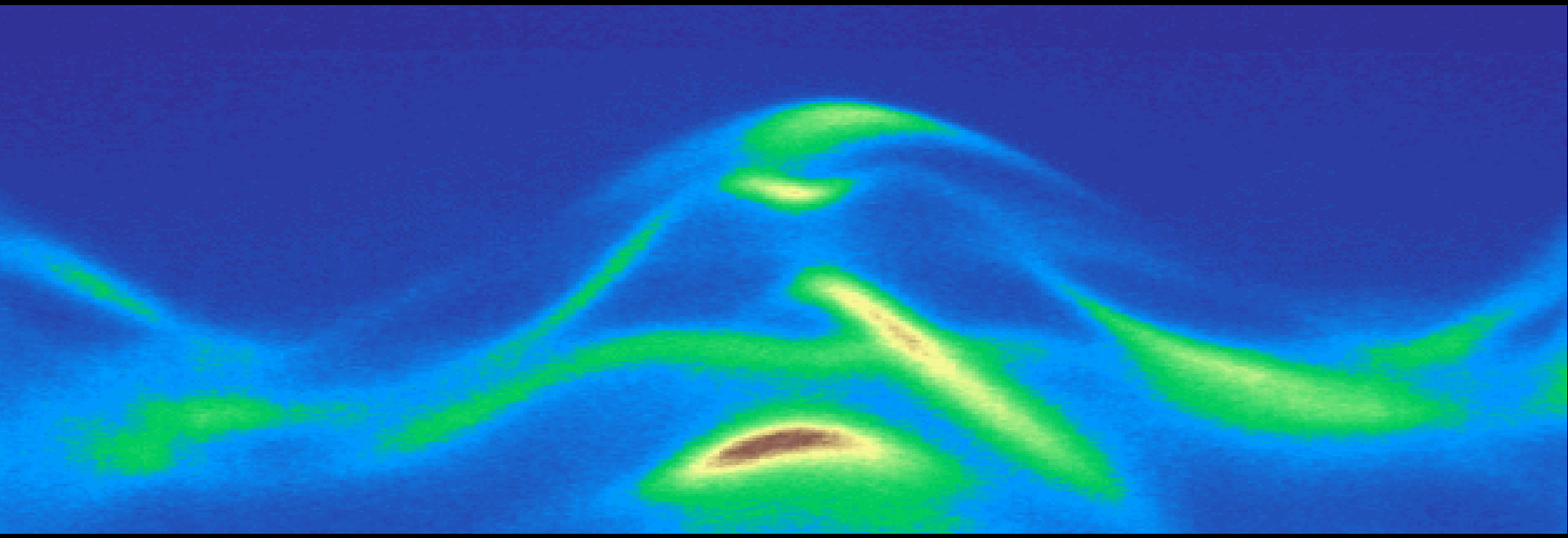
Does the normal normal state in 2D metals ever sets in?



