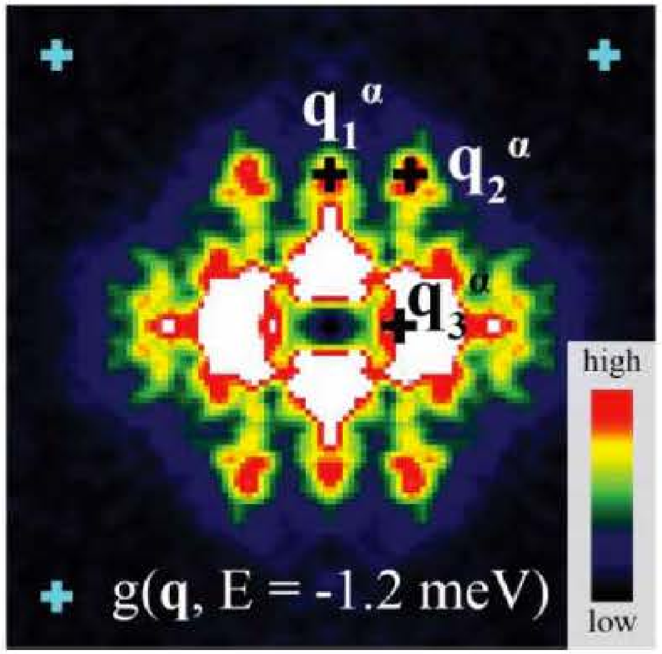
# FeSe measurement

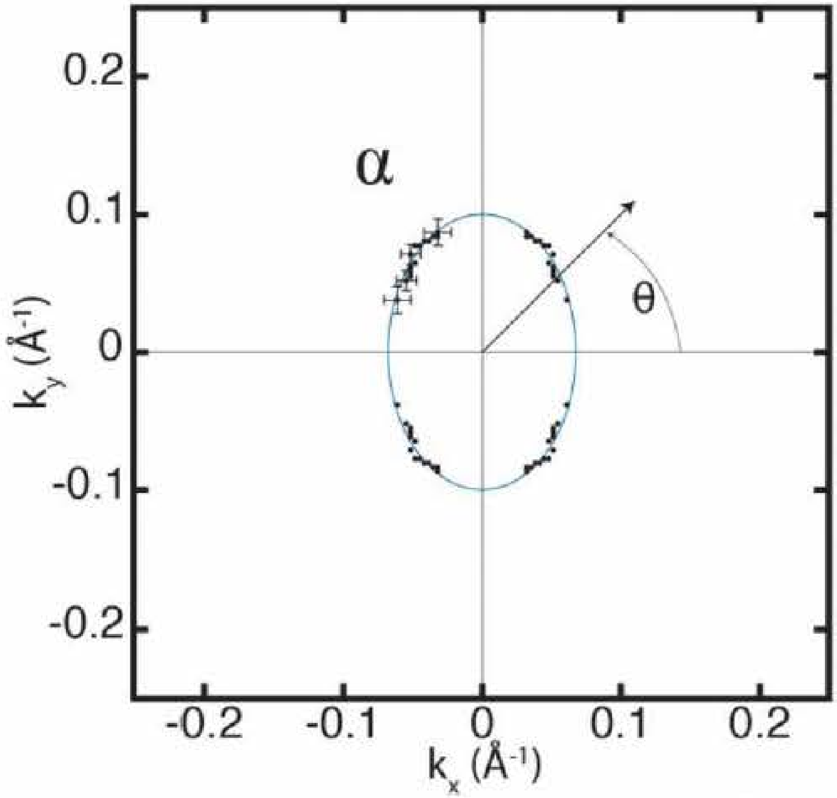
Cornell group (Sprau et al Science 2017)



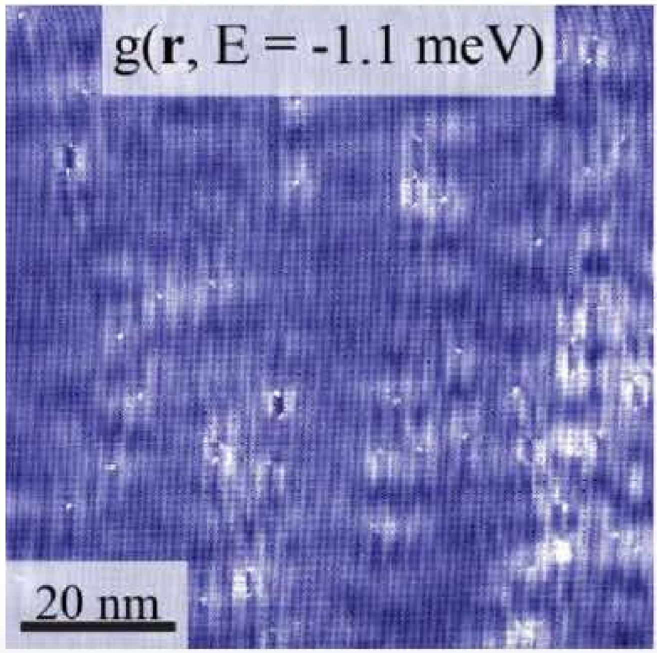
Conductance maps

FT

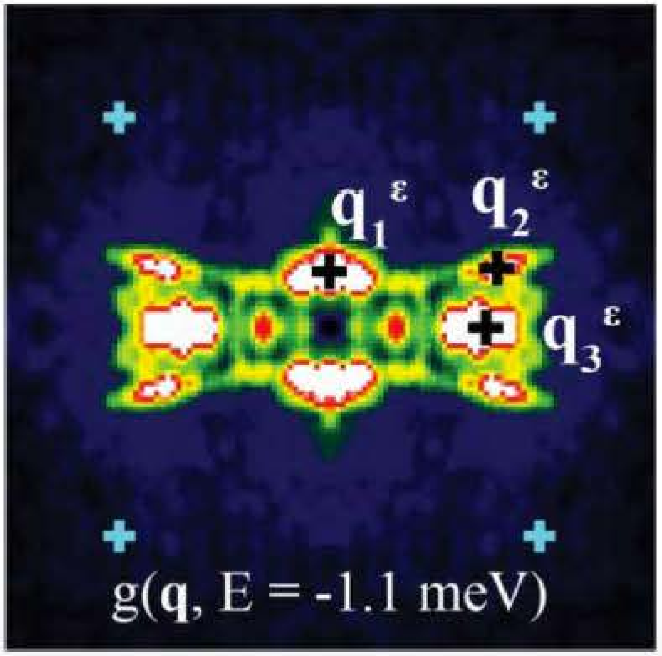


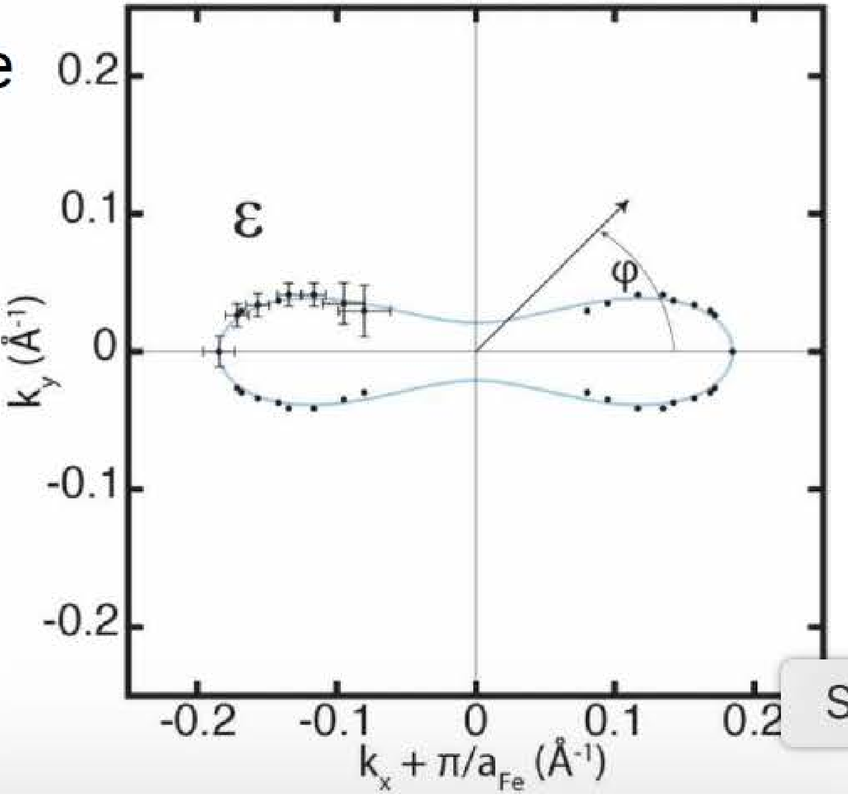


Trace back Fermi surface



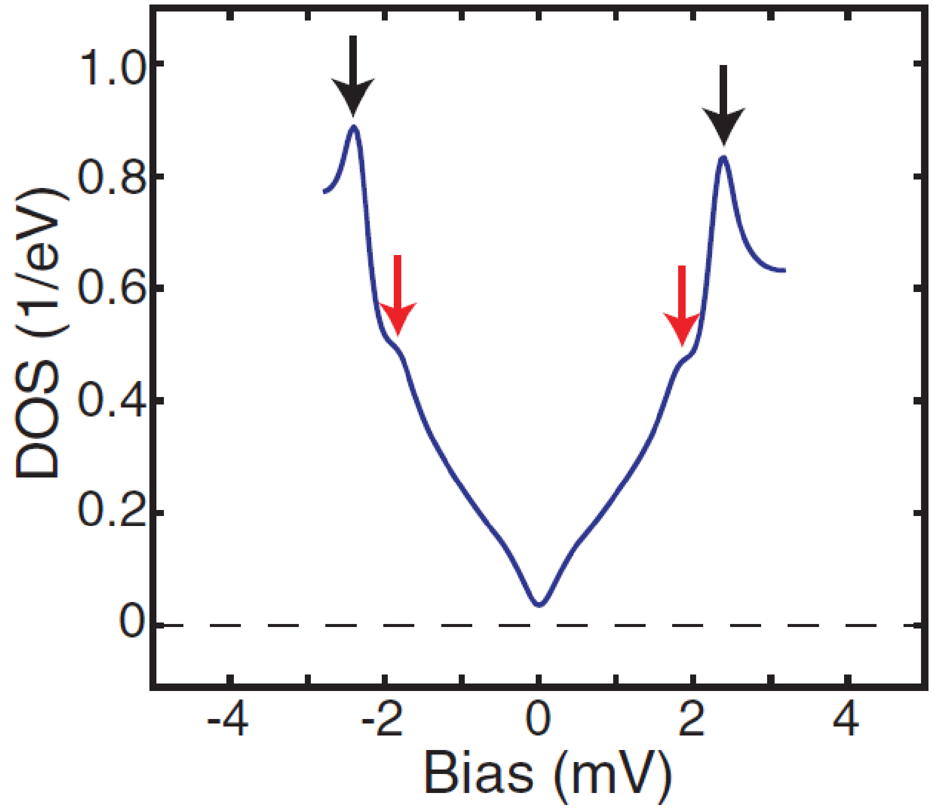
FT

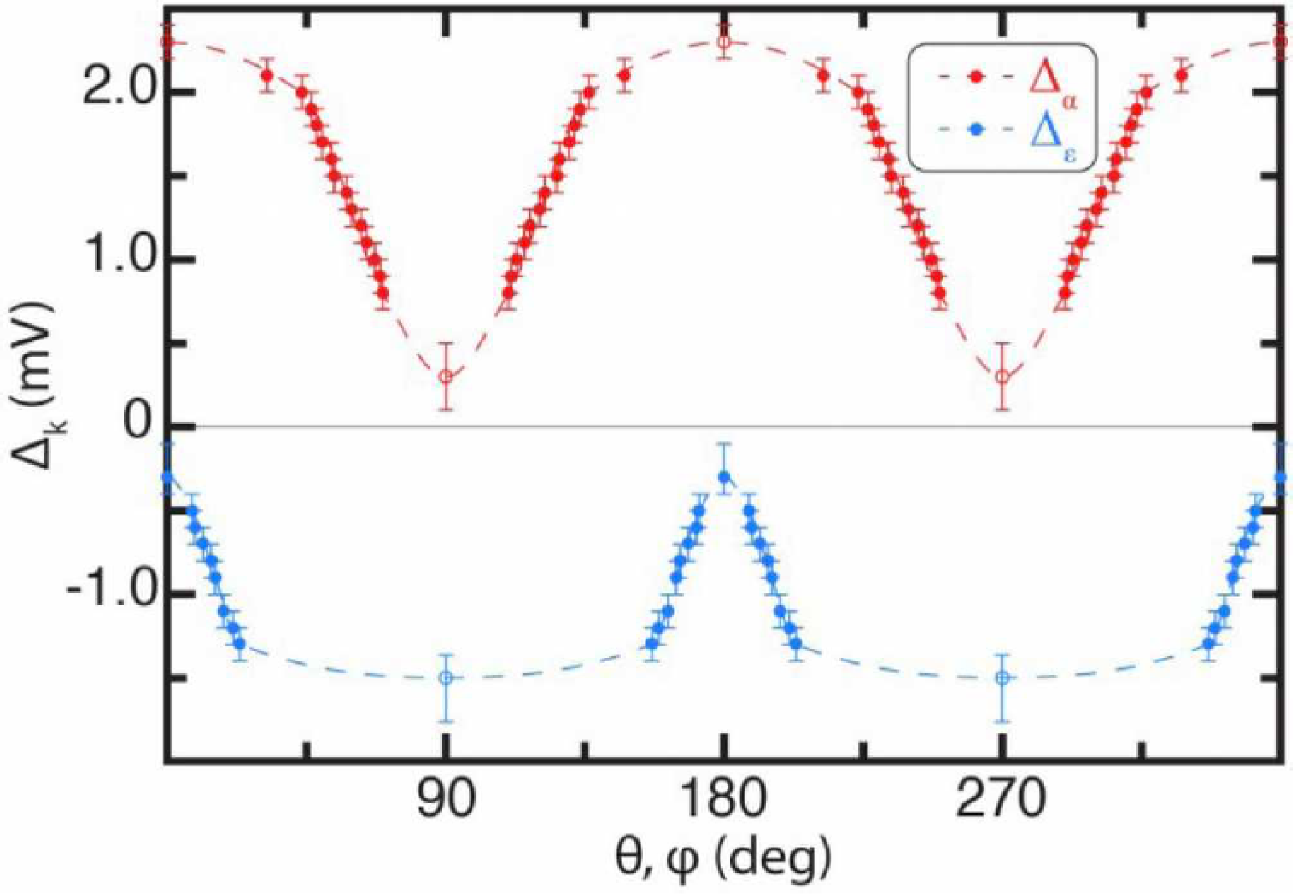




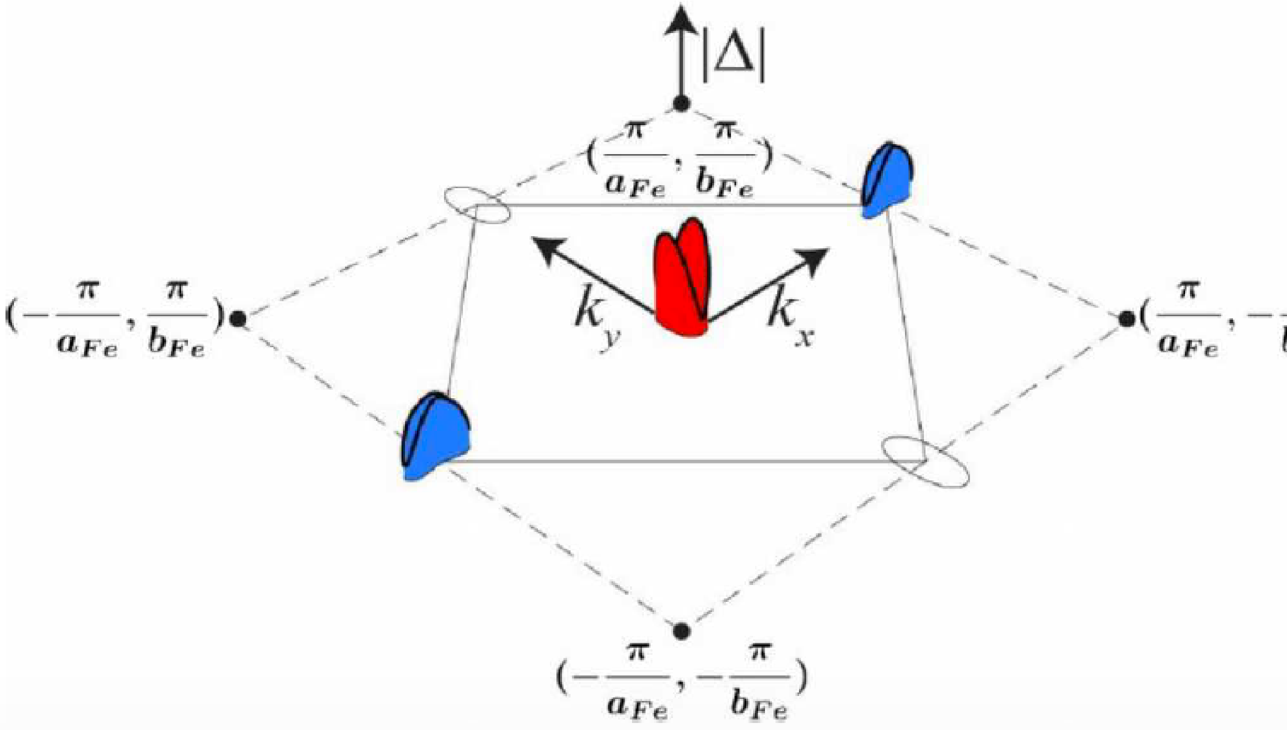
# Superconducting gap

- highly anisotropic order parameter, 2 band
- “antiphase” oscillation

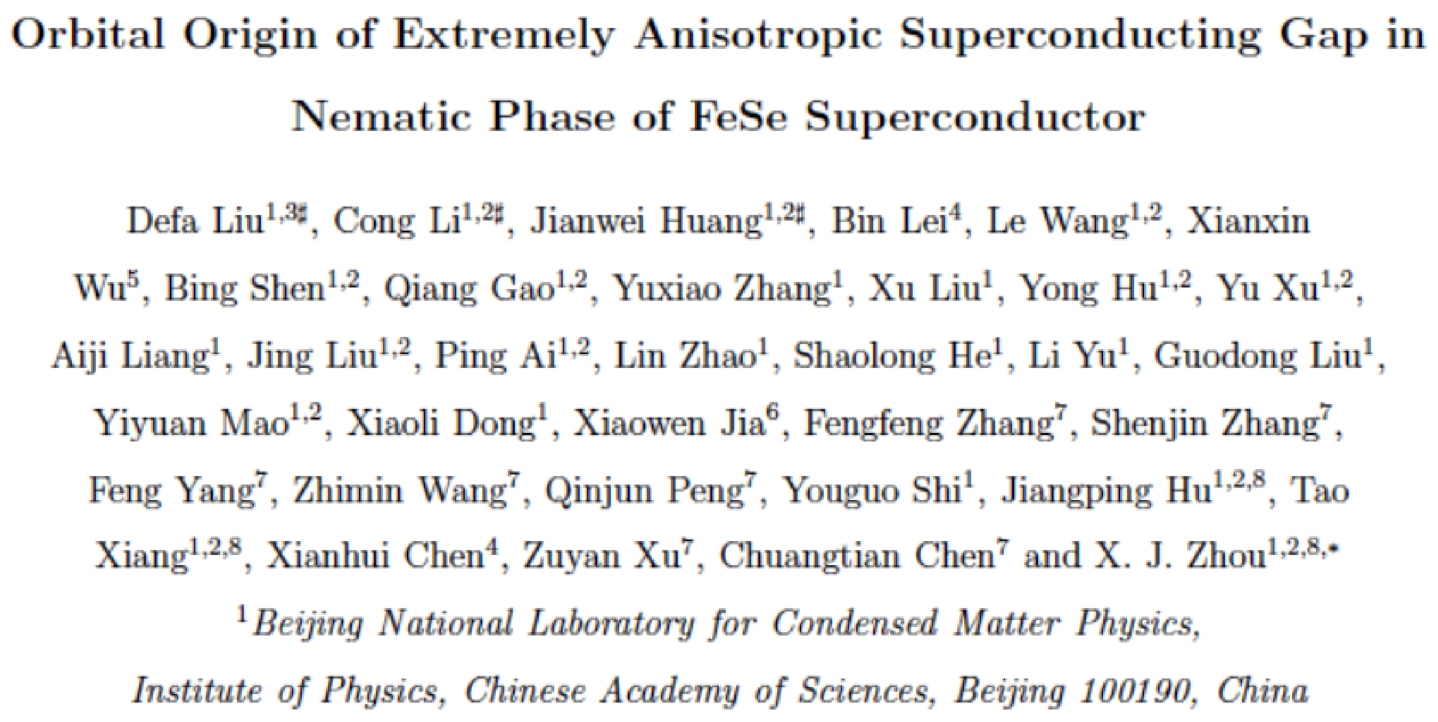




Sign change?!



