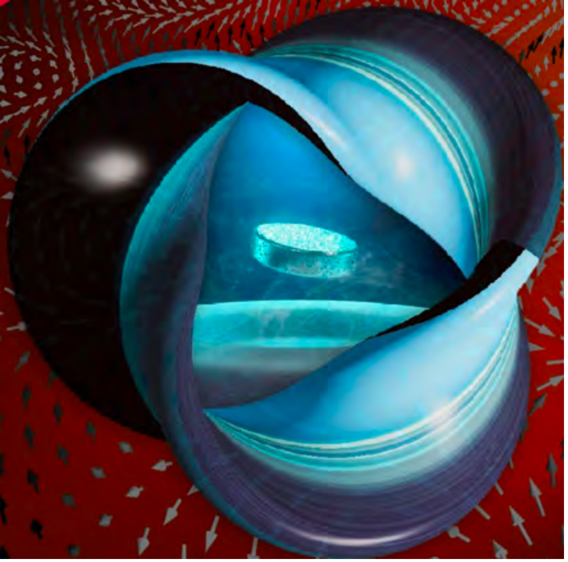
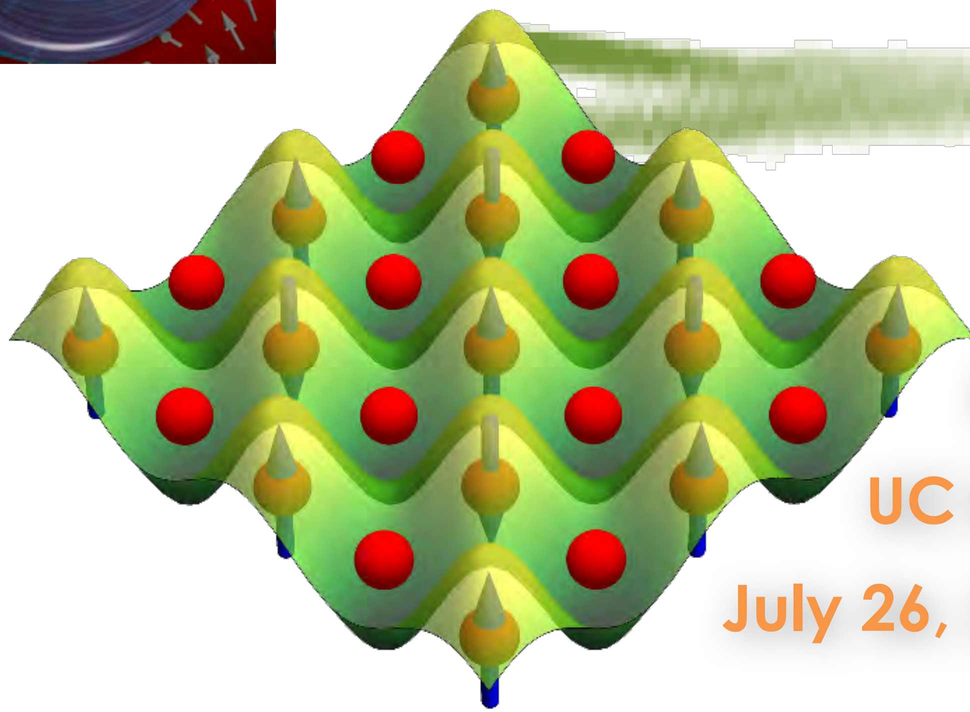


Finding Orders in Iron-based Superconductors

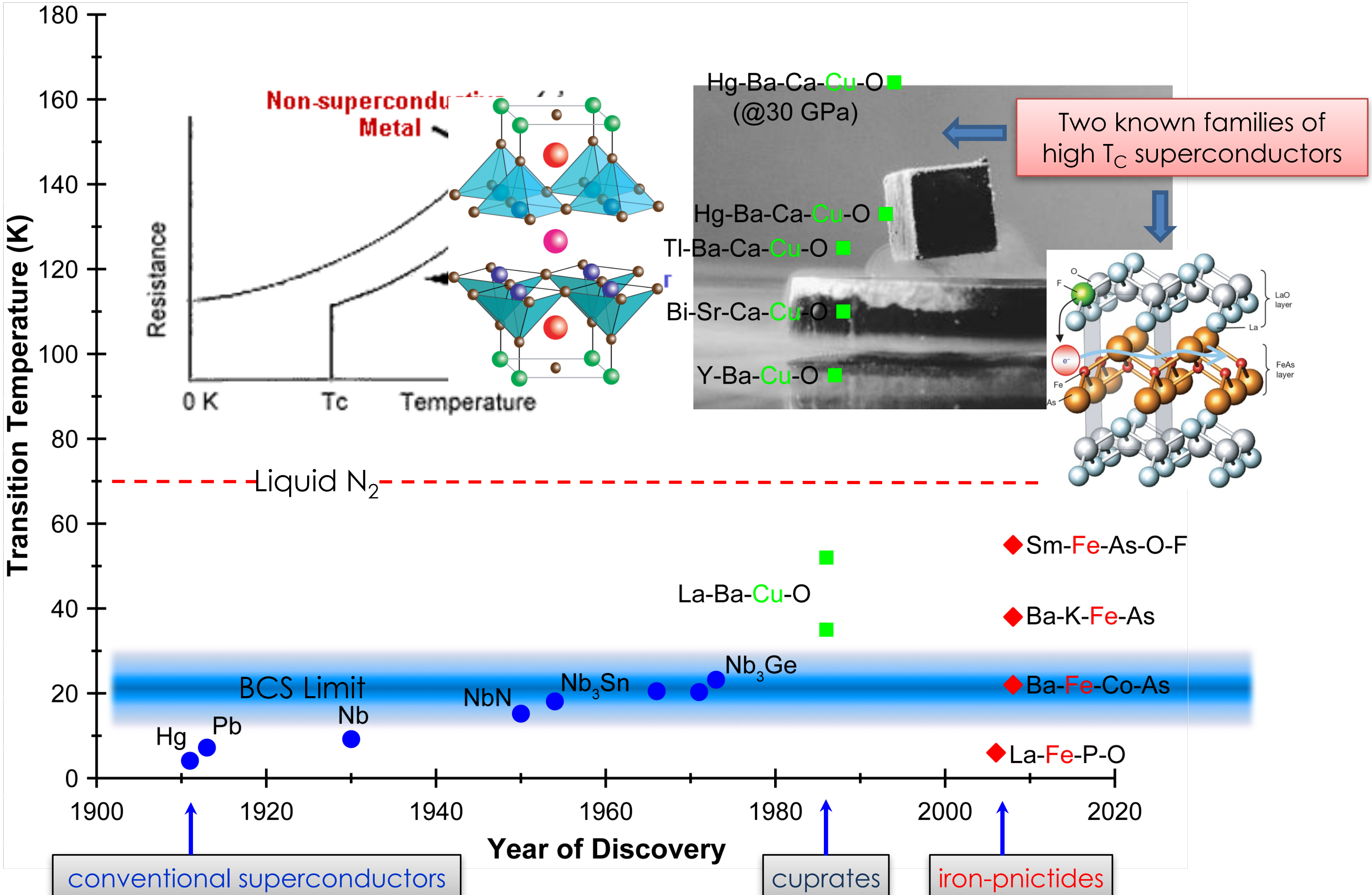


Ming Yi

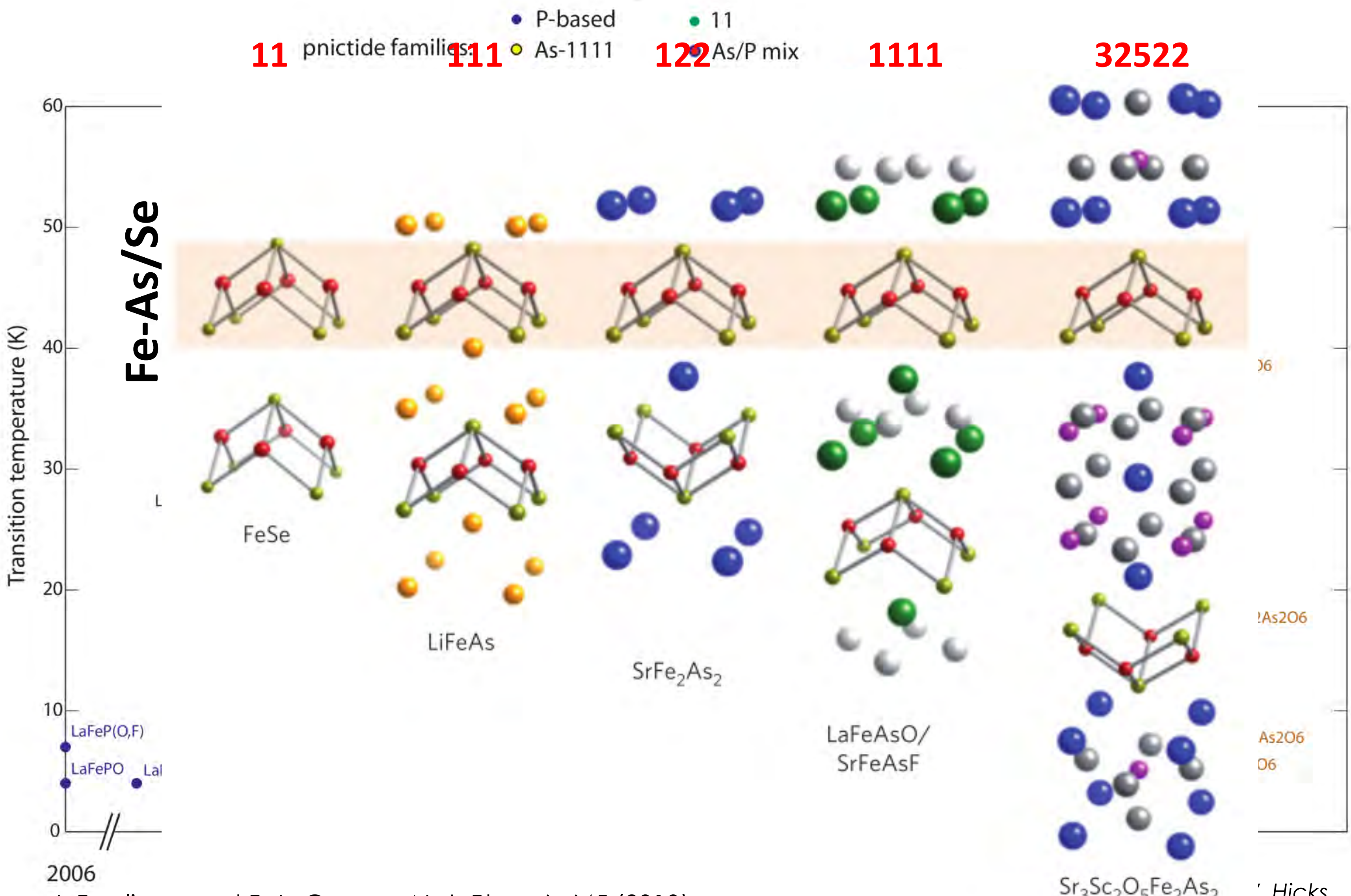
UC Berkeley

July 26, 2017

History of superconductivity



The families of iron-based superconductors



J. Paglione and R. L. Greene. Nat. Phys. 6, 645 (2010).

Outline

- Importance of *correlations* to superconductivity
  - Bandwidth-tuned superconductivity in $RbFe_2Se_2$
  - Overall correlation trends in FeSCs
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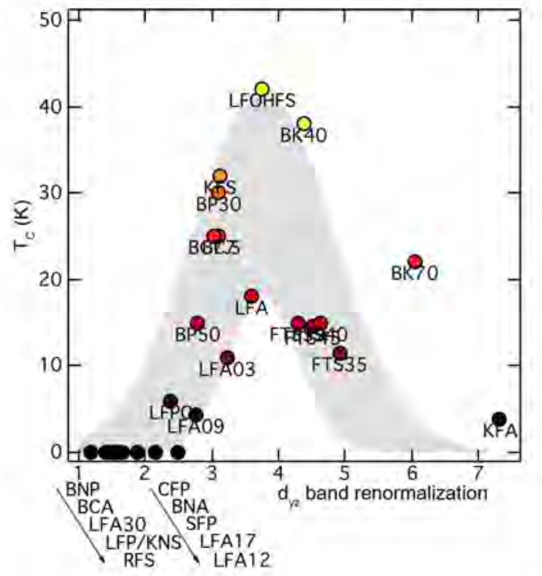
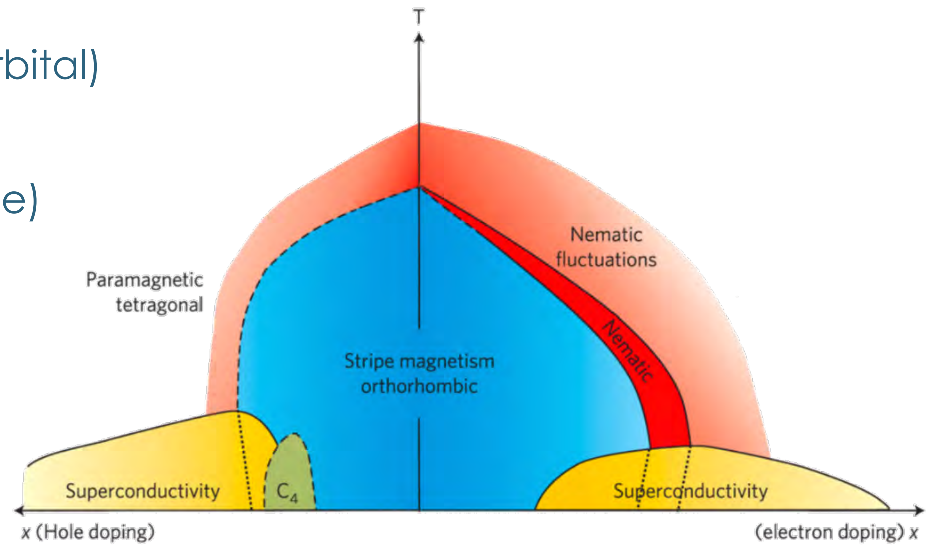
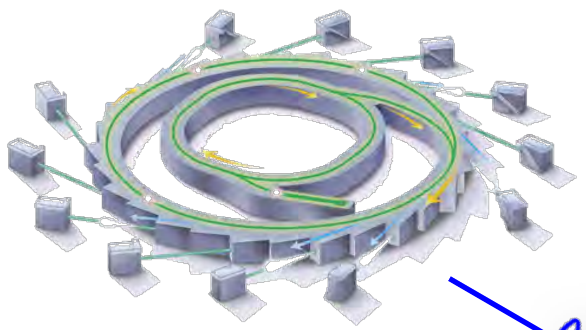
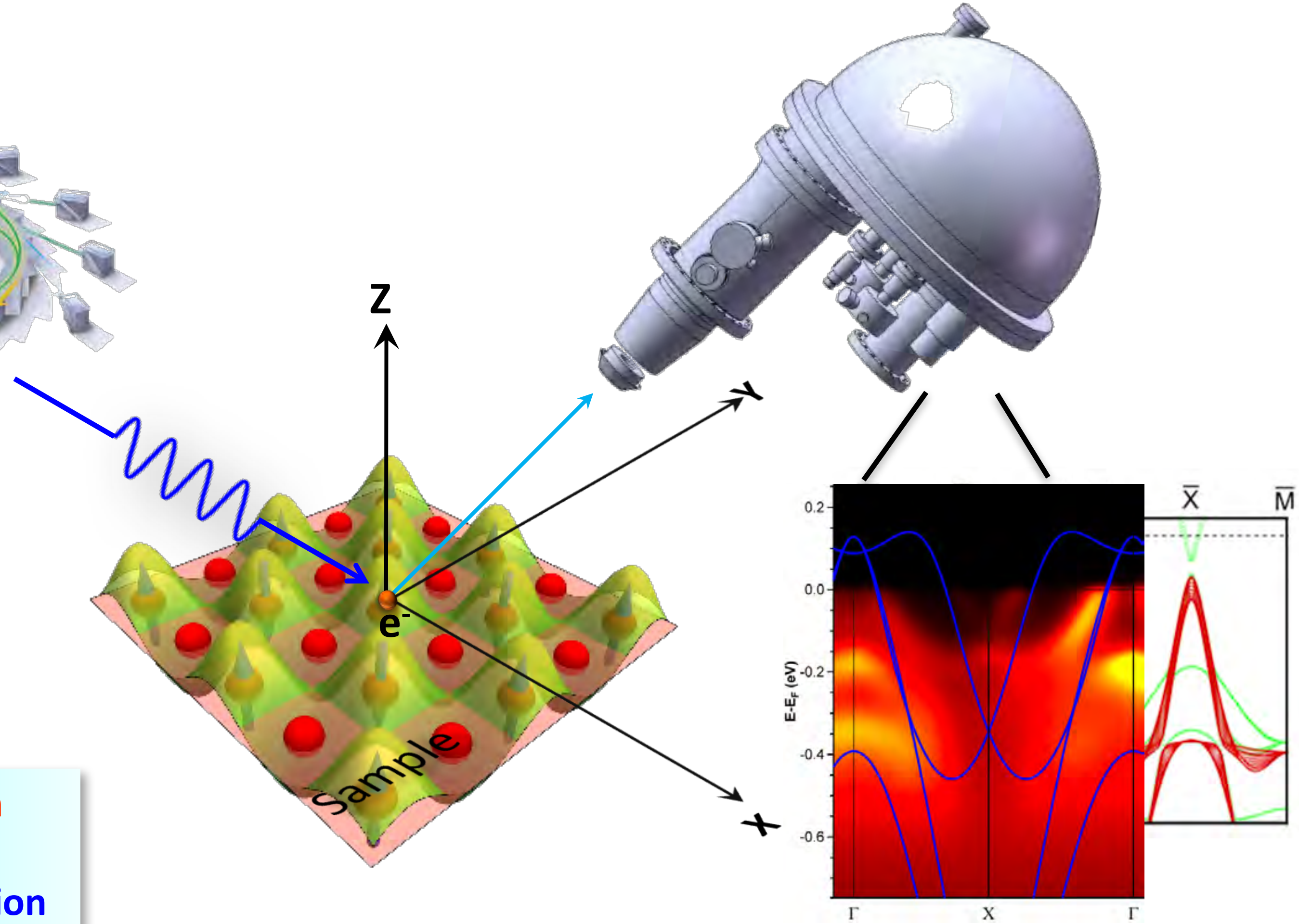
  - Orbital anisotropy (spin coupling to orbital)
  - Charge order (spin coupling to charge)





Angle-Resolved PhotoEmission Spectroscopy (ARPES)





Energy Conservation

$E_B = h\nu - E_{kin} - \Phi$

Momentum Conservation

$K_{\parallel} = k_{\parallel} + G_{\parallel}$

Direct measure of electronic structures

D. Lu, M. Yi et al. Nature 455, 81 (2008).

What ARPES measures

Photoemission Intensity:

$$I(k,w)=I_0|M(k,w)|^2 f(w)A(k,w) \otimes R(\Delta k, \Delta\omega)$$

Single-particle spectral function

$$A(\mathbf{k},\omega) \propto \frac{\operatorname{Im}\Sigma(\mathbf{k},\omega)}{[\omega - \varepsilon_{\mathbf{k}} - \operatorname{Re}\Sigma(\mathbf{k},\omega)]^2 + [\operatorname{Im}\Sigma(\mathbf{k},\omega)]^2}$$

bare band dispersions

$$\Sigma(\mathbf{k},\omega) = \Sigma'(\mathbf{k},\omega) + i\Sigma''(\mathbf{k},\omega)$$

The "self-energy" captures the effects of interactions

Damascelli, Hussain, Shen, Rev. Mod. Phys. 75, 473 (2003)

What ARPES measures

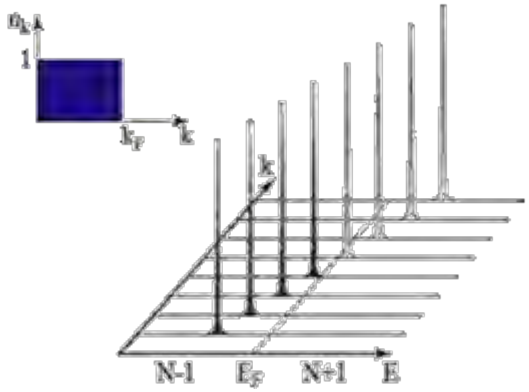
Photoemission Intensity:

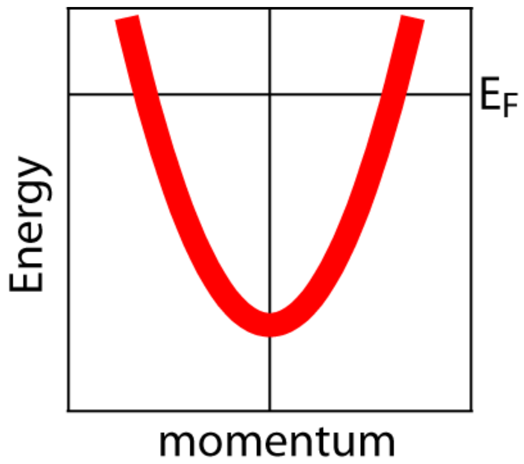
$$I(k,w)=I_0|M(k,w)|^2 f(w)A(k,w) \otimes R(\Delta k, \Delta\omega)$$

Single-particle spectral function

$$A(\mathbf{k},\omega) = \delta(\omega - \varepsilon_k)$$

Non-interacting electron system





Damascelli, Hussain, Shen, Rev. Mod. Phys. 75, 473 (2003)

What ARPES measures

Photoemission Intensity:

$$I(k,w)=I_0|M(k,w)|^2 f(w) A(k,w) \otimes R(\Delta k, \Delta\omega)$$

Single-particle spectral function

$$A(\mathbf{k},\omega) = Z_\mathbf{k} \frac{\Gamma_\mathbf{k}/\pi}{(\omega-\varepsilon_\mathbf{k})^2+\Gamma_\mathbf{k}^2} + A_{incoh}$$

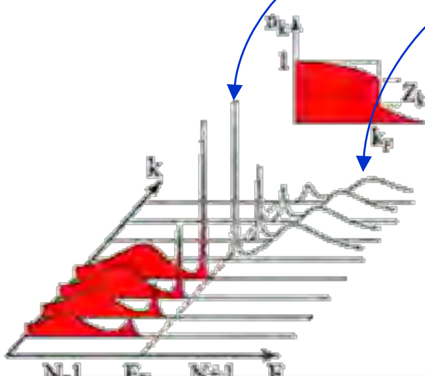
Coherence Factor:

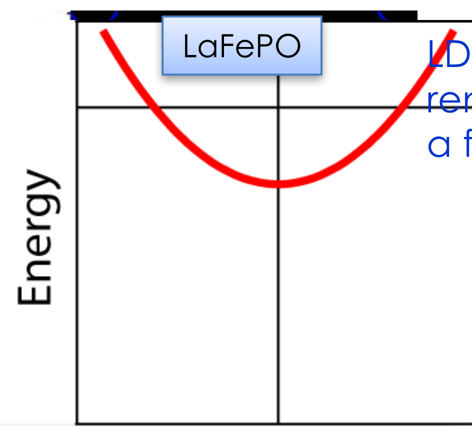
$$Z_\mathbf{k} = (1-\partial\Sigma'/\partial\omega)^{-1} < 1$$

$$\varepsilon_\mathbf{k} = Z_\mathbf{k}(e_\mathbf{k}+\Sigma')$$

1. reduces overall spectral weight
2. renormalizes (scales) band dispersions by a factor. Electrons become more localized.

Fermi liquid system



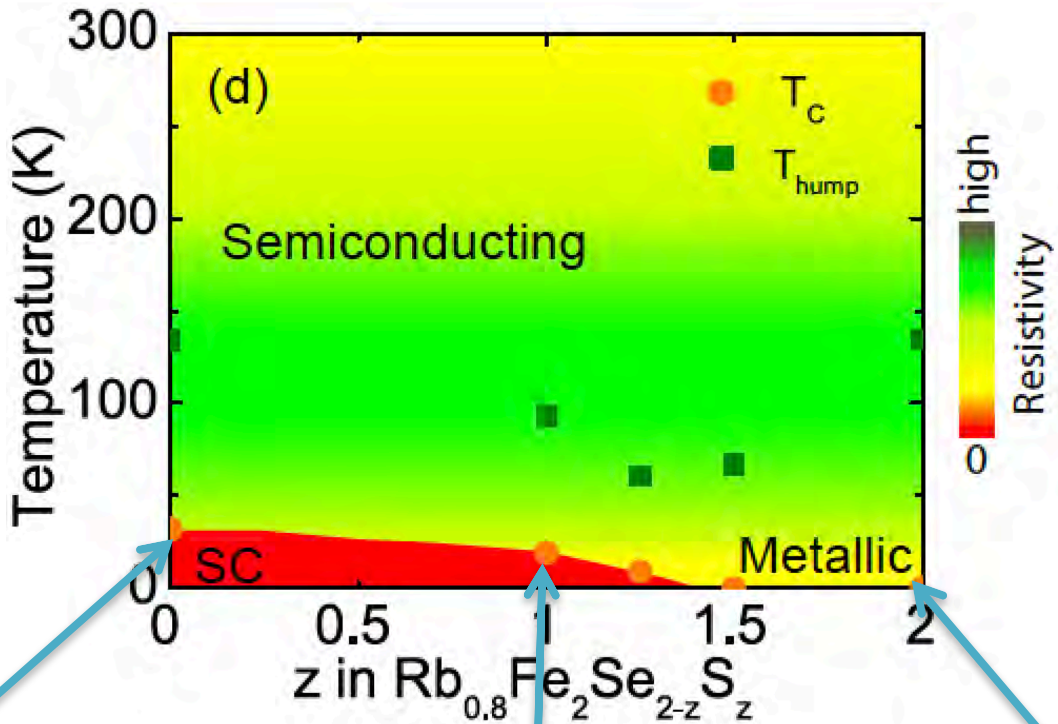


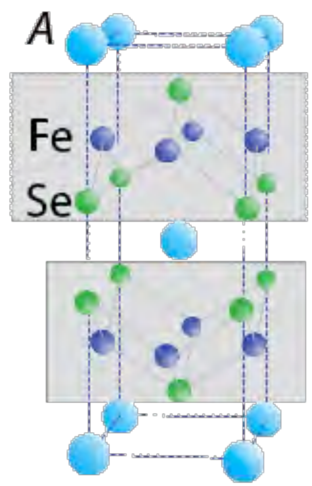
LDA renormalized by a factor of 2.2

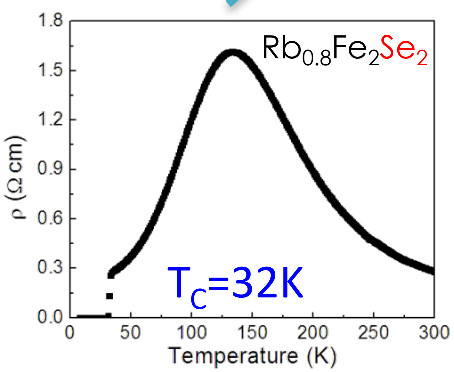
A measure of electron correlations

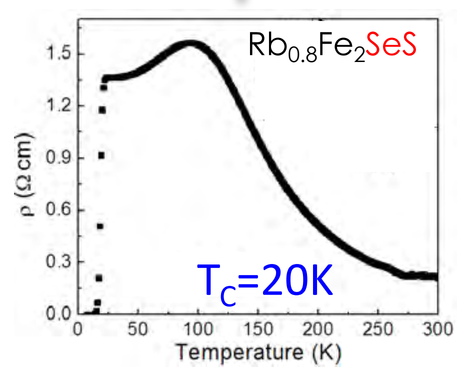
Why do we care about correlations?

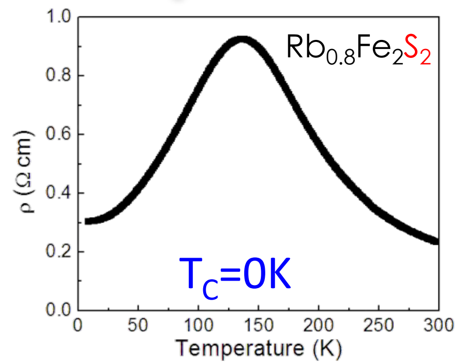
Correlation-tuned superconductivity in $Rb_xFe_2Se_2$







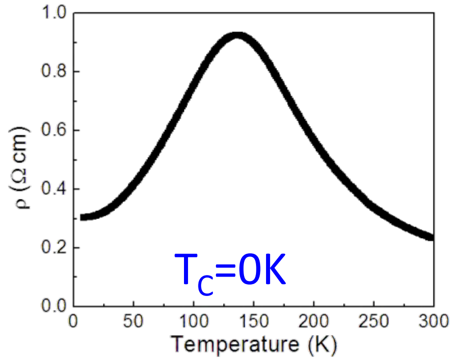




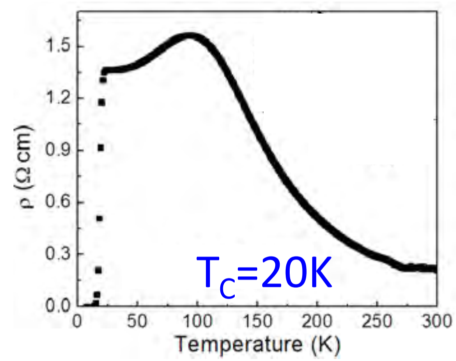
M. Wang, M. Yi *et al*. PRB 93, 075155 (2016)

Same Fermi surface topology

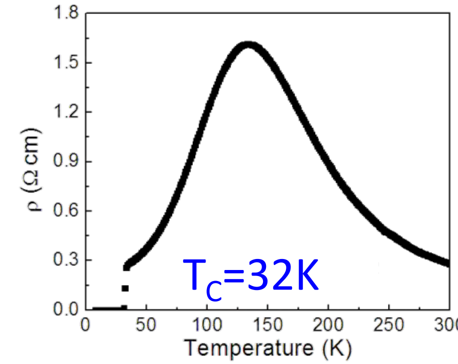
$Rb_{0.8}Fe_2S_2$



$Rb_{0.8}Fe_2SeS$

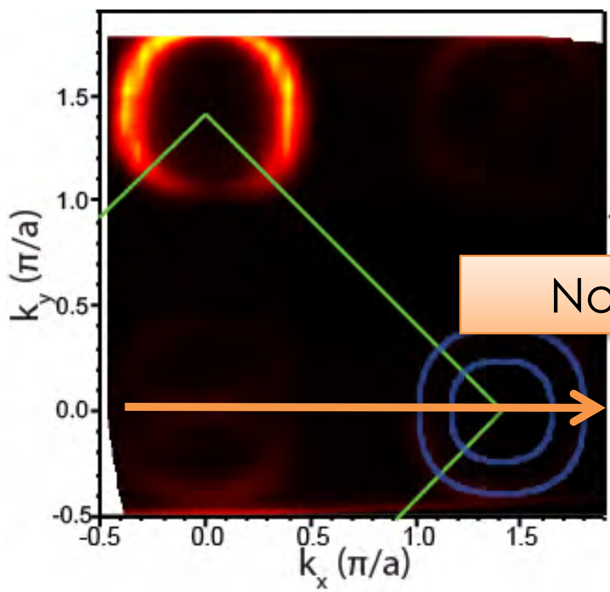


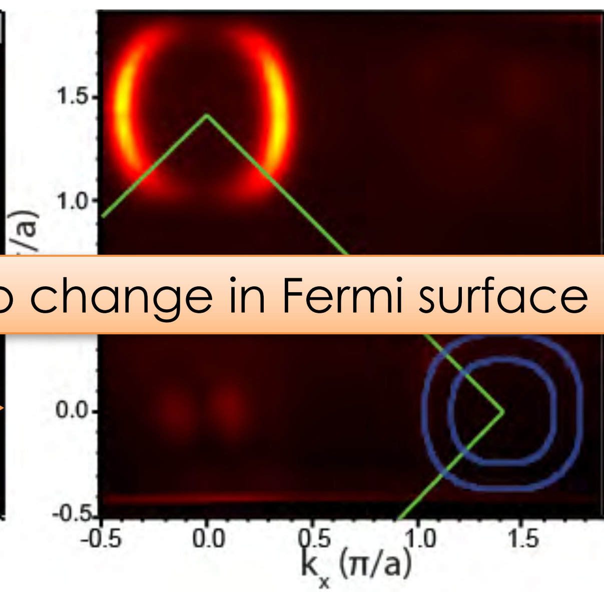
$Rb_{0.8}Fe_2Se_2$

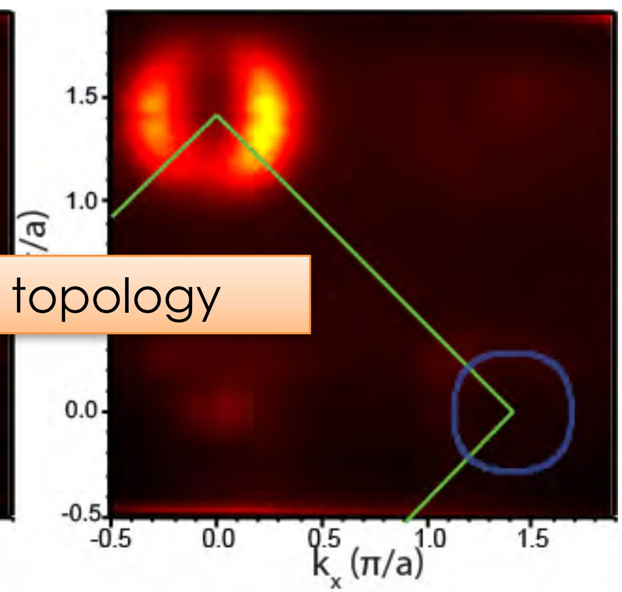


Metallic

Superconducting



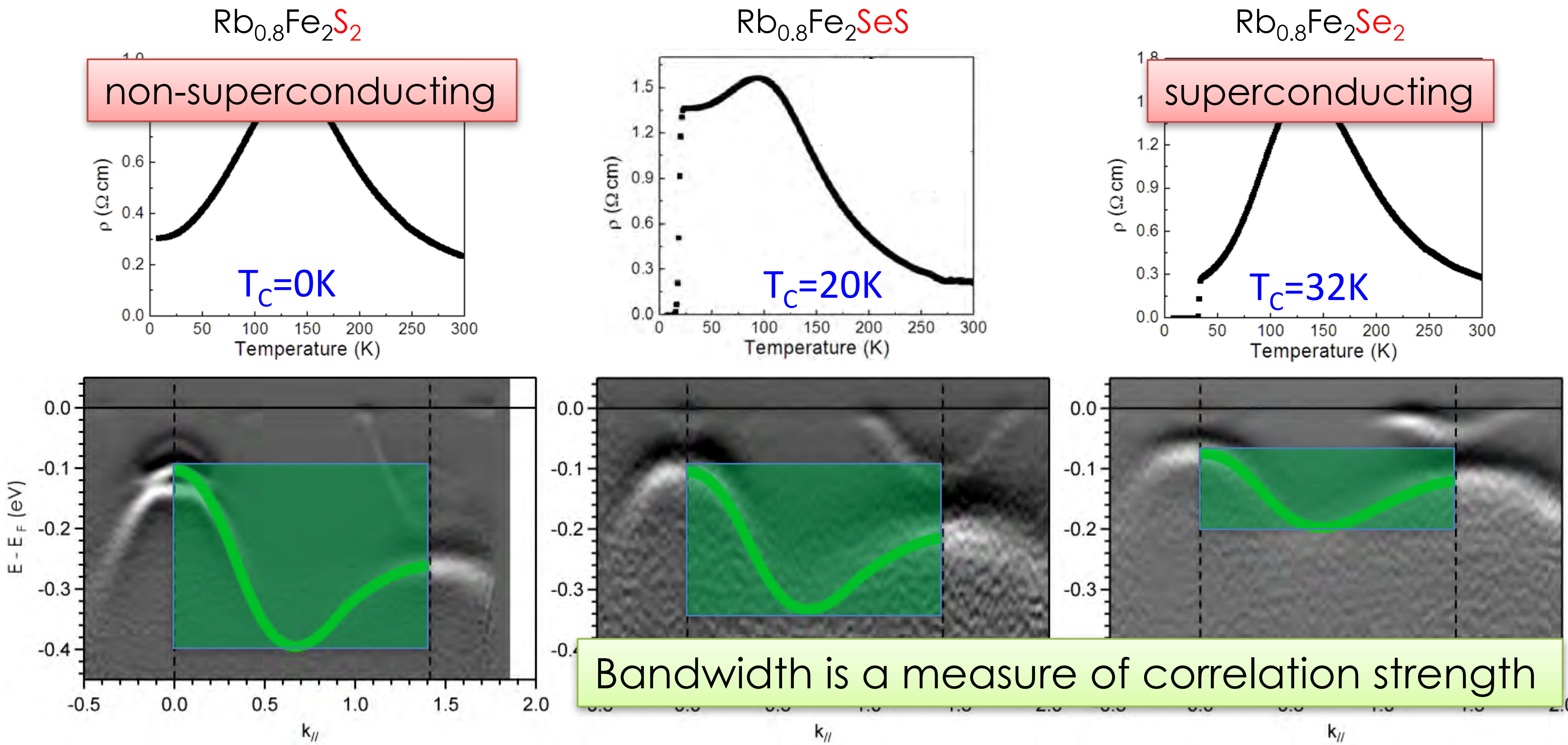




No change in Fermi surface topology

M. Yi *et al*. PRL 115, 256403 (2015)

Very different correlation strength!