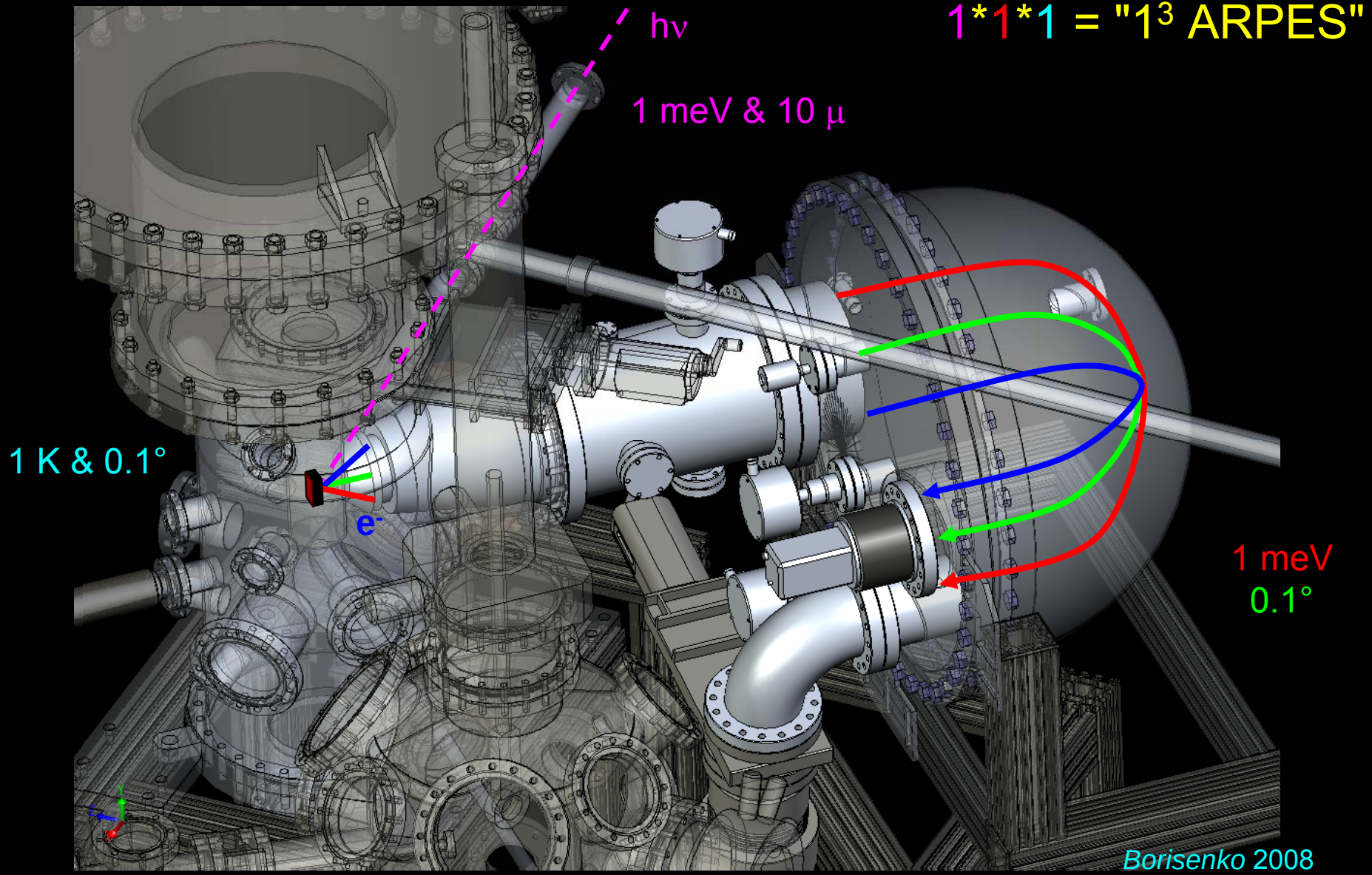
A. A. Kordyuk
IFW Dresden

Outline

I. New ARPES
   - wide acceptance angle
   - ultimate resolution
   - lowest temperature

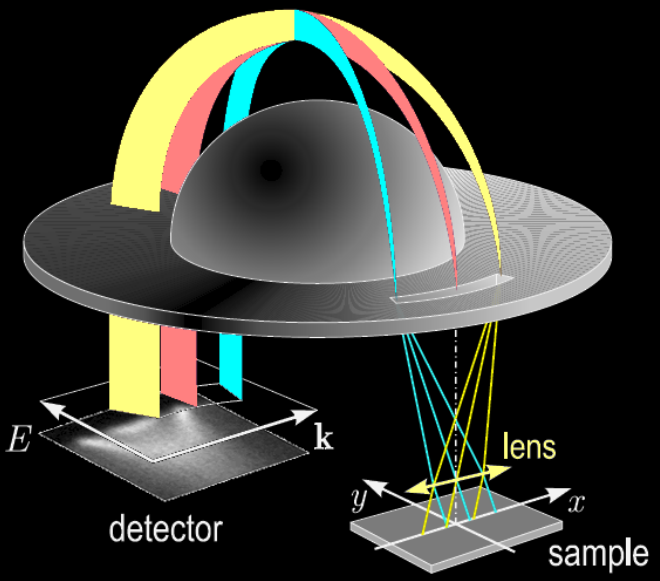
II. Ordering in
   - dichalcogenides
   - cuprates & etc.
   - pnictides