# ARPES finds same gap structure

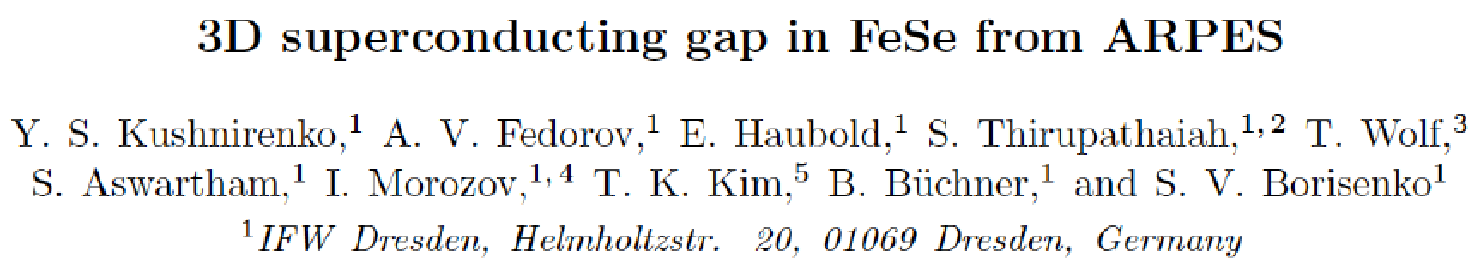


### Orbital Origin of Extremely Anisotropic Superconducting Gap in Nematic Phase of FeSe Superconductor

Defa Liu[1,3♯], Cong Li[1,2♯], Jianwei Huang[1,2♯], Bin Lei[4], Le Wang[1,2], Xianxin Wu[5], Bing Shen[1,2], Qiang Gao[1,2], Yuxiao Zhang[1], Xu Liu[1], Yong Hu[1,2], Yu Xu[1,2], Aiji Liang[1], Jing Liu[1,2], Ping Ai[1,2], Lin Zhao[1], Shaolong He[1], Li Yu[1], Guodong Liu[1], Yiyuan Mao[1,2], Xiaoli Dong[1], Xiaowen Jia[6], Fengfeng Zhang[7], Shenjin Zhang[7], Feng Yang[7], Zhimin Wang[7], Qinjun Peng[7], Youguo Shi[1], Jiangping Hu[1,2,8], Tao Xiang[1,2,8], Xianhui Chen[4], Zuyan Xu[7], Chuangtian Chen[7] and X. J. Zhou[1,2,8,*]

[1]*Beijing National Laboratory for Condensed Matter Physics,*
*Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

ArXiv:1802.02940

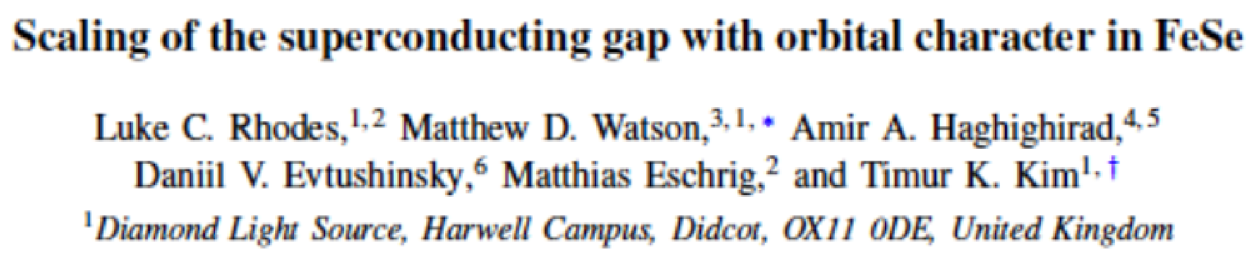


### 3D superconducting gap in FeSe from ARPES

Y. S. Kushnirenko,[1] A. V. Fedorov,[1] E. Haubold,[1] S. Thirupathaiah,[1,2] T. Wolf,[3] S. Aswartham,[1] I. Morozov,[1,4] T. K. Kim,[5] B. Büchner,[1] and S. V. Borisenko[1]

[1]*IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany*

ArXiv:1802.08668



### Scaling of the superconducting gap with orbital character in FeSe

Luke C. Rhodes,[1,2] Matthew D. Watson,[3,1,*] Amir A. Haghighirad,[4,5] Daniil V. Evtushinsky,[6] Matthias Eschrig,[2] and Timur K. Kim[1,†]

[1]*Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, United Kingdom*

ArXiv:1804.01436

# Theory: band structure modeling

- Tight binding model

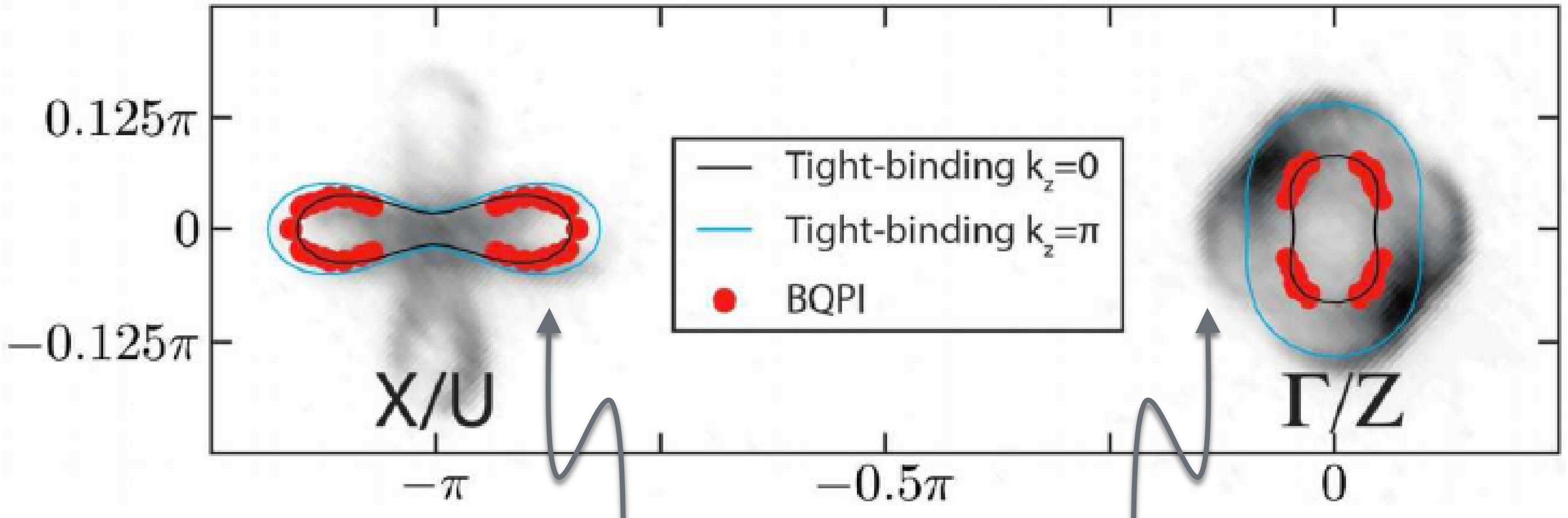
$$H_N = H_0 + H_{OO} + H_{SOC}$$

$$H_0 = \sum_{\mathbf{r},\mathbf{r}',a,b} t^{ab}_{\mathbf{r}-\mathbf{r}'} c^{\dagger}_{a,\mathbf{r}} c_{b,\mathbf{r}'}$$

site+bond
centered
orbital order

$$H_{SOC} = \lambda \boldsymbol{L} \cdot \boldsymbol{S}$$

needed for consistent splitting at Gamma



Twinned ARPES

Fit to ARPES, QO expts

Mukherjee et al PRL 2015

Kreisel et al PRB 2016

Sprau et al Science 2017

$$H_{OO} = \Delta_b \sum (\cos k_x - \cos k_y)(n_{xz}(\mathbf{k}) + n_{yz}(\mathbf{k})) + \Delta_s \sum_{\mathbf{k}} (n_{xz}(\mathbf{k}) - n_{yz}(\mathbf{k}))$$

# Tight binding model

$$H_N = H_0 + H_{OO} + H_{SOC}$$

$$H_0 = \sum_{\mathbf{r},\mathbf{r}',a,b} t^{ab}_{\mathbf{r}-\mathbf{r}'} c^\dagger_{a,\mathbf{r}} c_{b,\mathbf{r}'}$$

site+bond
centered
orbital order

$$H_{SOC} = \lambda \boldsymbol{L} \cdot \boldsymbol{S}$$

needed for consistent
splitting at Gamma

+

$$\begin{aligned} H_U = {} & U \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + U' \sum_{i,\ell'<\ell} n_{i\ell} n_{i\ell'} \\ & + J \sum_{i,\ell'<\ell} \sum_{\sigma,\sigma'} c^\dagger_{i\ell\sigma} c^\dagger_{i\ell'\sigma'} c_{i\ell\sigma'} c_{i\ell'\sigma} \\ & + J' \sum_{i,\ell'\neq\ell} c^\dagger_{i\ell\uparrow} c^\dagger_{i\ell\downarrow} c_{i\ell'\downarrow} c_{i\ell'\uparrow}, \end{aligned}$$

Hubbard-Kanamori:
multiple orbitals, onsite only

# Superconductivity: Ingredients of model

- Interactions (standard)
- Electronic structure (measured)
- Pairing mechanism?

$$H = H_0 + U \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + U' \sum_{i,\ell'<\ell} n_{i\ell} n_{i\ell'}$$

$$+ J \sum_{i,\ell'<\ell} \sum_{\sigma,\sigma'} c^\dagger_{i\ell\sigma} c^\dagger_{i\ell'\sigma'} c_{i\ell\sigma'} c_{i\ell'\sigma}$$

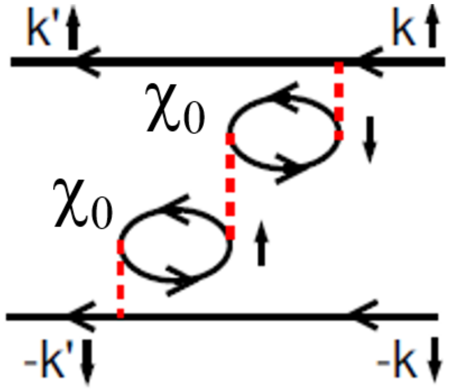
$$+ J' \sum_{i,\ell'\neq\ell} c^\dagger_{i\ell\uparrow} c^\dagger_{i\ell\downarrow} c_{i\ell'\downarrow} c_{i\ell'\uparrow},$$

$$\chi^0_{\ell_1\ell_2\ell_3\ell_4}(q) = -\sum_{k,\mu\nu} M^{\mu\nu}_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{q}) G^\mu(k+q) G^\nu(k)$$

$$\Gamma_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}') = \left[\frac{3}{2}\bar{U}^s \chi_1^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^s + \frac{1}{2}\bar{U}^s - \frac{1}{2}\bar{U}^c \chi_0^{\mathrm{RPA}}(\mathbf{k}-\mathbf{k}')\bar{U}^c + \frac{1}{2}\bar{U}^c\right]_{\ell_1\ell_2\ell_3\ell_4}$$

$$\Gamma_{\nu\mu}(\mathbf{k},\mathbf{k}') = \mathrm{Re} \sum_{\ell_1\ell_2\ell_3\ell_4} a_\nu^{\ell_1,*}(\mathbf{k}) a_\nu^{\ell_4,*}(-\mathbf{k}) \times \Gamma_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}')\, a_\mu^{\ell_2}(\mathbf{k}') a_\mu^{\ell_3}(-\mathbf{k}')$$

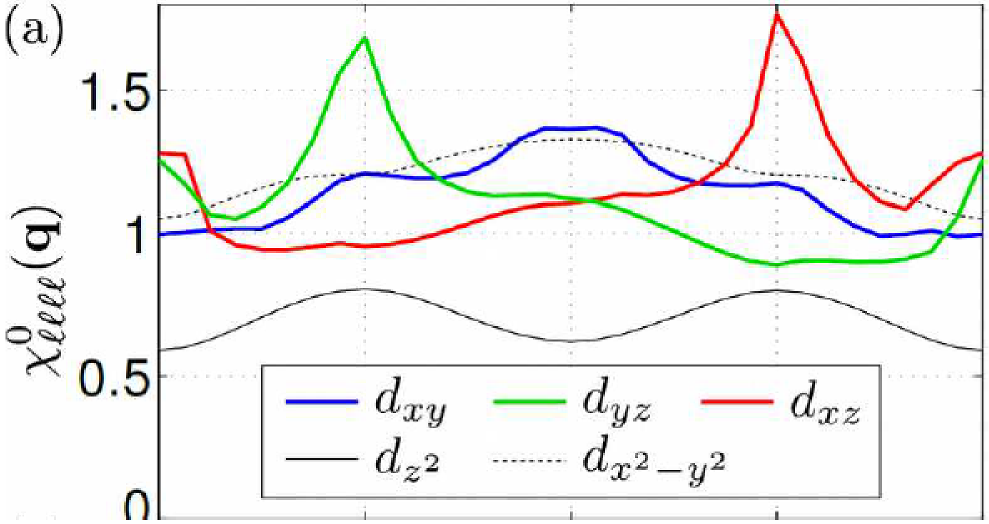
(spin fluctuation pairing vertex)