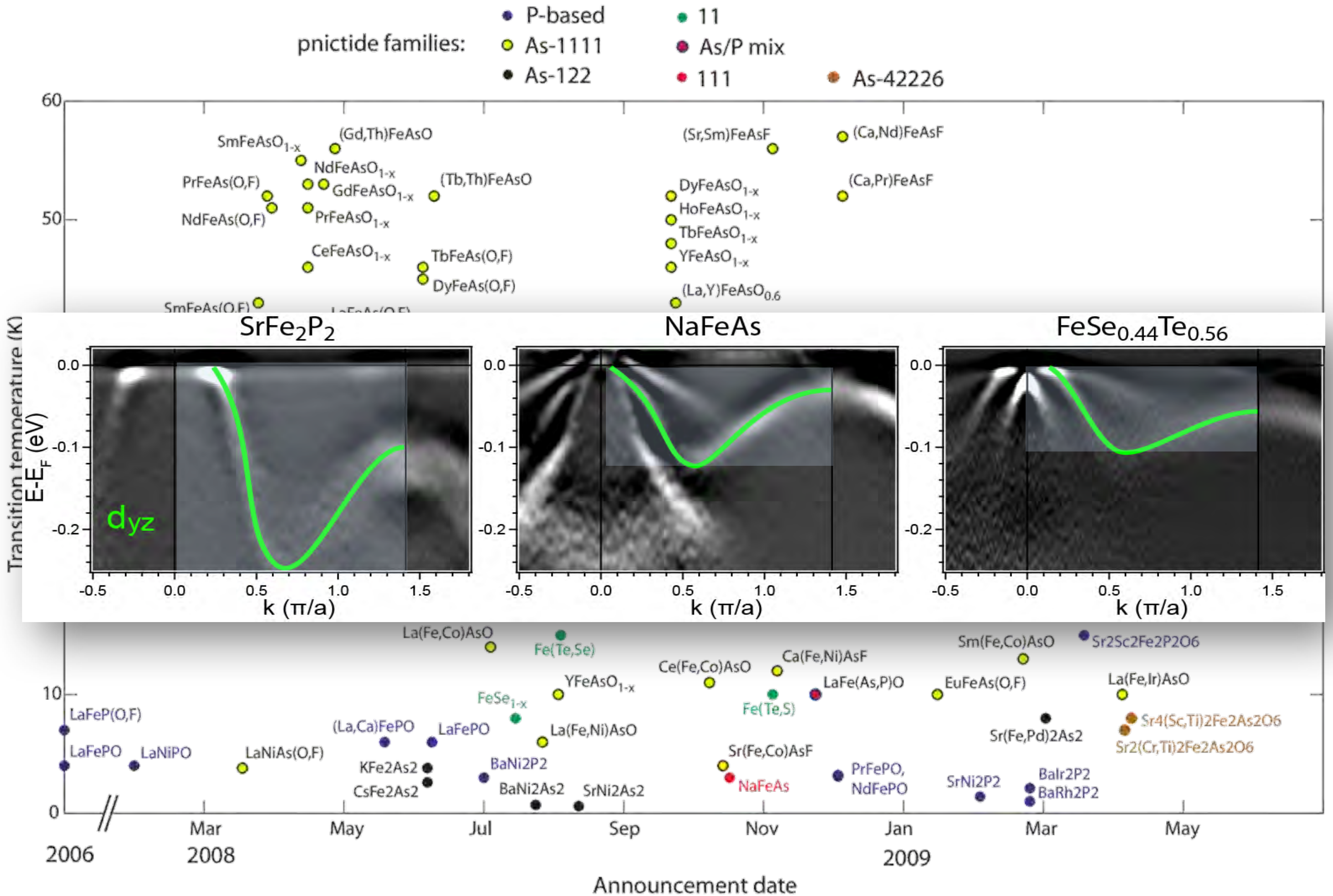
faster electrons
– weak correlations

band slope ~ electron velocity

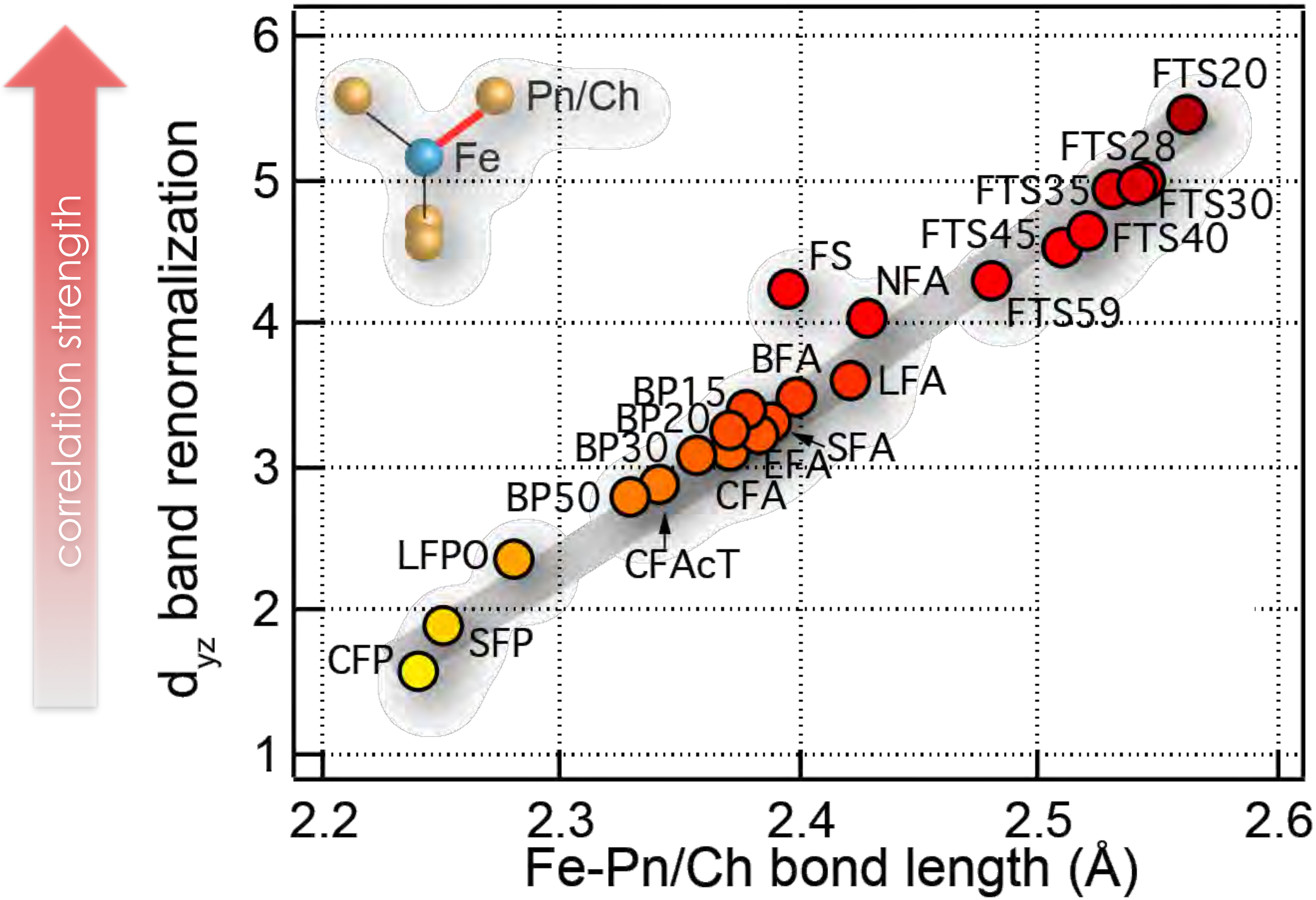
slower electrons
– strong correlations

Electron correlation is important for high temperature superconductivity!

Correlation trends in all iron-pnictides

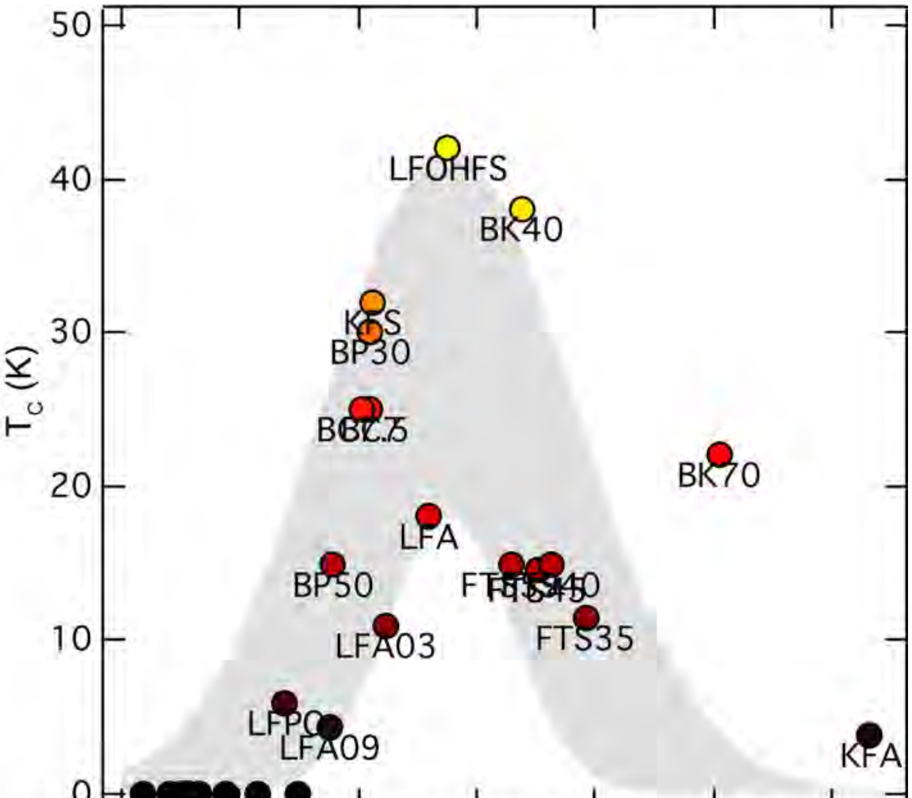


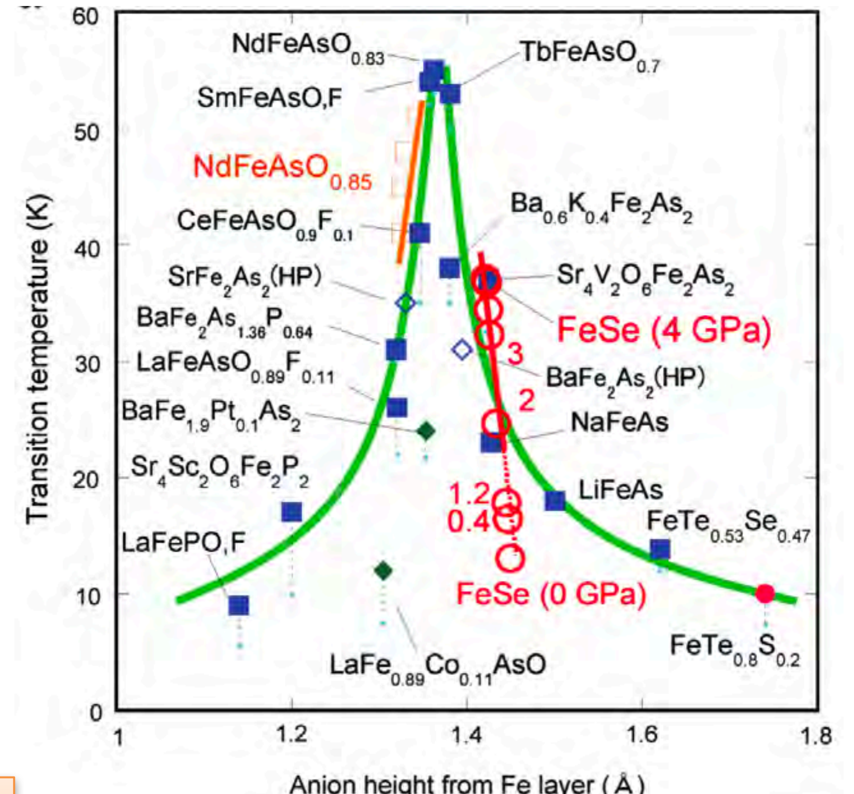
Bandwidth of all iron-based superconductors



**acknowledging ARPES groups around the world*

Superconductivity and correlation strength





Y Mizuguchi. Supercond Sci Technol 2010; 23: 054013

Some electron correlation is needed for optimal superconductivity,
But too much of it kills superconductivity

correlation strength

Outline

- Importance of *correlations* to superconductivity
  - Bandwidth-tuned superconductivity in $RbFe_2Se_2$
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  - Orbital anisotropy (spin coupling to orbital)
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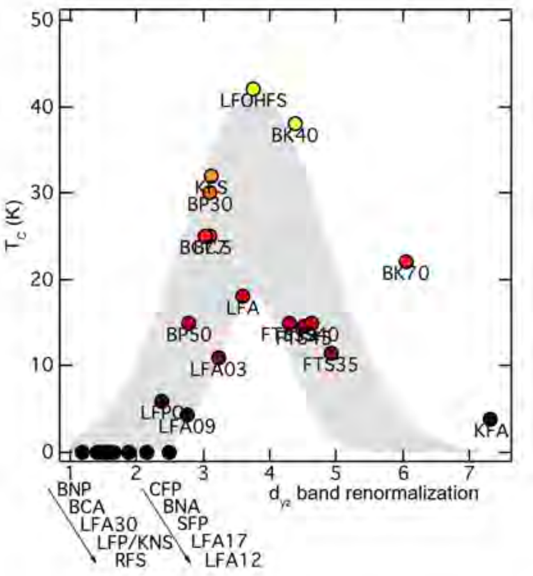
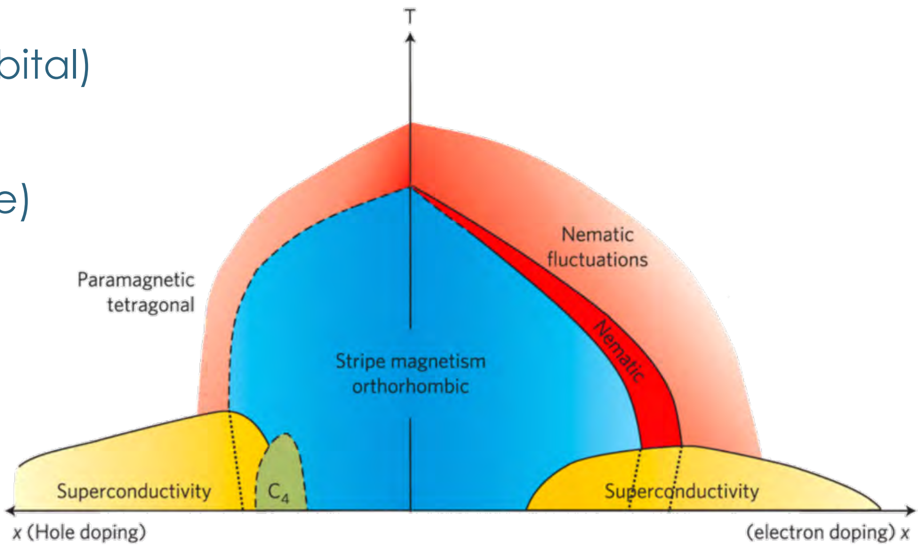
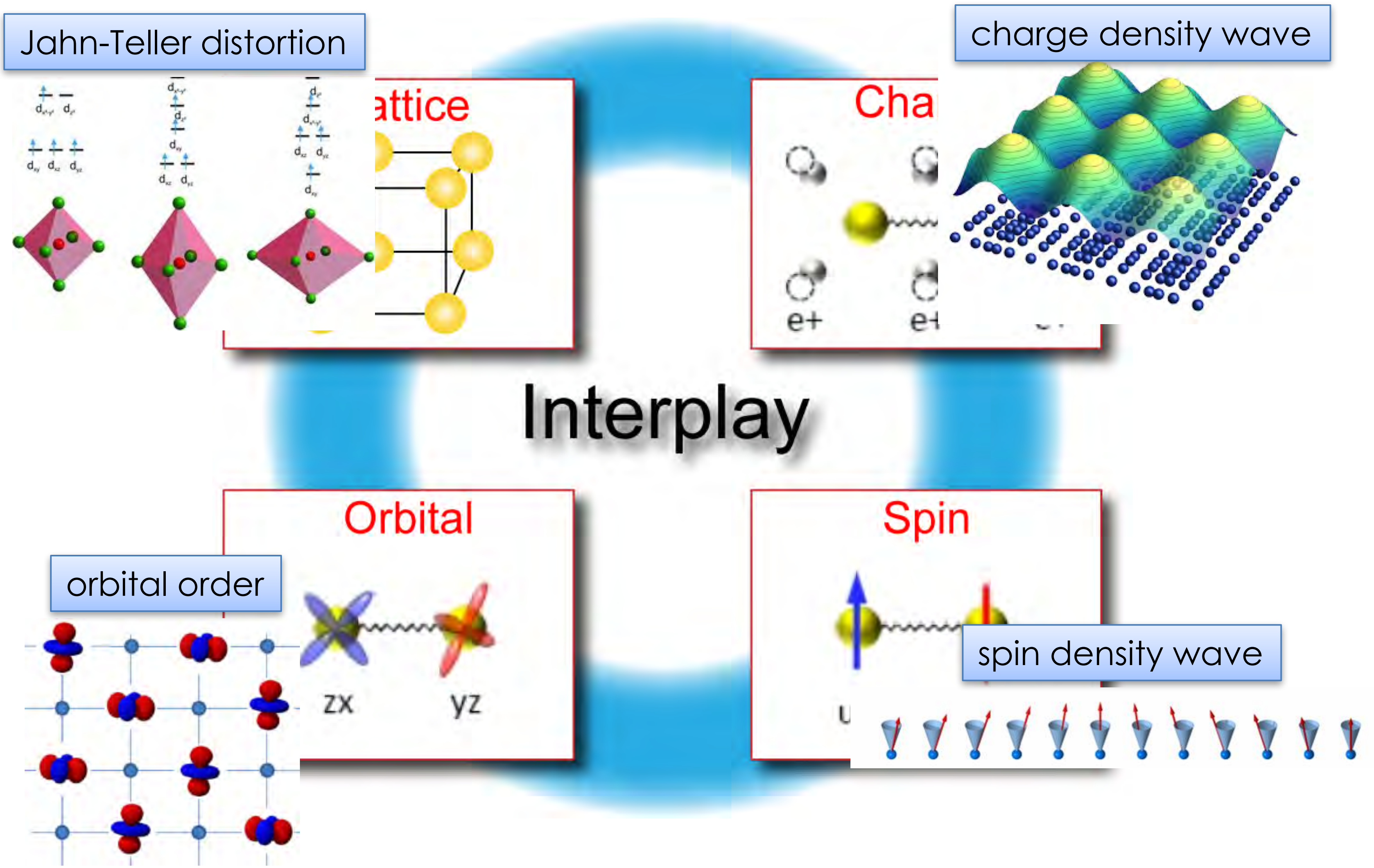
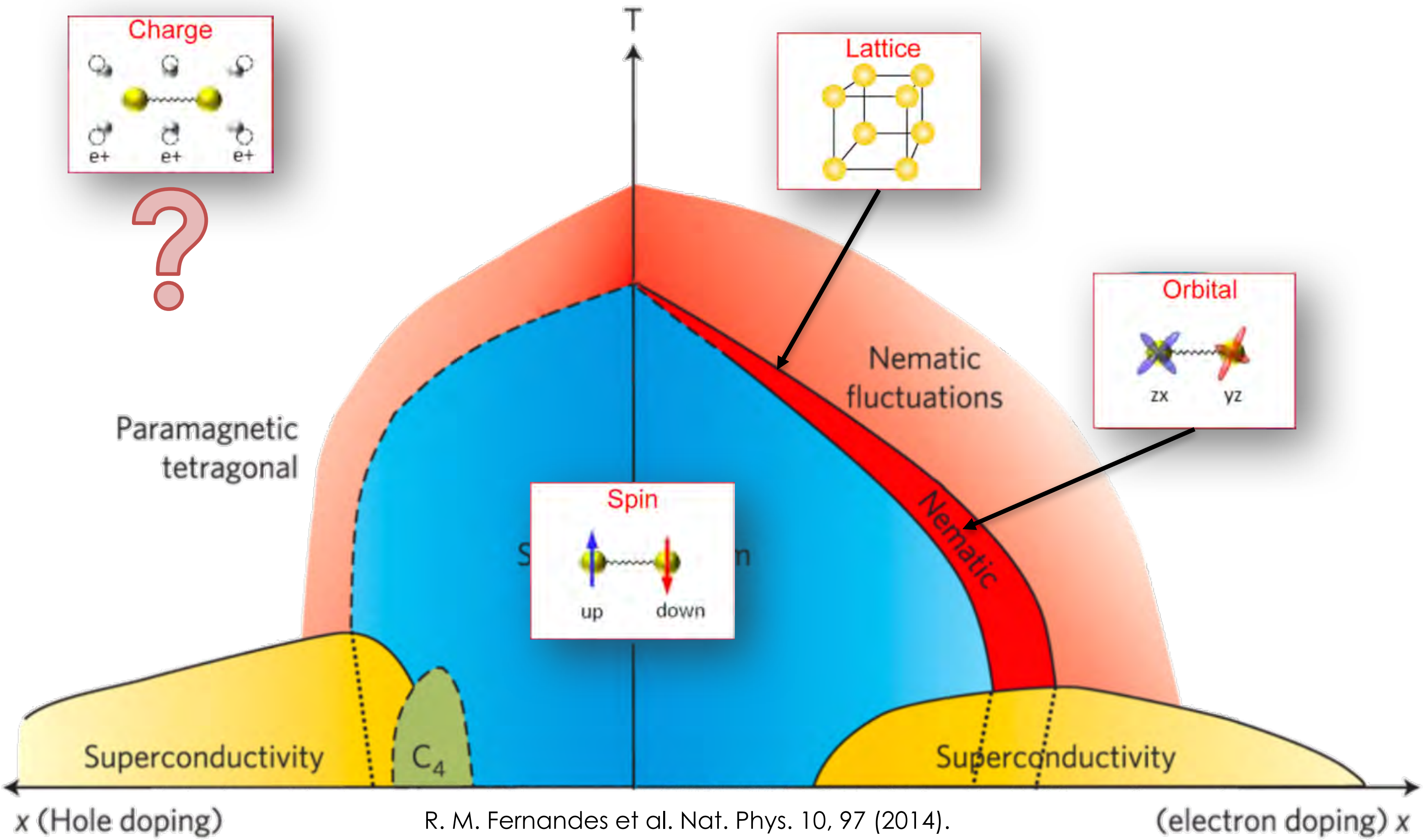




Emergence – fundamental degrees of freedom

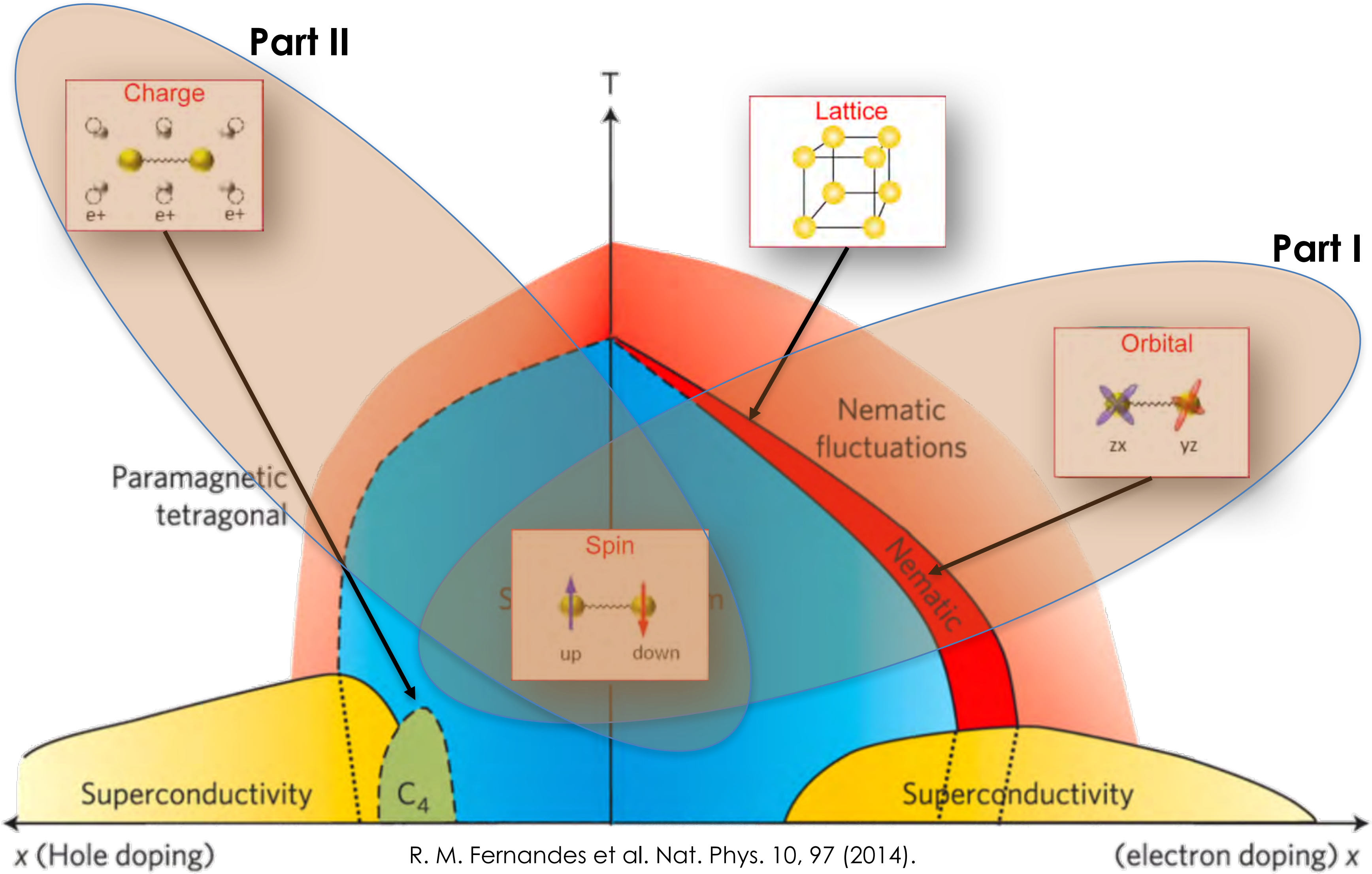


Re-introducing Iron-based superconductors



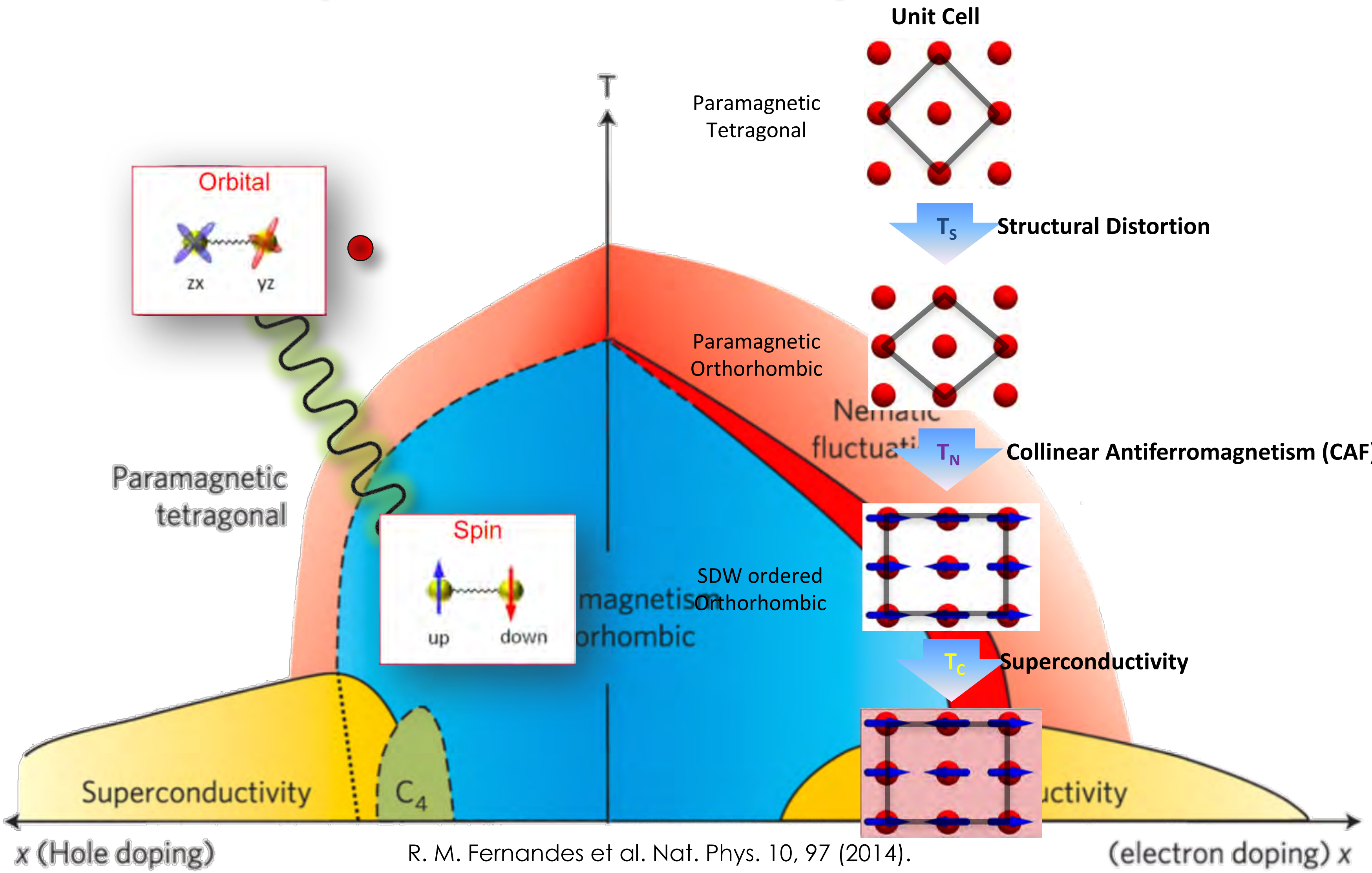
R. M. Fernandes et al. Nat. Phys. 10, 97 (2014).