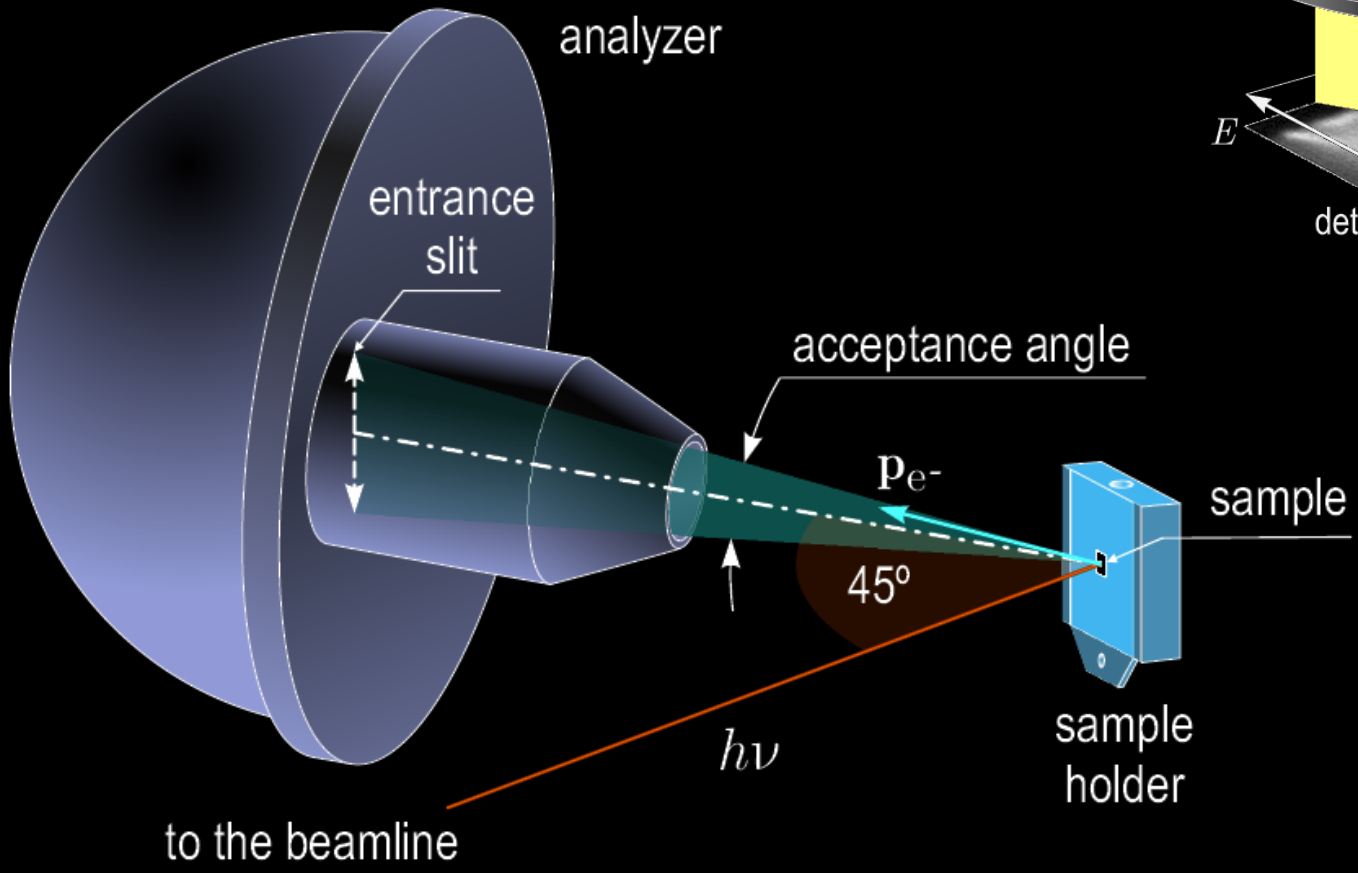
ARPES anatomy



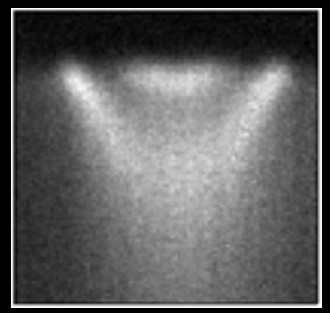
Borisenko 2008

Photoelectric effect + SES

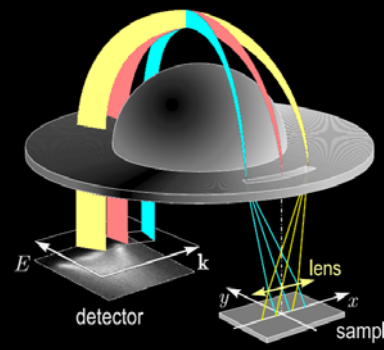