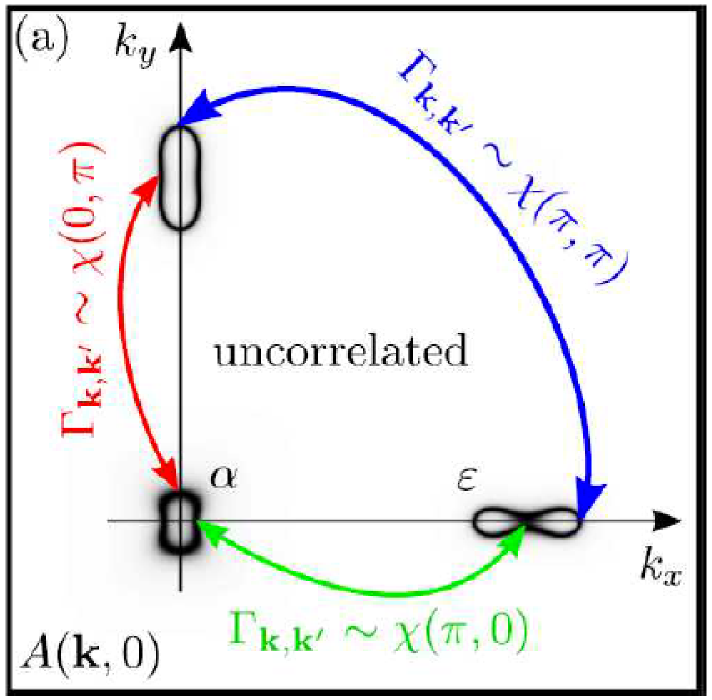
etc…

# Pairing from spin-fluctuation theory?

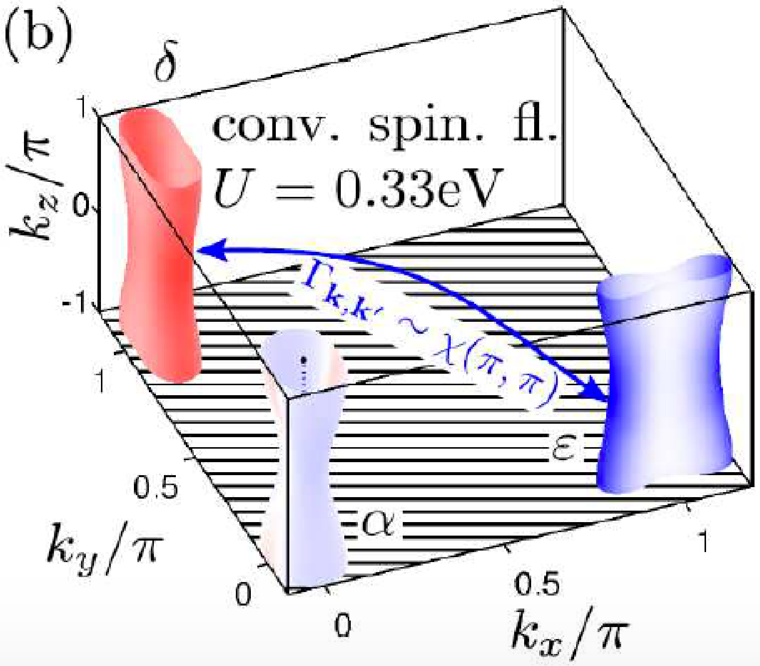
- Susceptibility

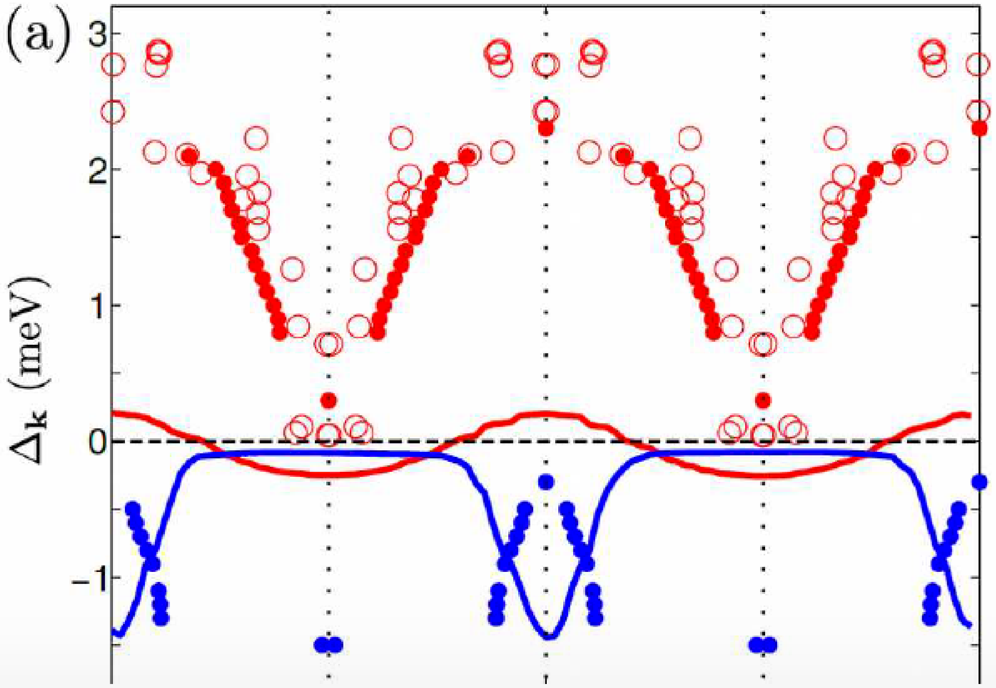


- Pairing glue



- Solution of BCS equation

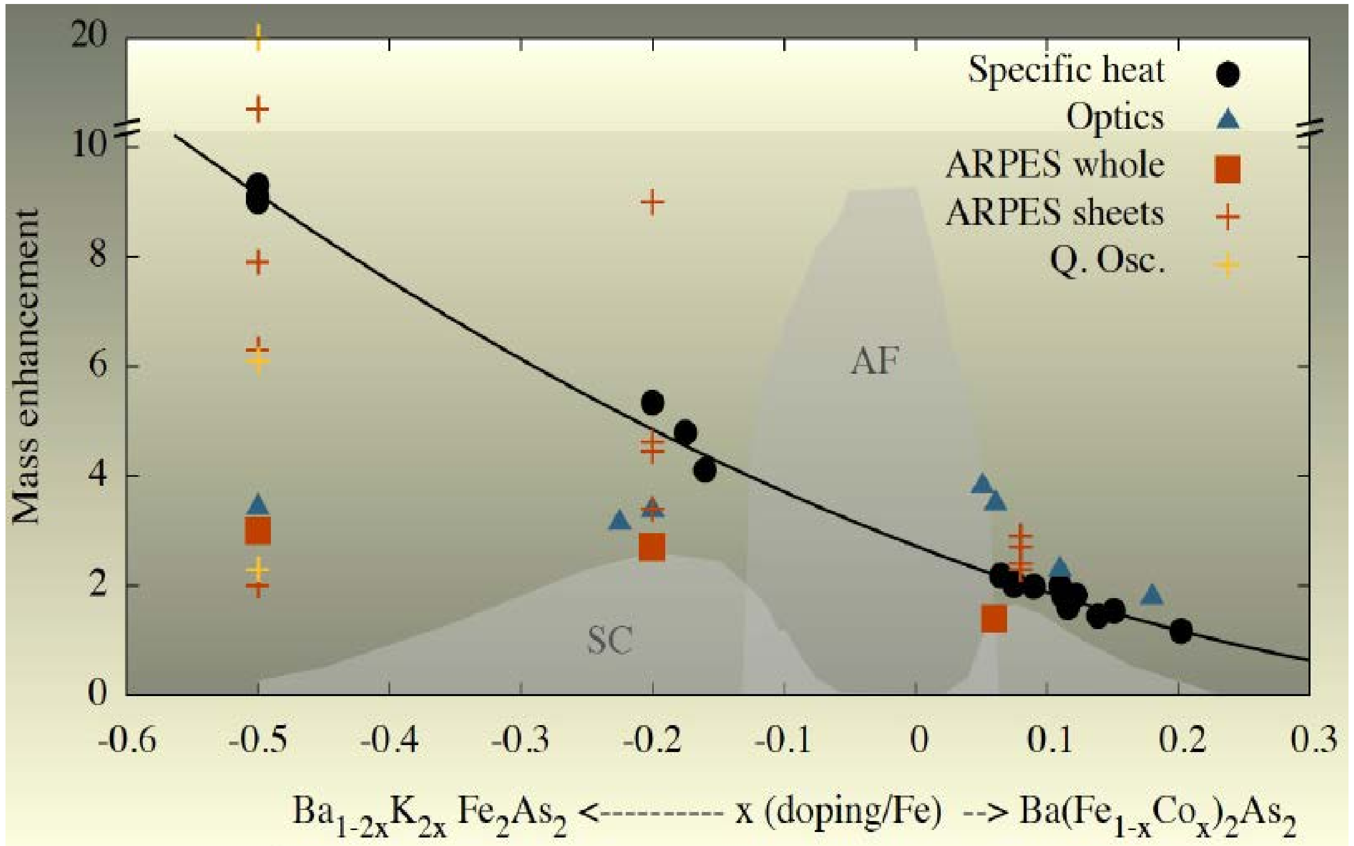




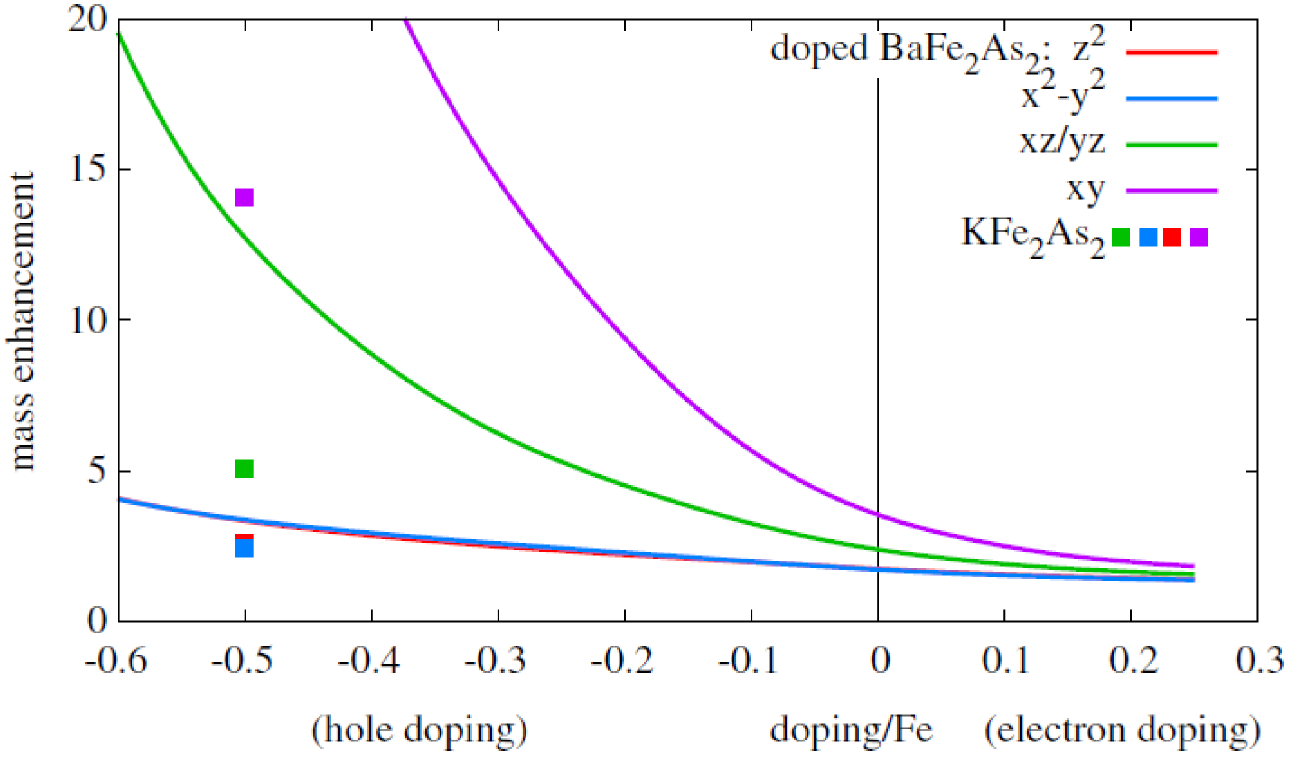
Does not work!
→ “in-phase” anisotropy
→ Small anisotropy on Gamma pocket!

# Orbital selective Mott picture

Yin et al 2011, Arakawa & Ogata 2011, de Medici et al 2011, Yu et al 2014



(all data in high-T tetragonal phase)



L. de Medici et al, PRL 2014

Sommerfeld coefficient

$$\gamma \sim N^*(E_F) = \sum_\alpha (m^*/m_b)_\alpha N_b^\alpha(E_F)$$

Optics: Drude contribution

$$D^* = \sum (m_b/m^*)_\alpha D_b^\alpha$$

⇒*selective* orbital mass enhancement

Recent reviews: Bascones et al CRAS 2016, Roekigham et al CRAS 2016, Yi et al npj Quantum Materials 2017

# Reminder: coherent & incoherent part of spectrum

**Renormalized Green's function:**

$$G^R(\mathbf{k}\sigma,\omega) = \frac{1}{\omega - \xi_{\mathbf{k}} - \Sigma^R(\mathbf{k}\sigma,\omega)}$$

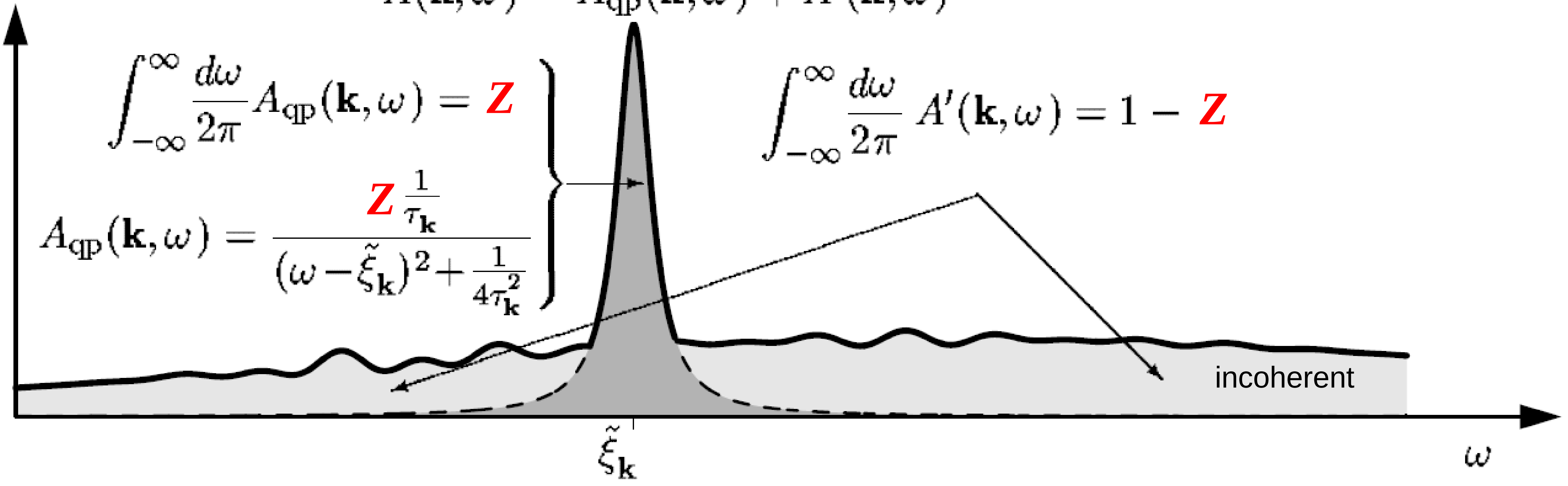
$$\equiv \quad Z\left[\omega - \tilde{\xi}_{\mathbf{k}} + \frac{i}{2\tilde{\tau}_{\mathbf{k}}(\omega)}\right]^{-1}$$

**Quasiparticle weight:**

$$Z^{-1} = 1 - \frac{\partial}{\partial\omega}\mathrm{Re}\,\Sigma(\tilde{k}_F,\omega)\Big|_{\omega=0}$$

**Spectral function:** $A(\mathbf{k},\omega) = -\frac{1}{\pi}\mathrm{Im}\,G^R(\mathbf{k},\omega)$

$$A(\mathbf{k},\omega) = A_{\mathrm{qp}}(\mathbf{k},\omega) + A'(\mathbf{k},\omega)$$



$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A_{\mathrm{qp}}(\mathbf{k},\omega) = Z$$

$$A_{\mathrm{qp}}(\mathbf{k},\omega) = \frac{Z\,\frac{1}{\tau_{\mathbf{k}}}}{(\omega-\tilde{\xi}_{\mathbf{k}})^2 + \frac{1}{4\tau_{\mathbf{k}}^2}}$$

$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A'(\mathbf{k},\omega) = 1 - Z$$

Bruus & Flensberg.

# Modified spin fluctuation pairing Ansatz

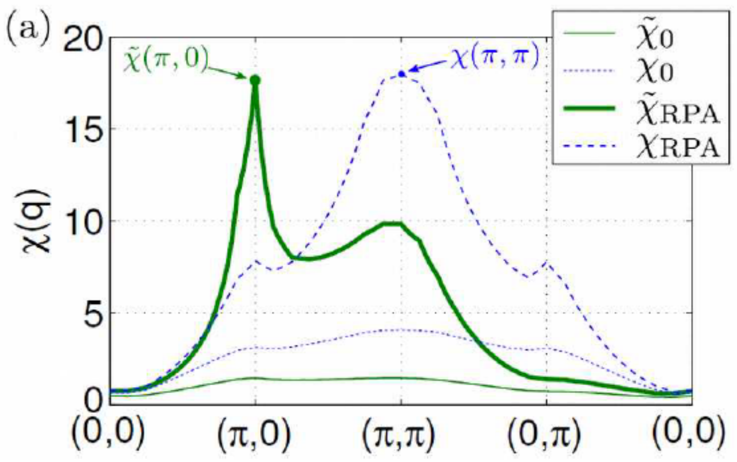
## (Sprau et al Science 2017, Kreisel et al PRB 2017)

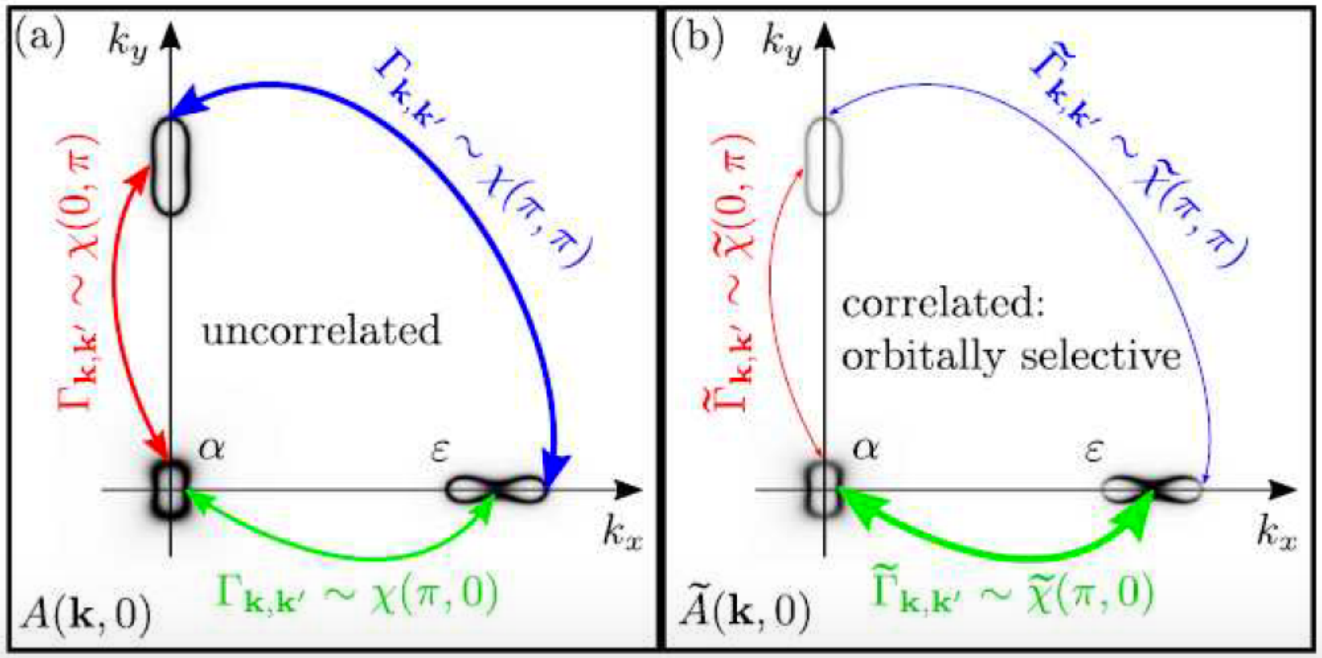
- “dressed susceptibility”

$$\tilde{\chi}^0_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{q}) = \sqrt{Z_{\ell_1}Z_{\ell_2}Z_{\ell_3}Z_{\ell_4}}\;\chi^0_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{q})$$

- Dressed pairing interaction

$$\tilde{\Gamma}_{\nu\mu}(\mathbf{k},\mathbf{k}') = \mathrm{Re}\sum_{\ell_1\ell_2\ell_3\ell_4}\sqrt{Z_{\ell_1}}\sqrt{Z_{\ell_4}}\,a_\nu^{\ell_1,*}(\mathbf{k})\,a_\nu^{\ell_4,*}(-\mathbf{k}) \times\tilde{\Gamma}_{\ell_1\ell_2\ell_3\ell_4}(\mathbf{k},\mathbf{k}')\,\sqrt{Z_{\ell_2}}\sqrt{Z_{\ell_3}}\,a_\mu^{\ell_2}(\mathbf{k}')\,a_\mu^{\ell_3}(-\mathbf{k}')$$





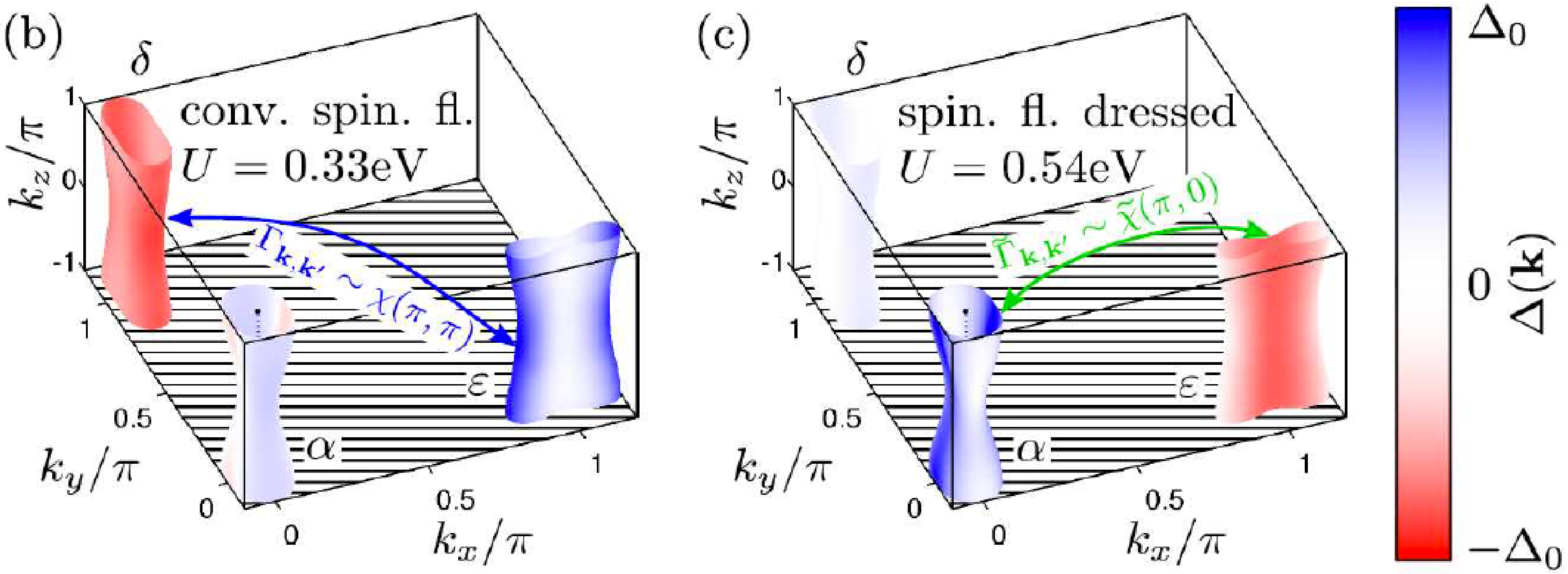
Dominant pairing in $d_{yz}$ orbital channel
→ orbital selective pairing

Remarks:

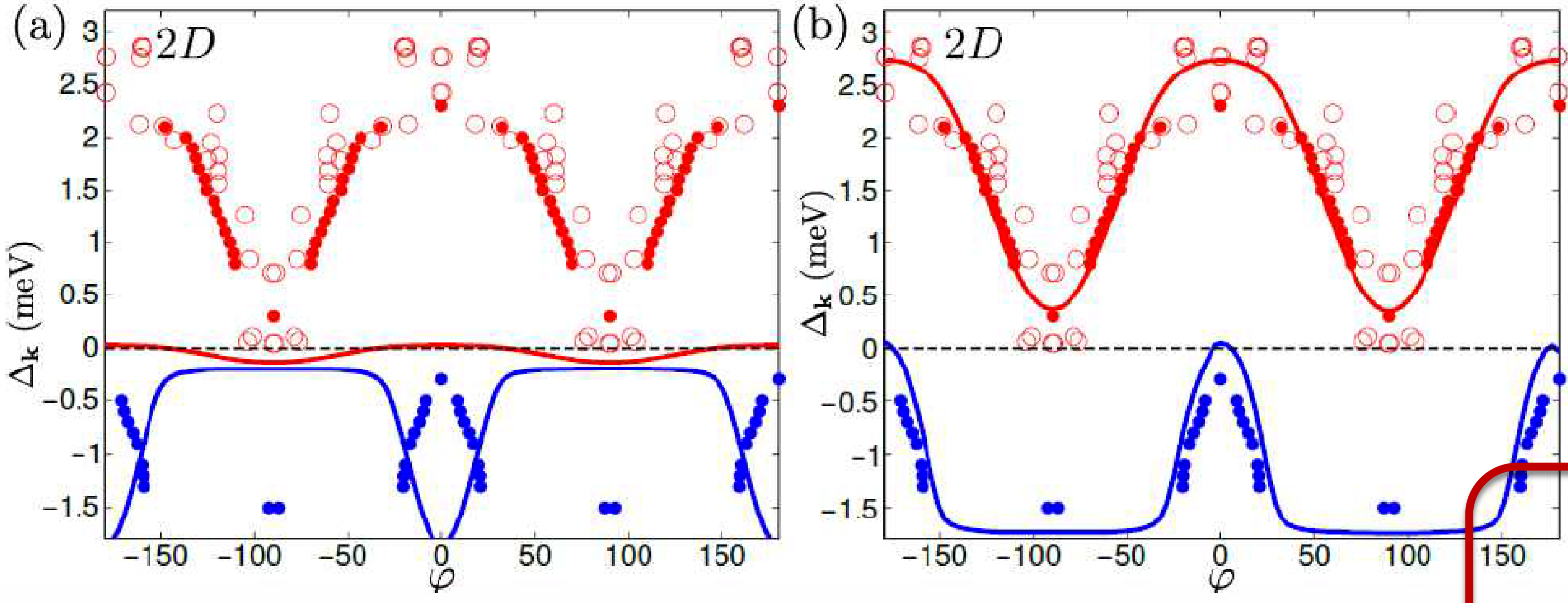
- bands fit to ARPES, QO, QPI contain already Σ’(k,0)
- Basic conclusion from STM – pairing on yz orbitals only -- *might* be explainable without Z’s
  - a) suppress xy, rely on nematic wave functions to kill xz (Kang et al aXv:2018)
  - b) suppress xy, take xz/yz shifts from nematic spin correlations (Fanfarillo et al aXv:2018)

# Pairing and gap structure

“uncorrelated” correlated



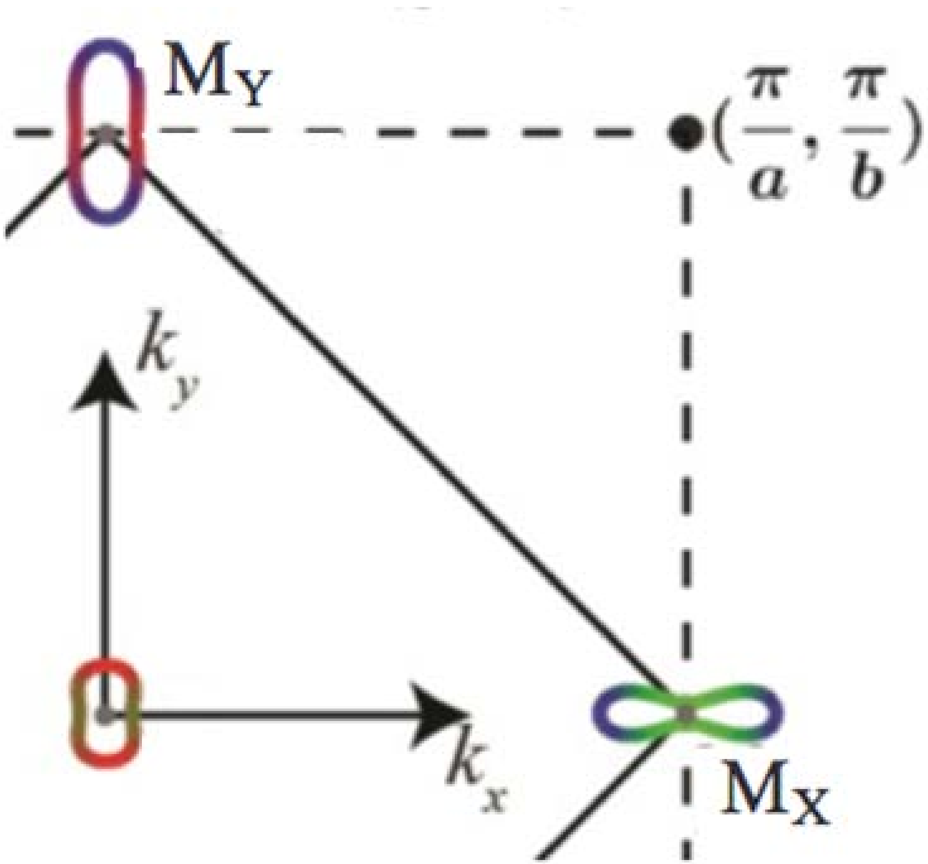
A. Kreisel et al, PRB 2017



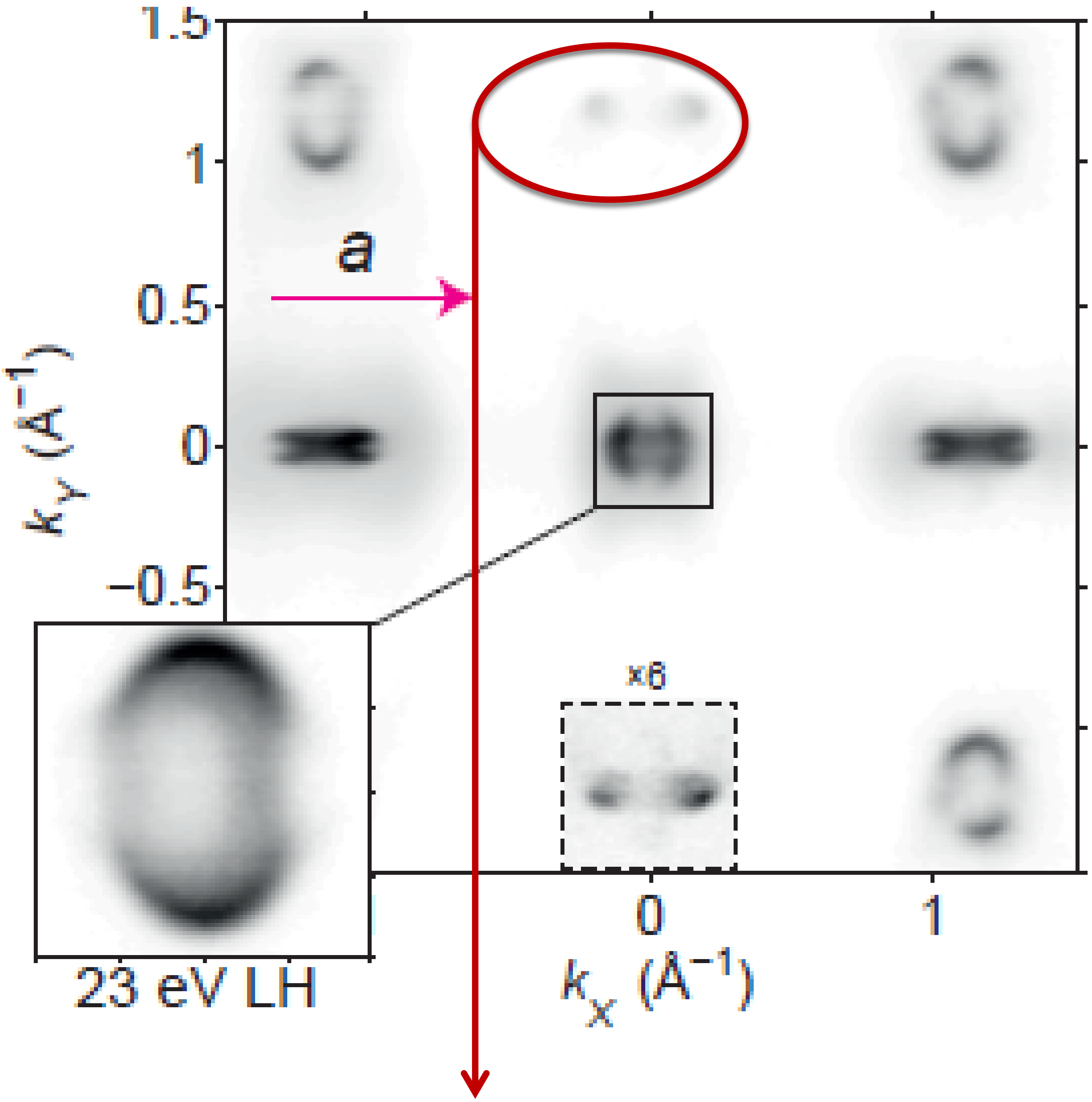
$$(d_{xy}, d_{x^2-y^2}, d_{xz}, d_{yz}, d_{3z^2-r^2})$$

$$\{\sqrt{Z_l}\} = [0.2715, 0.9717, 0.4048, 0.9236, 0.5916]$$

# Consistency of untwinned ARPES with orbital selective pairing ansatz



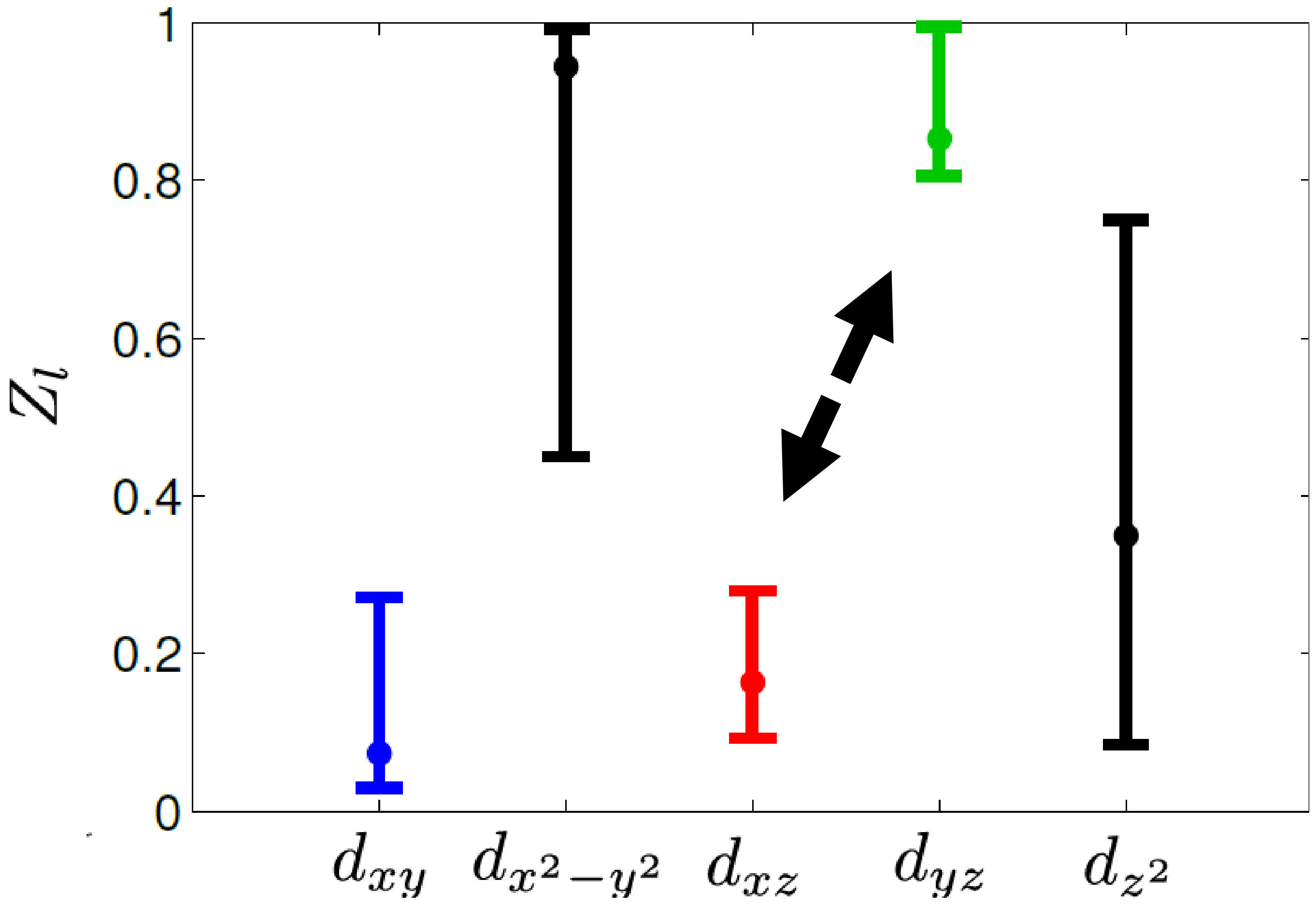
Expected from “red-blue shift” alone

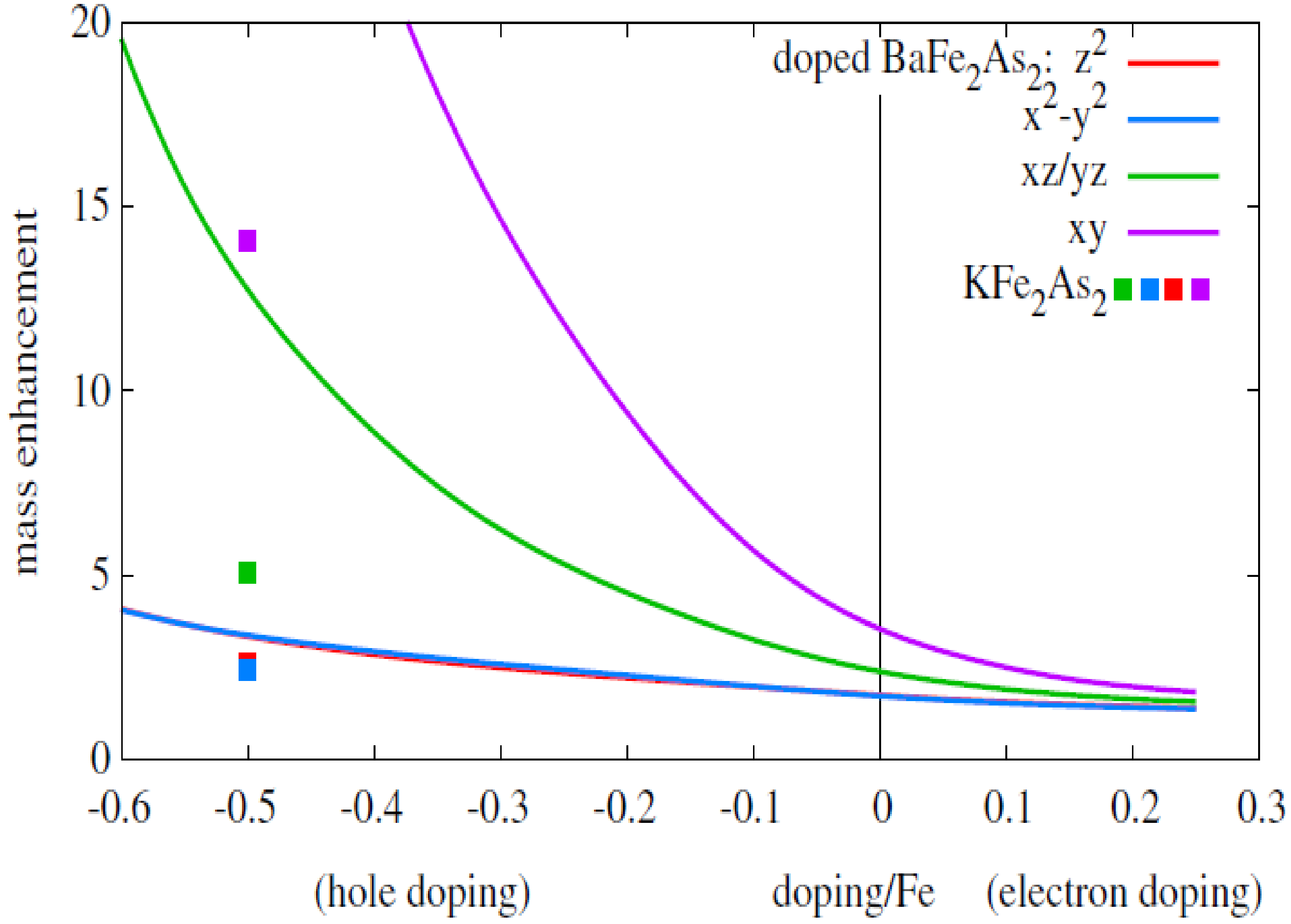


M. Watson et al, PRB 2017

No xz weight!!!!!