Conclusion: discovery of a charge order



R. M. Fernandes et al. Nat. Phys. 10, 97 (2014).

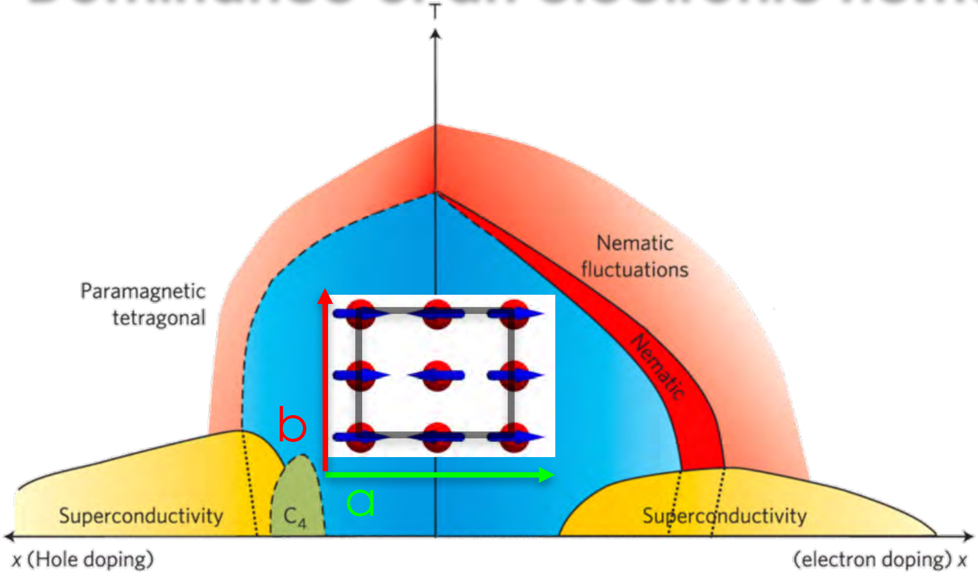
Iron-based superconductors: known phases

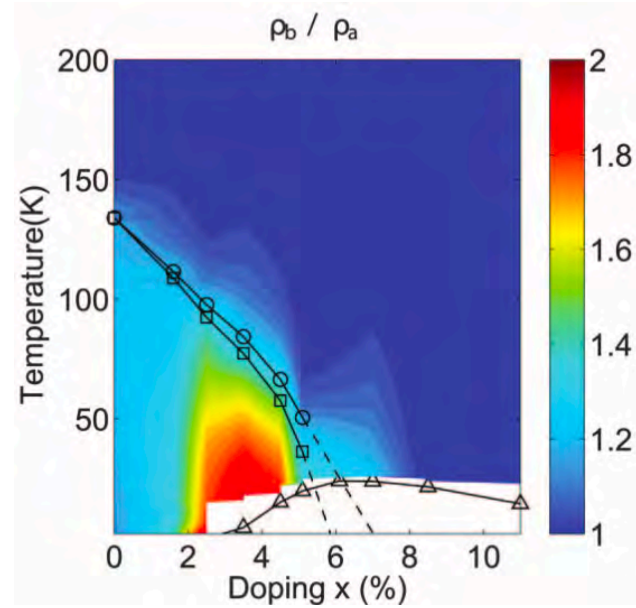


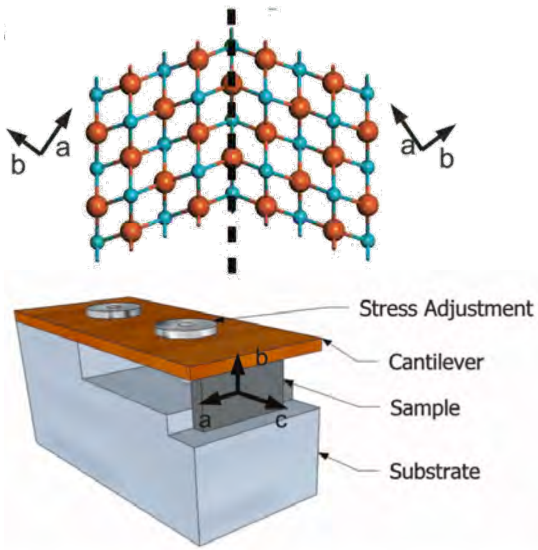
R. M. Fernandes et al. Nat. Phys. 10, 97 (2014).

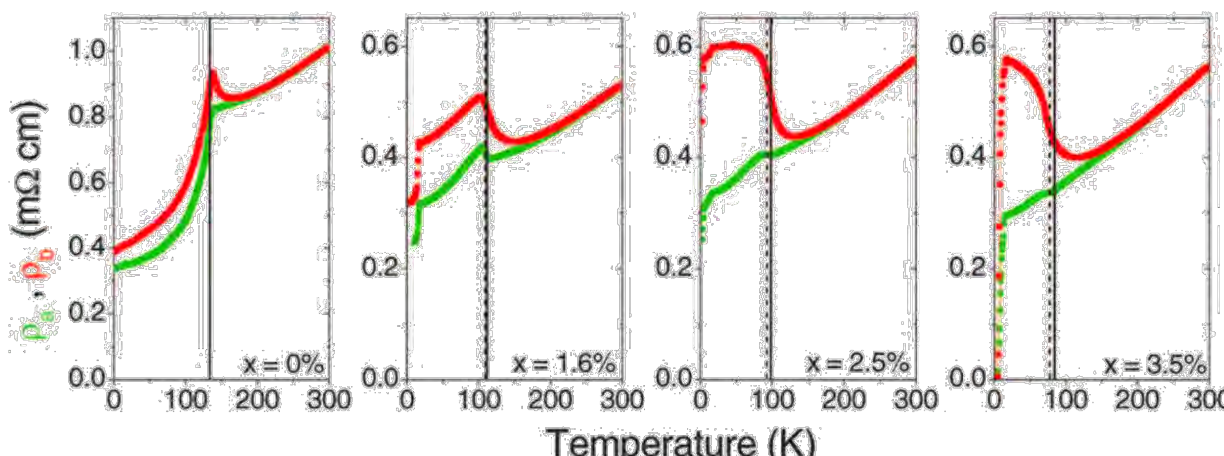
Berkeley UNIVERSITY OF CALIFORNIA

Dominance of an electronic nematic phase: resistivity



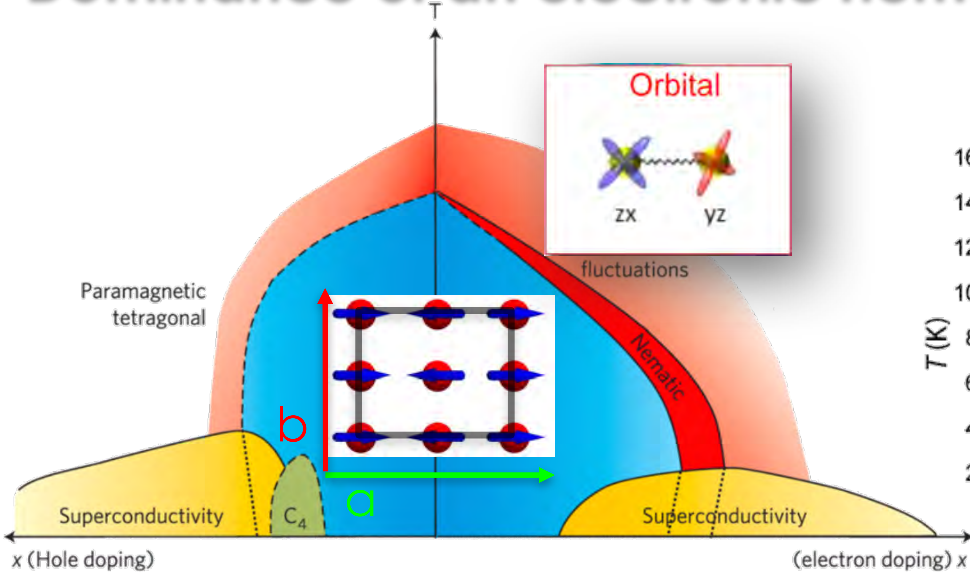


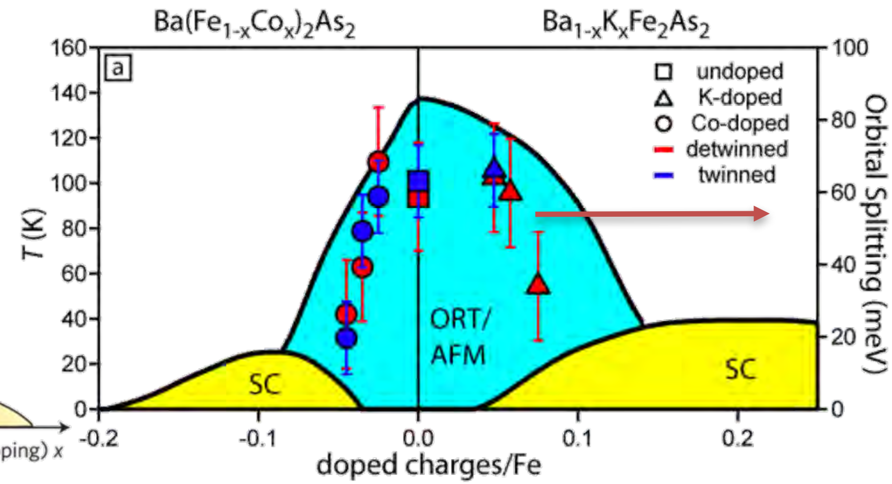


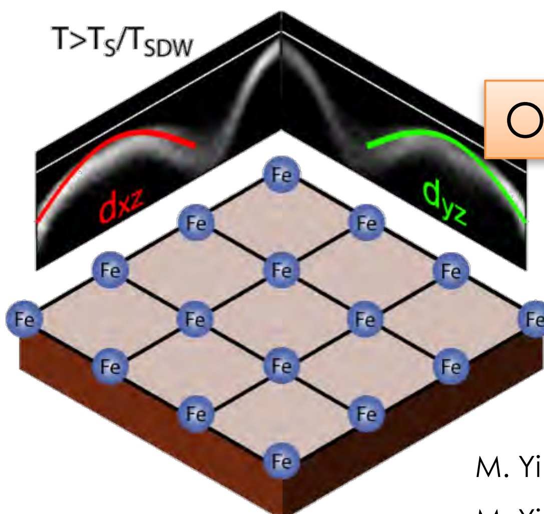


J.-H. Chu *et al*. Science 329, 824 (2010)

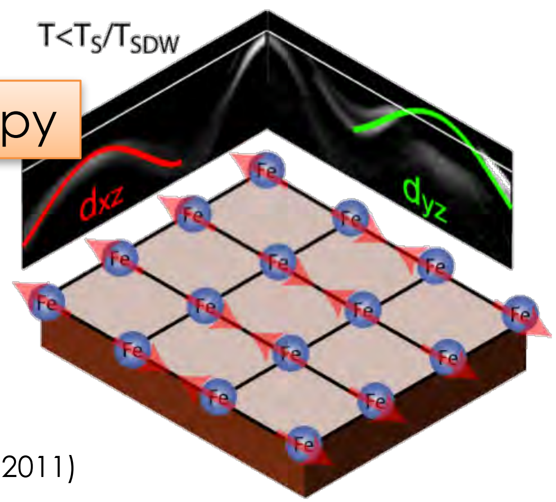
Dominance of an electronic nematic phase: ARPES







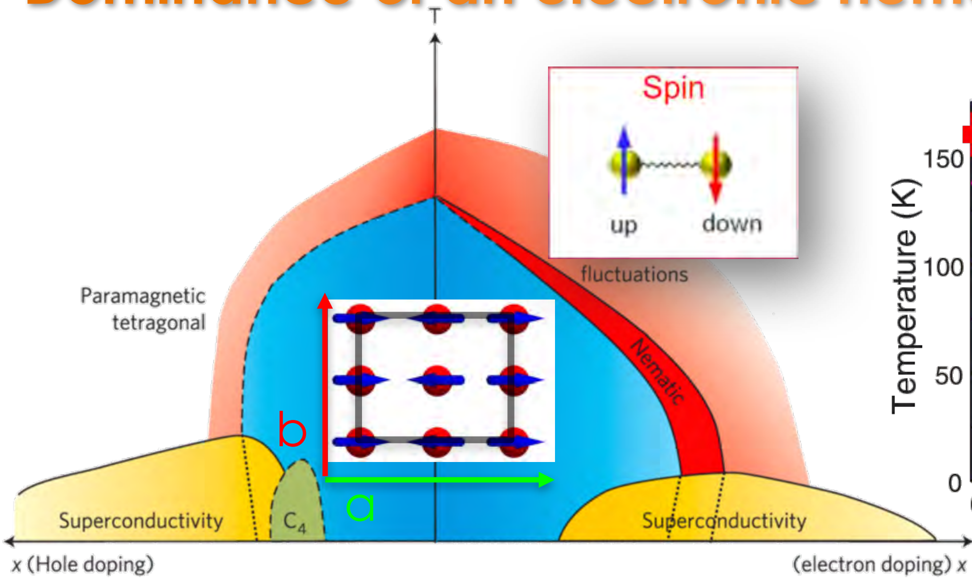
Orbital anisotropy

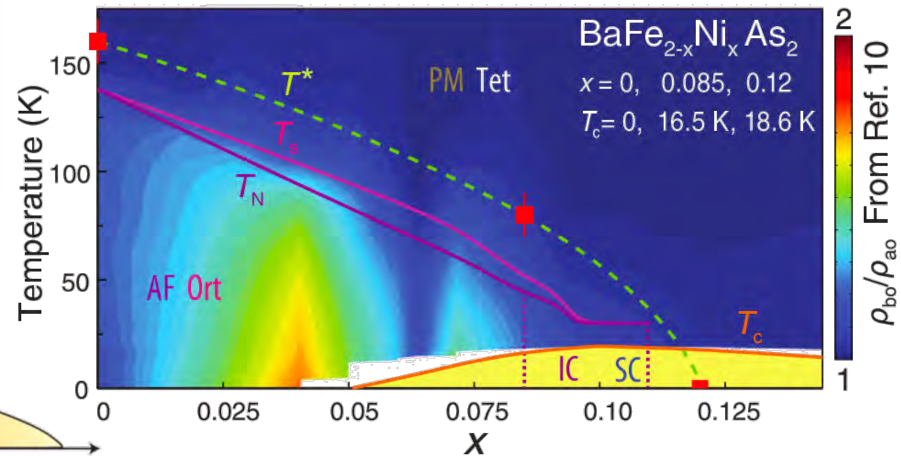


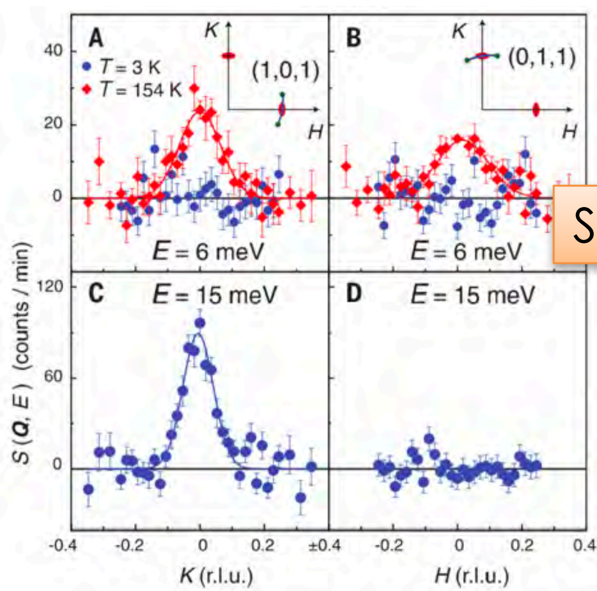
M. Yi *et al*. PNAS 108, 6878 (2011)

M. Yi *et al*. Nat. Comm. 5, 3711 (2014)

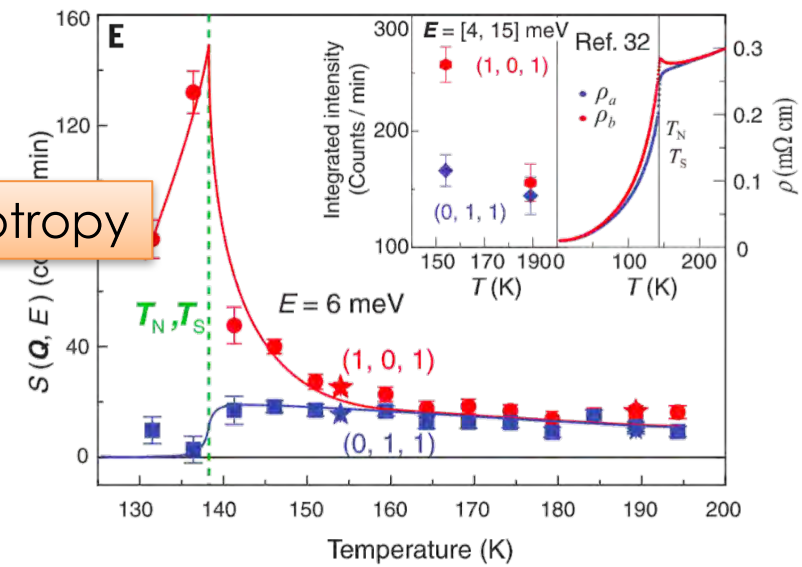
Dominance of an electronic nematic phase: neutron





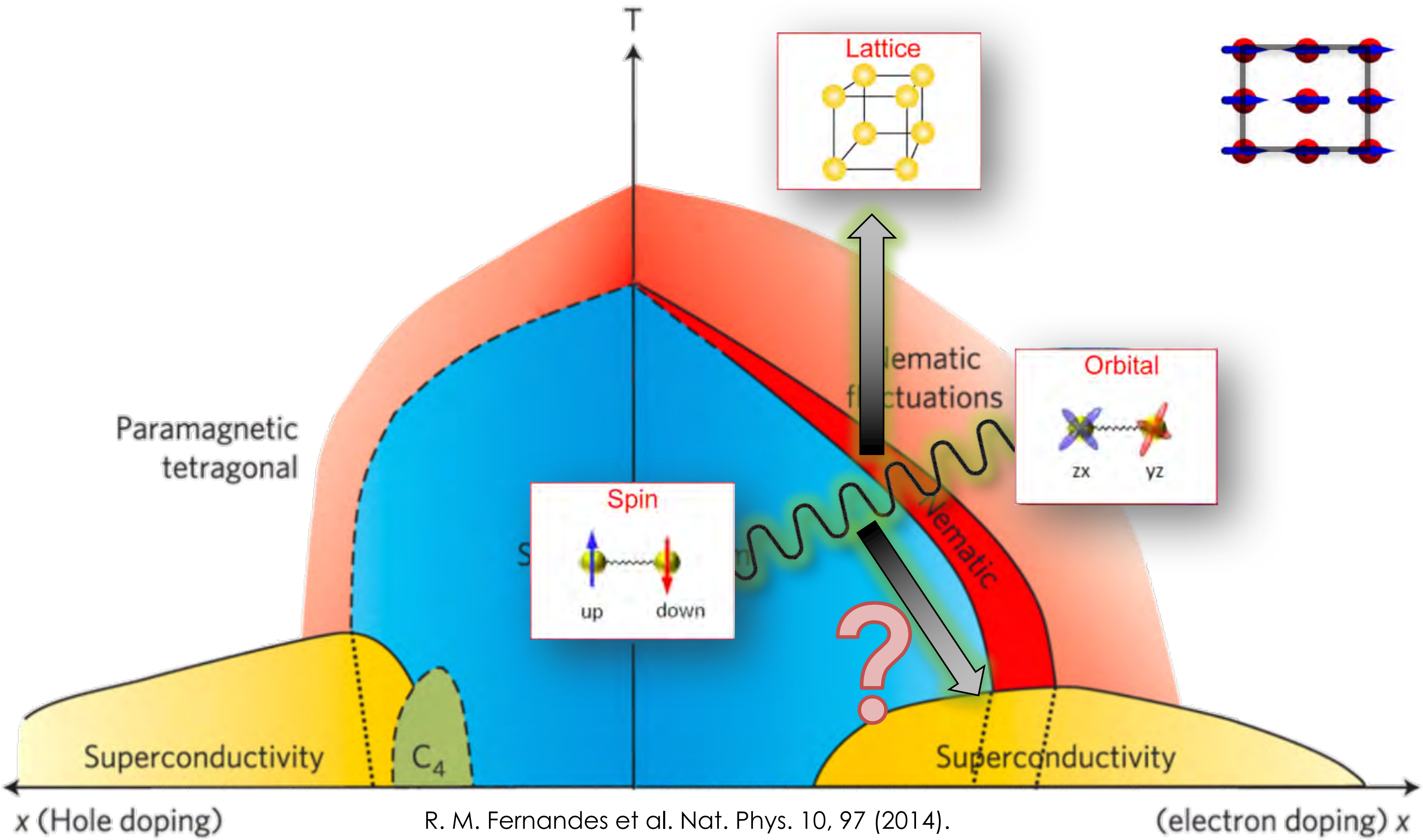


Spin anisotropy



X. Lu *et al*. Science 345, 657 (2014)

Strong coupling of the spin and orbital degrees of freedom



R. M. Fernandes et al. Nat. Phys. 10, 97 (2014).

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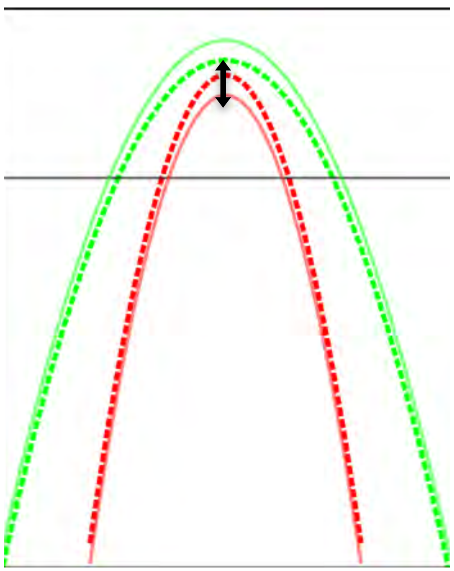
Distinct signatures of different order parameters

Nematicity

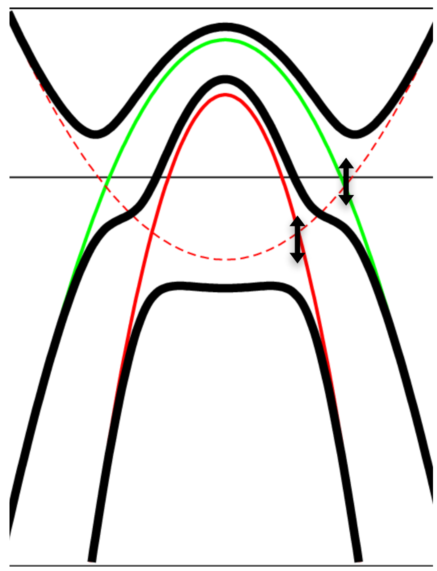
Δ_S



Orbital-dependent *band shift* associated with T_S

Spin Density Wave

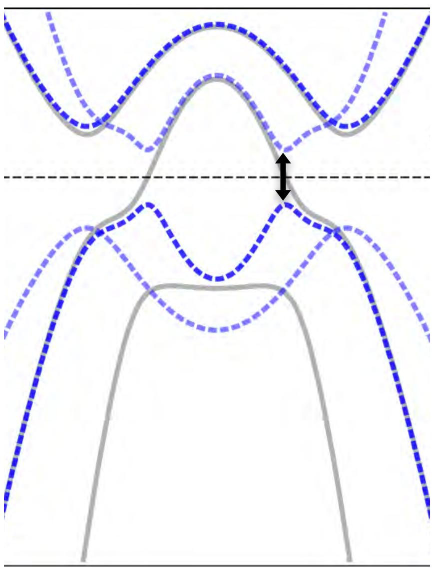
Δ_{SDW}



particle-hole asymmetric gap associated with T_{SDW}

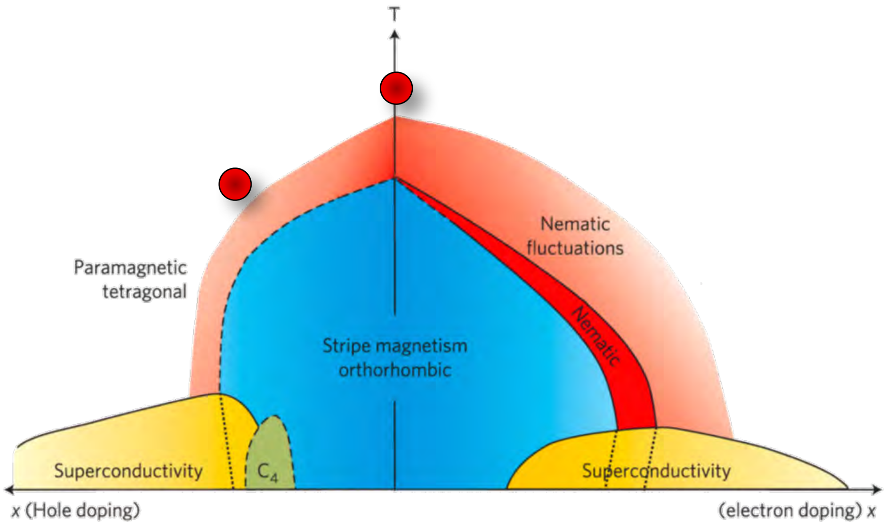
Superconductivity

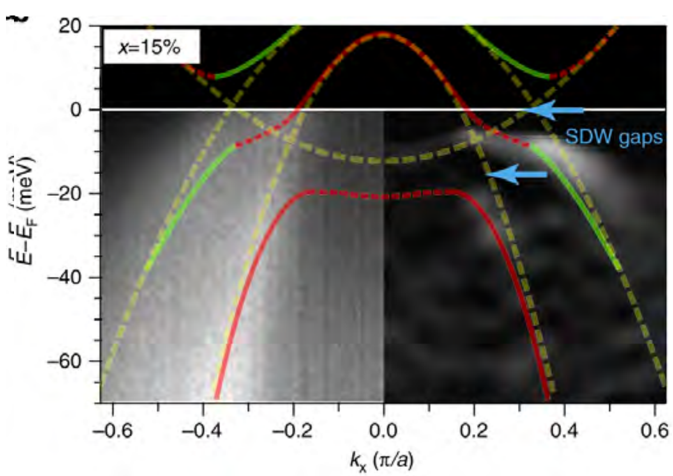
Δ_{SC}

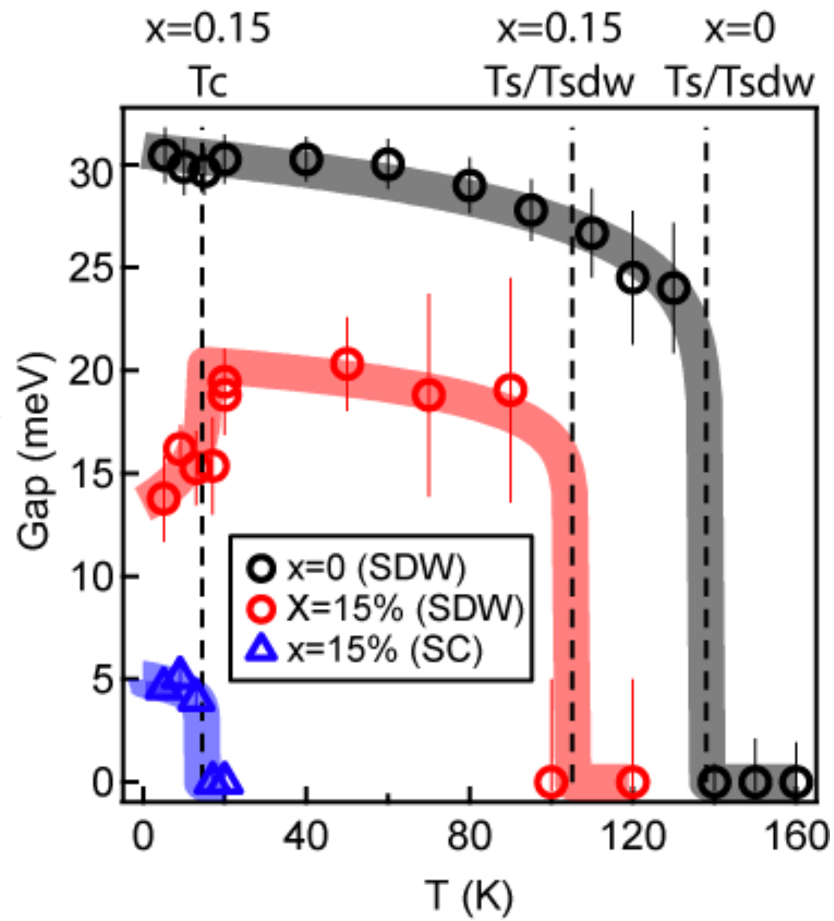


particle-hole symmetric gap associated with T_C

Competition of the magnetic order with superconductivity



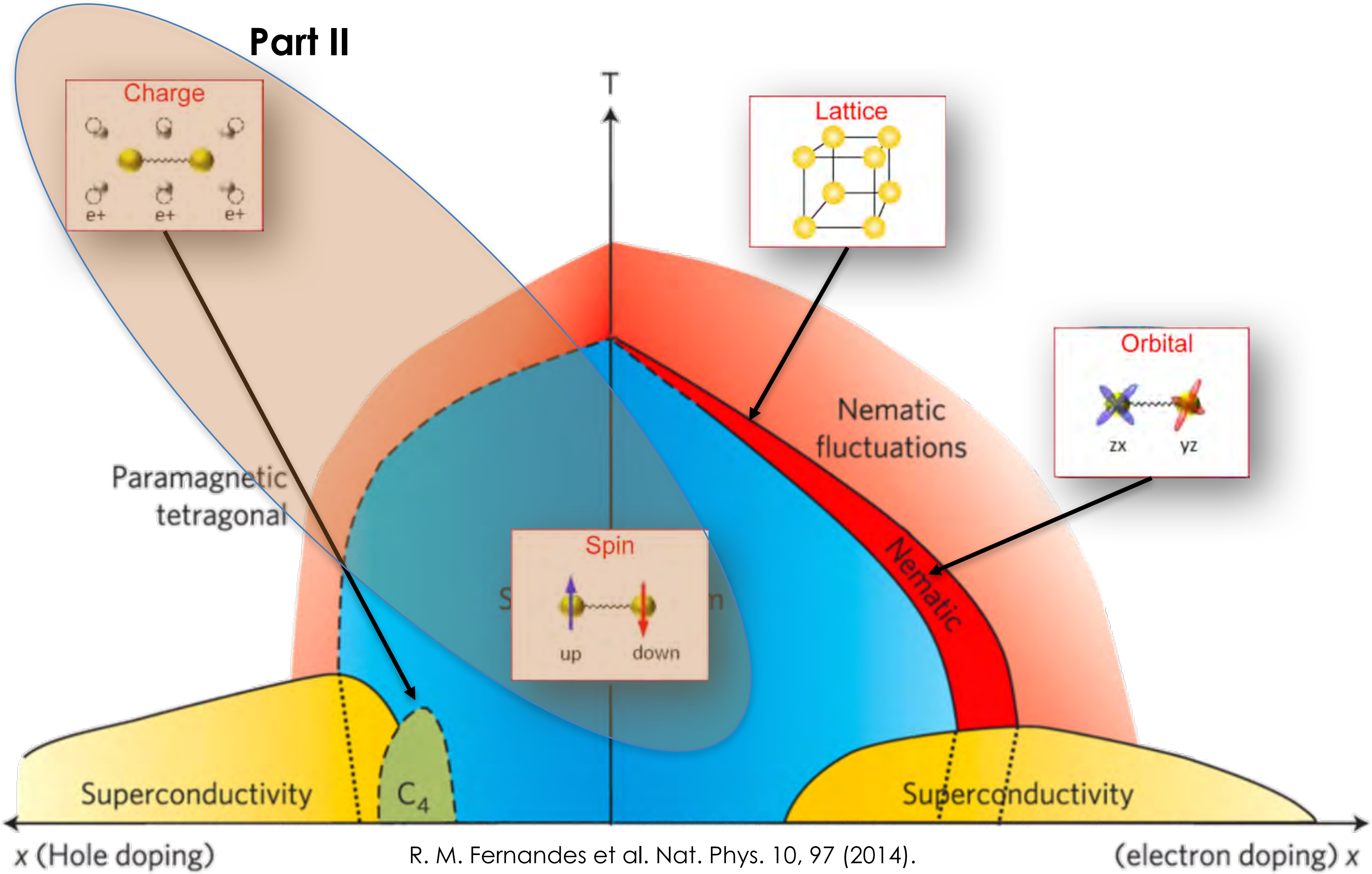




magnetism and superconductivity coexist and compete

M. Yi *et al*. Nat. Comm. 5, 3711 (2014)

Part II: evidence for a charge order

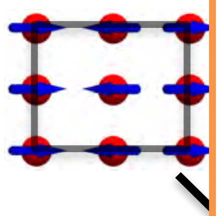


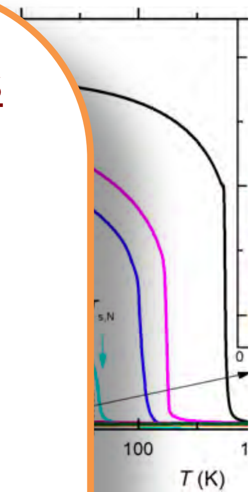
R. M. Fernandes et al. Nat. Phys. 10, 97 (2014).