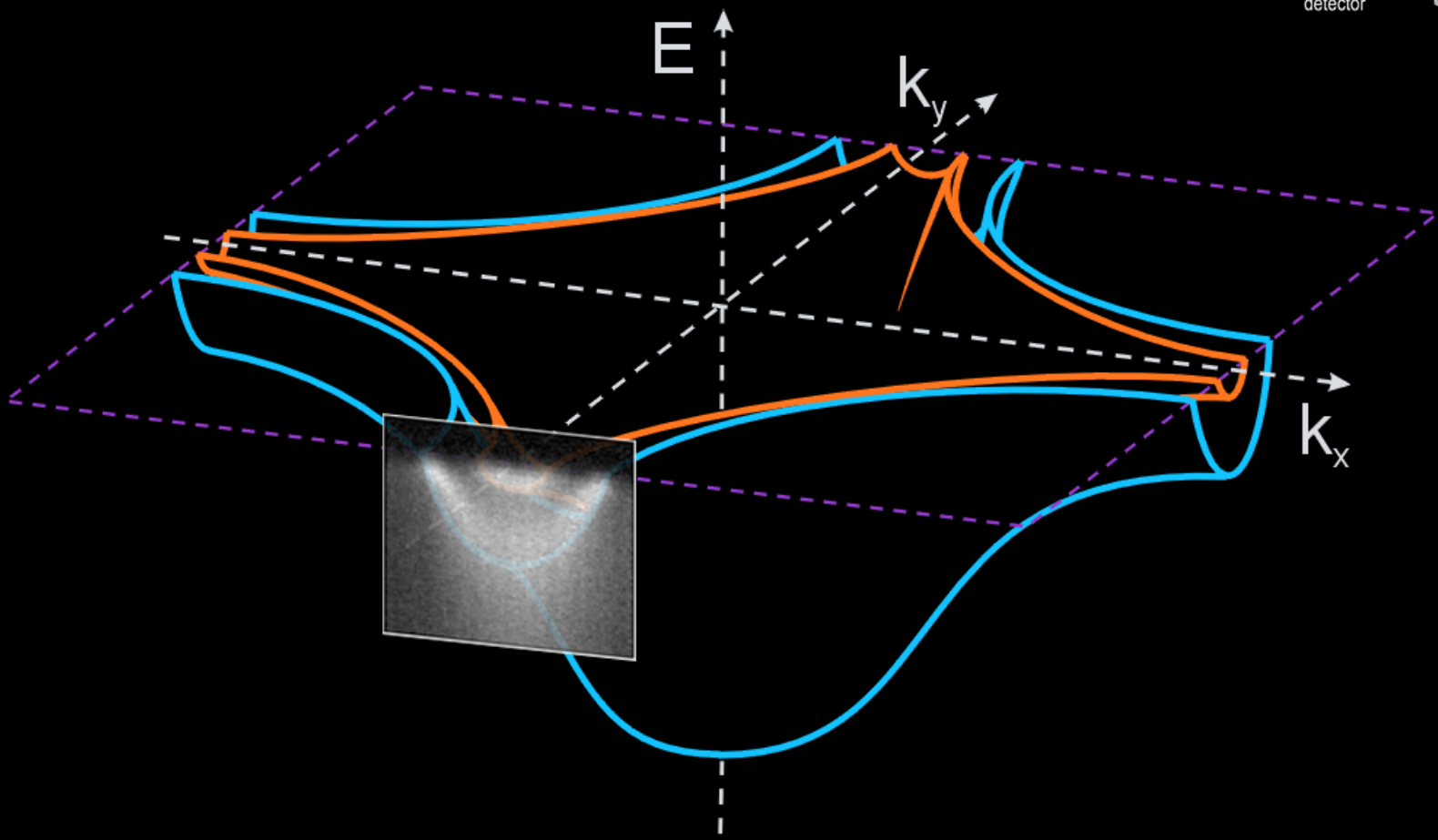


ARPES Image

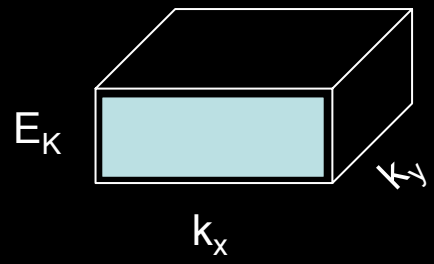


ARPES Image → ARPES Space

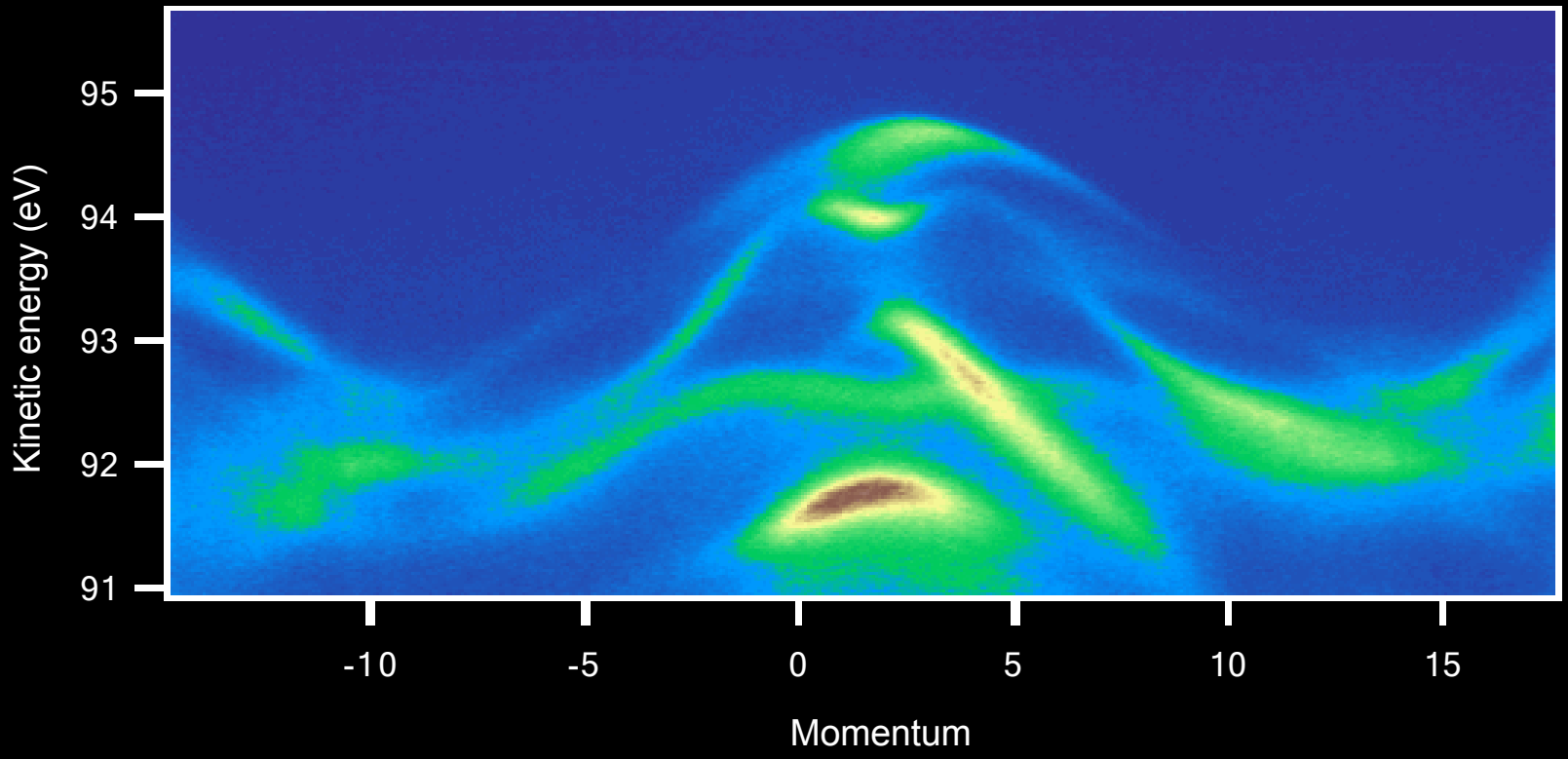