# Are renormalizations found from fit sensible?





“Error bars” consistent with SC gap fit

Note a) xy must be smallest

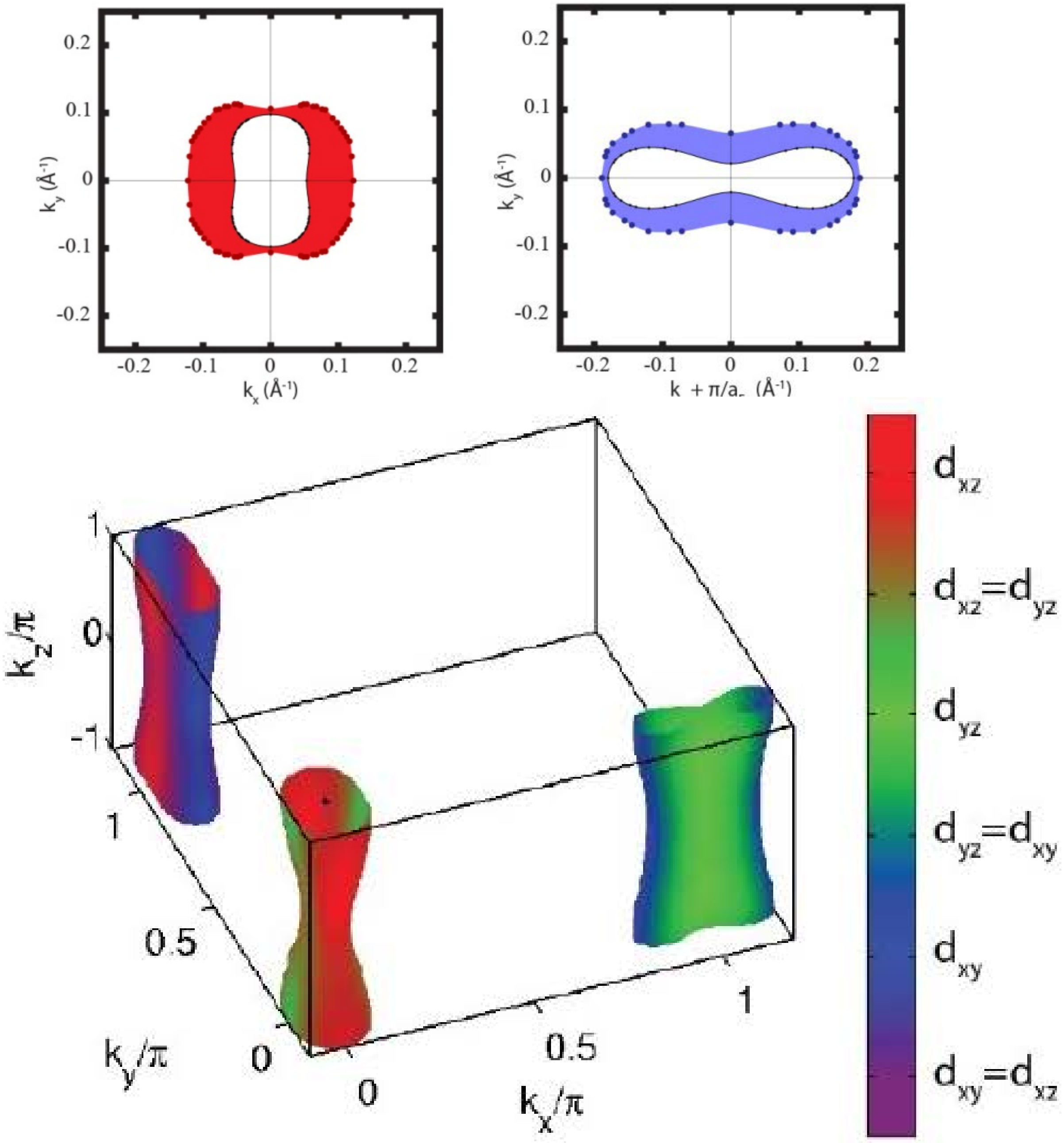
b) xz, yz, must be quite different

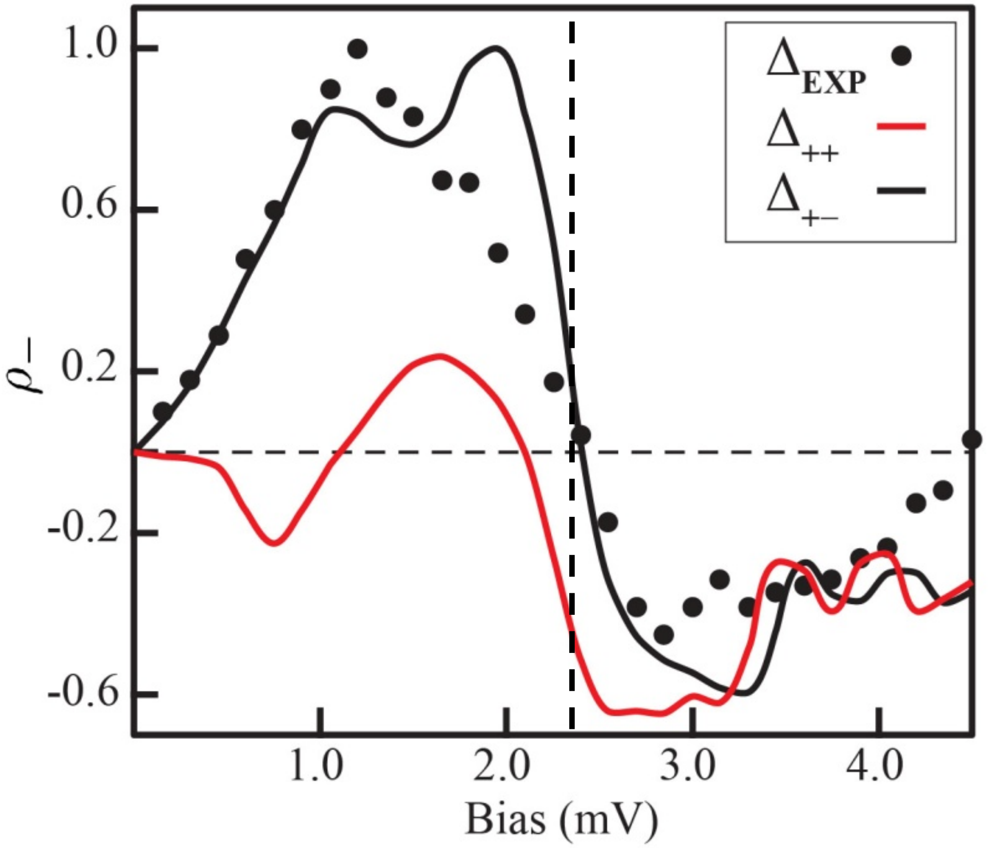
Cf. Yu et al arXiv 2018

# New technique to detect gap sign change from QPI: FeSe

## Is the SC state $s_{++}$, à la DL Feng?

$$\boldsymbol{\delta}\rho_-(E) = \sum_{\vec{q}_{inter}} \boldsymbol{\delta}\rho_-(\vec{p}_1 + \delta\vec{q}, E)$$



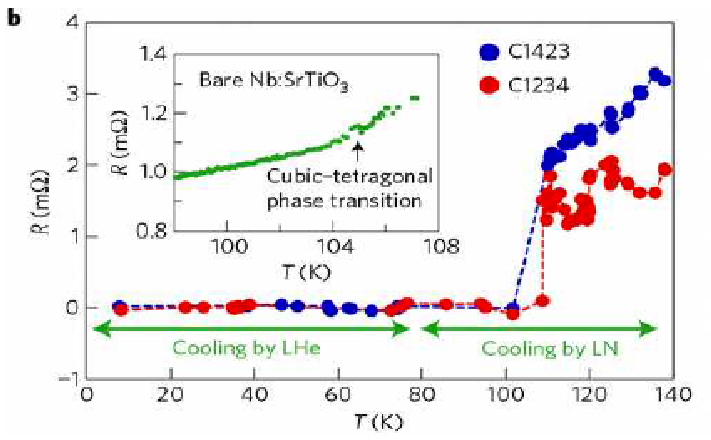


No zero crossing between gaps, as predicted for sign-changing SC:

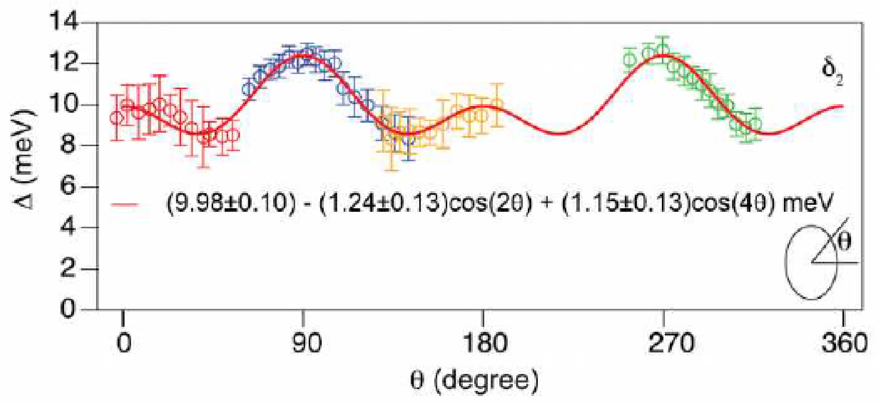
$\Delta(\vec{k})$ changes sign between the hole-like and electron-like pocket.

Sprau et al Science 357, 75 (2017)

# Other systems: FeSe monolayer

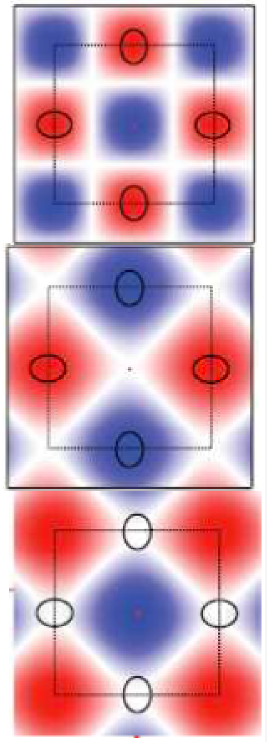


Ge et al. Nat. Mater. **14**, 285 (2015)

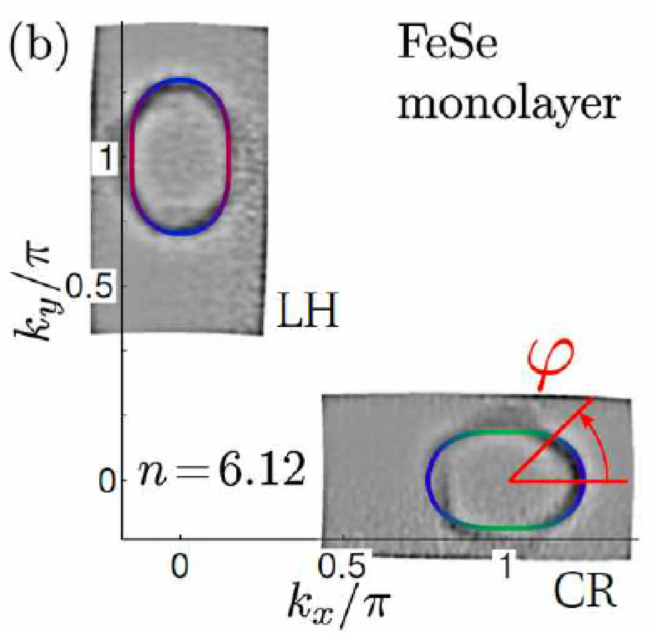


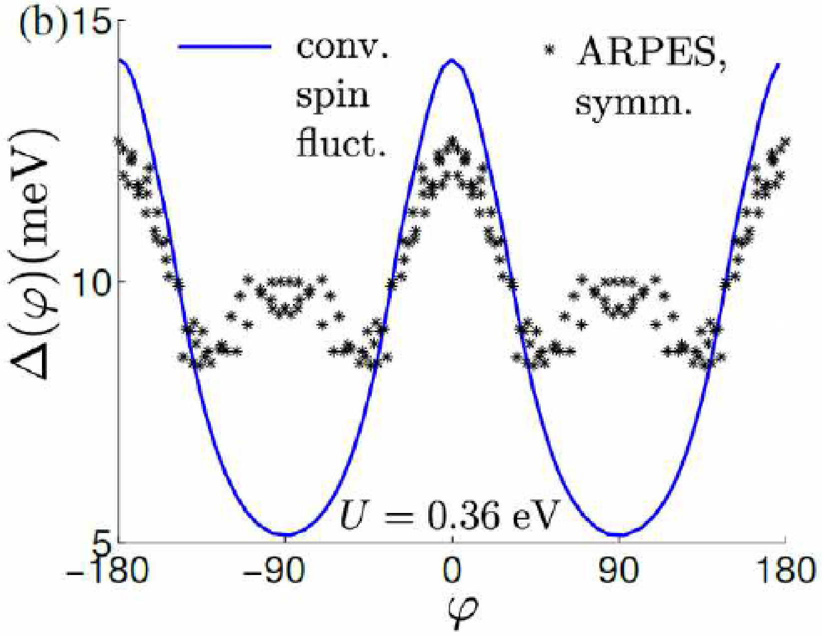
Zhang, et al., Phys. Rev. Lett. **117**, 117001 (2016)

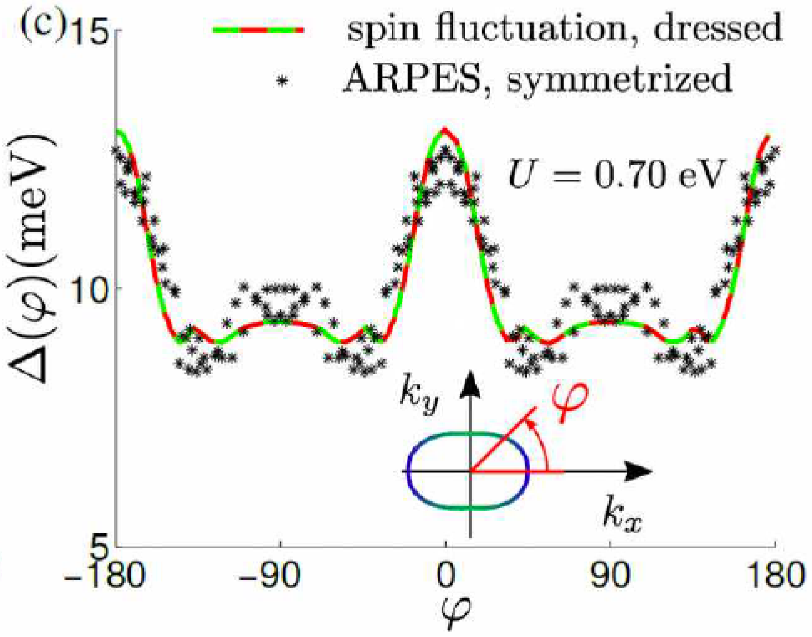
No explanation of the two maxima structure by conventional approaches



- Same model, but: 2D, no orbital order, rigid shift







$$\{\sqrt{Z_l}\} = [0.4273, 0.8000, 0.9826, 0.9826, 0.700]$$

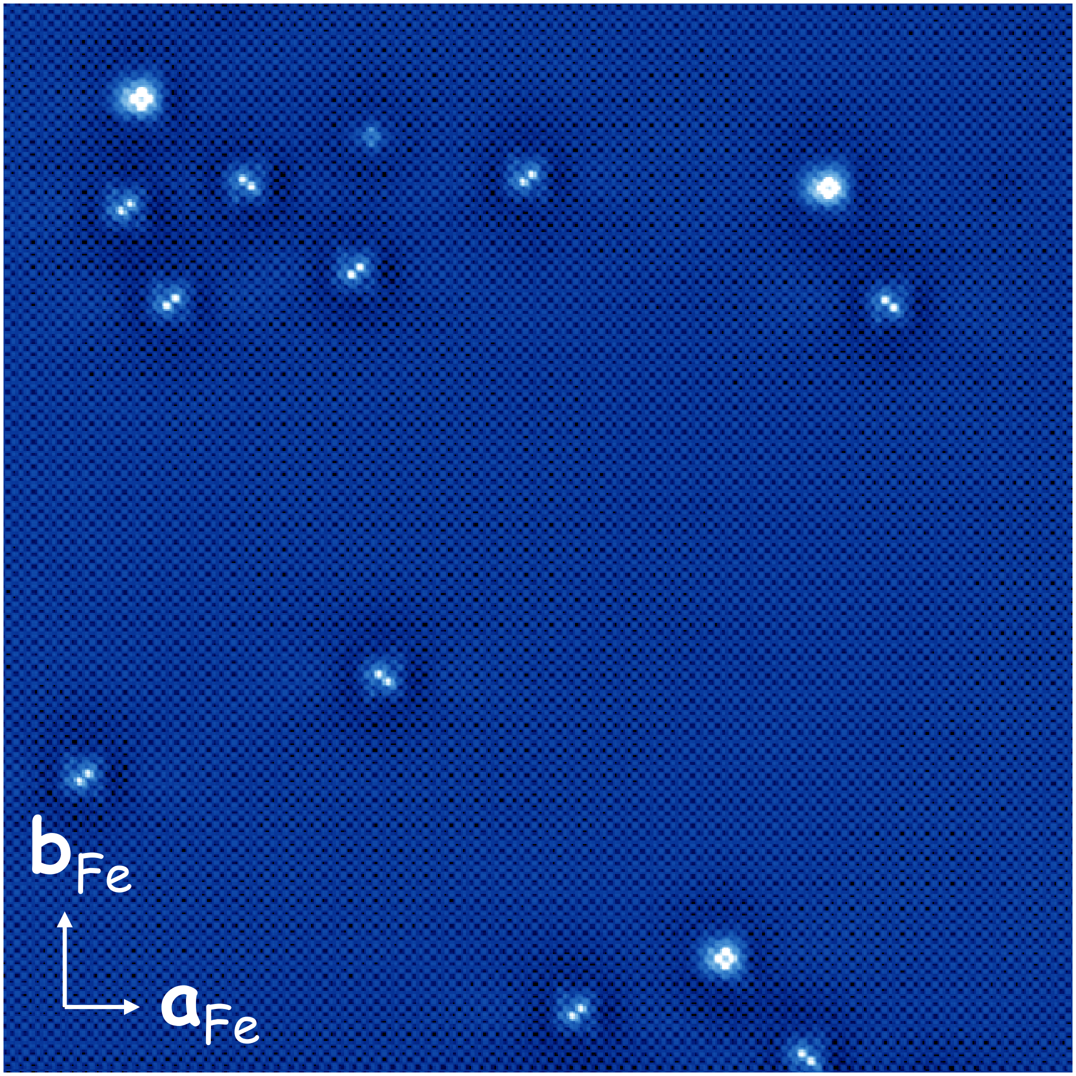
$$(d_{xy}, d_{x^2-y^2}, d_{xz}, d_{yz}, d_{3z^2-r^2})$$

Kreisel et al PRB 2017

# Quasi-particle interference in FeSe

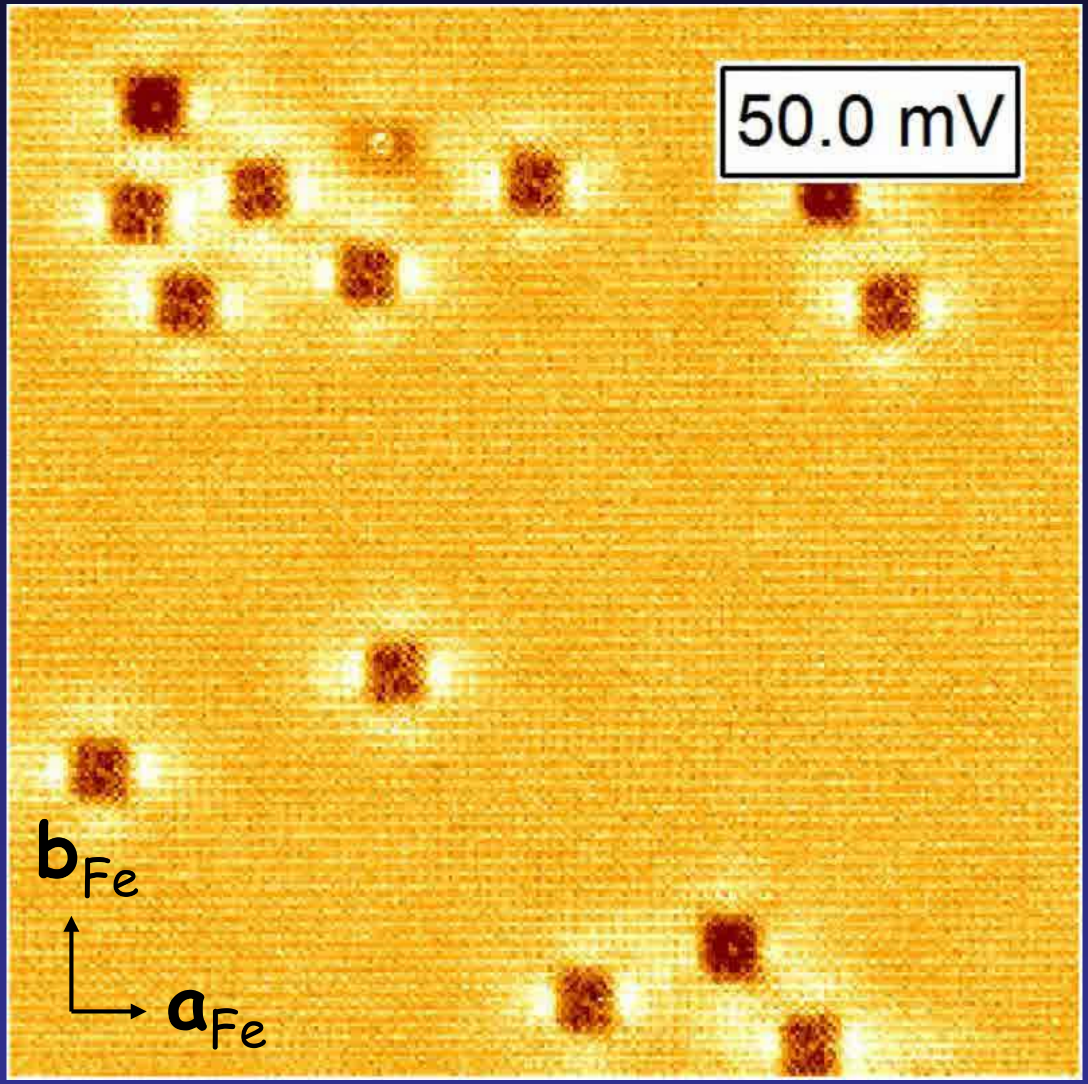
S. Kasahara *et al.*, PNAS **111**, 16309 (2014).