The curious C_4 phase

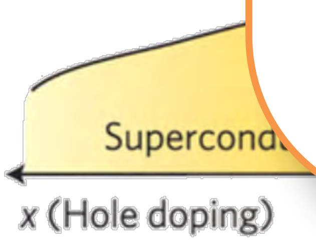
Rotational C_4 symmetry is restored

Magnetism most...
broken ro...
Strongly...





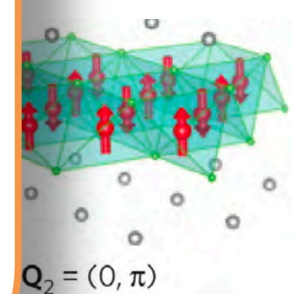
Param...
tet...



Universal feature of hole-doped 122 pnictides

$Ba_{1-x}Na_xFe_2As_2$
$Ba_{1-x}K_xFe_2As_2$
$Sr_{1-x}Na_xFe_2As_2$
$Ca_{1-x}Na_xFe_2As_2$
…

S. Avci *et al*. Nat. Comm. 5, 3845 (2014)
F. Waber *et al*. PRB 91, 060505(R) (2015)
A. Böhmer *et al*. Nat. Comm. 6, 7911 (2015)
J. Allred *et al*. Nat. Phys. 12, 493 (2016)
K. M. Taddei, *et al*. PRB 93, 134510 (2016)
L. Wang *et al*. PRB 93, 014514 (2016)
K. M. Taddei, *et al*. PRB 95, 064508 (2017)
…

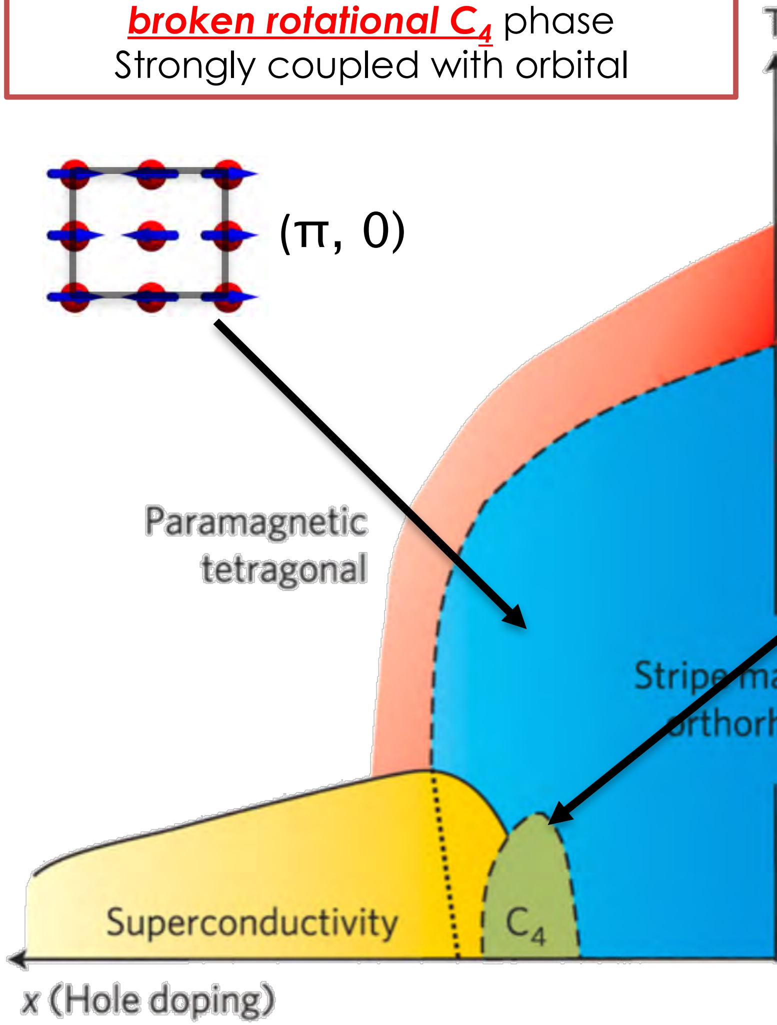


...nder
...nmetry

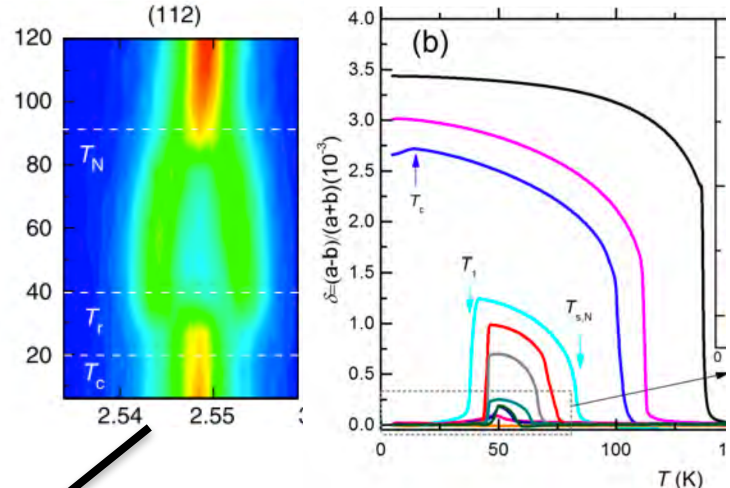
S. Avci *et al*. Nat. Comm. 5, 3845 (2014)
L. Wang *et al*. PRB 93, 014514 (2016)

The curious C_4 phase

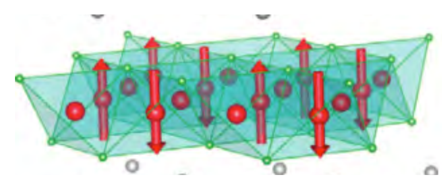
Magnetism mostly appeared in
broken rotational C_4 phase
Strongly coupled with orbital



Rotational C_4 symmetry is restored



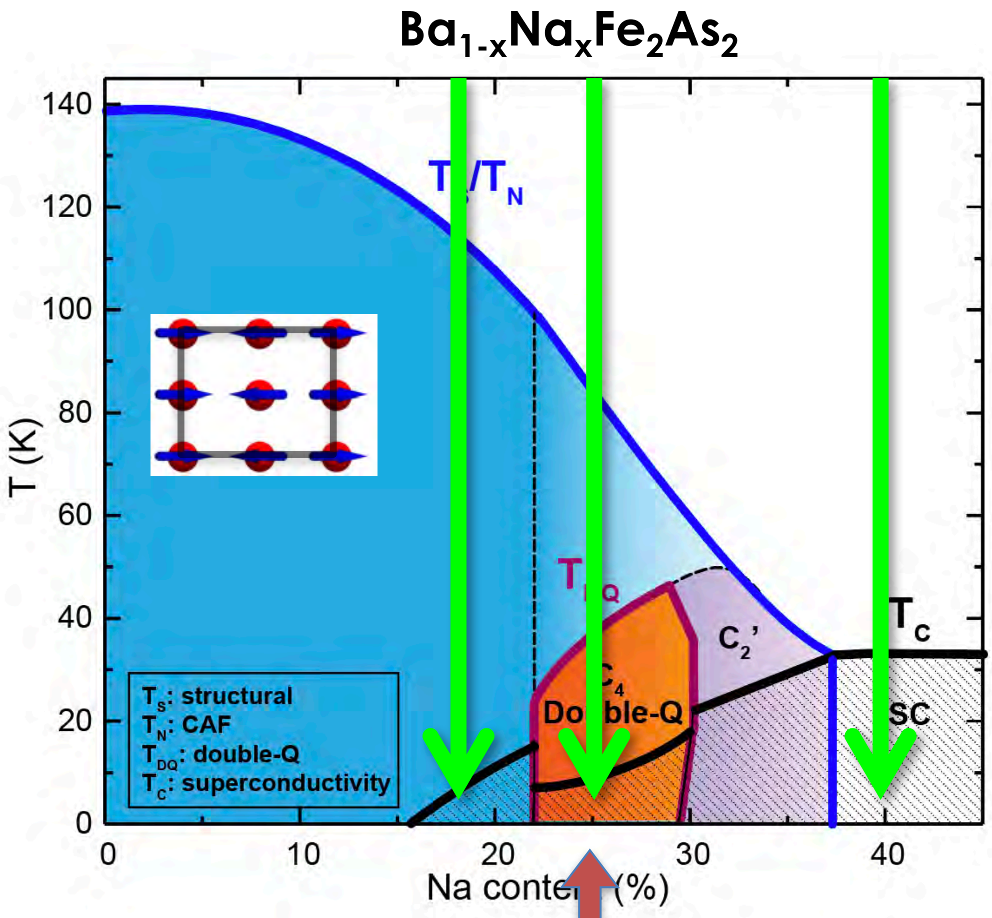
Double-Q order

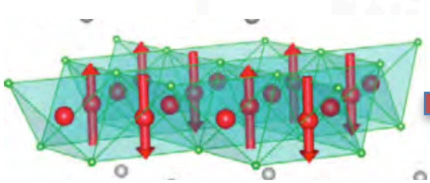


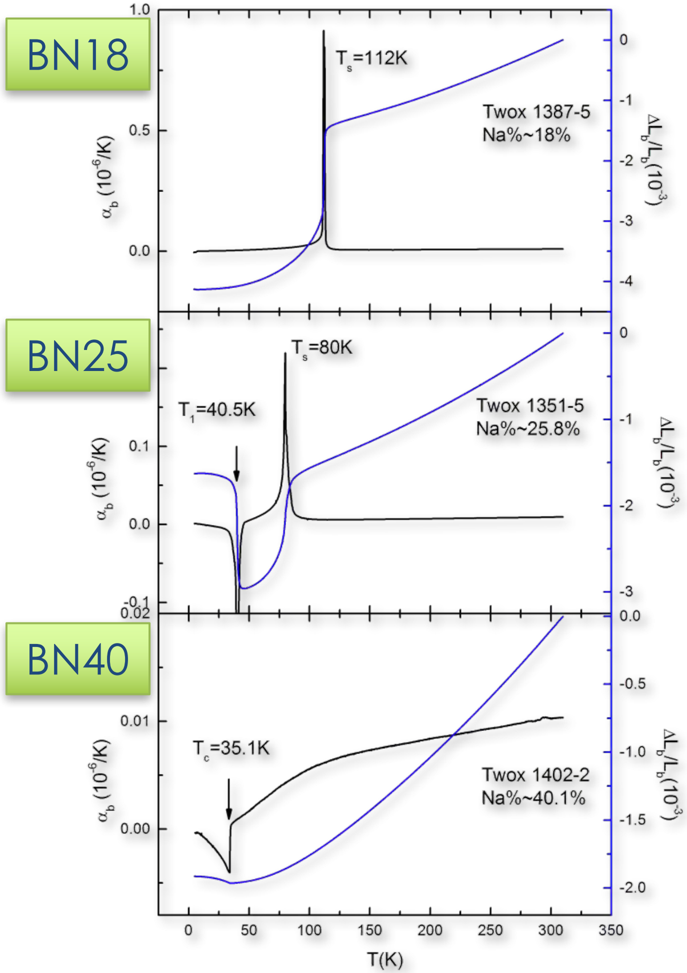
Magnetic order under
preserved C_4 symmetry

S. Avci *et al*. Nat. Comm. 5, 3845 (2014)
L. Wang *et al*. PRB 93, 014514 (2016)

Three doping regimes measured

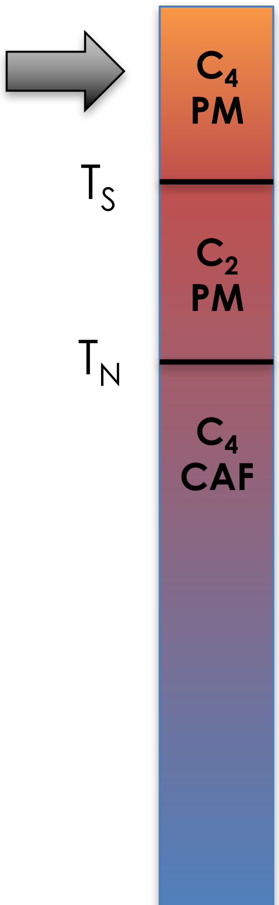


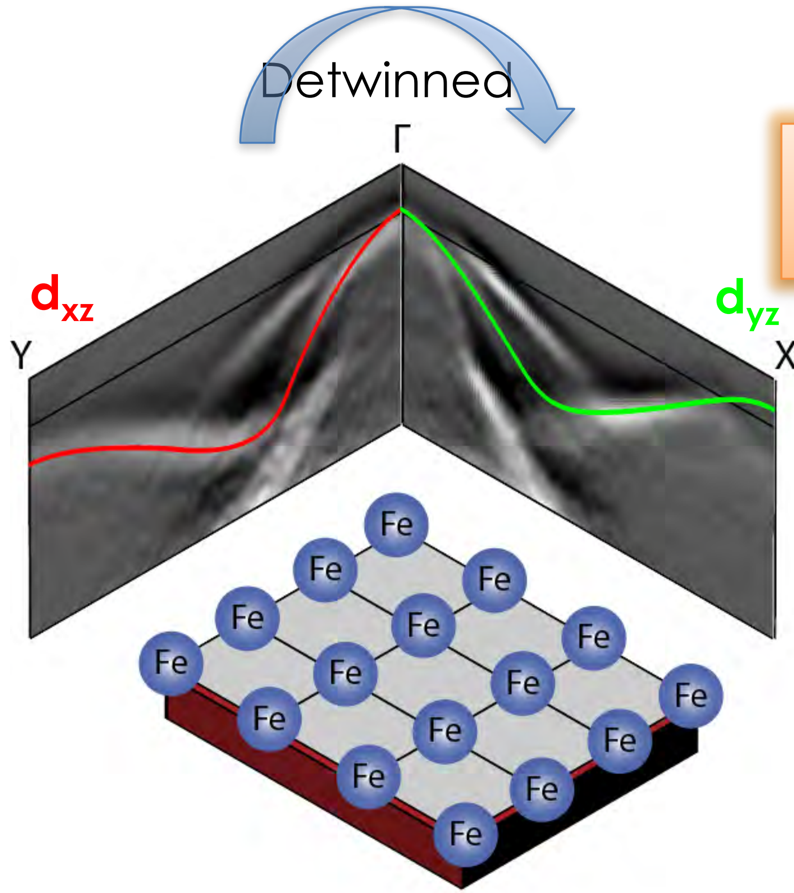




L. Wang *et al*. PRB 93, 014514 (2016)

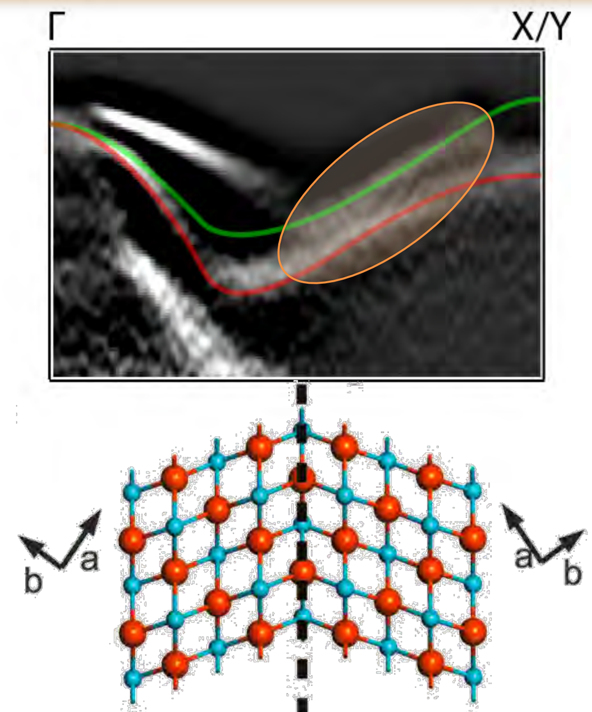
A word on twinning effect



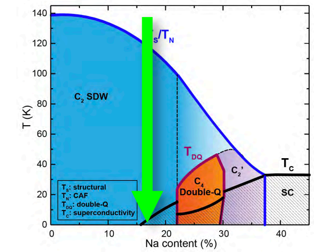


Twinned

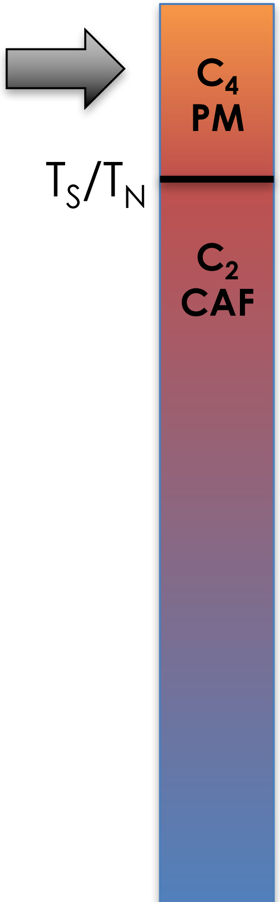
Apparent splitting on twinned sample
=
rotational symmetry breaking