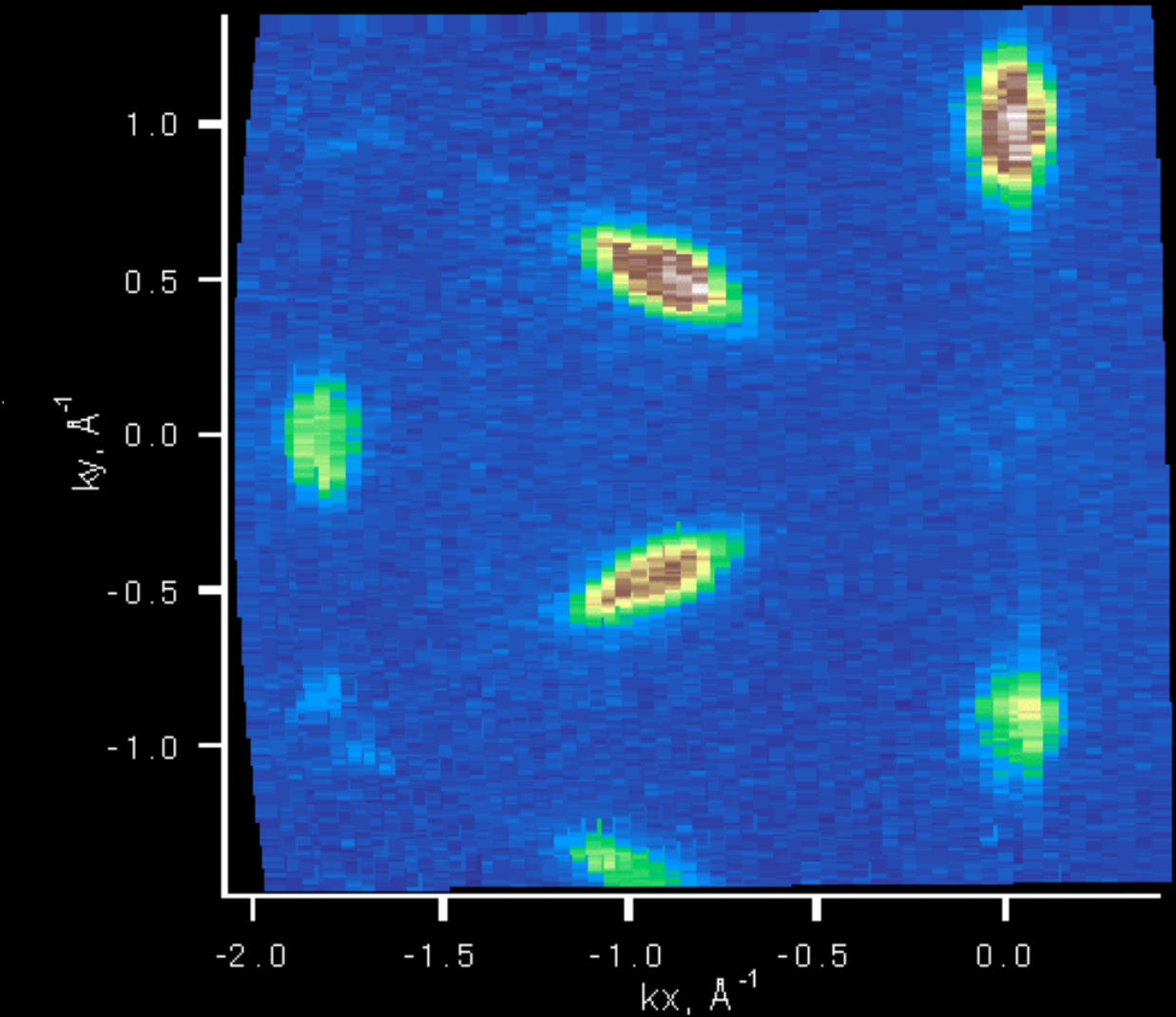
Wide - acceptance lens

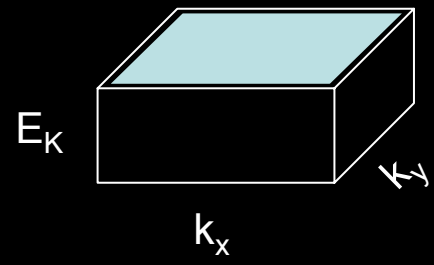


$TiSe_2$

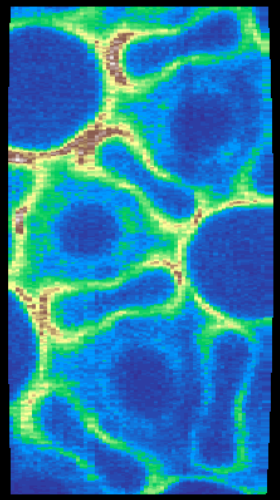