Topograph $T$ ~ 1.5 K



45 nm × 45 nm, +50 mV/100 pA

*dI/dV/(I/V)*



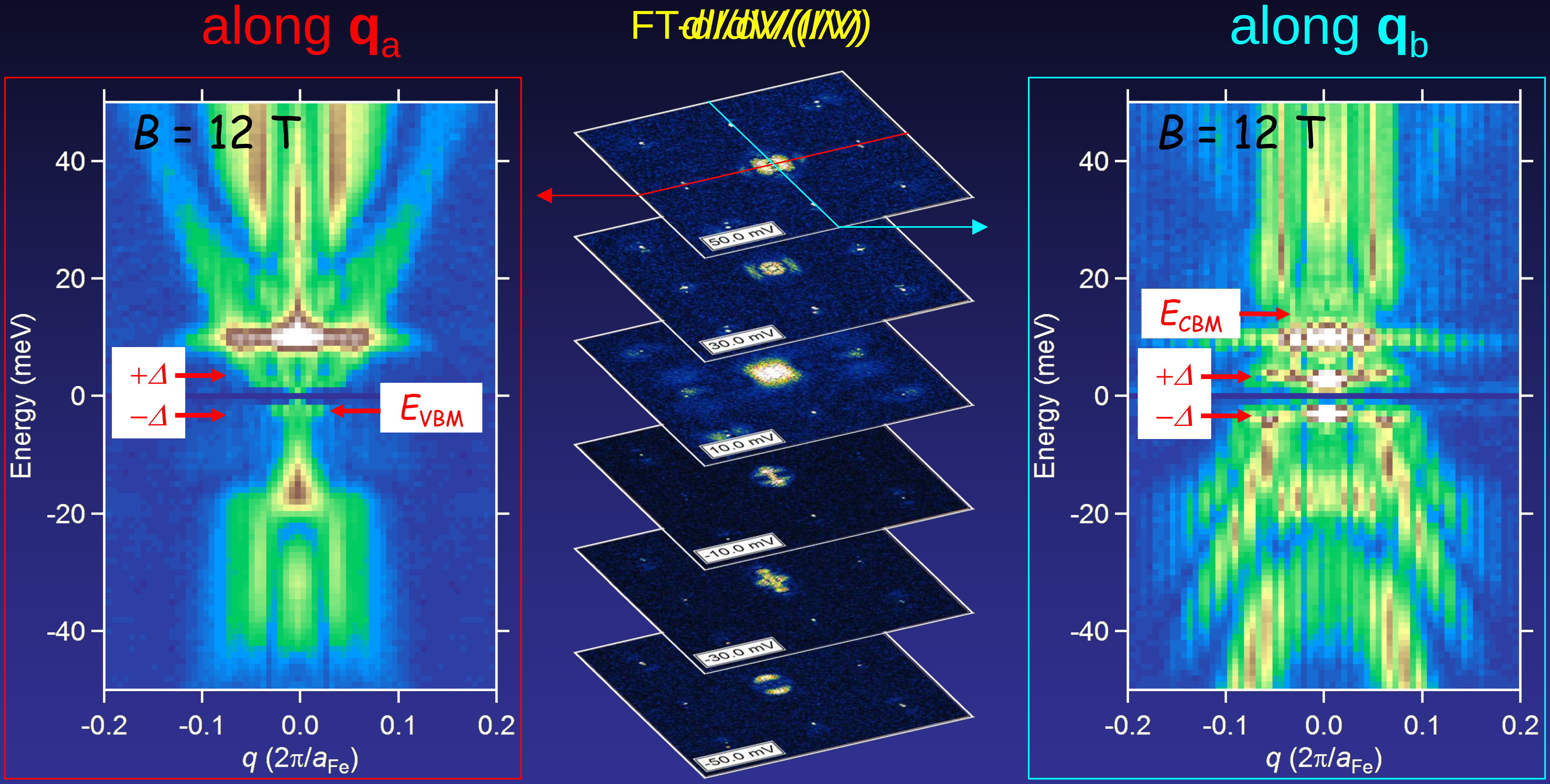
Unidirectional dispersing features

cf. NaFeAs: E. P. Rosenthal *et al.*,
Nat. Phys. **10**, 225 (2014).

Thanks to T. Hanaguri

# Rotation of QPI patterns at high energy

S. Kasahara *et al.*, PNAS **111**, 16309 (2014).



along $\mathbf{q}_a$

FT-*dI*/*dV*(*I*/*V*)

along $\mathbf{q}_b$

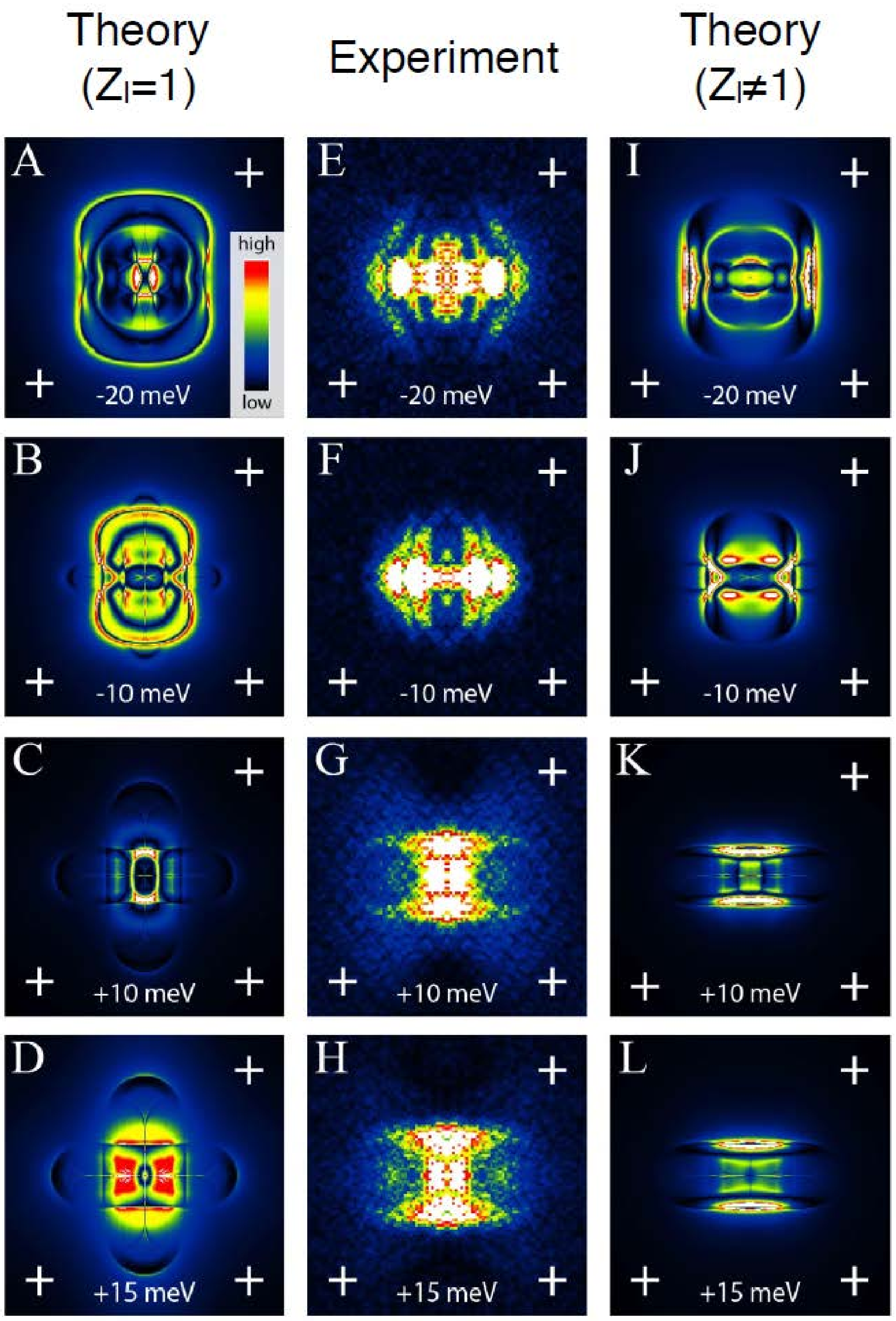
Electron-like

Hole-like

- Orthogonal electron- and hole-like dispersions
- Extremely small $|E_{BM} - E_F| \sim D$, long $\lambda_F \sim x$

Thanks to T. Hanaguri

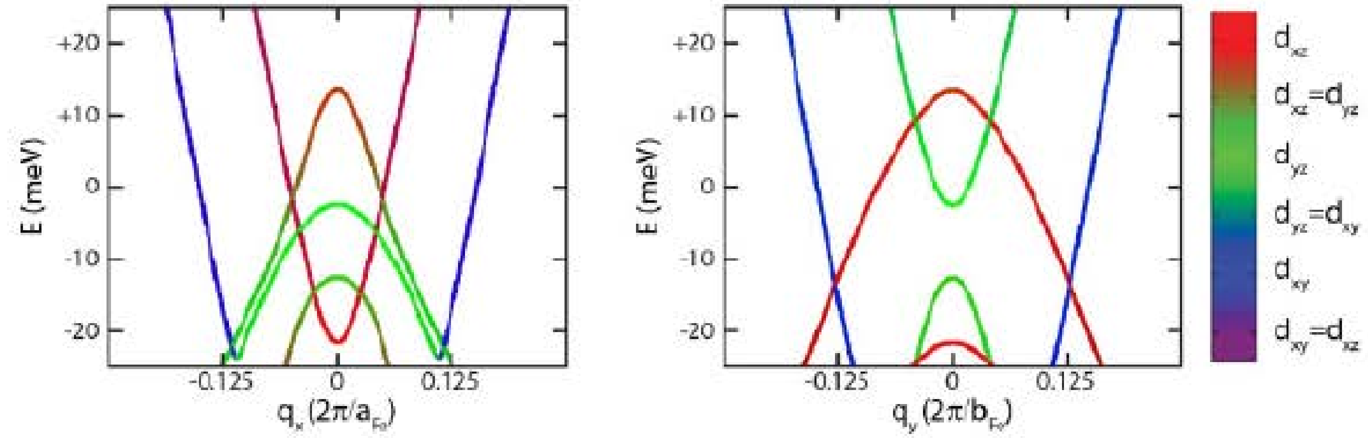
# Consistency with other observables?
# “Normal state” QPI



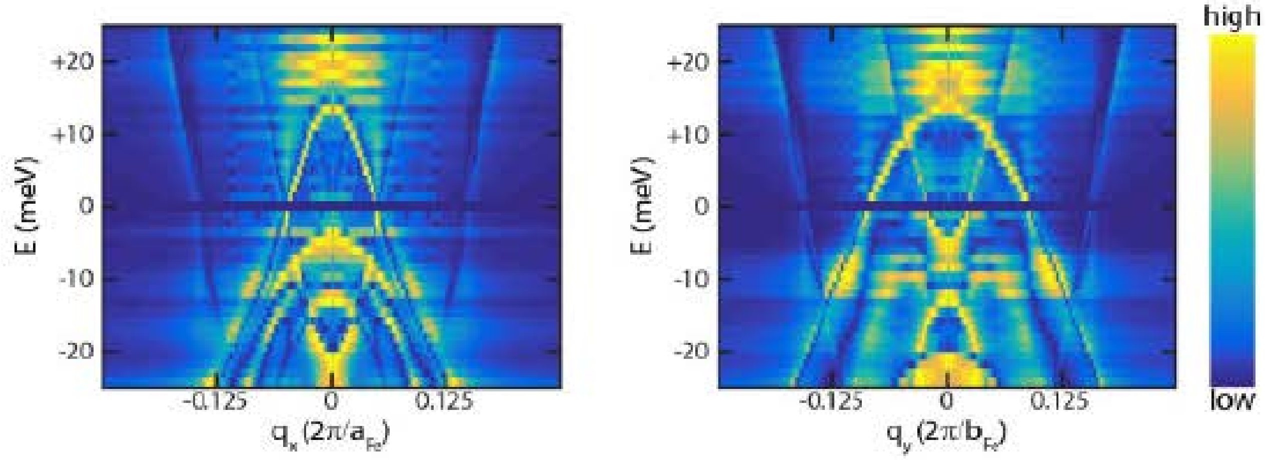
*Same Z’s as*
*Sprau et al.*

Note 1D character seen well above energies E~$T_s$

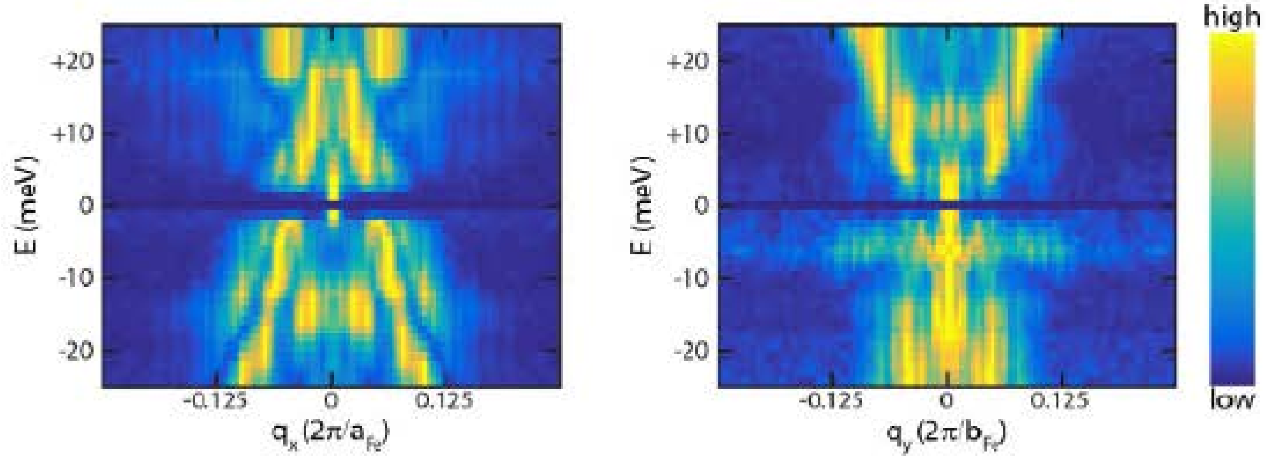
Kostin et al
ArXiv:1802.02266,
Nat. Mat. 2018



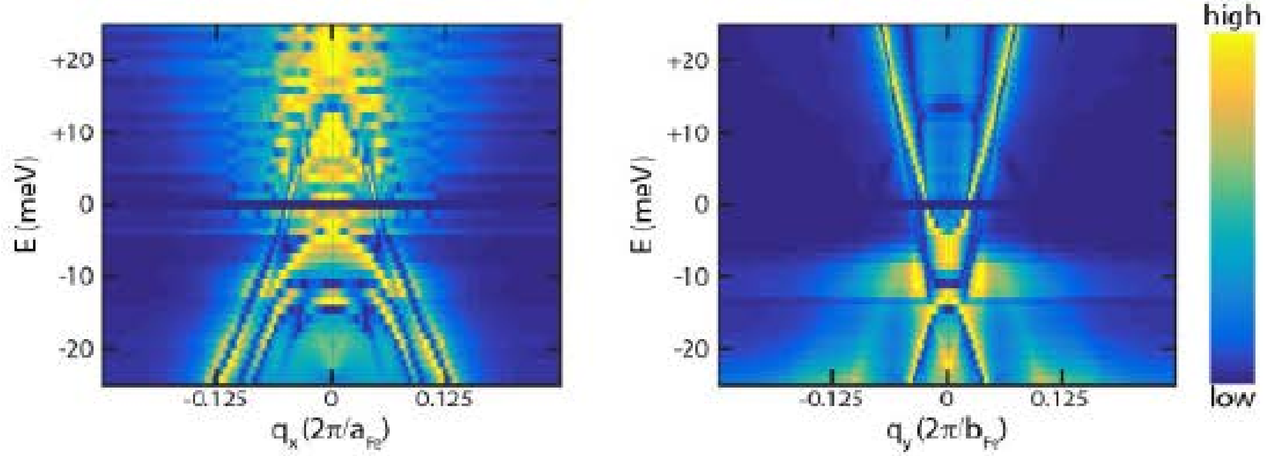
Theory: QPI maxima as given from the band structure



Theory: QPI, all Z=1



Experiment. See also papers by T. Hanaguri et al. (S. Kasahara et al, PNAS 2014)



Theory: QPI, orbital selective Z

# Friedel oscillations rotate around a single Fe-centered defect

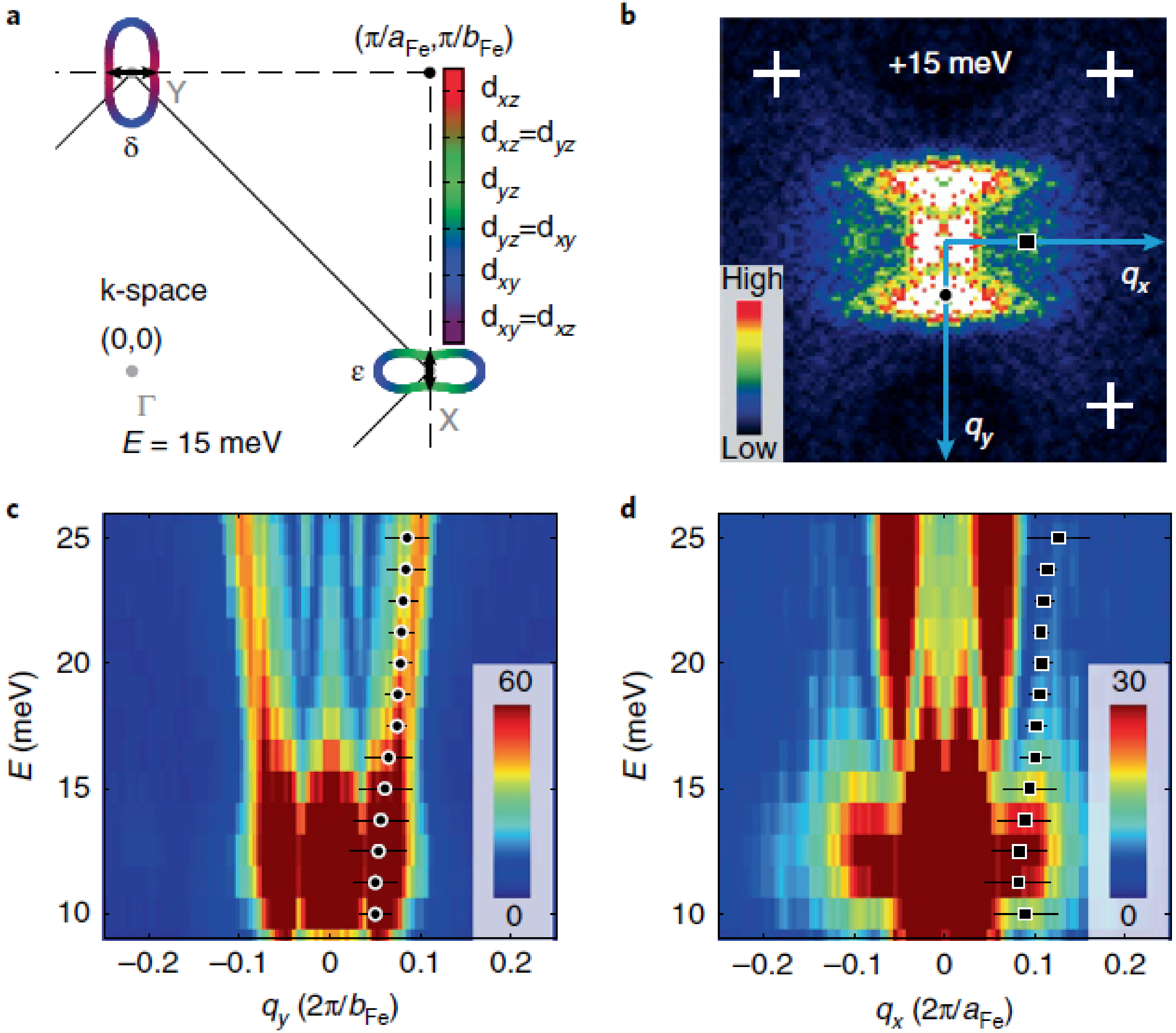
Theory Z=1

Expt.Kostin et al

OS Theory Z<1

Remarkable rotation of $C_2$ pattern with bias is due to orbital differentiation – dominance of yz states

Where is the d pocket?