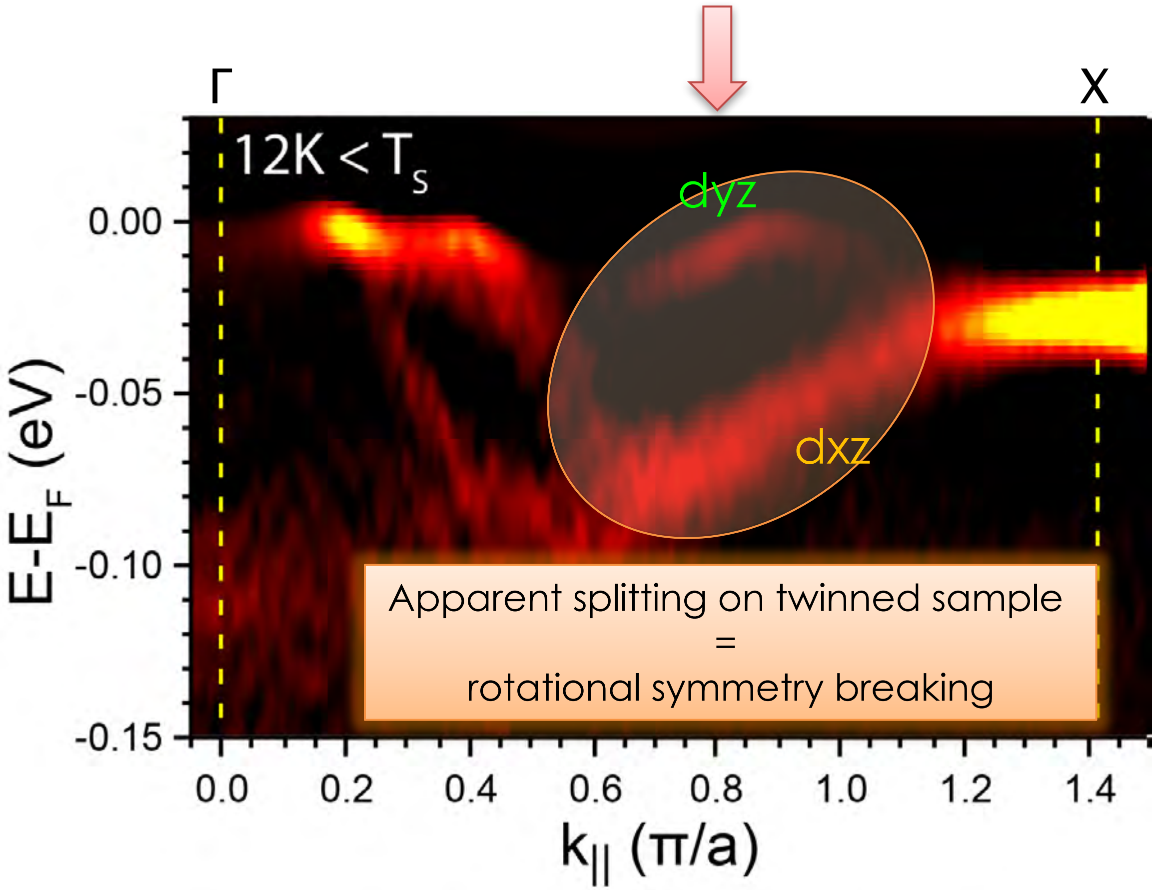


M. Yi, *et al*. PNAS 108, 6878 (2011)
M. Yi, *et al*. NJP 14, 073019 (2012)

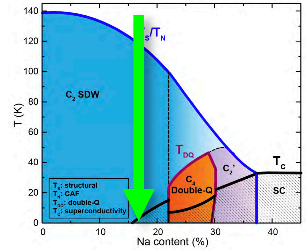


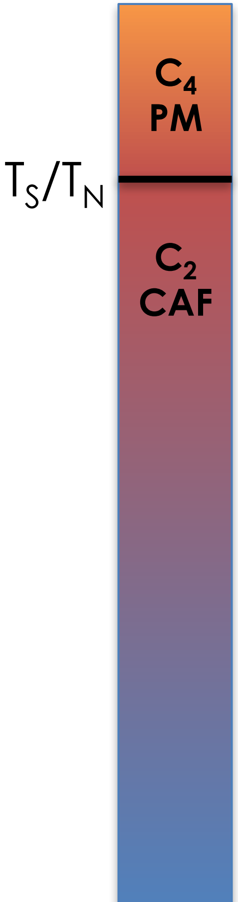
BN18: expected nematicity

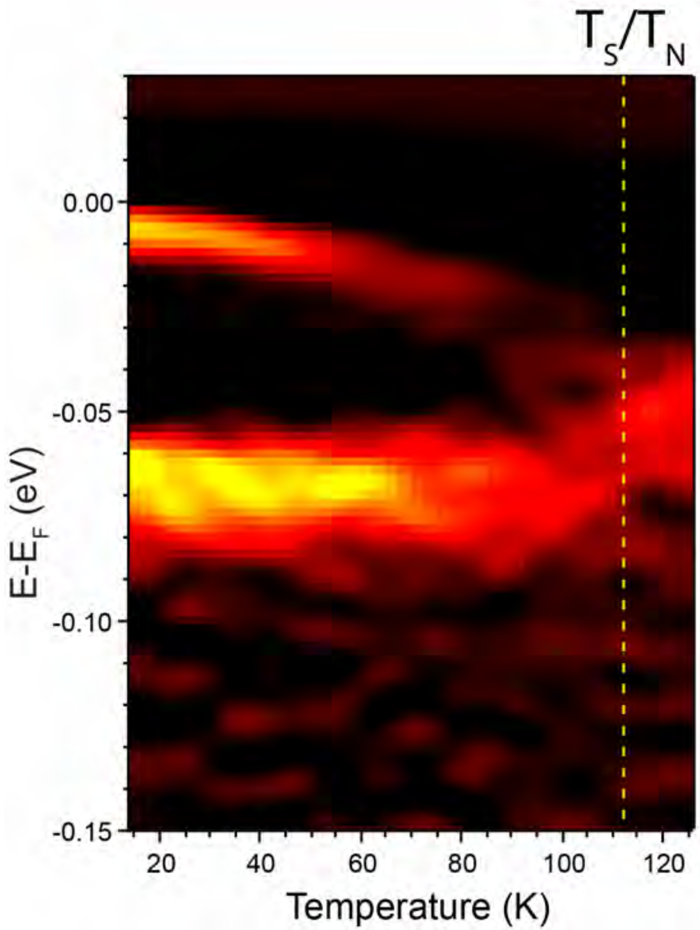


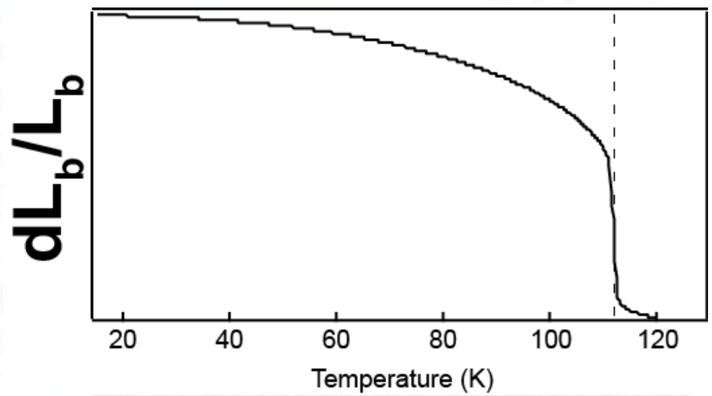


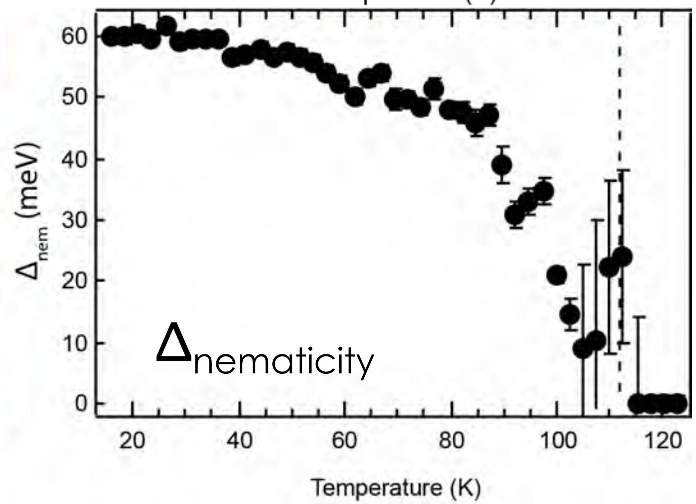
BN18: expected nematicity



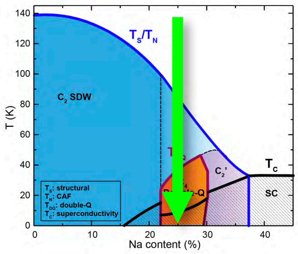


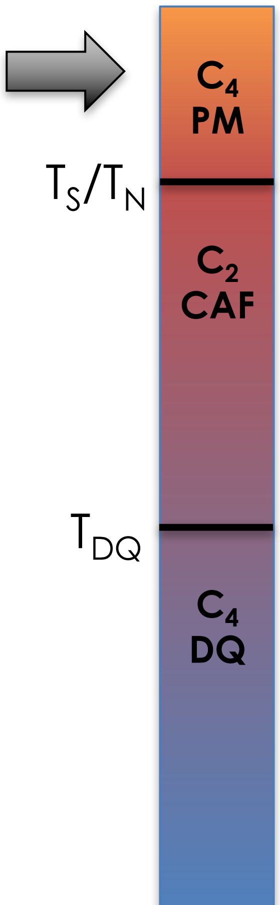


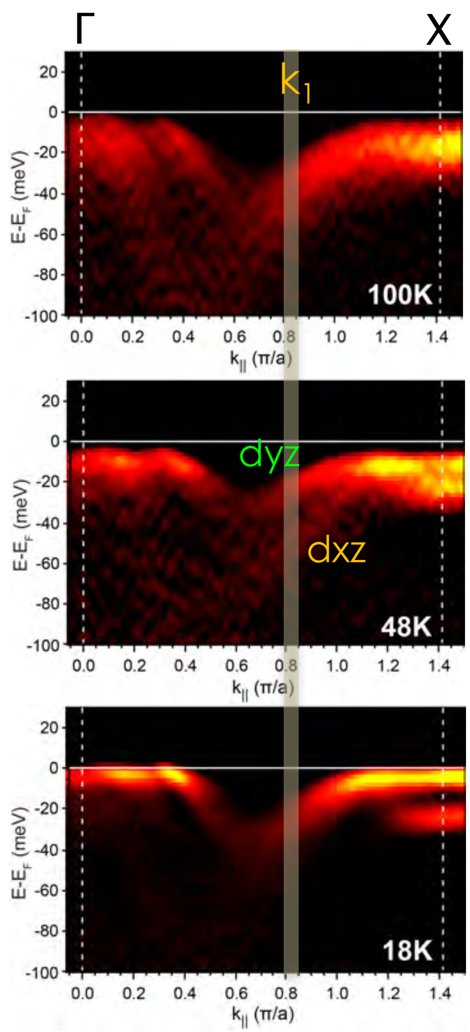


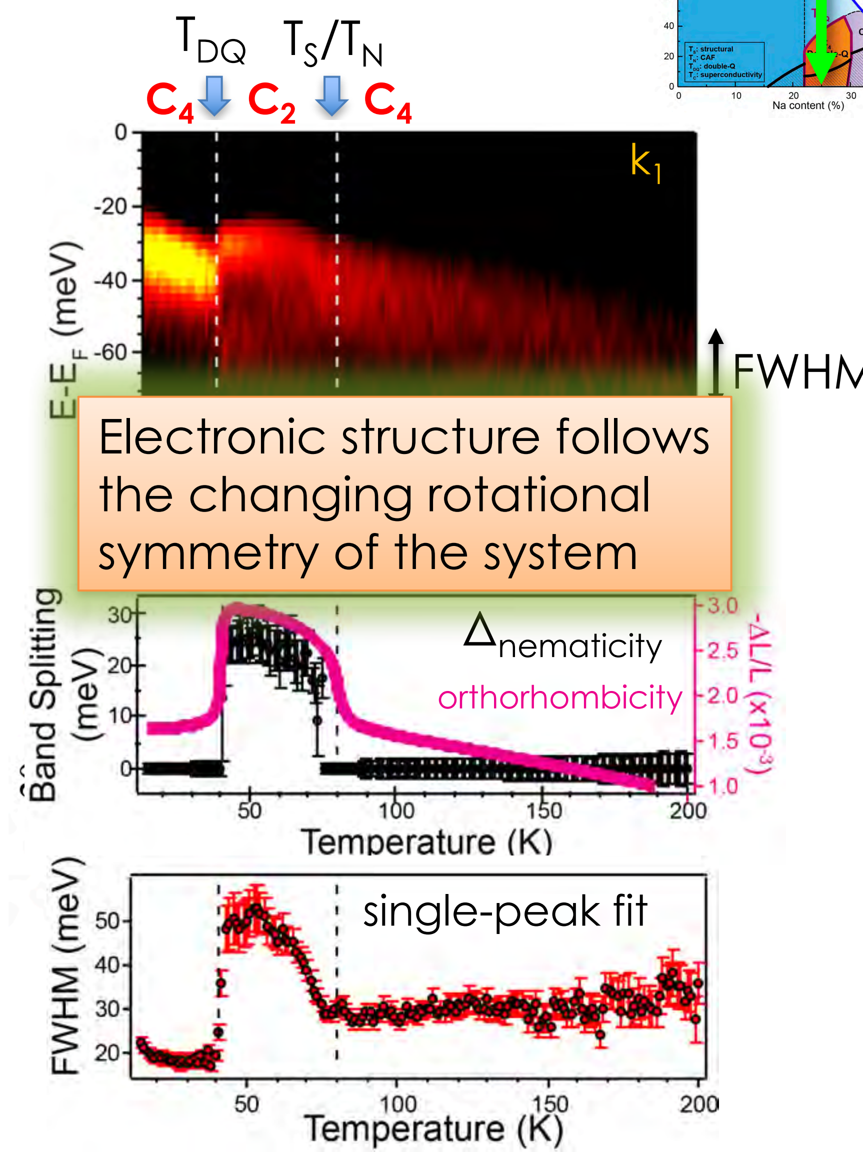


BN25: expected nematicity



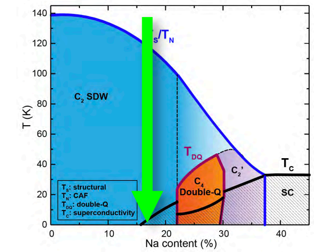


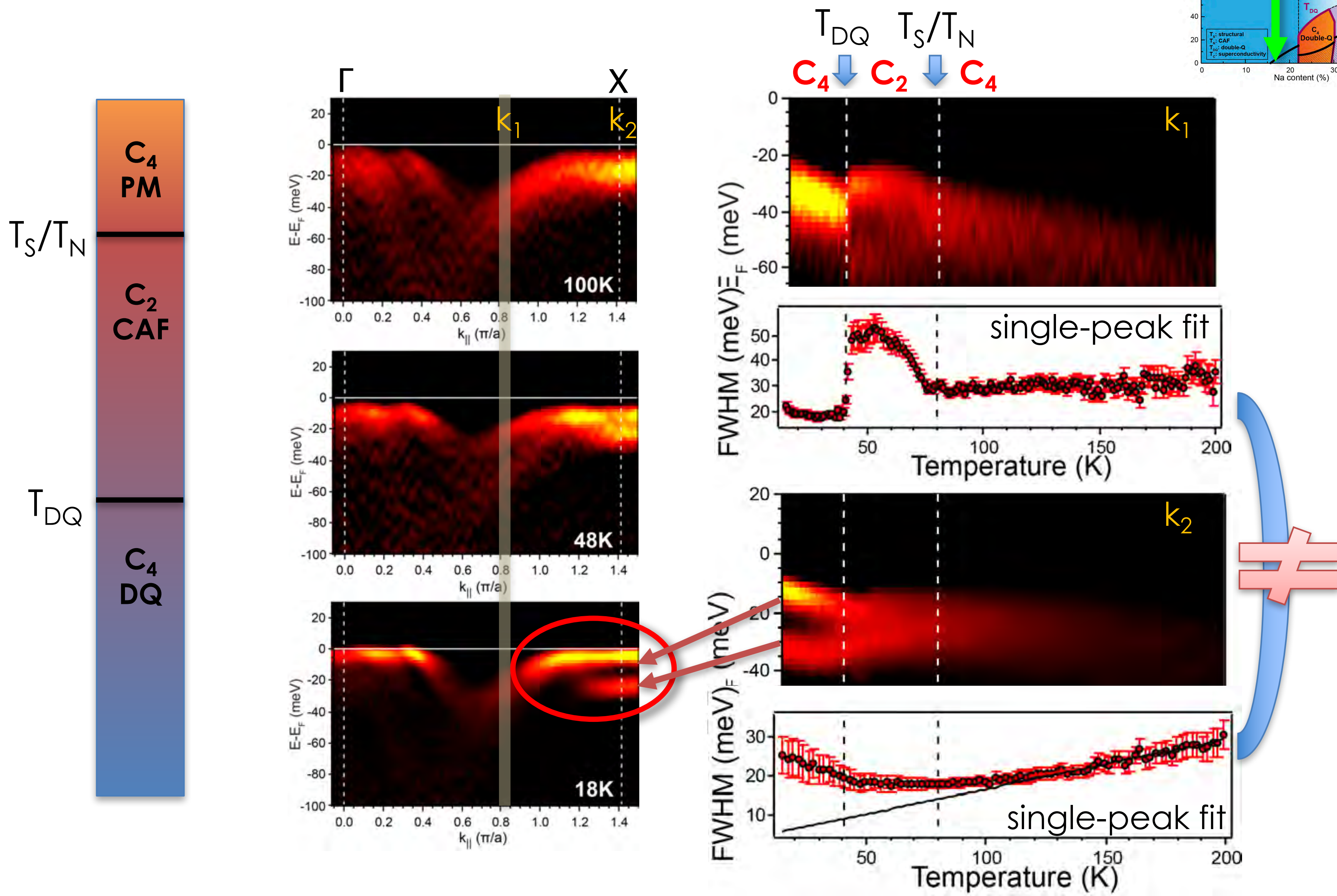




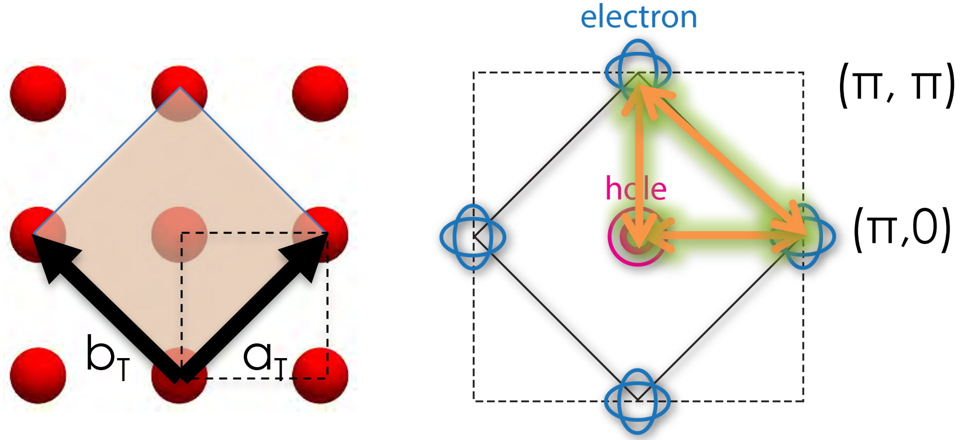
Electronic structure follows the changing rotational symmetry of the system

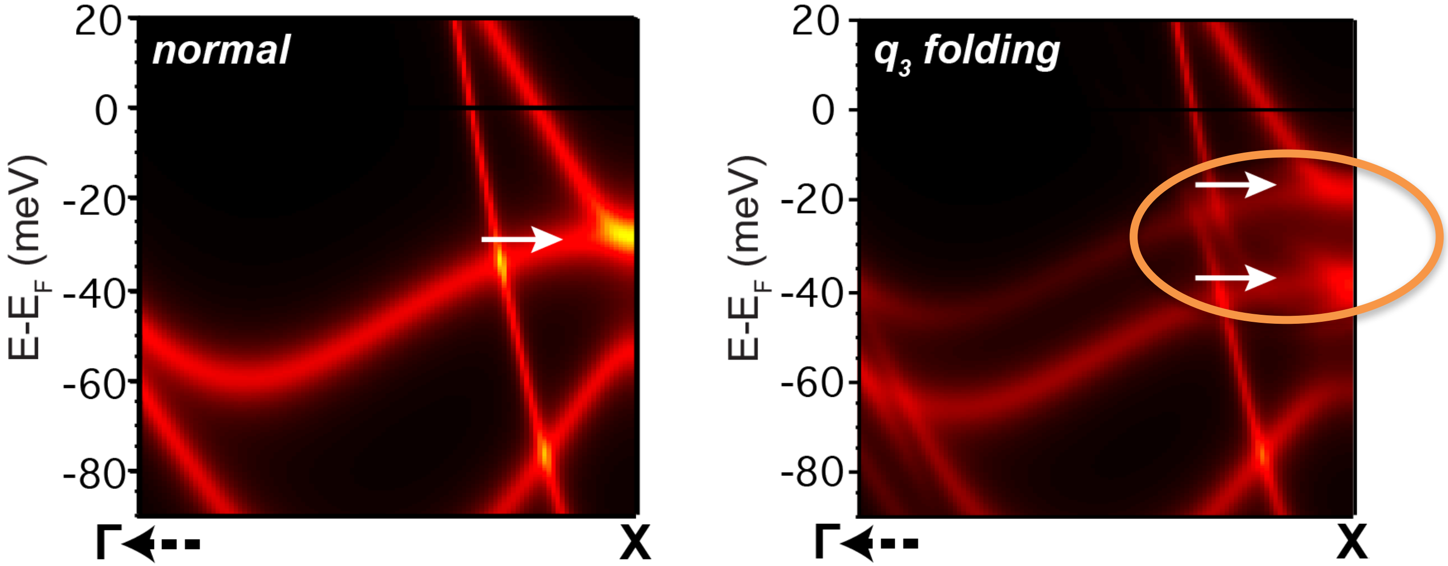
BN25: unexpected band splitting



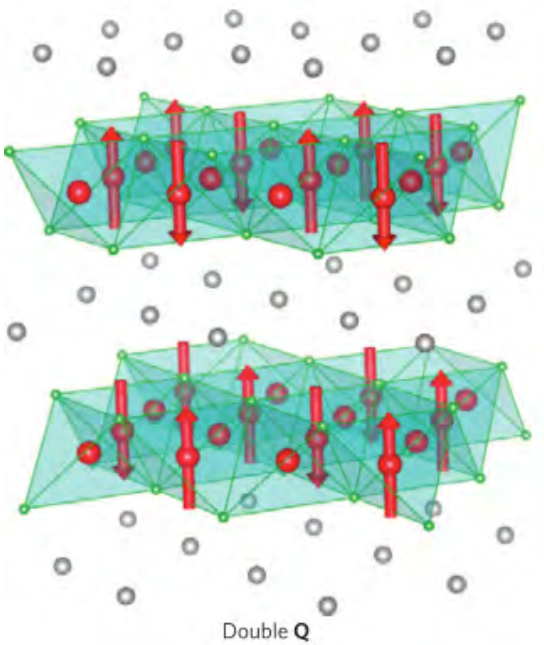


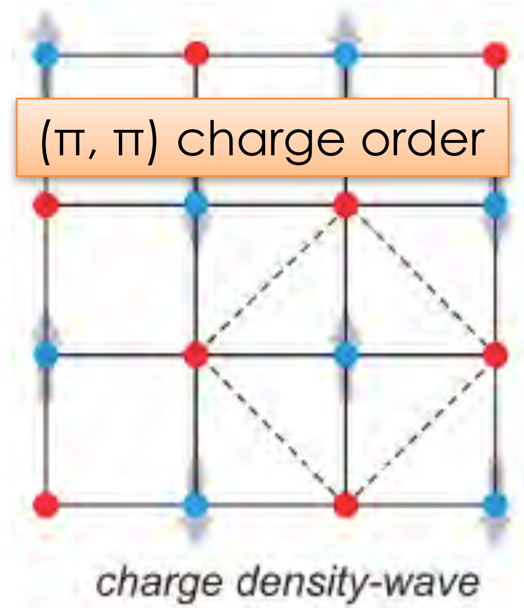
Simulations to identify the origin of the band doubling





(π, π) charge order accompanying the double-Q order

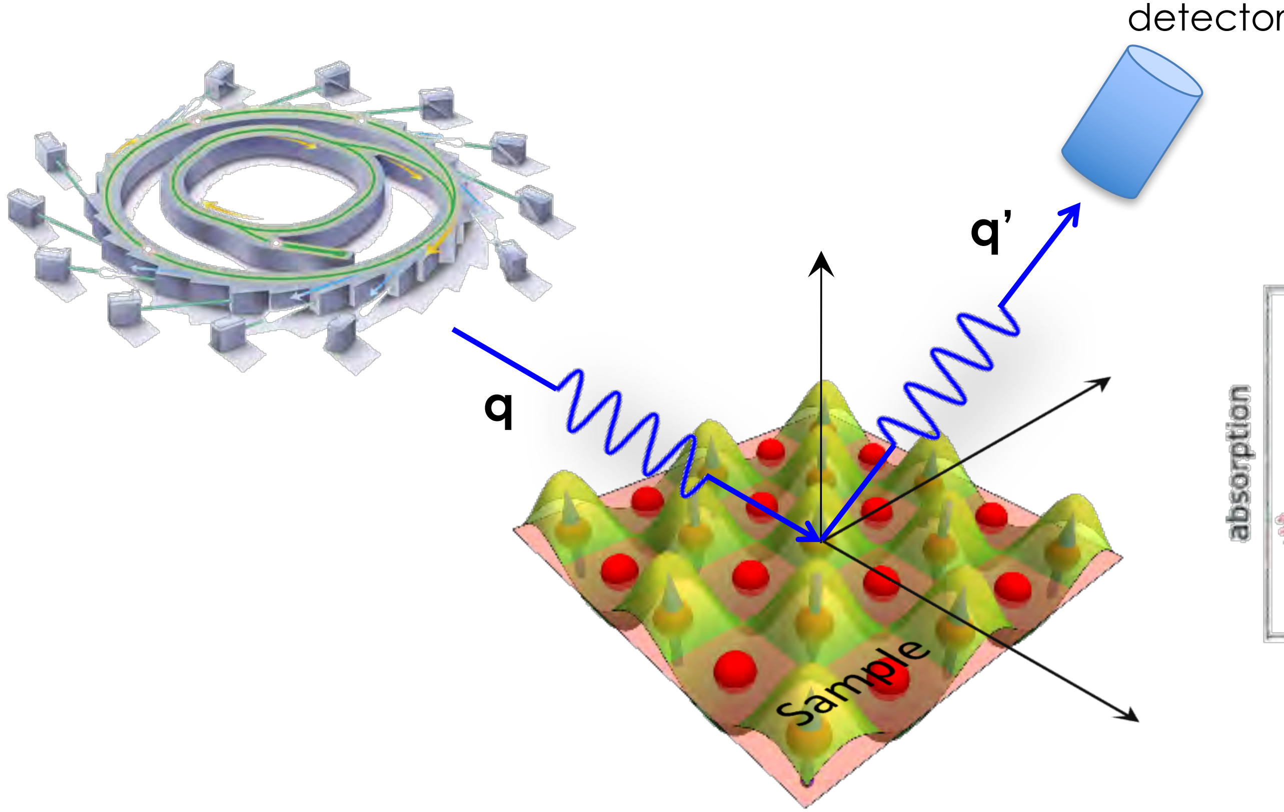


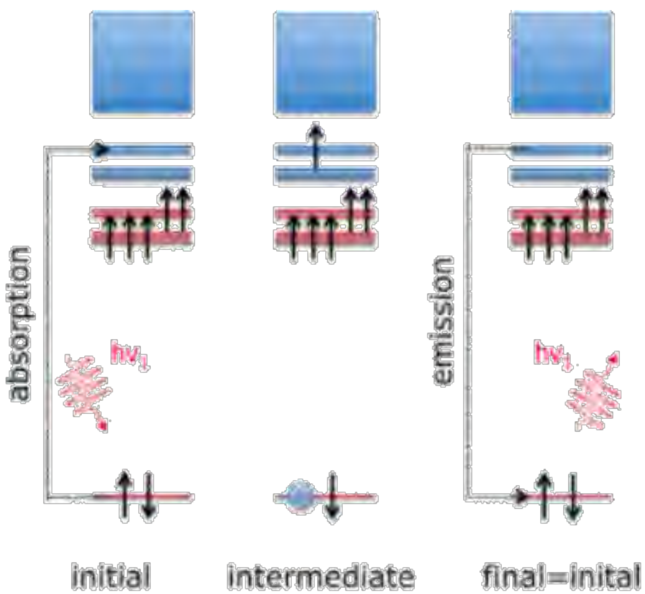


Blue sublattice: antiferromagnetic
Red sublattice: no moments
Unequal charges on blue/red sublattices

M. Gastiasoro, B. M. Andersen. PRB 92, 140506(R) (2015)
R. Fernandes, S. Kivelson, E. Berg. PRB 93, 014511 (2016)

Resonant Elastic X-ray Scattering (REXS)

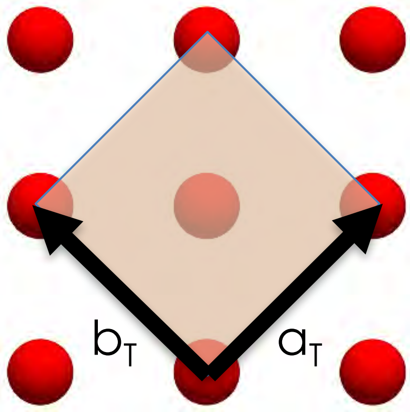


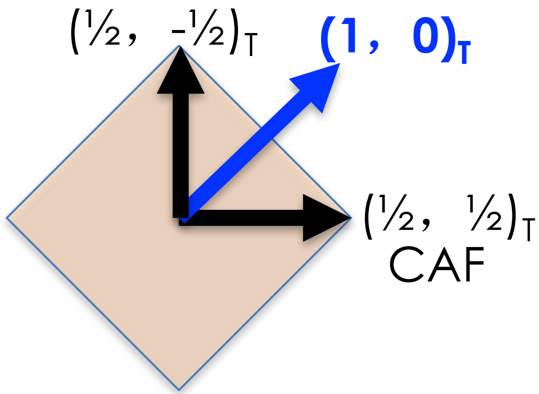


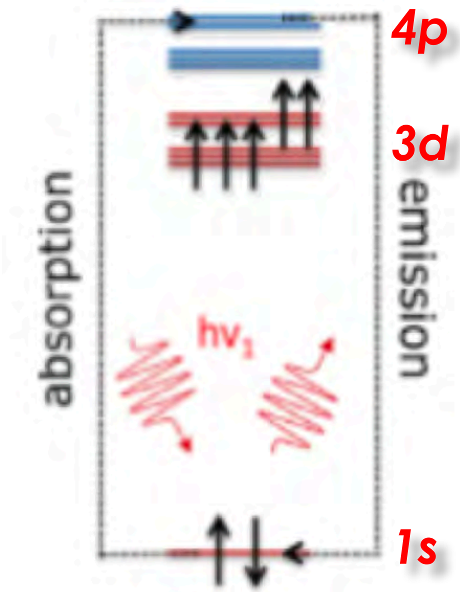
Probe orders with vector: **Q = q – q'**

Enhanced on resonance: $I_{RXS} \propto \Im(\lim_{\Gamma \to 0} \langle i| \boldsymbol{R}^\dagger \frac{1}{\omega - \omega_i - H + i\Gamma/2} \boldsymbol{R} |i\rangle)$

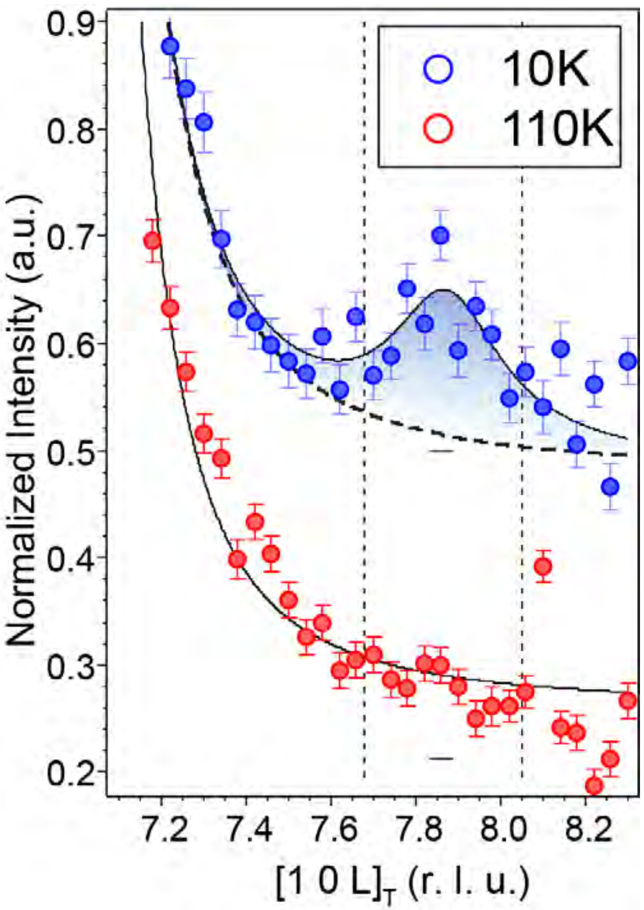
Hard X-Ray RXS at Fe *K* edge

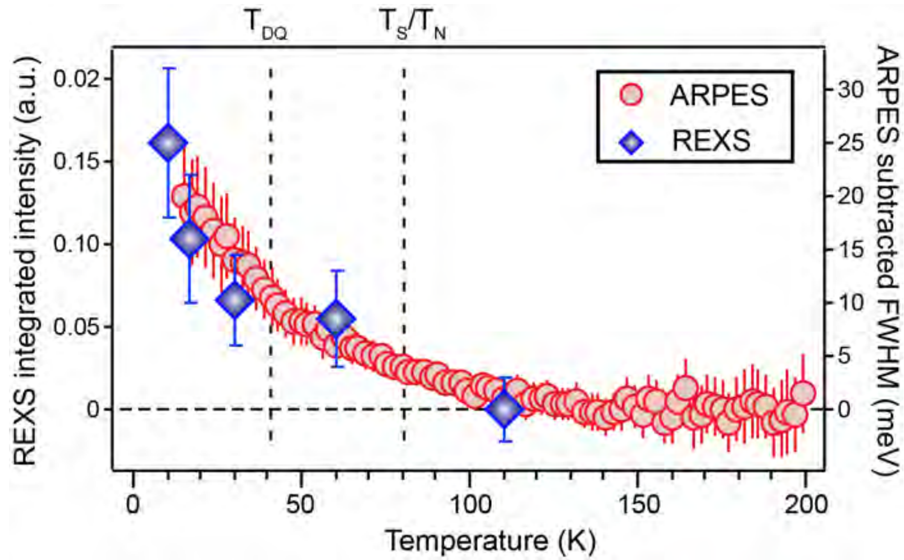


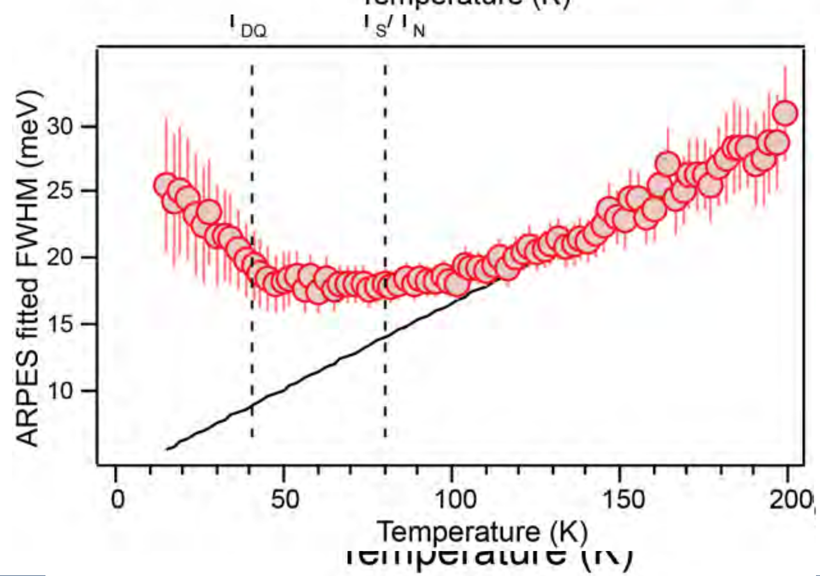




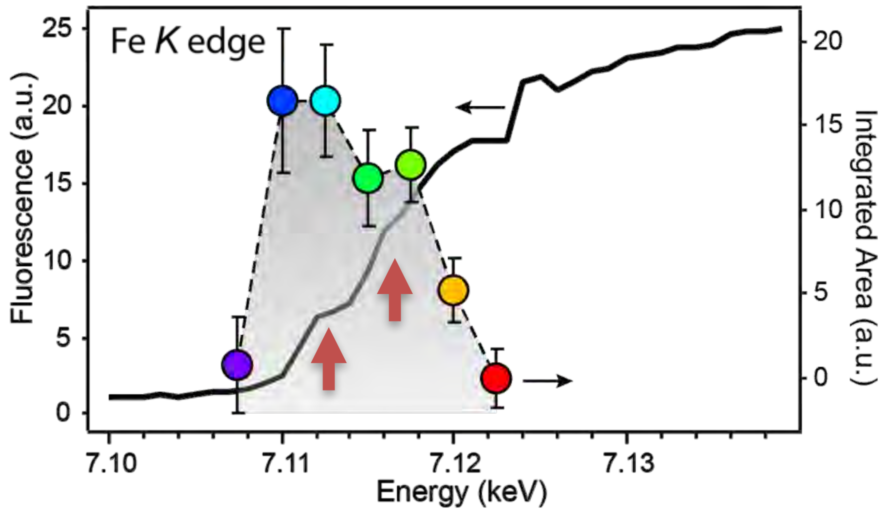
New peak emerges corresponding to (π, π) order



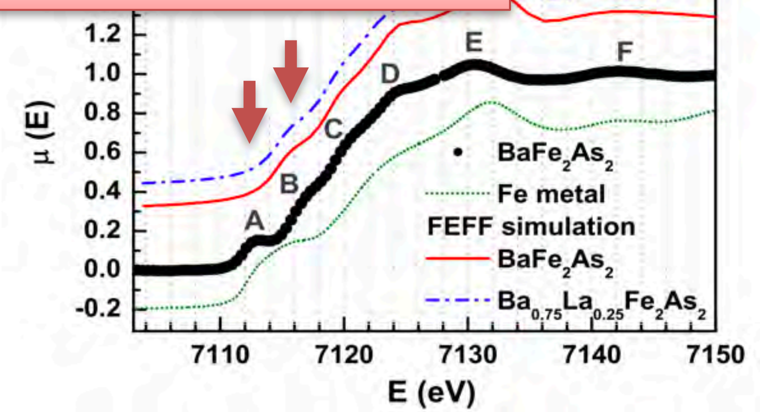




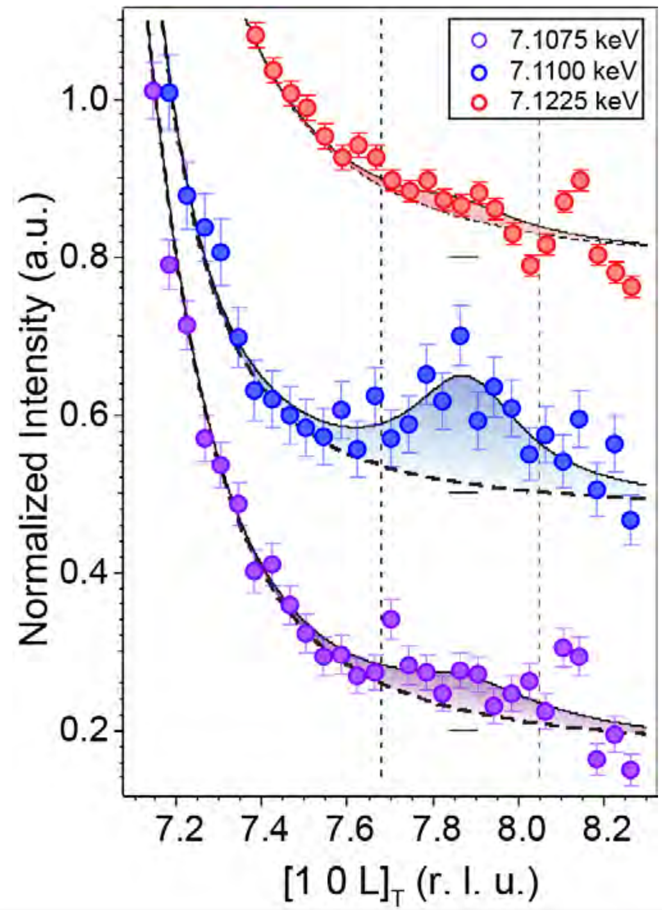
(π, π) order peak resonance behavior



Transitions involving 3d states

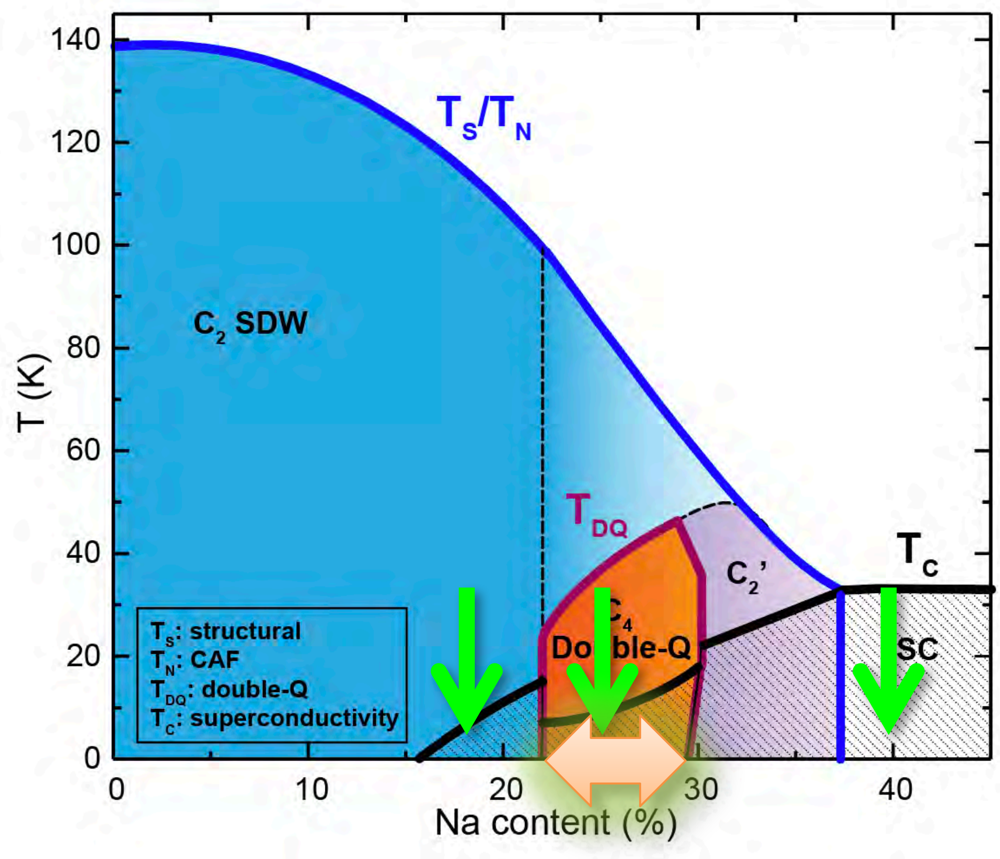


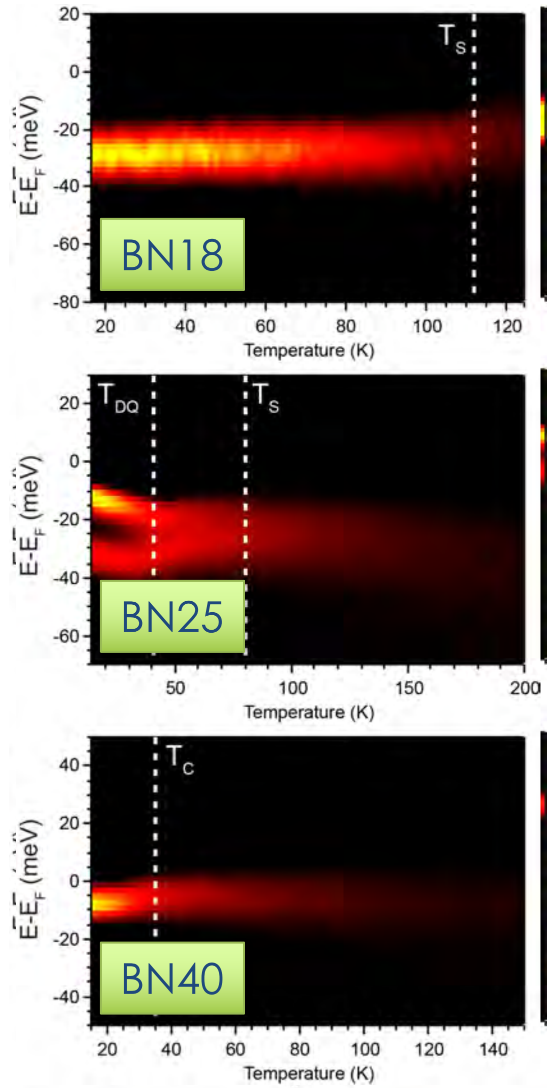
E. M. Bittar *et al*. PRL 107, 267402 (2011)



Charge order mostly involves Fe 3d states near the Fermi level.