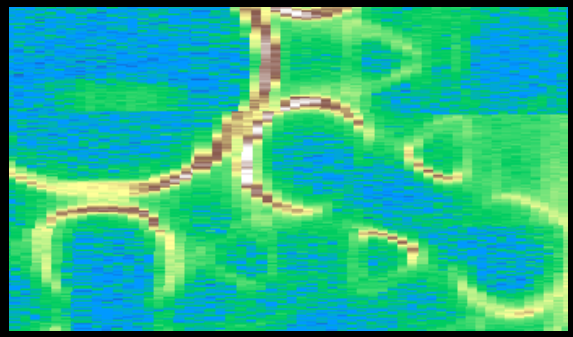
Wide acceptance lens

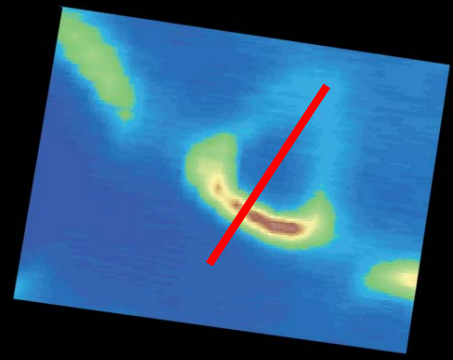


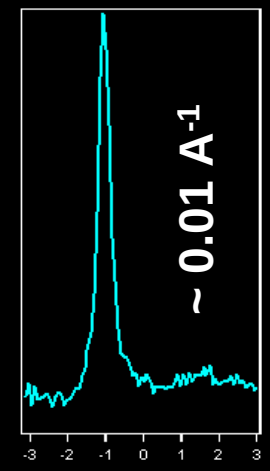


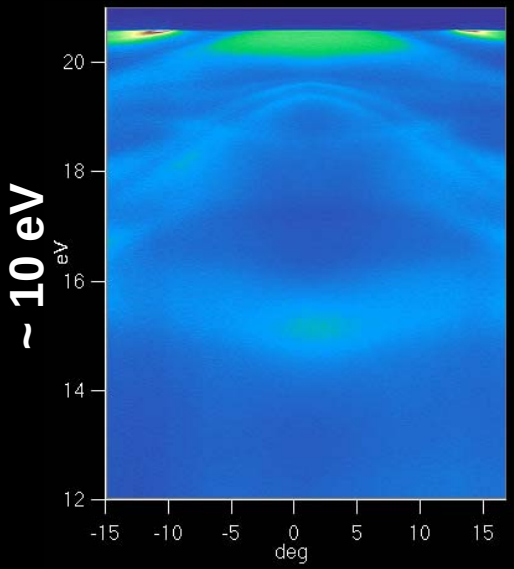