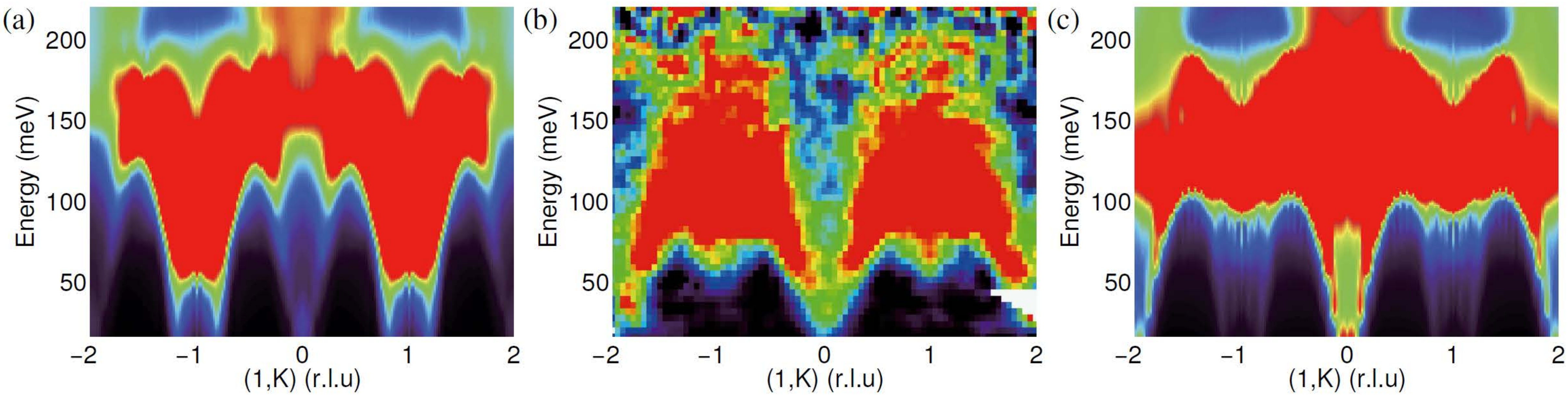
# Inelastic neutron scattering (twinned)

## RPA dynamical susceptibility with and without qp weight renormalizations

No Z’s: π,π fluctuations
too strong

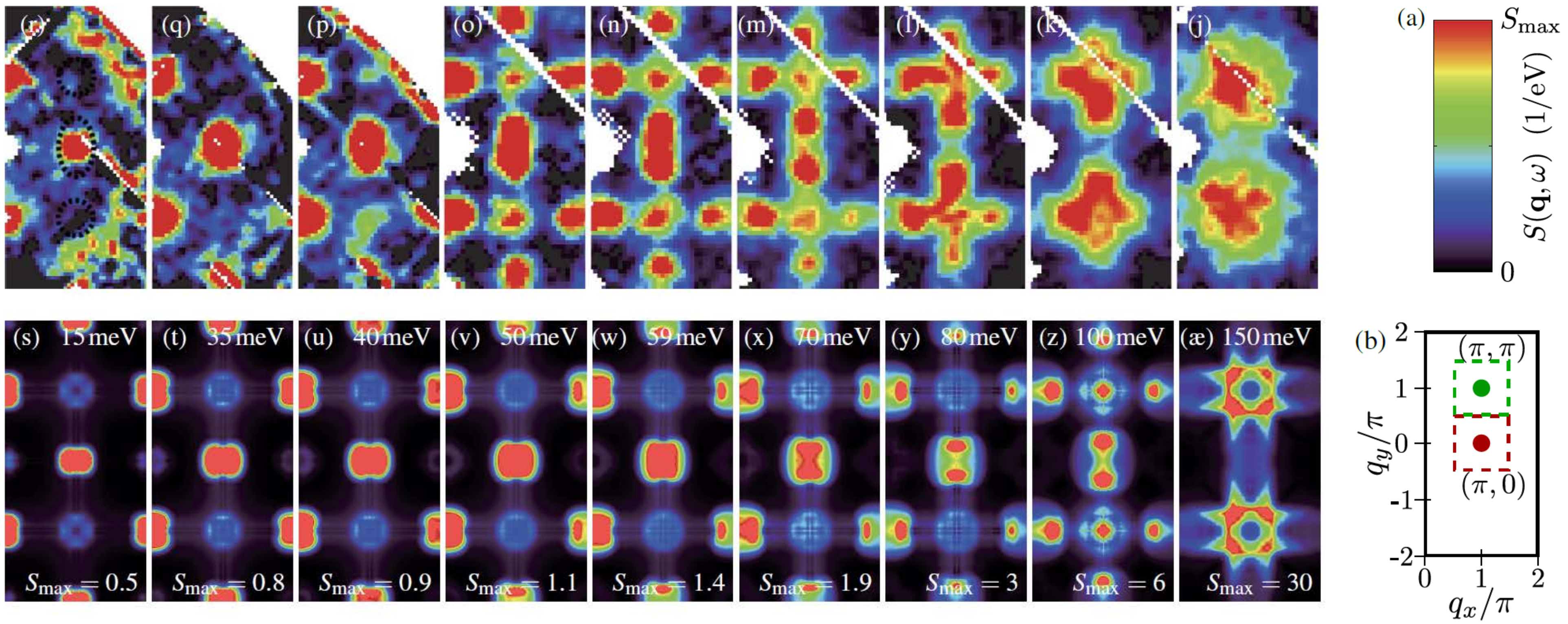
Q. Wang et al
Nat. Comm. 2016

With Z’s: π,π fluctuations
weakened at low E: spin gap

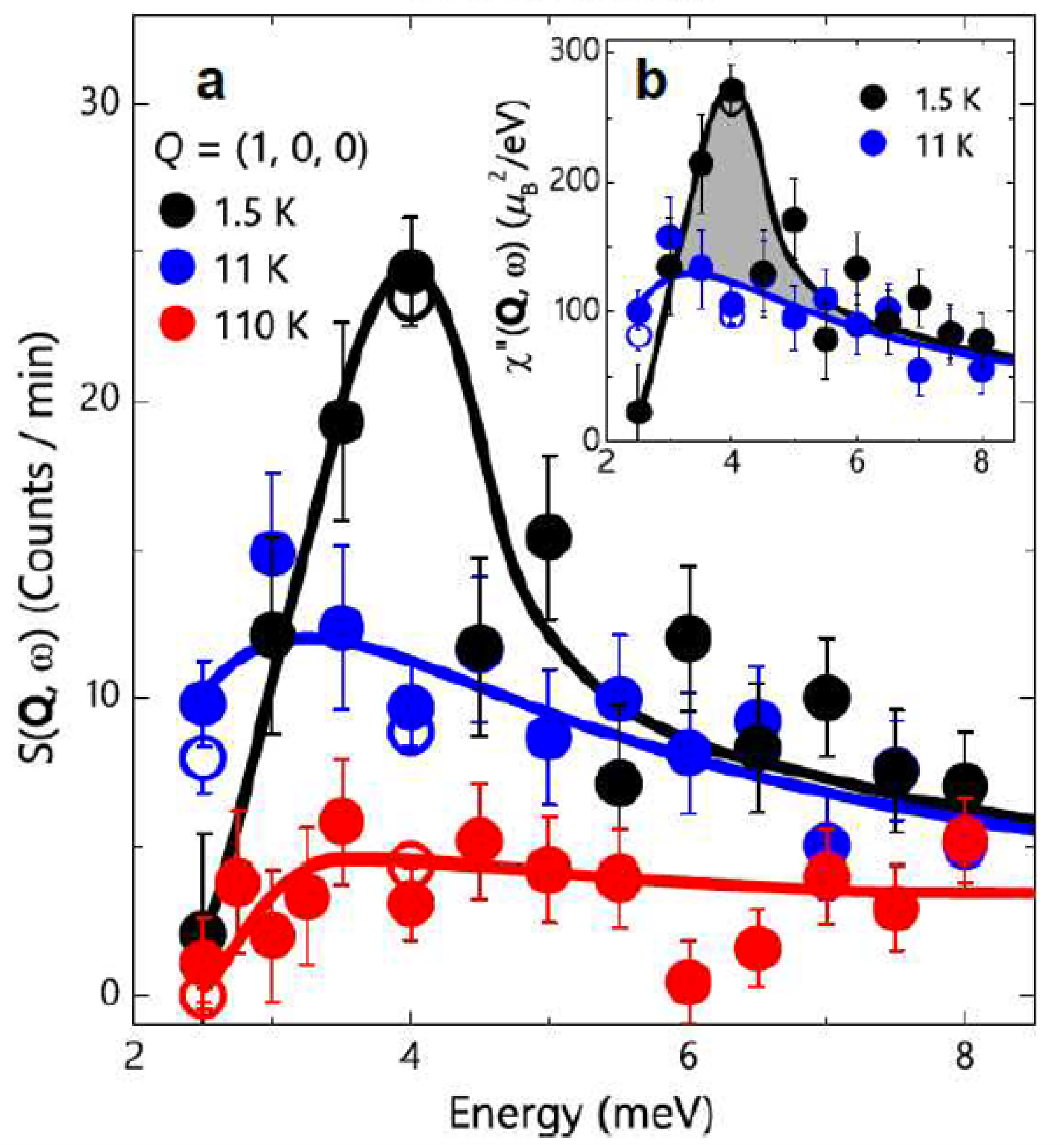


expt

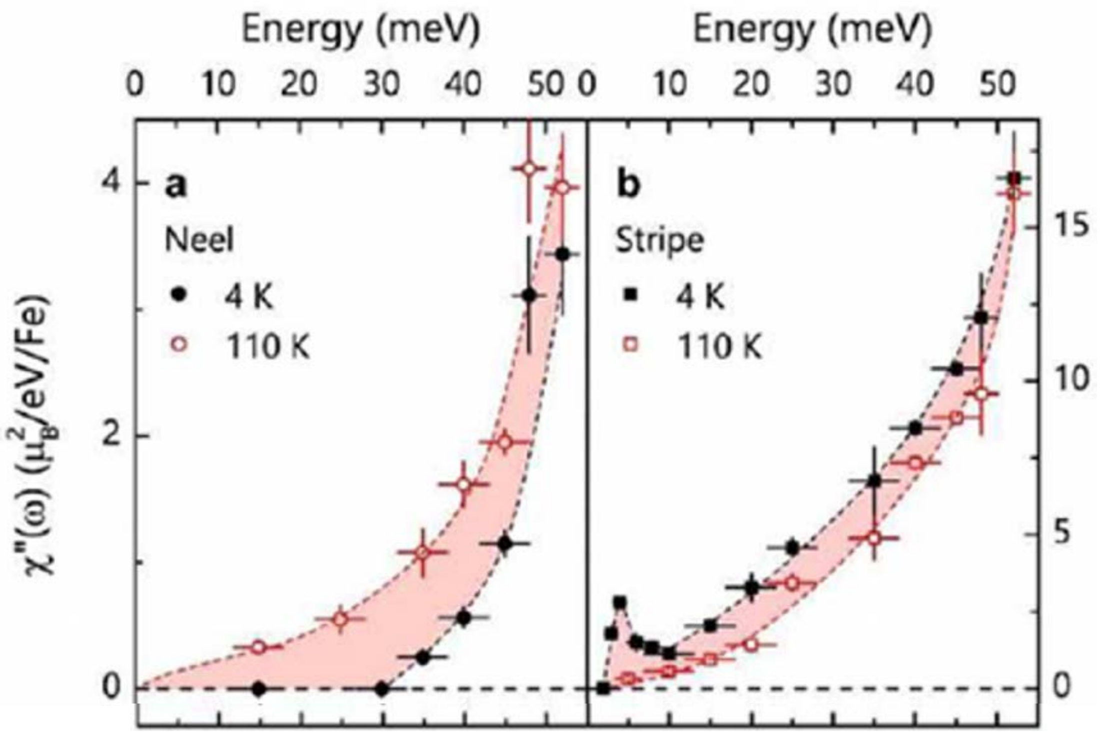
thy w/ Z’s

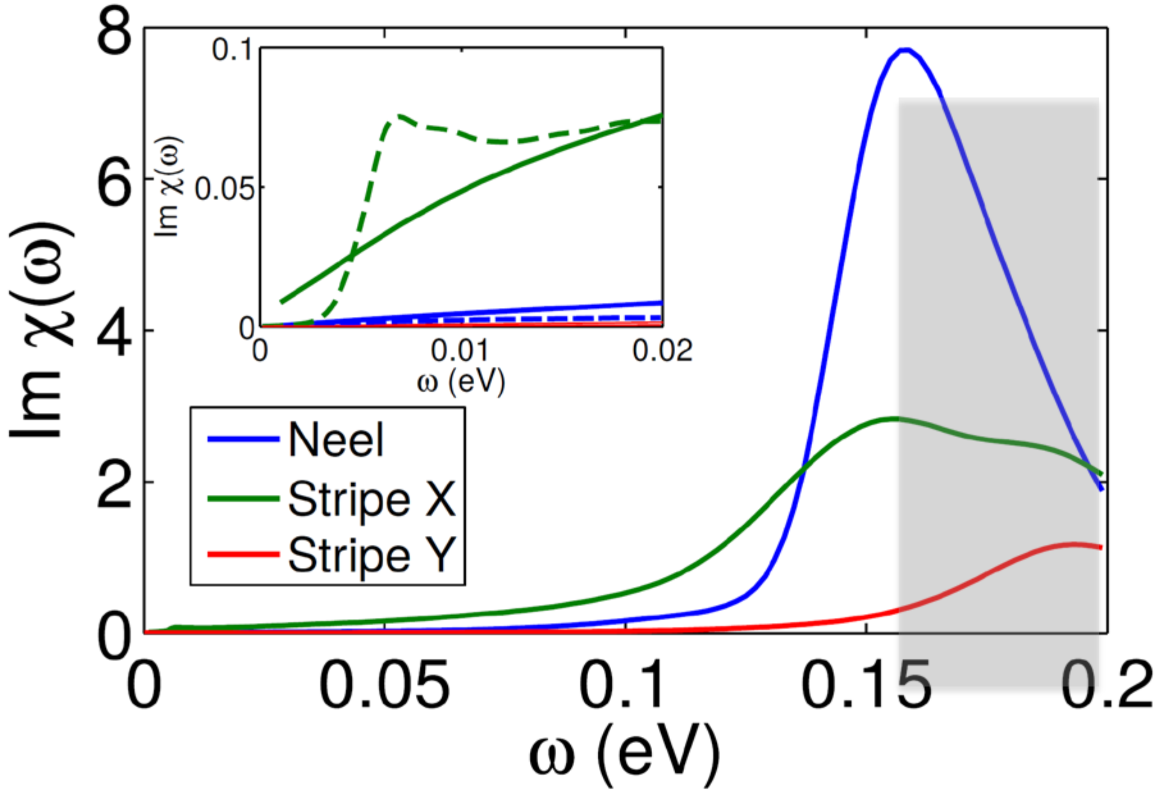


# Inelastic neutron scattering (twinned): SC state



Wang *et al.*, Nature Materials **15**, 159 (2016)

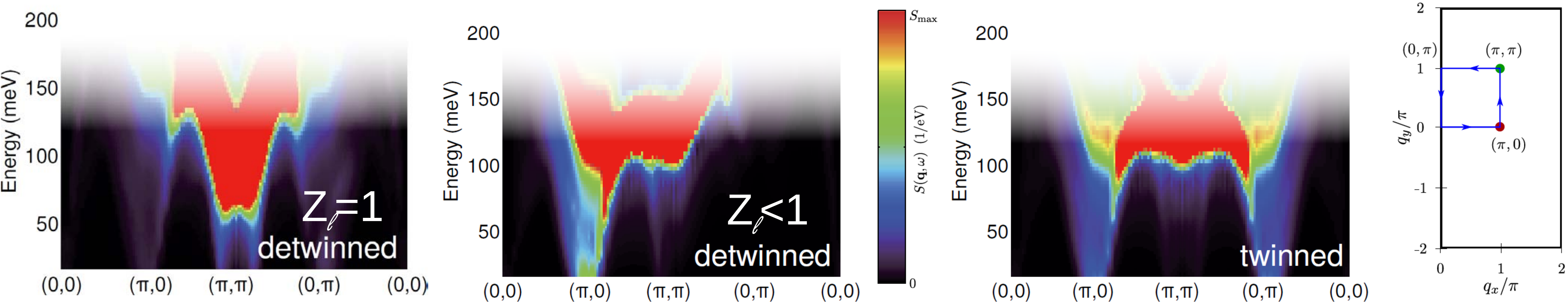




**A. Kreisel, et al PRB 2015; arXiv:1807.09482**

Quasiparticle weights make π,π excitations commensurate, suppress intensity at low T – “spin gap”

# Inelastic neutron scattering: predictions for untwinned samples



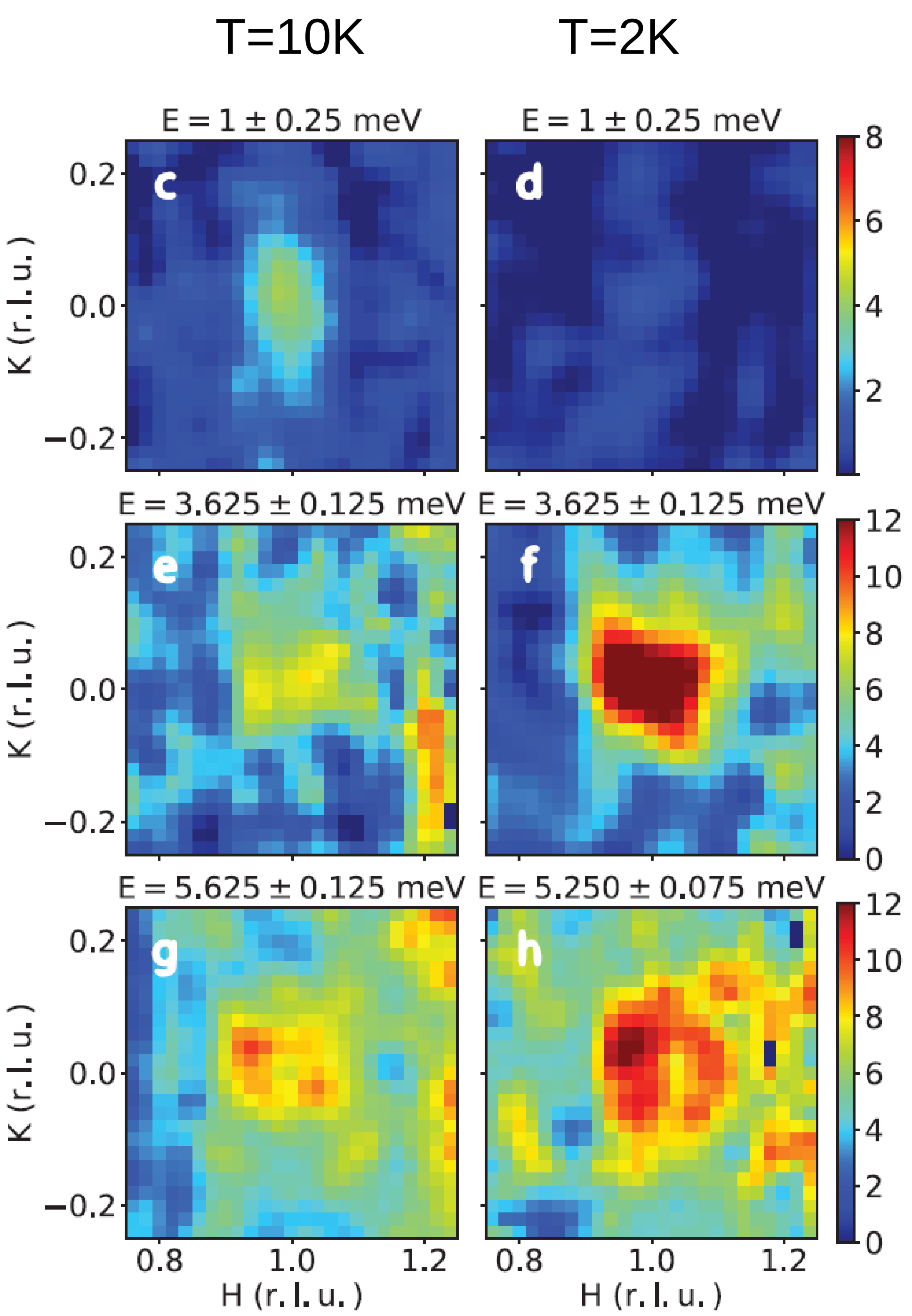
Remarks:

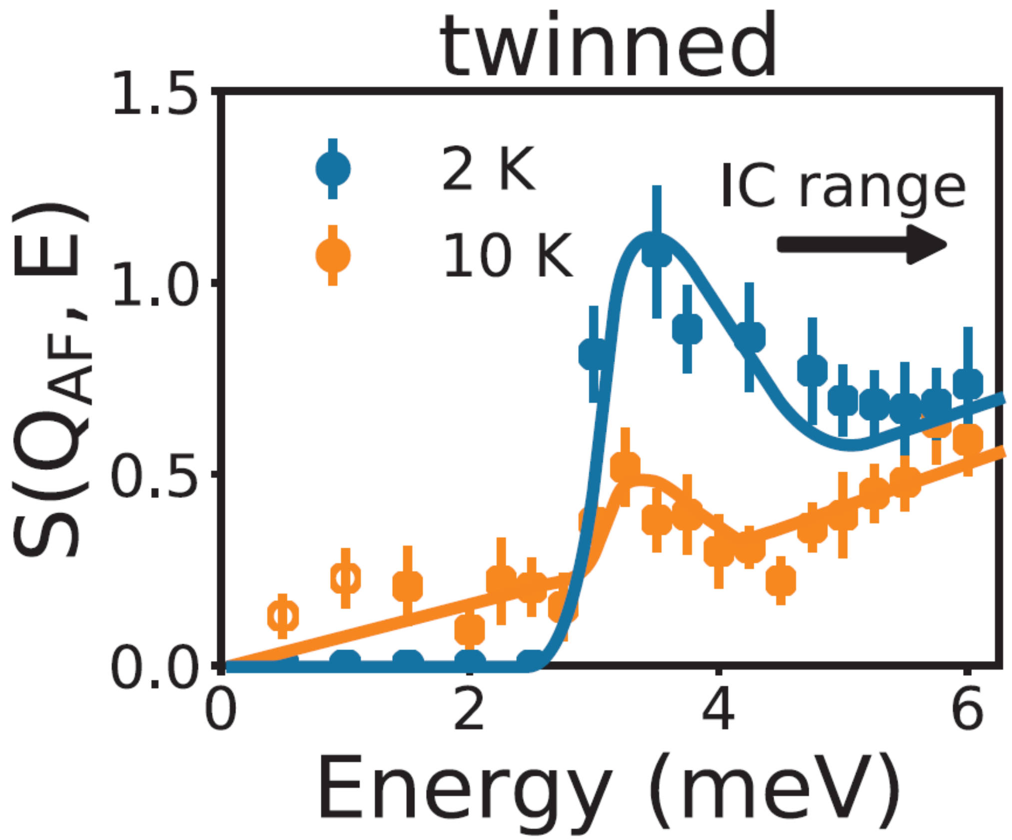
- Current approach breaks down at higher energies because 1) band structure incorrect; 2) Z-factors increase w/ energy, not accounted for; 3) RPA inadequate
- Virtually no weight at (0,π) expected at low energies, in contrast to unrenormalized band.

See also: She et al arXiv 2017, Lai et al 2017 – predicted strong π,0/0,π anisotropy in localized models

# Inelastic neutron scattering: recent results for *twinned* samples

Chen et al 2018 (Dai & Broholm groups; Kreisel, Andersen and PJH)

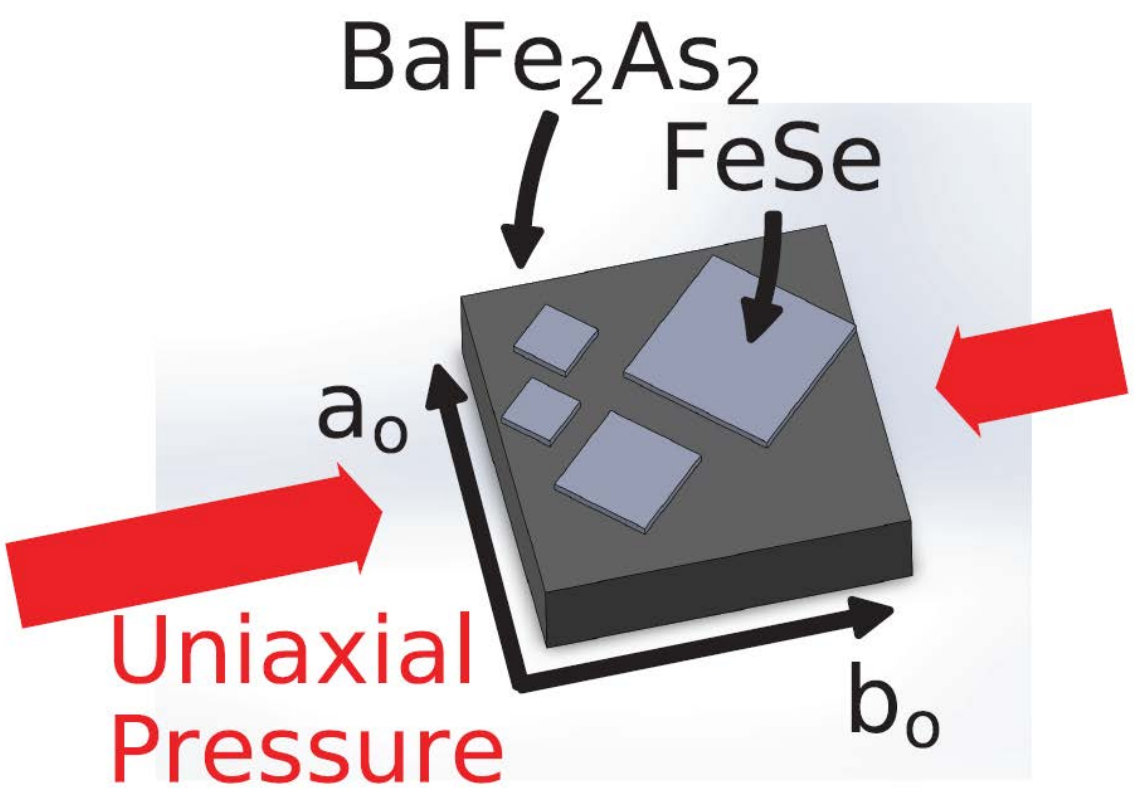


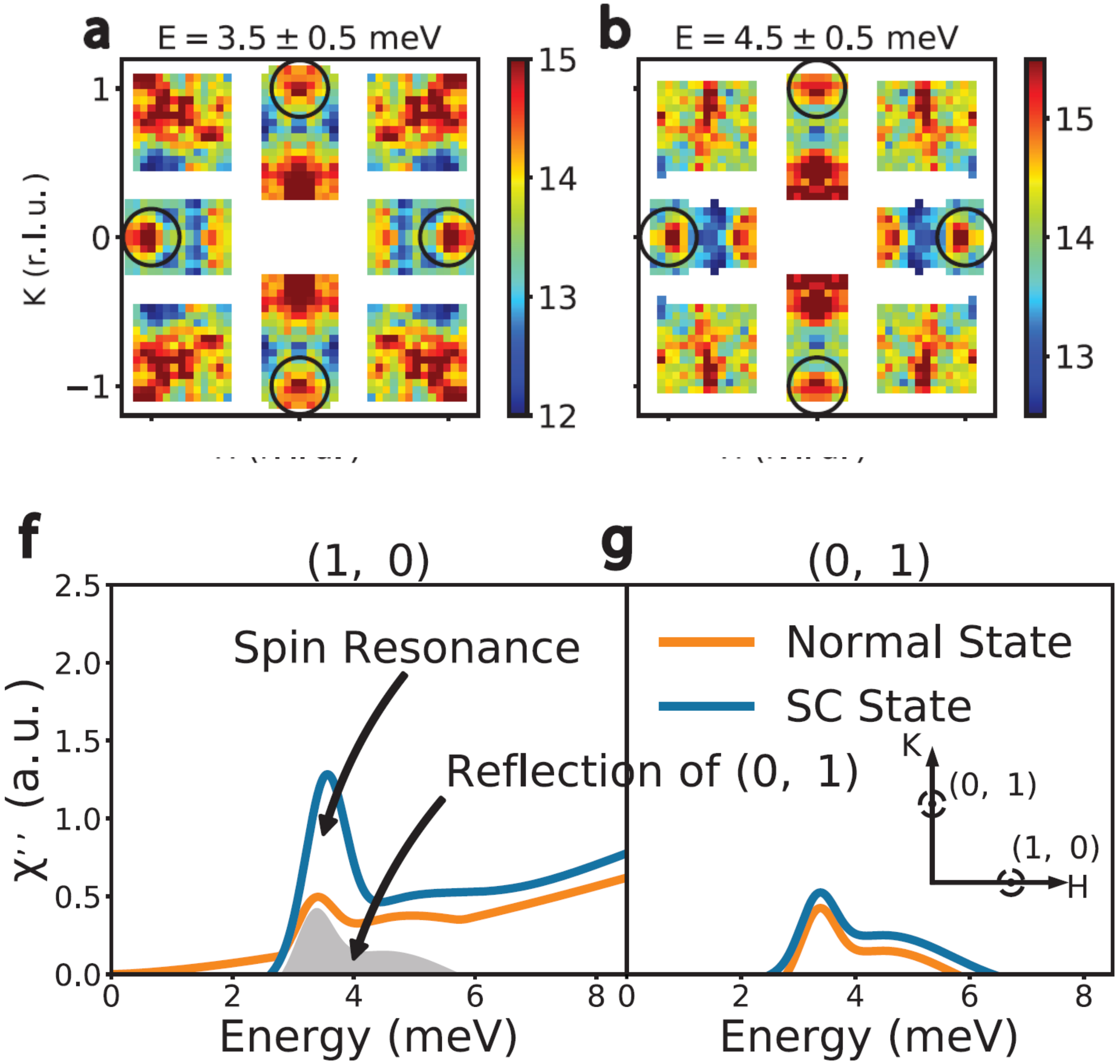


No low-E spin gap except in SC state
Incommensurate ringlike excitations at ~5mev
(near resonance energy)

# Inelastic neutron scattering: recent results for *untwinned* samples

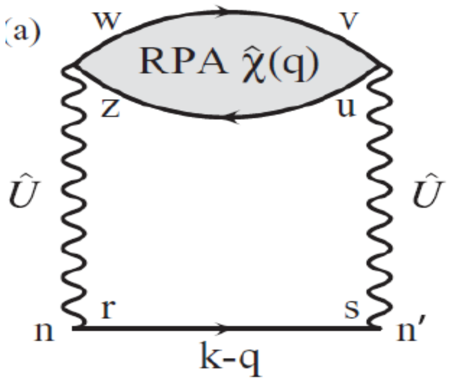
Chen et al 2018 (Dai & Broholm groups; Kreisel, Andersen and PJH)

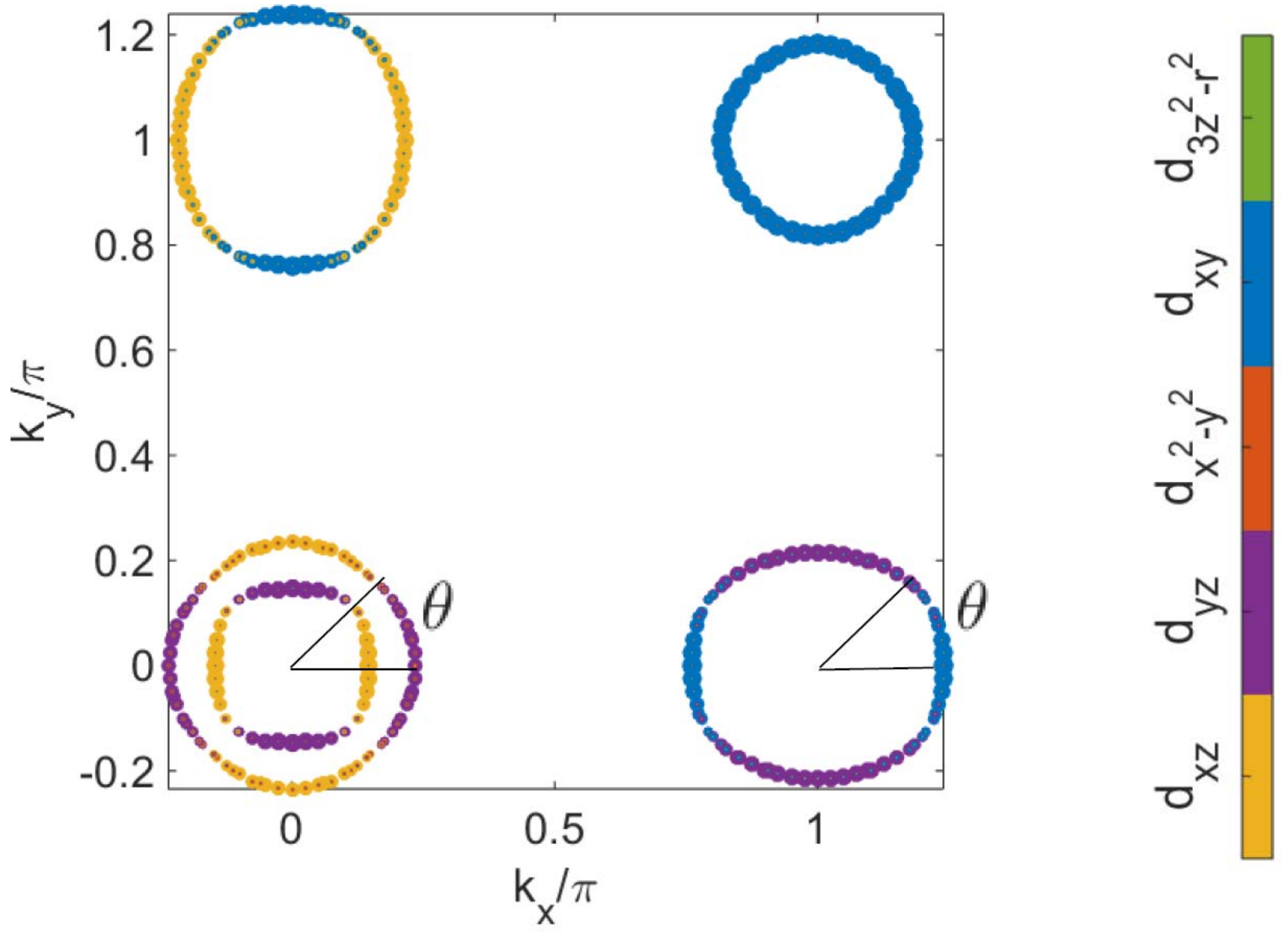


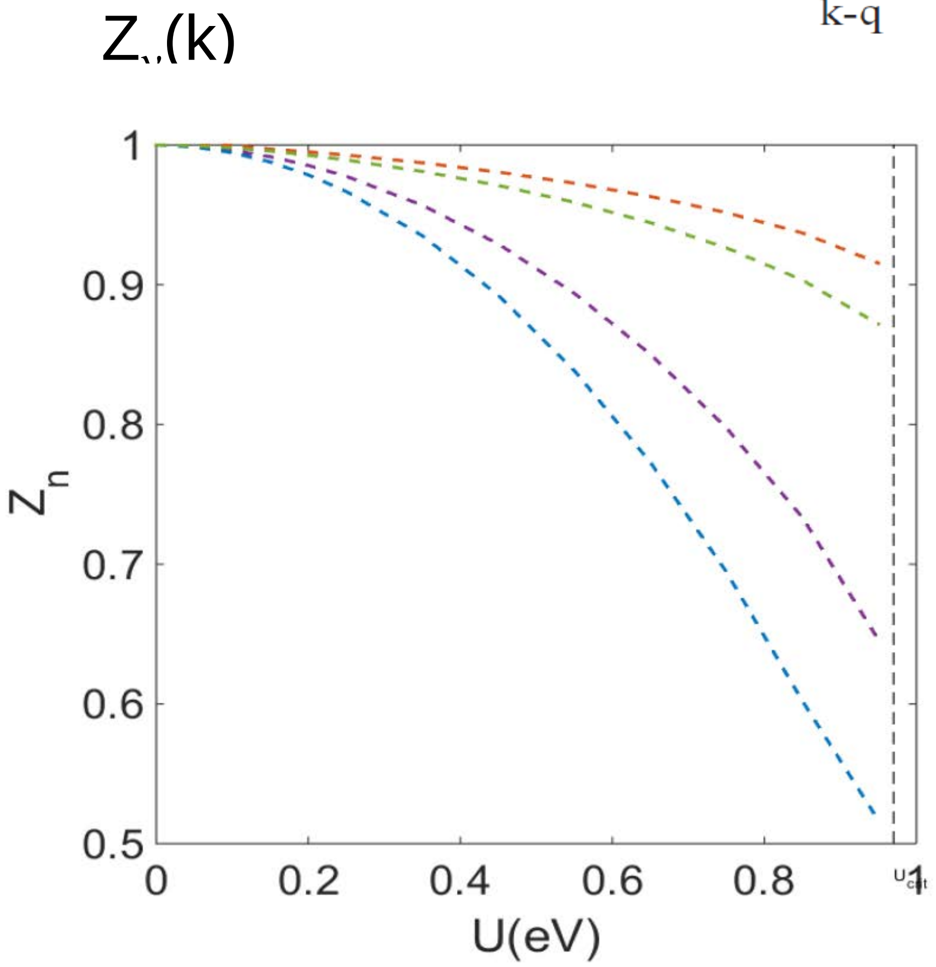


# Momentum-dependence of self-energy

Ikeda et al 2009 band structure for 1111 $n = 6.0$







working on FeSe…

# Conclusions/questions

1) FeSe exhibits orbital-selective Cooper pairing, crucial for fundamental theory of Fe-based superconductivity

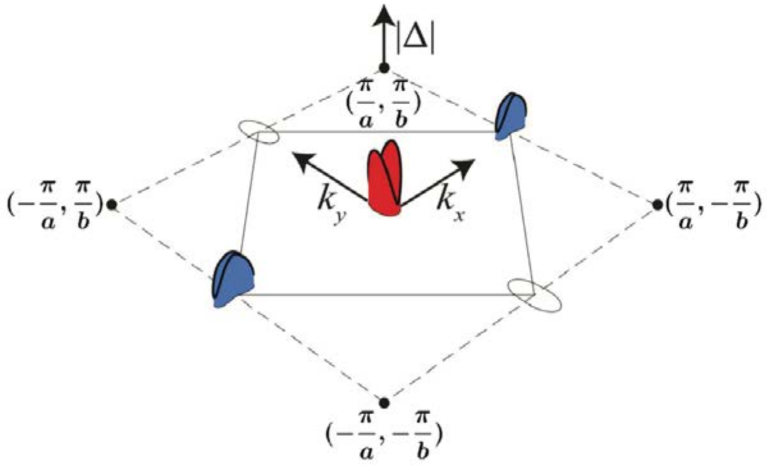
2) Modified spin-fluctuation theory that allows for orbitally dependent quasiparticle weights provides a quantitative description of normal state excitations, gap structure

3) Same procedure works for Fe/STO monolayers, LiFeAs

4) Novel QPI analysis suggests sign-changing states in FeSe, FeSe intercalates with electron pockets only

5) Strong anisotropy between p,0 and 0,pi spin fluctuations predicted in theory, seen in experiment, along with unusual localized mode.

6)



⟹

Superconductivity in Fe-chalcogenides has the same origin as Fe-pnictides – spin fluctuations

Can one achieve essentially the same story without xz/yz qp incoherence?
cf. Chubukov-Fernandes, Benfatto…