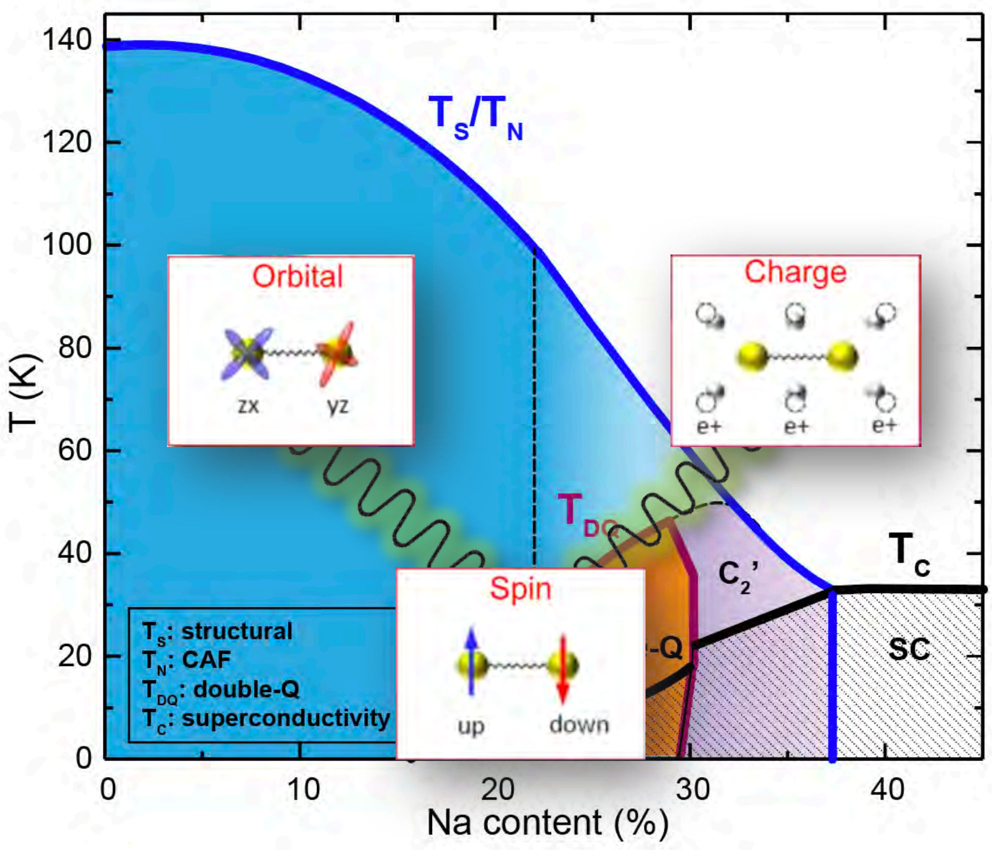
Charge order doping dependence





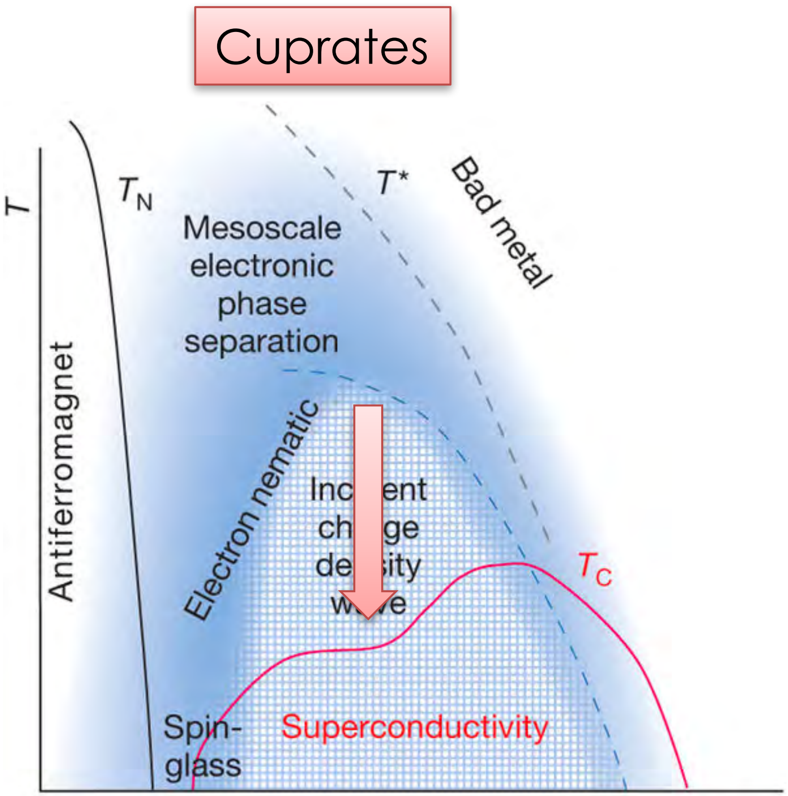
The charge order is predominantly coupled to the double-Q magnetic order.

Summary – strong coupling of spin and charge

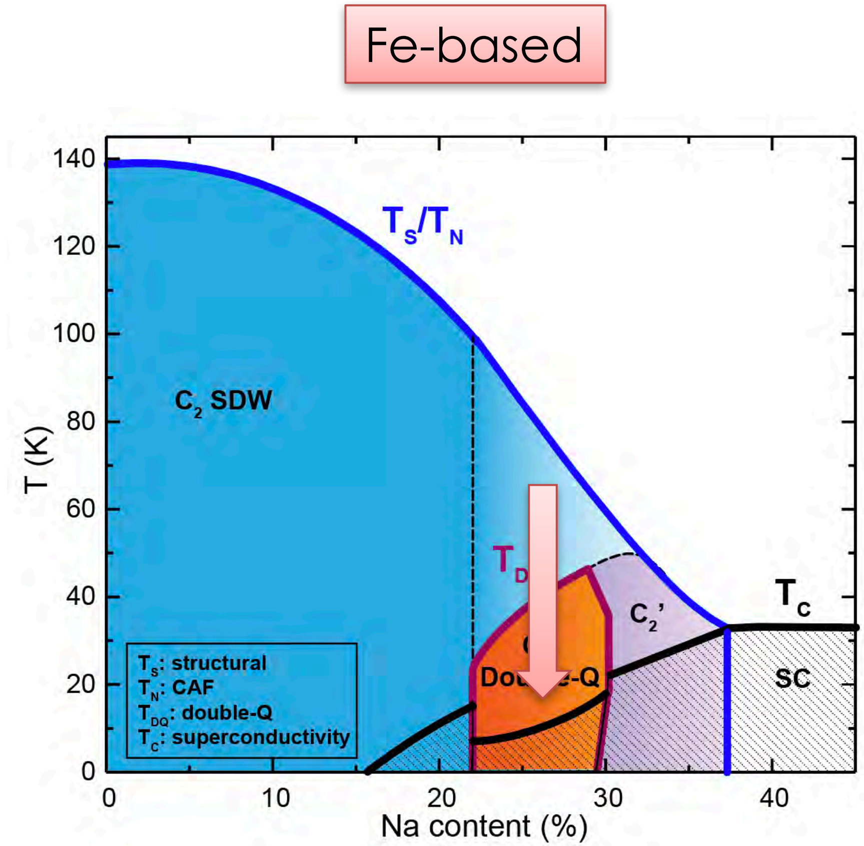


- Observed evidence of (π, π) *charge order*
  - Band folding (ARPES)
  - Ordering peak (REXS)
  - Resonant at the Fe K-edge involving transitions into the *3d* states
- Charge order couples to the double-Q magnetic order analogously as the nematic order to the collinear antiferromagnetic order
- Strong coupling of spin and charge

Commonalities in high temperature superconductors



Fradkin and Kivelson, Nat. Phys. 8, 864–866 (2012)



- Magnetically ordered parent phase
- Electronic nematic phase
- Charge order creating a dip in the superconducting dome

Collaborators

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Dung-Hai Lee
Bob Birgeneau

Stanford University
Yu He
Zhi-Xun Shen

Karlsruhe Institute of Technology
Liran Wang
Mingquan He
Frederic Hardy
Peter Schweiss
Peter Adelmann
Thomas Wolf
Matthieu Le Tacon
Anna Böhmer
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North Carolina State University
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Rice University
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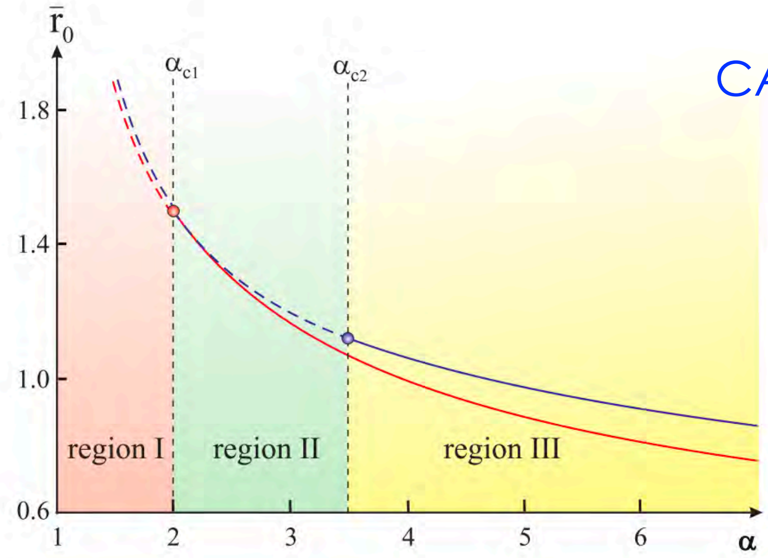
Renmin University
Rong Yu

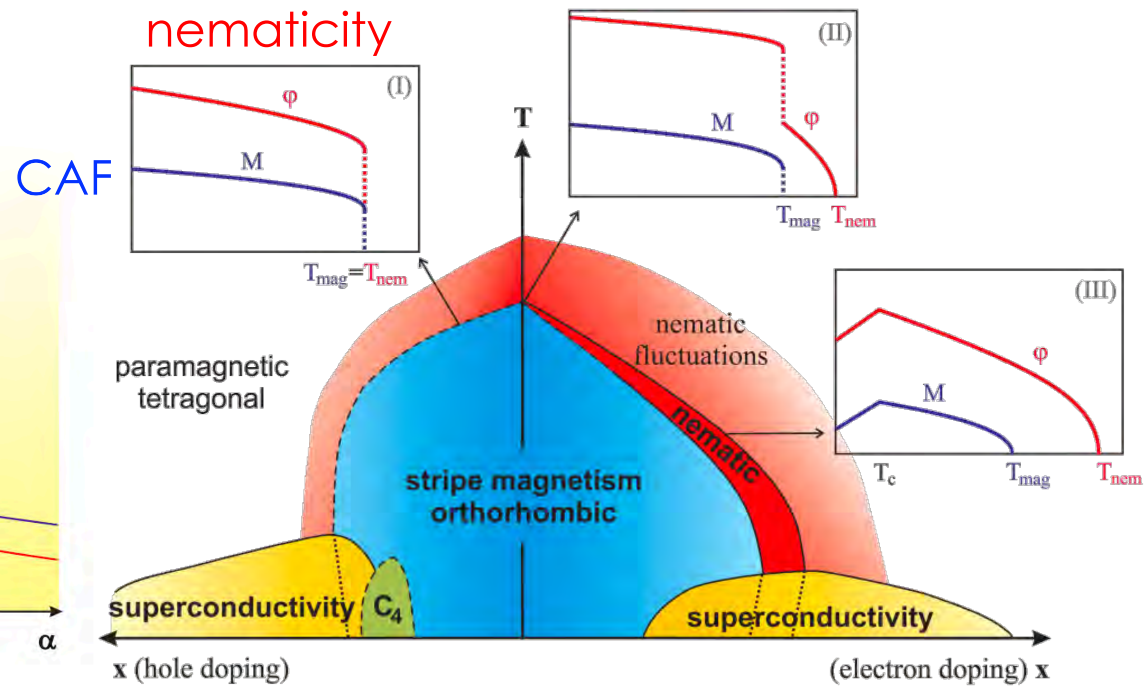
Stanford Synchrotron Radiation Lightsource
Donghui Lu
Makoto Hashimoto

Advanced Light Source
Sung-Kwan Mo
Zahid Hussain

National Synchrotron Light Source II
Christie Nelson

CO/Double-Q analogous to nematicity/CAF



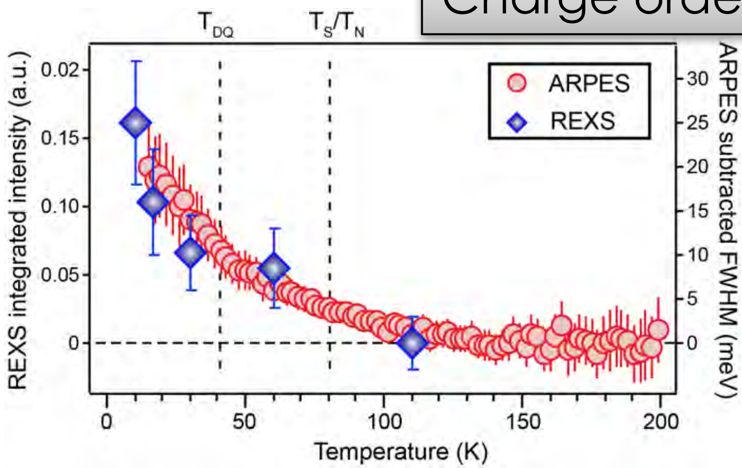


What about CO and double-Q magnetic order?

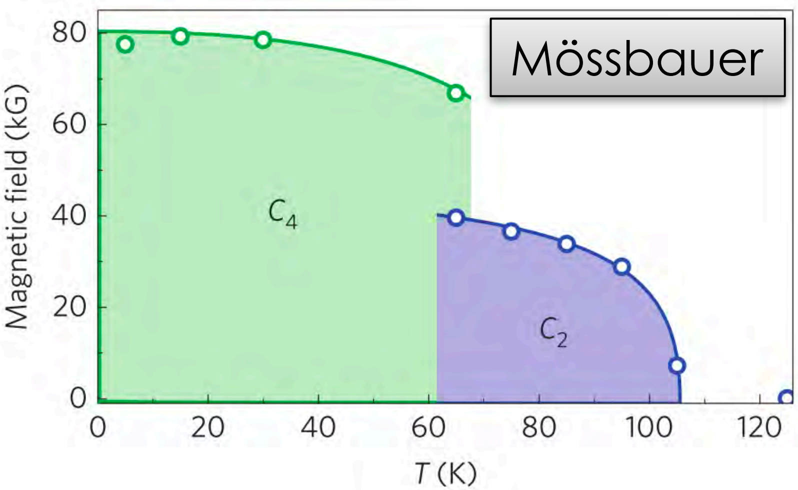
R. M. Fernandes et al. Nat. Phys. 10, 97 (2014).

CO appearing above double-Q magnetic order?

Charge order



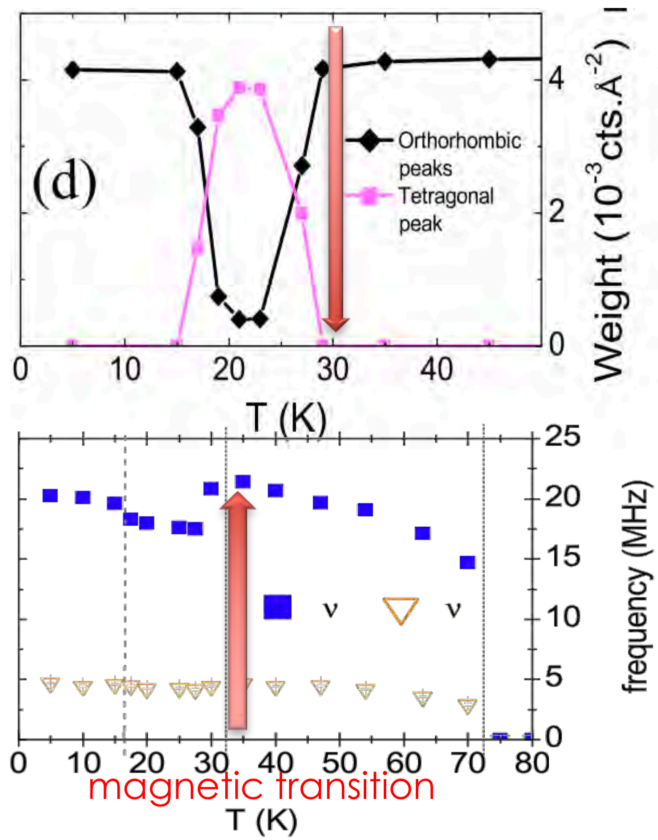
Mössbauer



J. M. Allred *et al*. Nat. Phys. 12, 493 (2016)

µSR

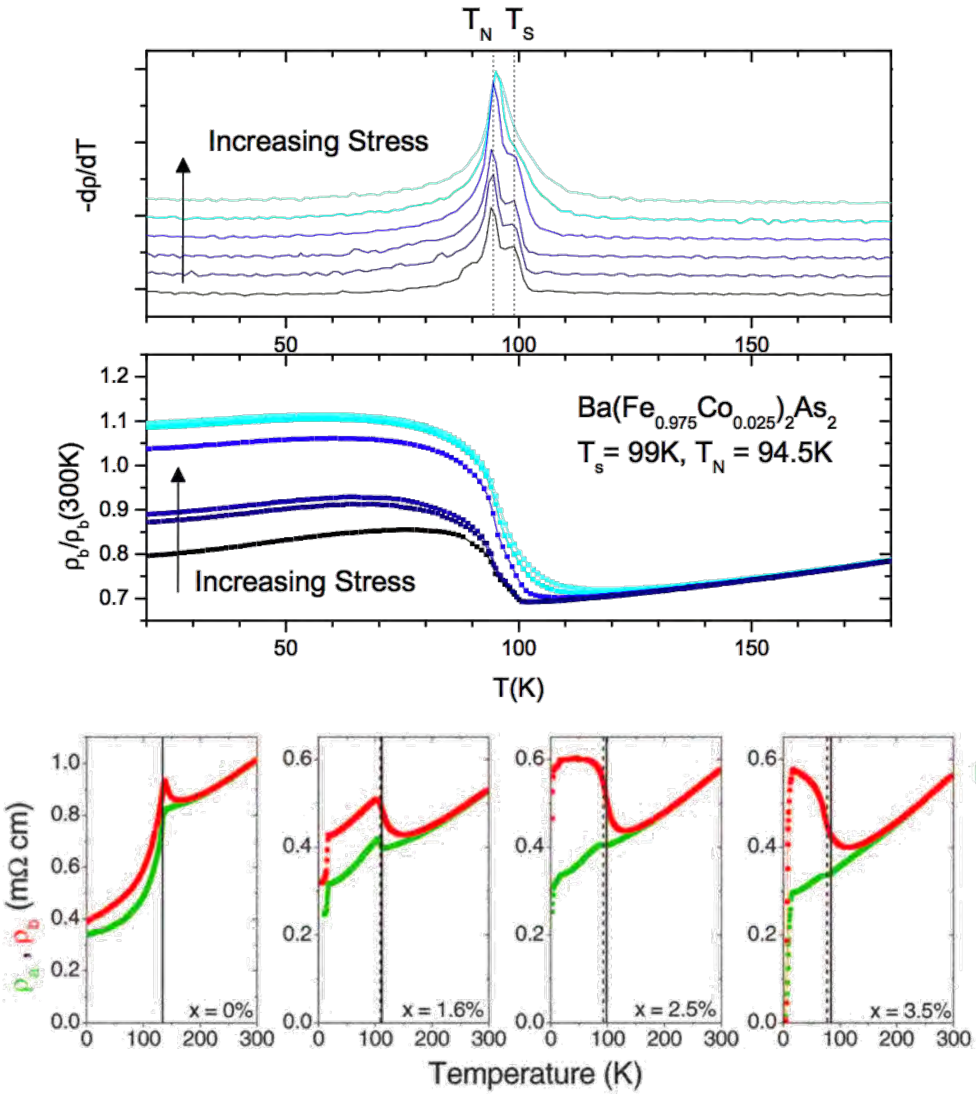
Structural transition



magnetic transition

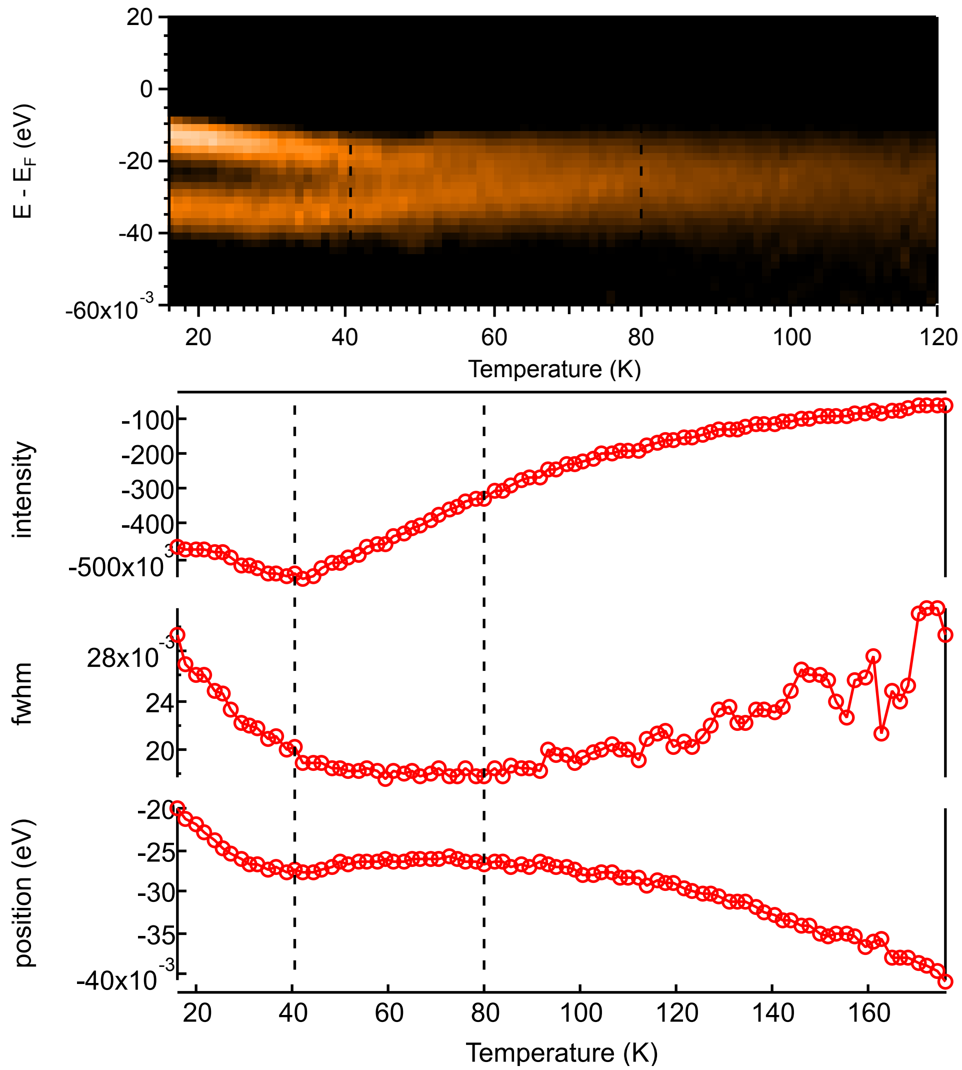
B. Mallet *et al*. arXiv: 1506.00786

Remember the strain effect on nematic order

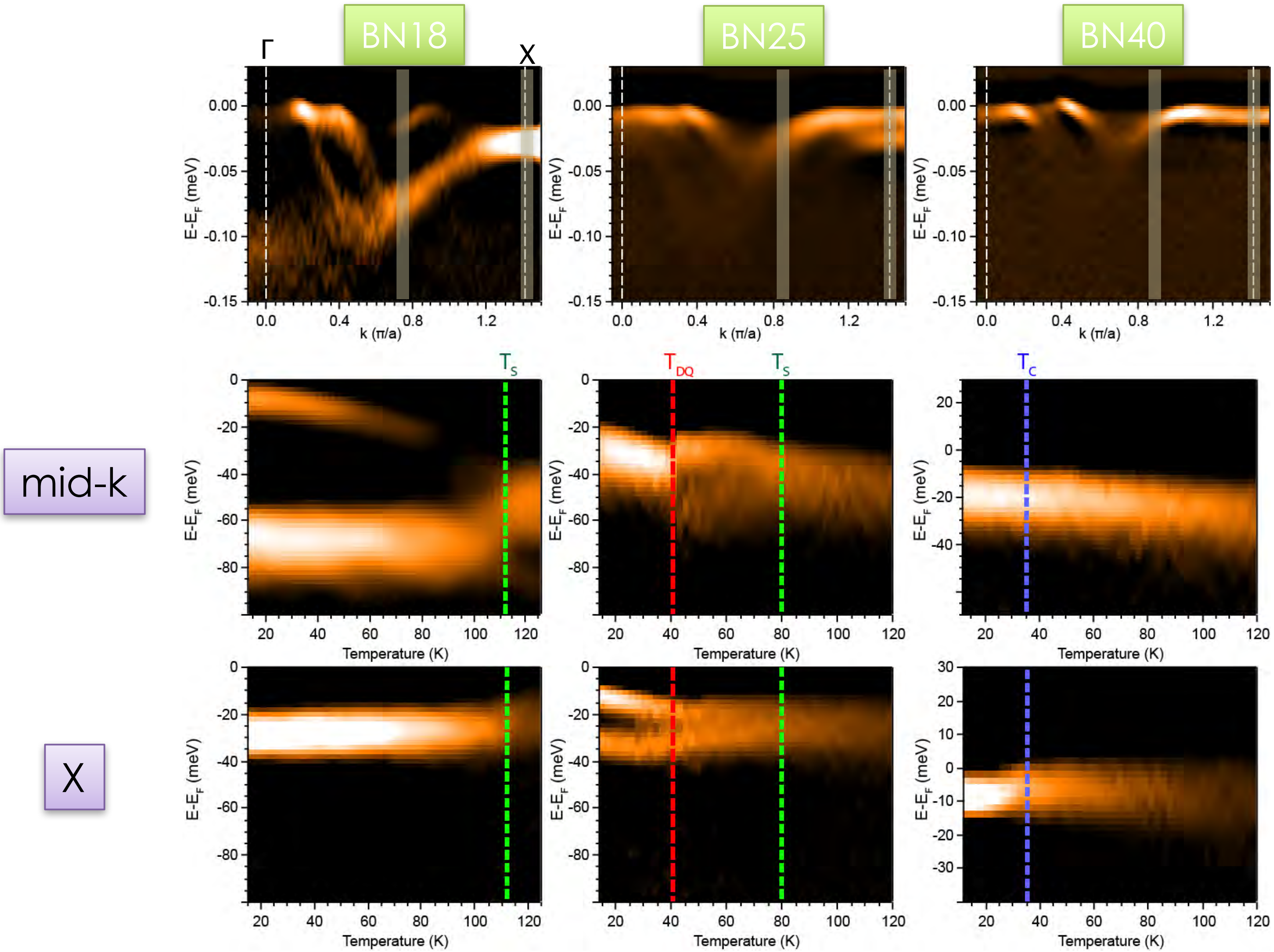


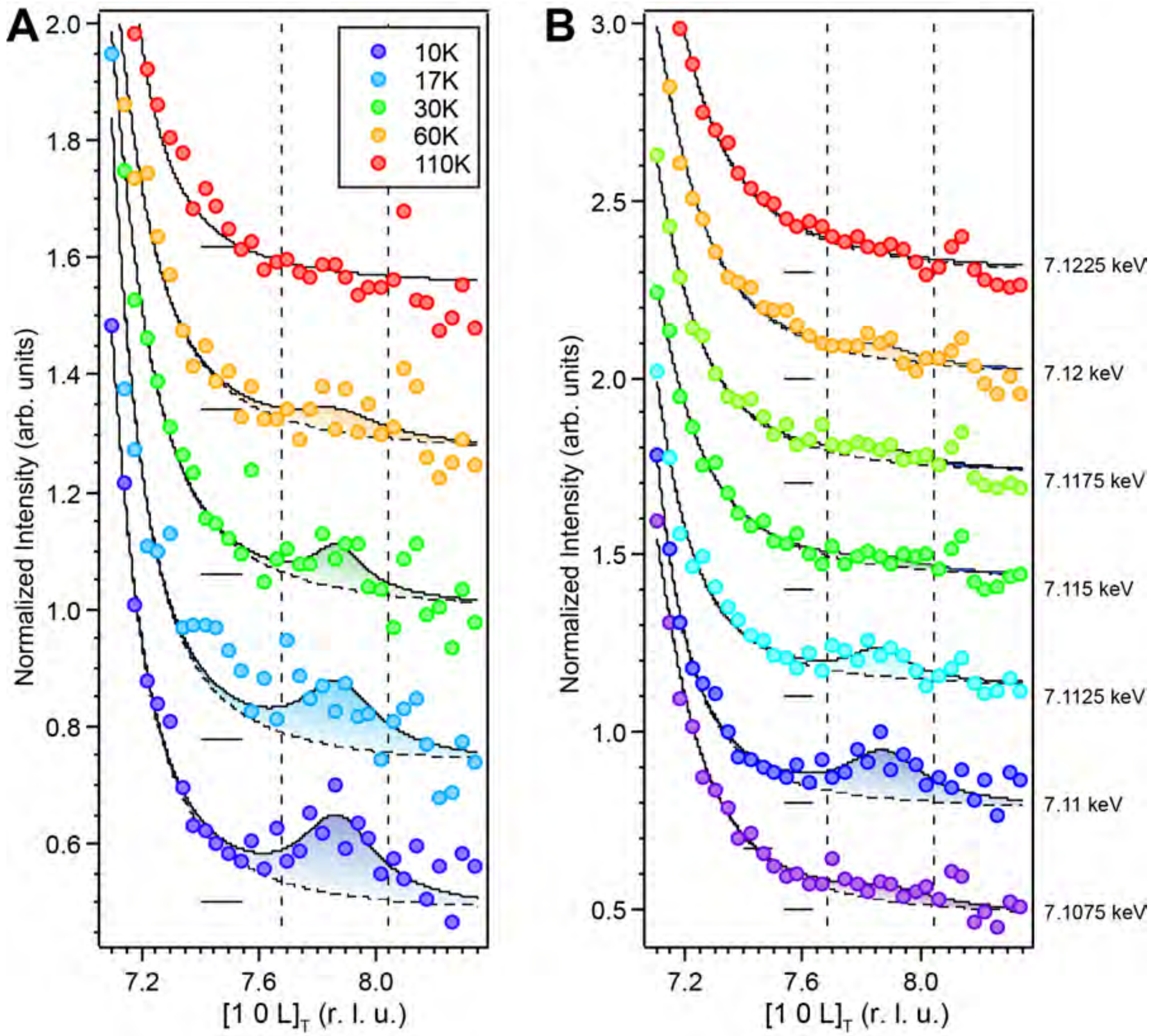
J.-H. Chu *et al*. Science 329, 824 (2010)

BN2 X, single gaussian fit



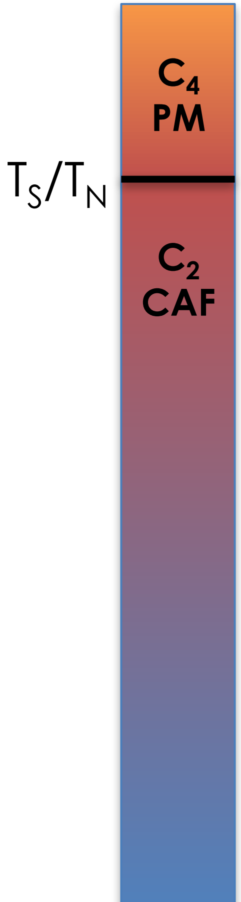
Temperature dependence at X- doping comparison