Zooming in…

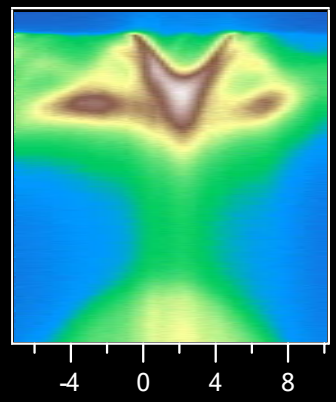

~ 10 A-1

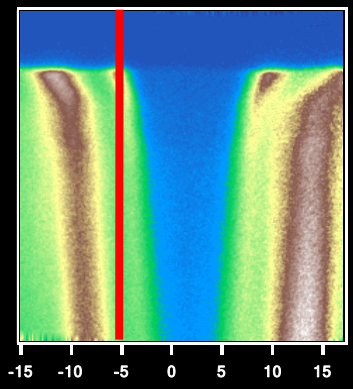

~ 1 A-1

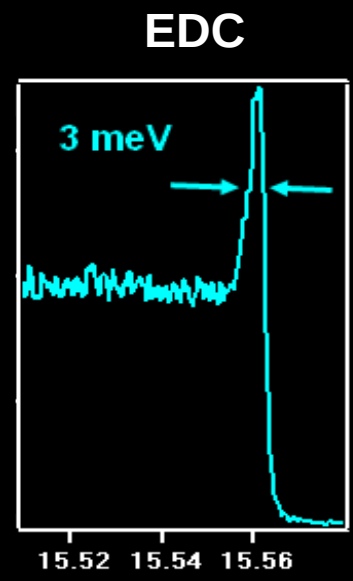