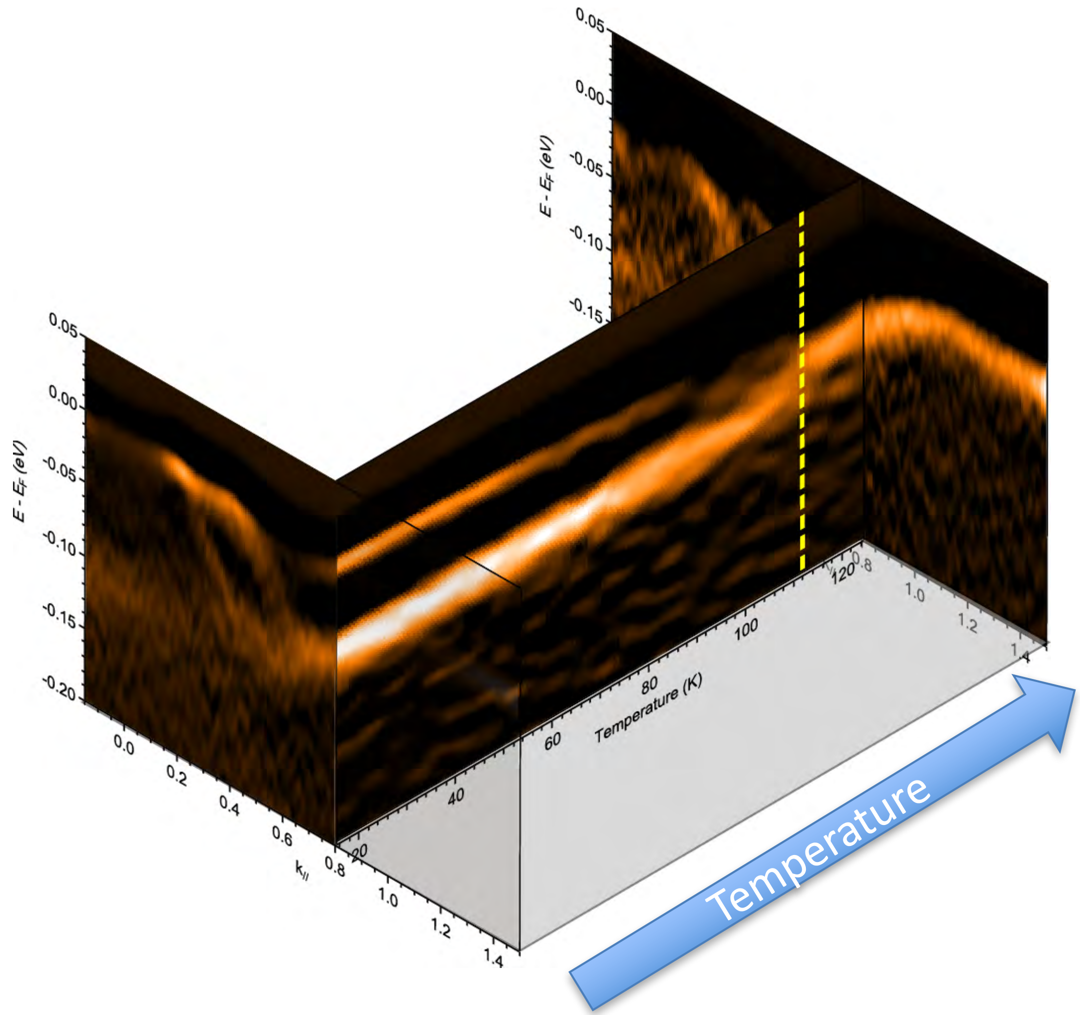


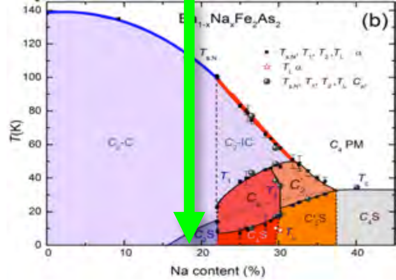


A
B
10K
17K
30K
60K
110K
Normalized Intensity (arb. units)
[1 0 L]T (r. l. u.)
7.1225 keV
7.12 keV
7.1175 keV
7.115 keV
7.1125 keV
7.11 keV
7.1075 keV

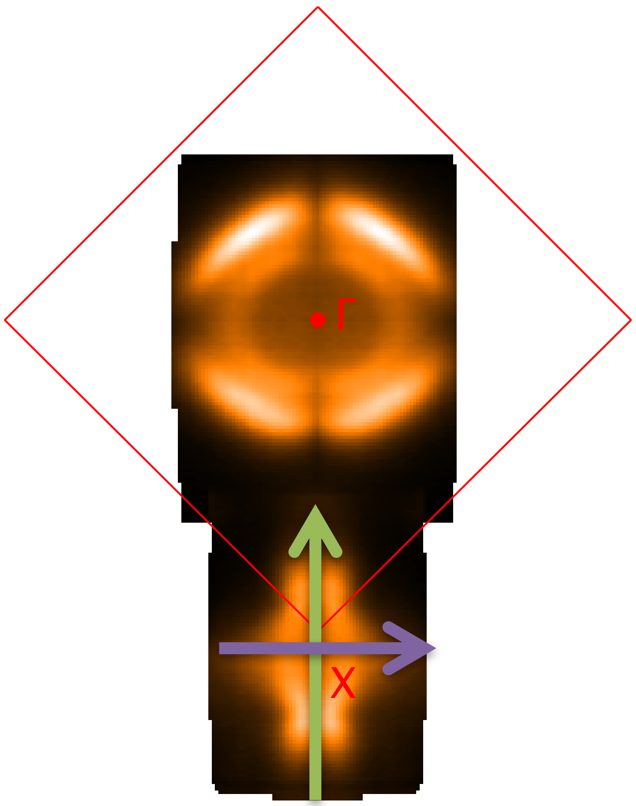
BN18: expected nematicity

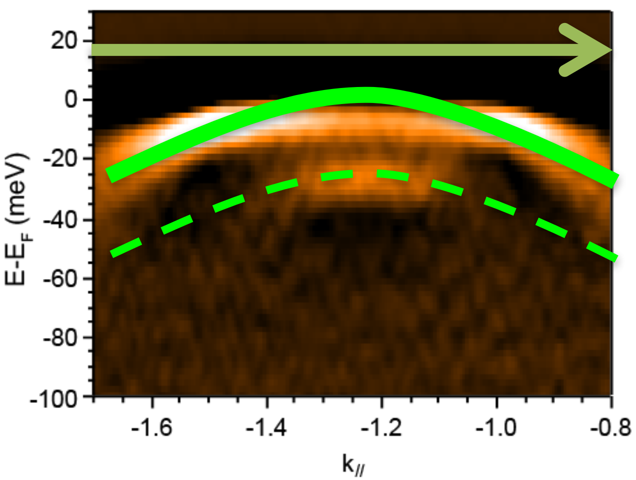




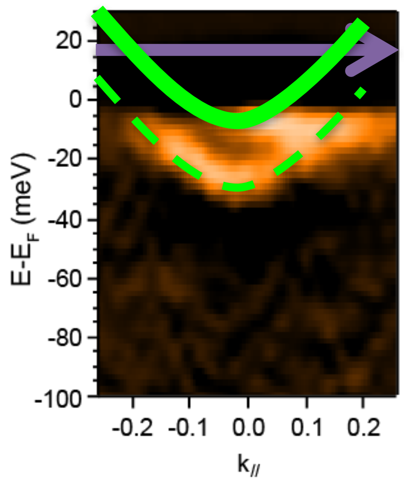


BN25: double sets of bands



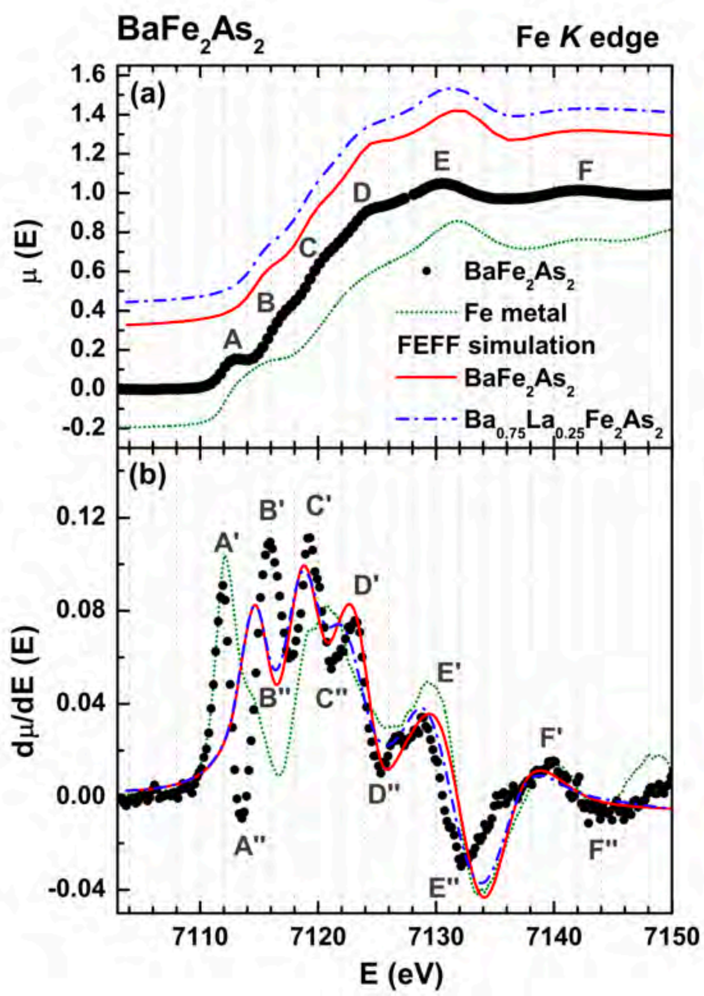


Hole-like



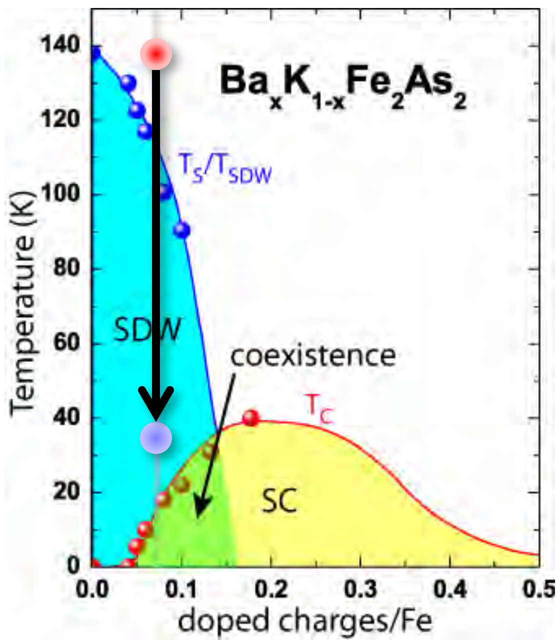
Electron-like

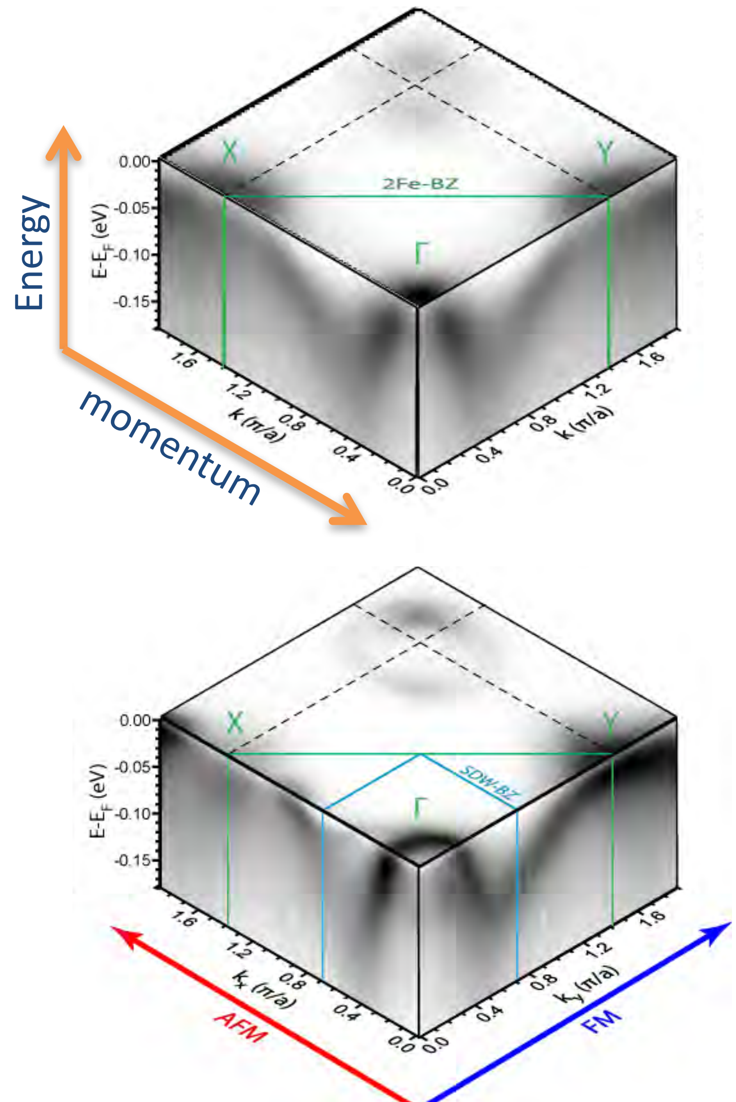
Appearance of a second copy of bands.



rivative are also shown in Fig. 2 (solid line). The calculated spectrum captures fairly well the observed $B-F$ features. The $C-F$ features above the edge are dipolar transitions to unoccupied Fe p projected states. An alternative simulation excluding $1s \rightarrow 3d$ quadrupolar transitions (not shown) shows a slightly weaker spectral weight for the B shoulder, demonstrating that it originates partly from such transitions and partly from dipolar transitions allowed by $4p-3d$ mixing in the Fe site without inversion symmetry [27,28]. The observed A preedge peak is completely absent in the simulation. This is possibly because charge-transfer effects in the absorption process, not fully taken into account in the simulation, pull down the $3d$ states yielding a combination of a well-screened peak B and a poorly screened peak A, as described in detail in Refs. [27,29].

Spectroscopic evidence for nematicity and SDW

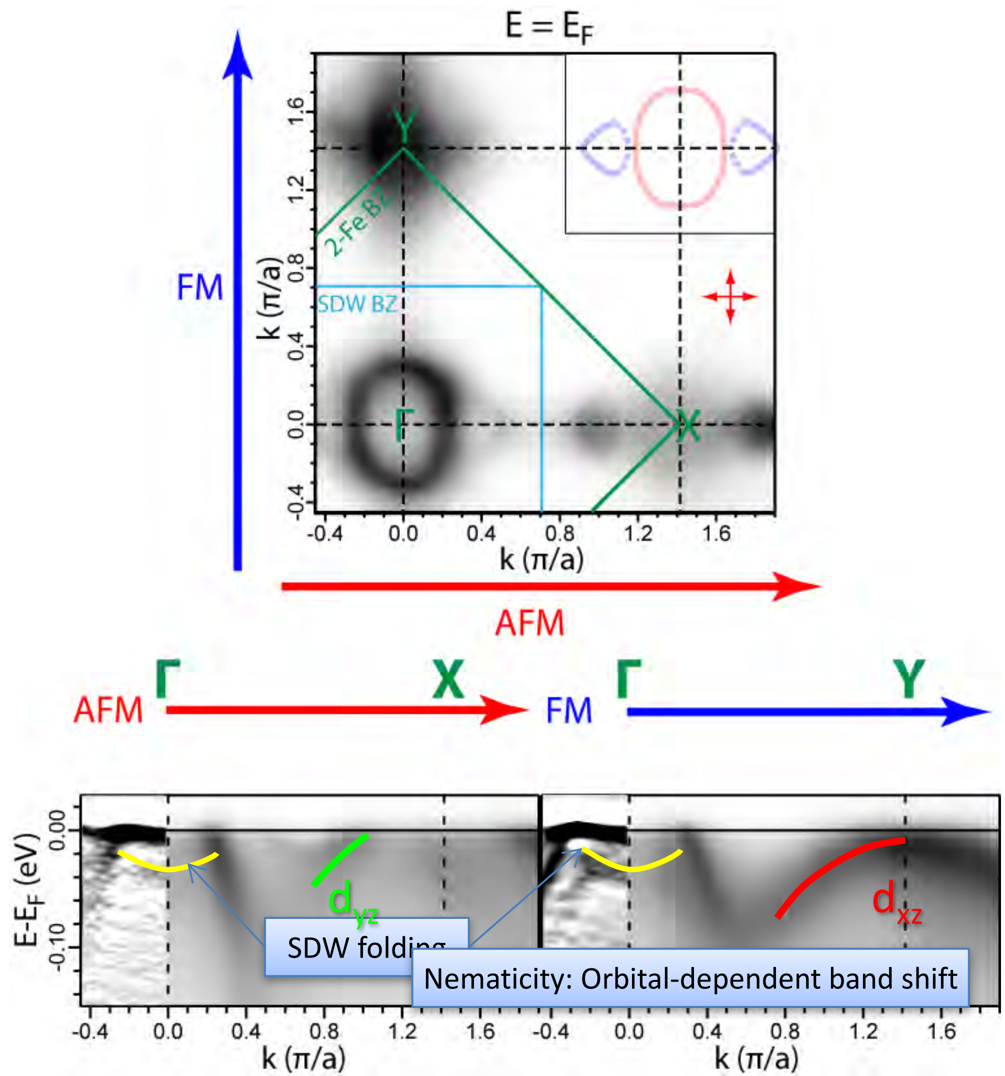




M. Yi *et al*. Nat. Comm. In revision.

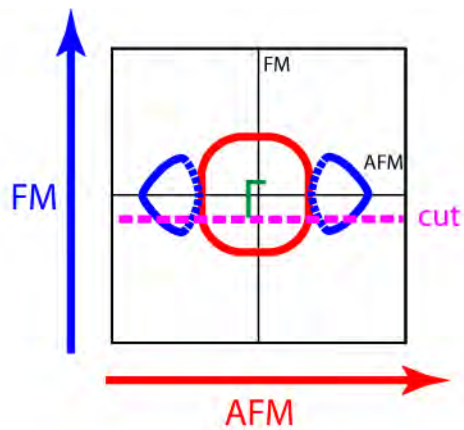
Berkeley
UNIVERSITY OF CALIFORNIA

Spectroscopic evidence for nematicity and SDW

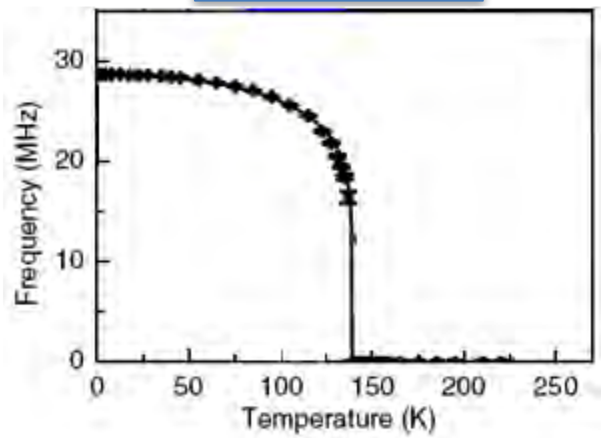


M. Yi *et al*. Nat. Comm. In revision.

Spin Density Wave gap

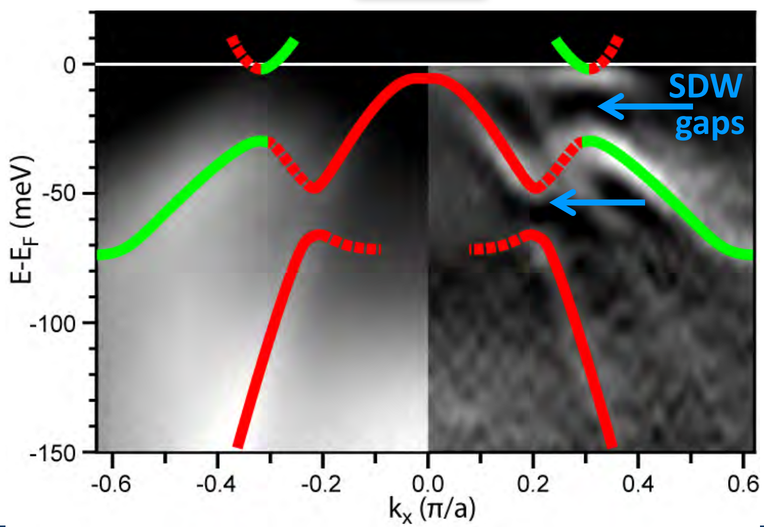


Magnetic moment

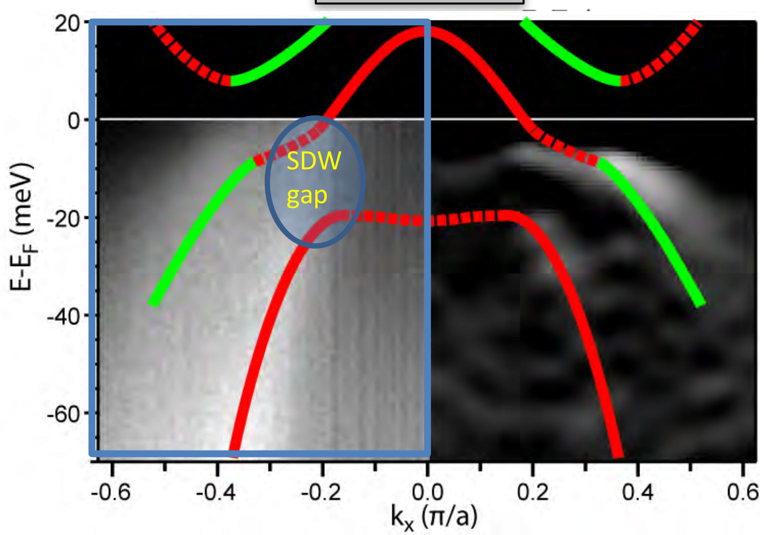


E. Wiesenmayer et al. PRL (2011)

X=0

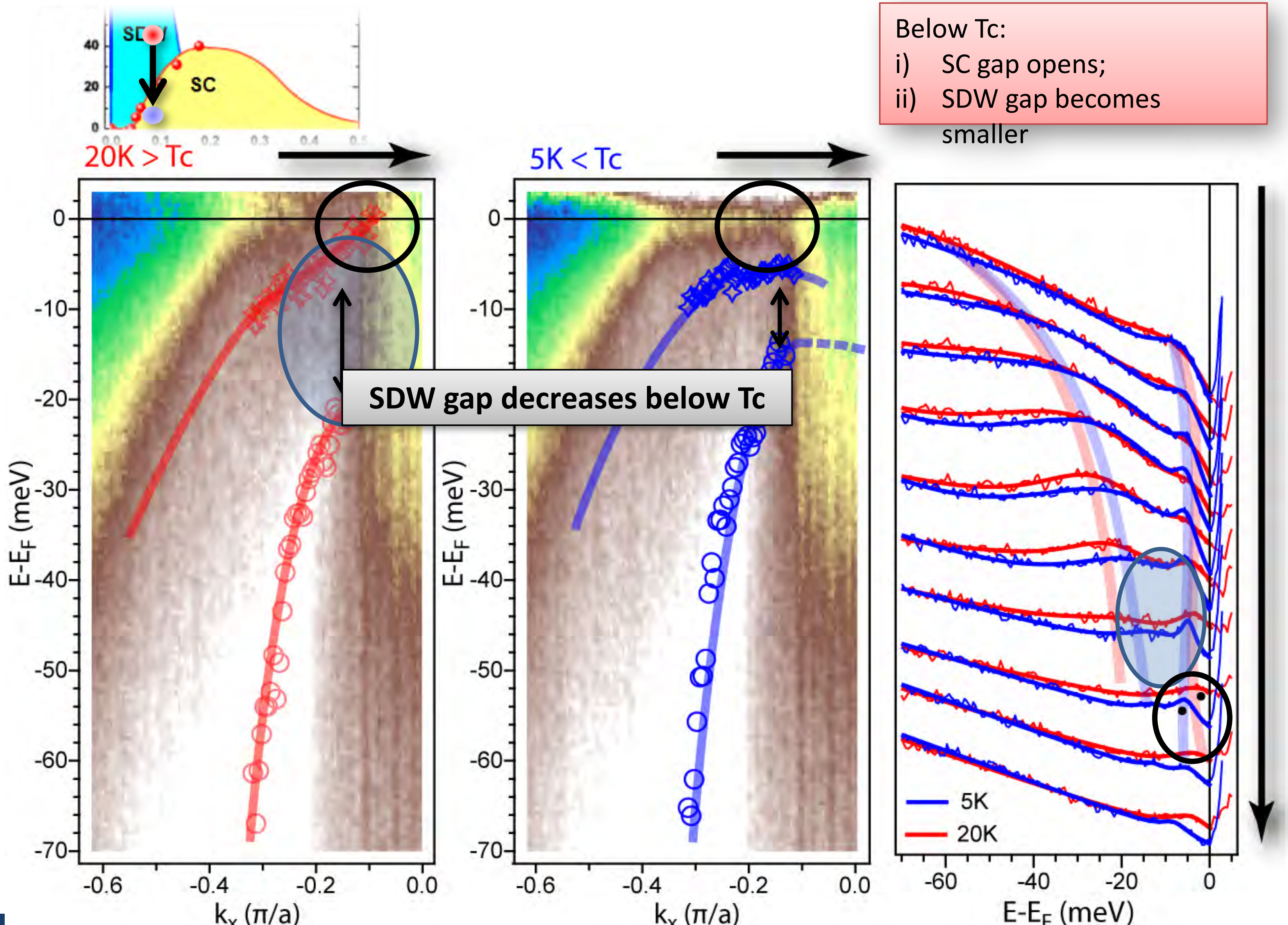


X=15%



M. Yi *et al*. Nat. Comm. In revision.

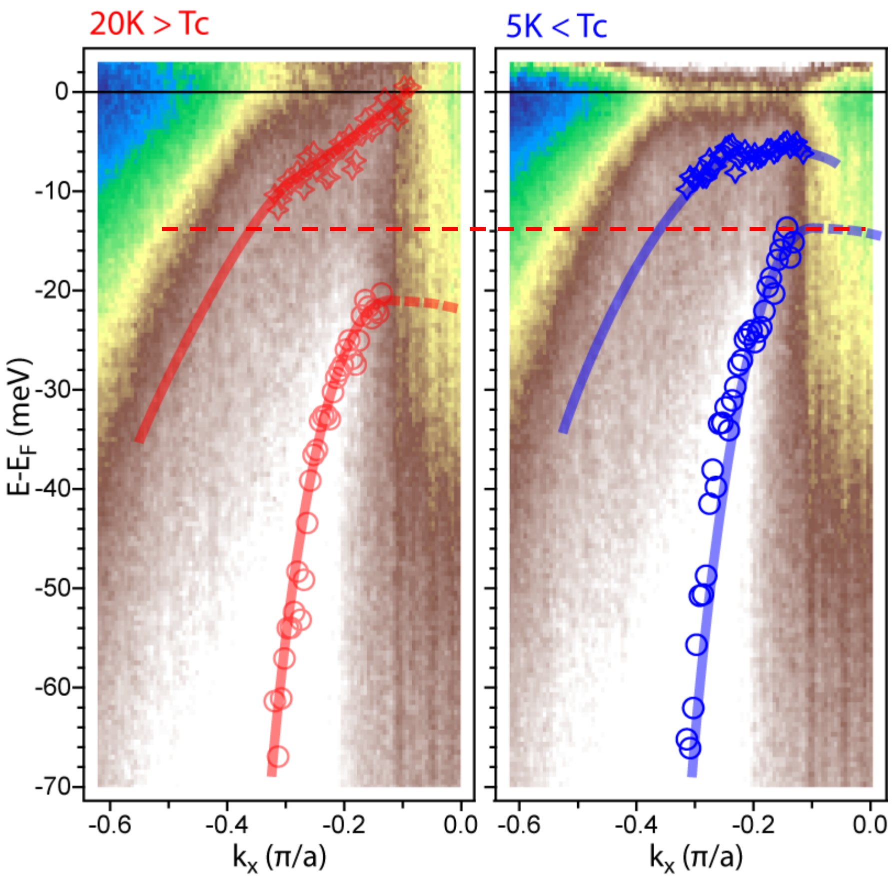
Electronic changes across T_C

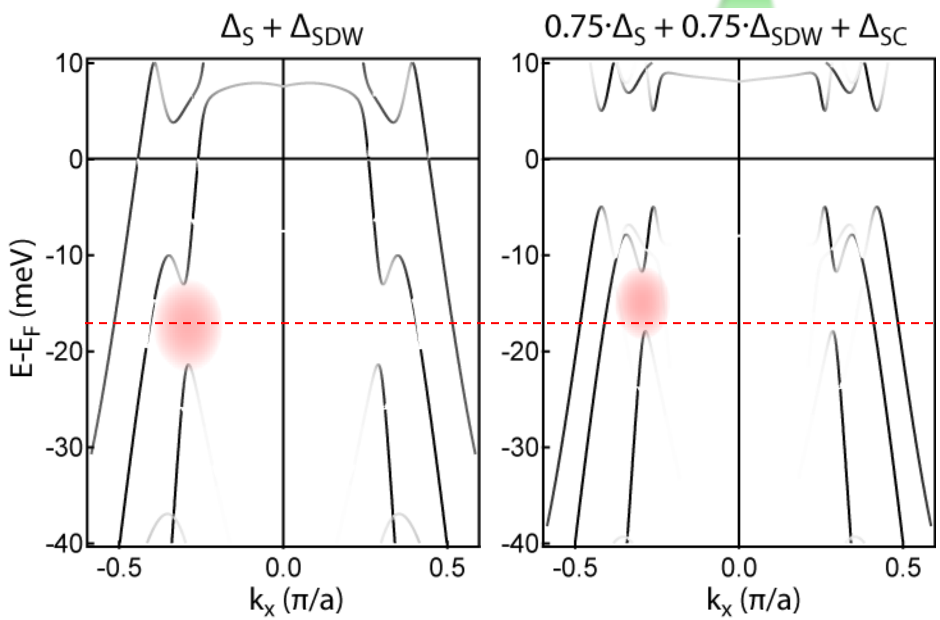


Below Tc:
i) SC gap opens;
ii) SDW gap becomes smaller

M. Yi *et al*. Nat. Comm. In revision.

Tight-binding model with Δ_S, Δ_{SDW}, and Δ_{SC}

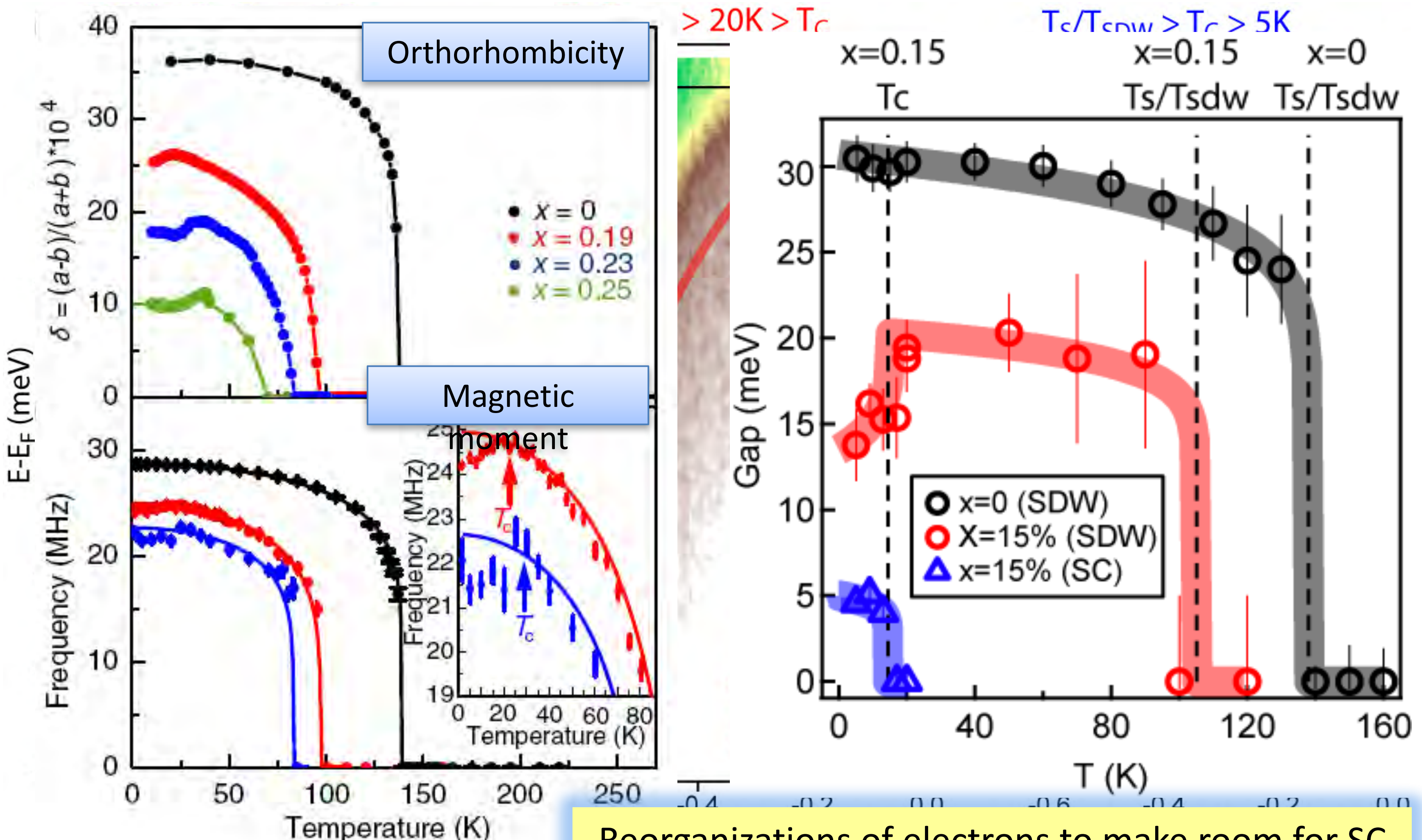




Calculations by Lex Kemper

Both nematic order and SDW order are suppressed with onset of SC
→ *SC and SDW/nematic orders compete!*

Δ_{SDW} and Δ_S: temperature dependence

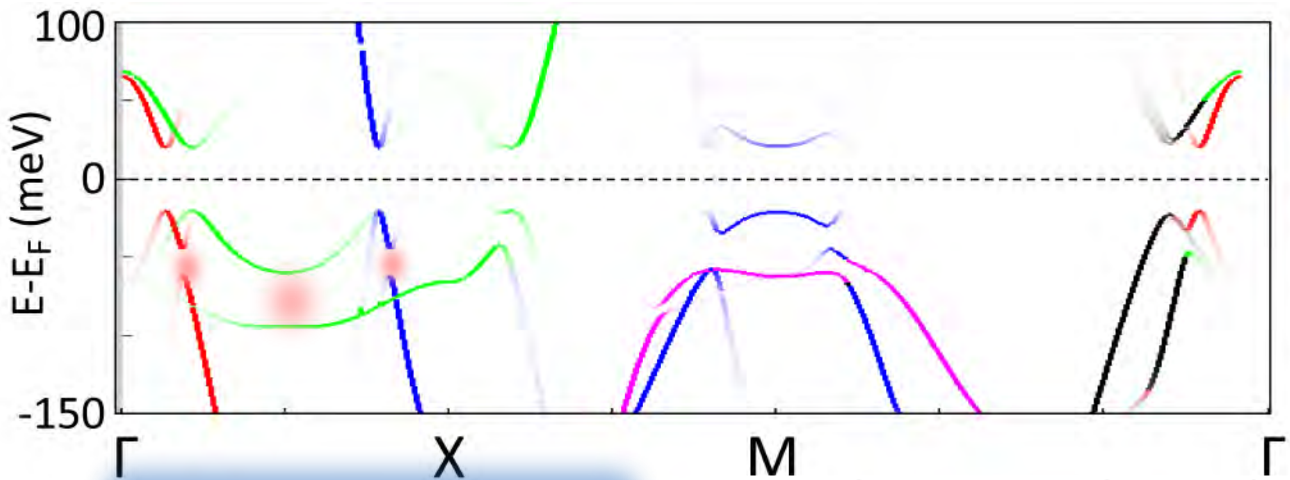


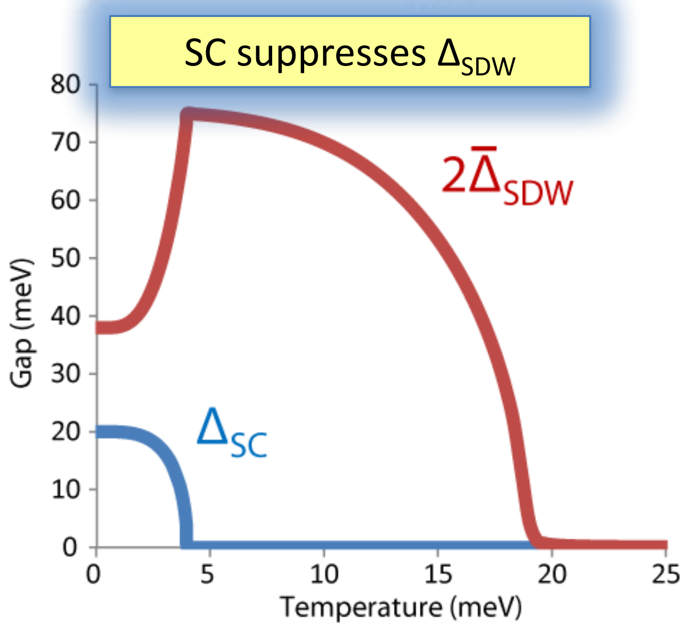
Reorganizations of electrons to make room for SC

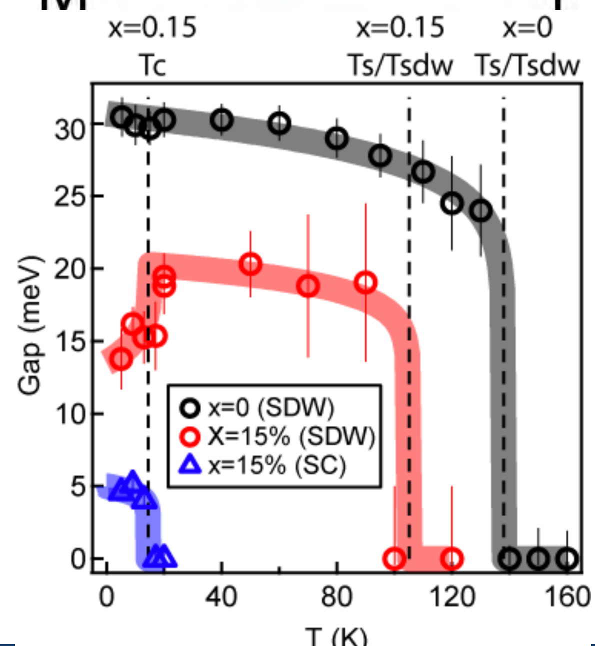
M. Yi *et al*. Nat. Comm. In revision.

Mean-Field calculations: competition of Δ_{SDW} and Δ_{SC}

SDW+SC



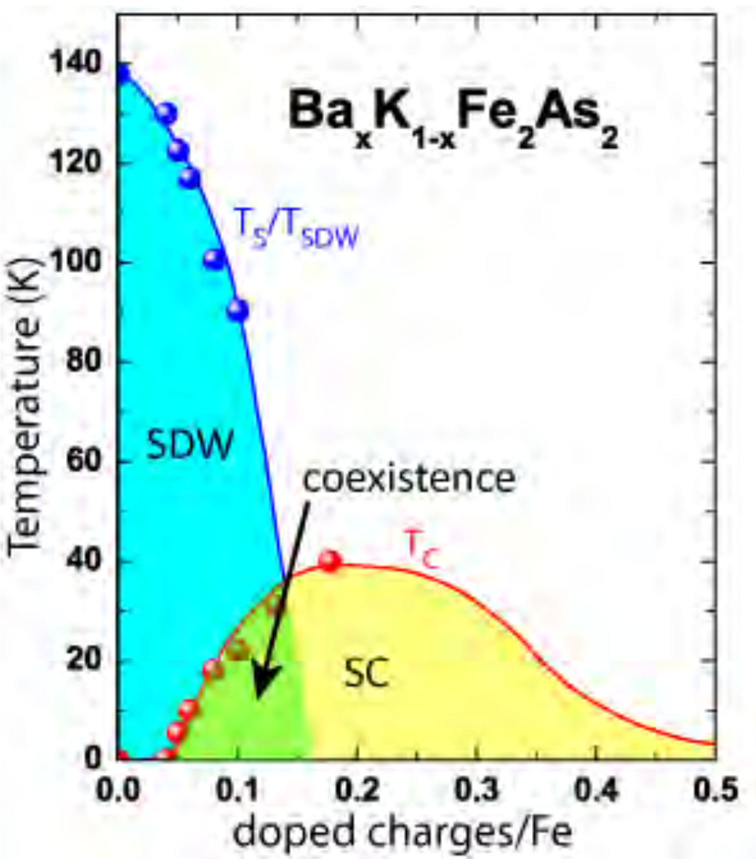


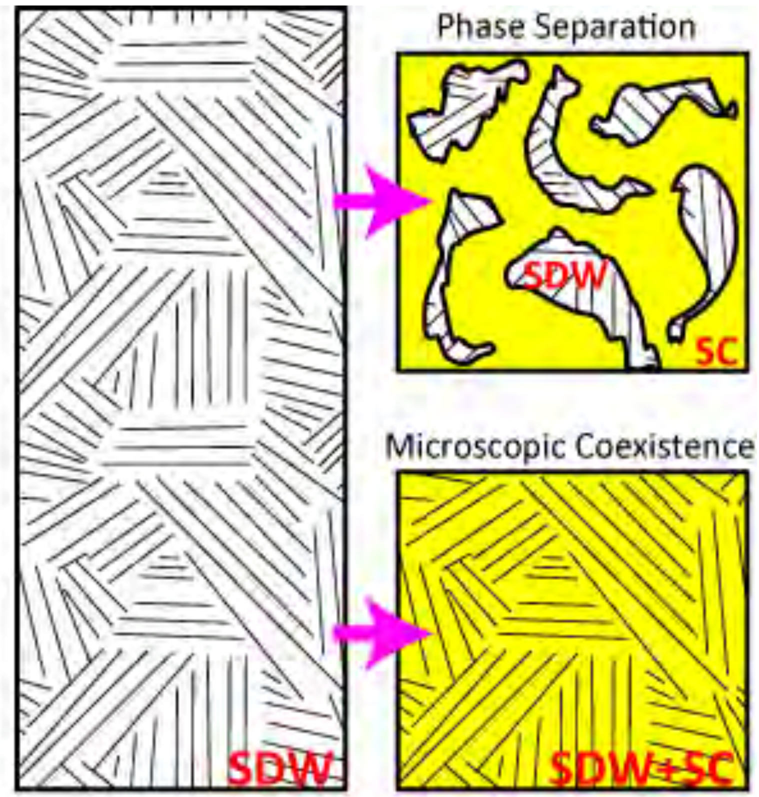


**Calculations by Nachum Plonka*

M. Yi *et al*. Nat. Comm. In revision.

Phase separation versus microscopic coexistence

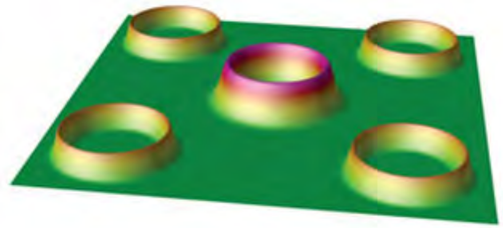


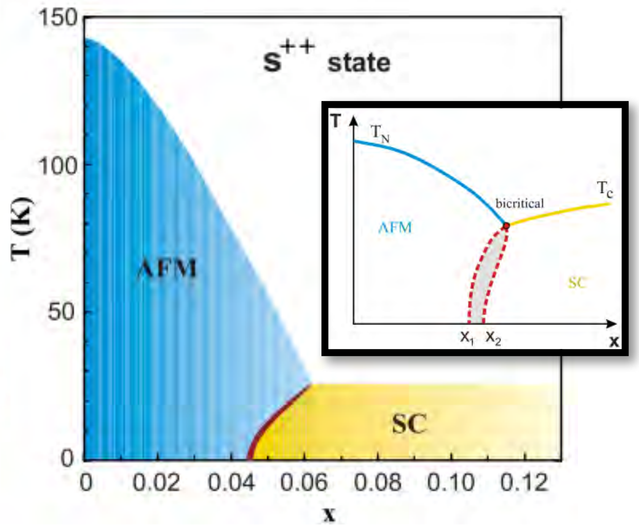


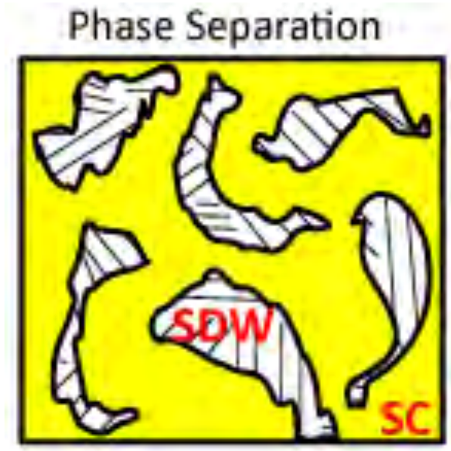
M. Yi *et al*. Nat. Comm. In revision.

Implications for superconductivity

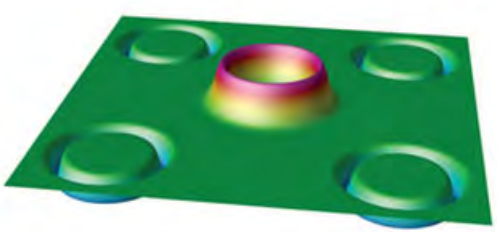
S++ pairing

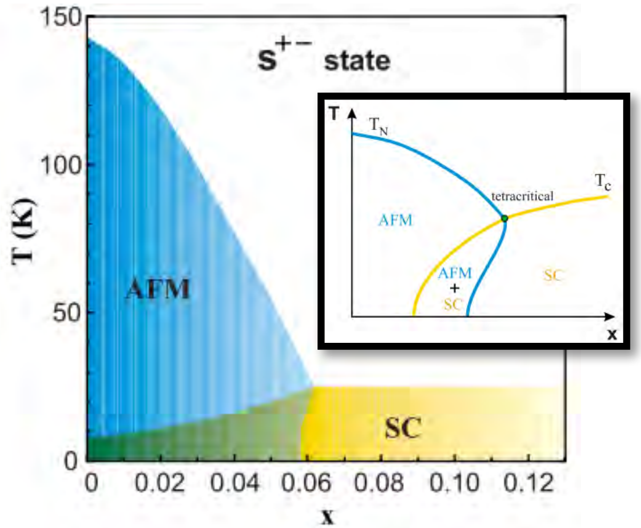


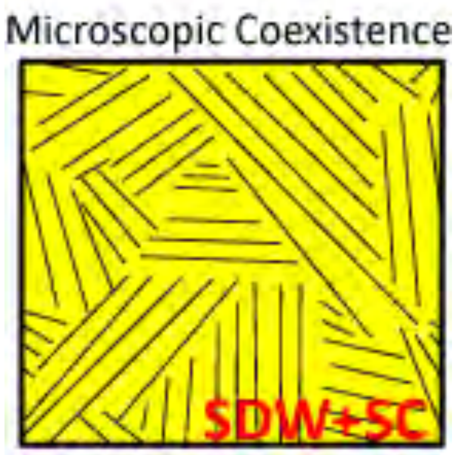




S+- pairing

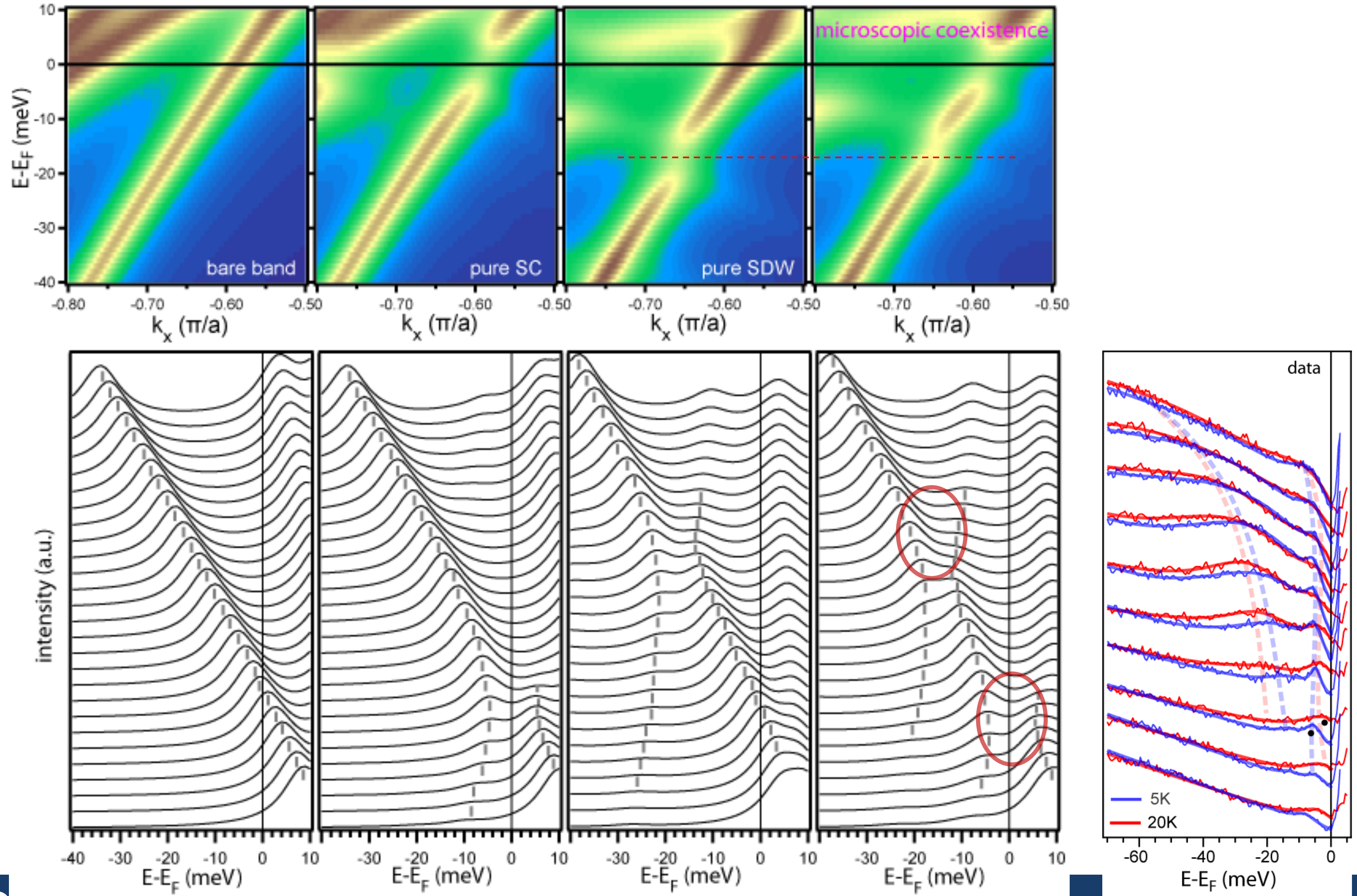






R.M. Fernandes and J. Schmalian. PRB 82, 014521 (2010)

Experimentally distinguishing the two scenarios



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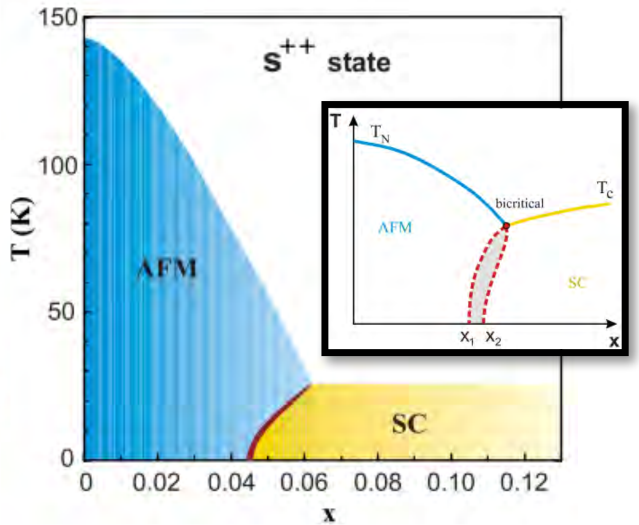
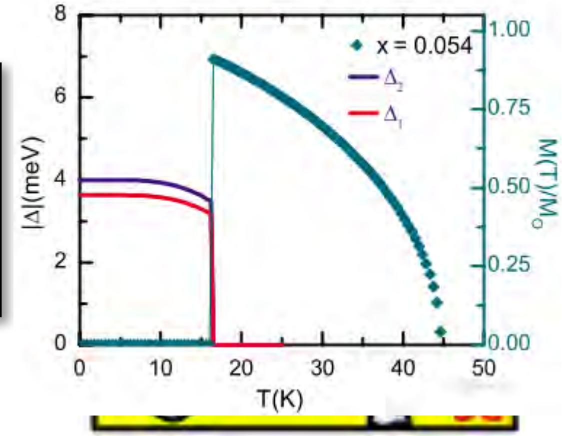
Implications for superconductivity

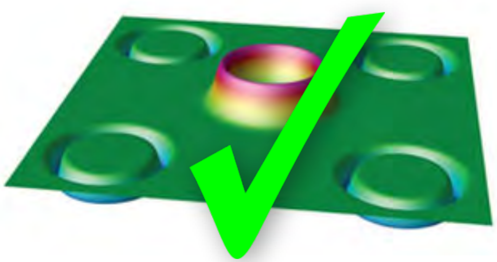
S^{++} pairing

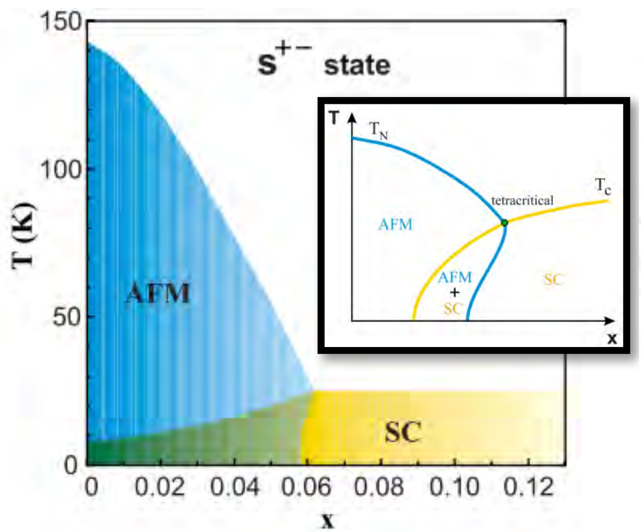


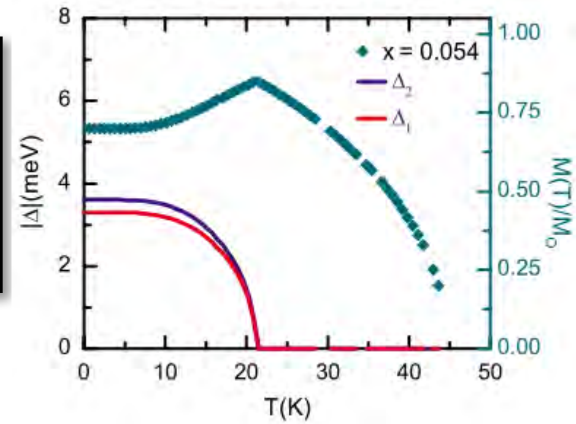


Microscopic Coexistence

S^{+-} pairing

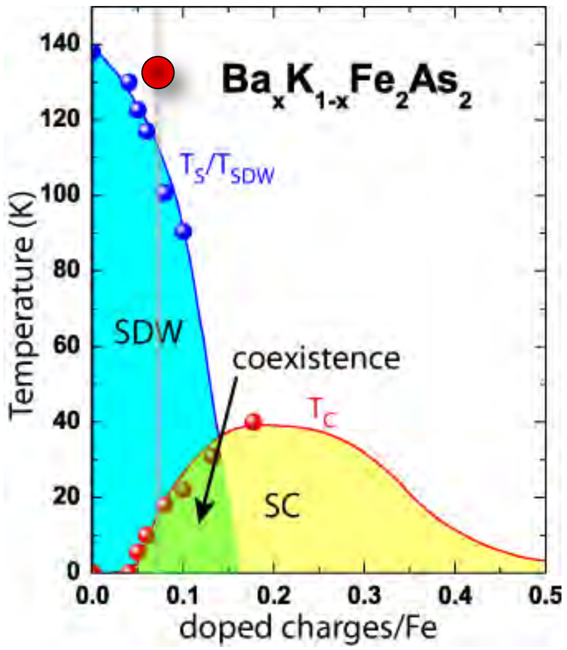


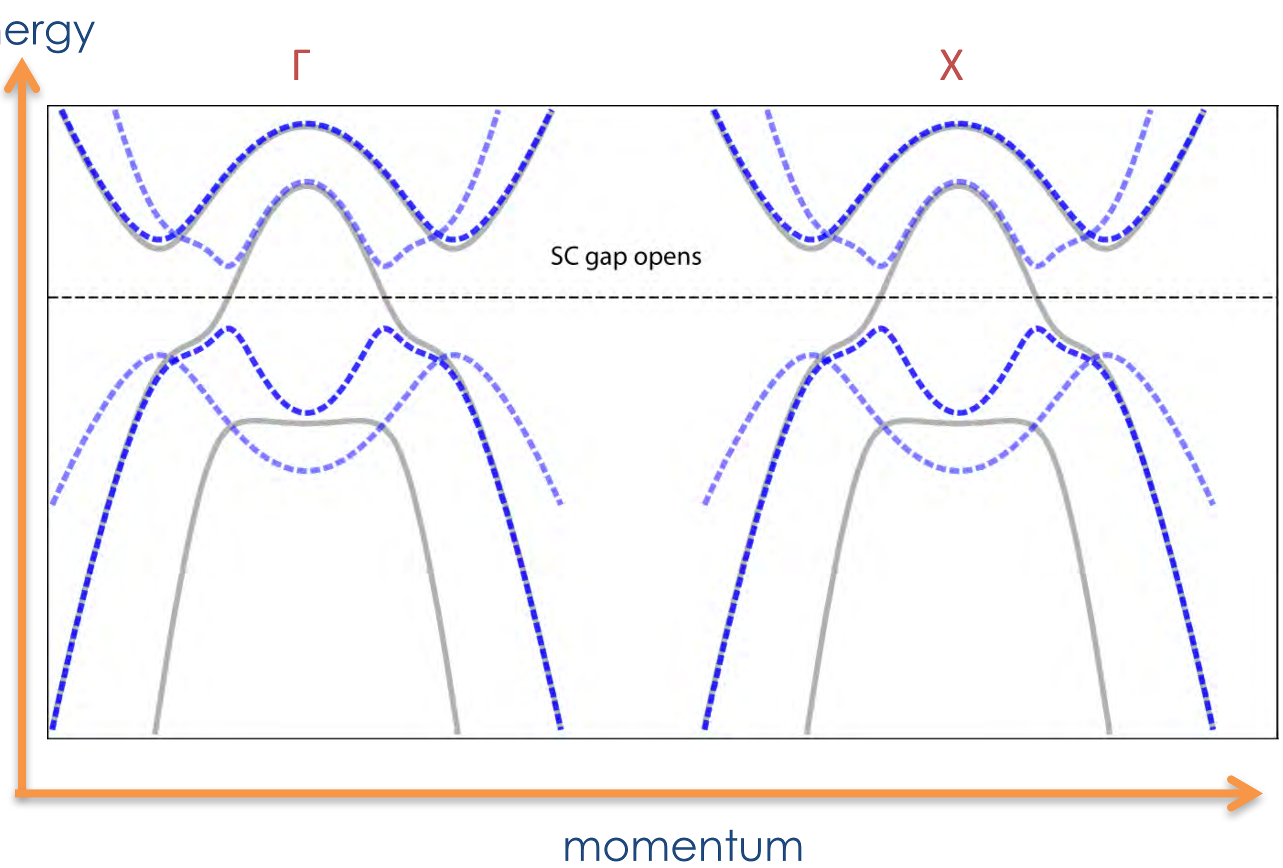




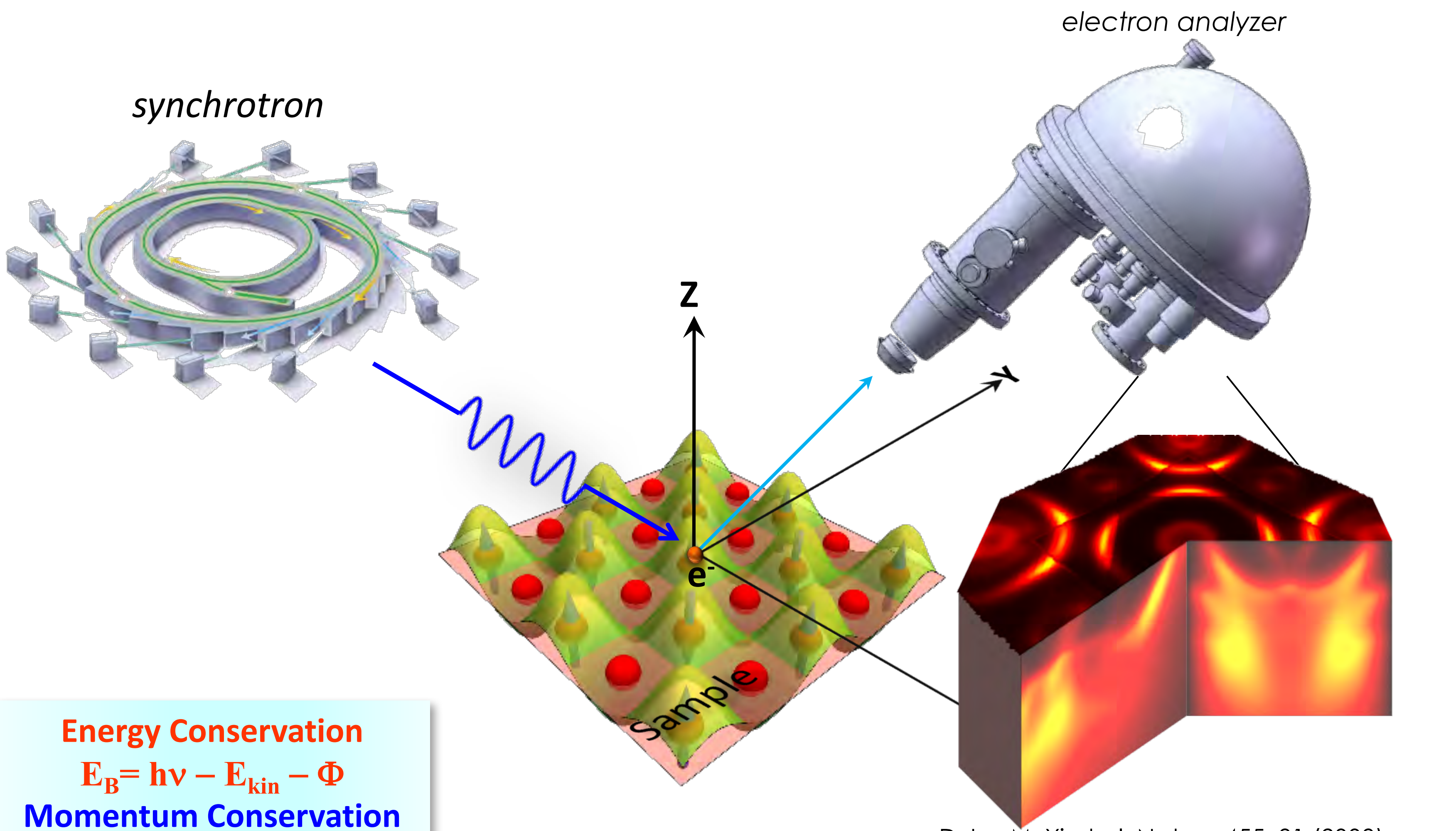
R.M. Fernandes and J. Schmalian. PRB 82, 014521 (2010)

Simplified schematic of electronic structure





Angle-Resolved PhotoEmission Spectroscopy (ARPES)



Energy Conservation

$E_B = h\nu - E_{kin} - \Phi$

Momentum Conservation

$K_{\parallel} = k_{\parallel} + G_{\parallel}$

D. Lu, M. Yi et al. Nature 455, 81 (2008).

Direct measure of electronic structures