~ 0.1 A-1


MDC
~ 0.01 A-1
-3 -2 -1 0 1 2 3

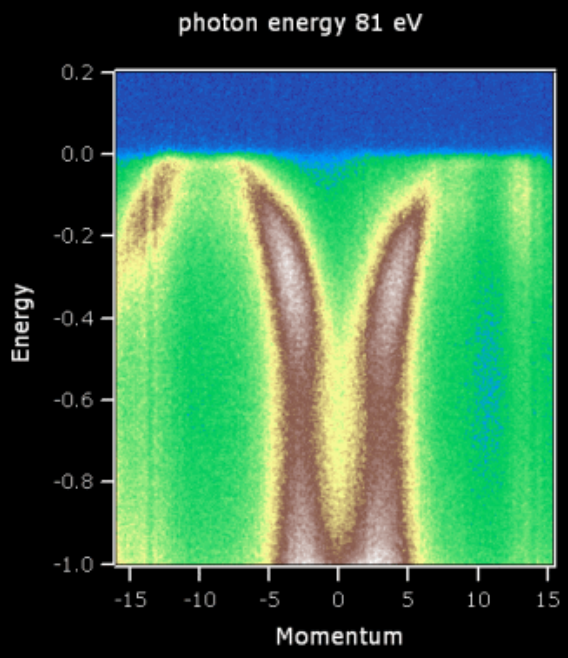

~ 10 eV
20
18
16
14
12
eV
-15 -10 -5 0 5 10 15
deg
Momentum


~ 1 eV
-4 0 4 8

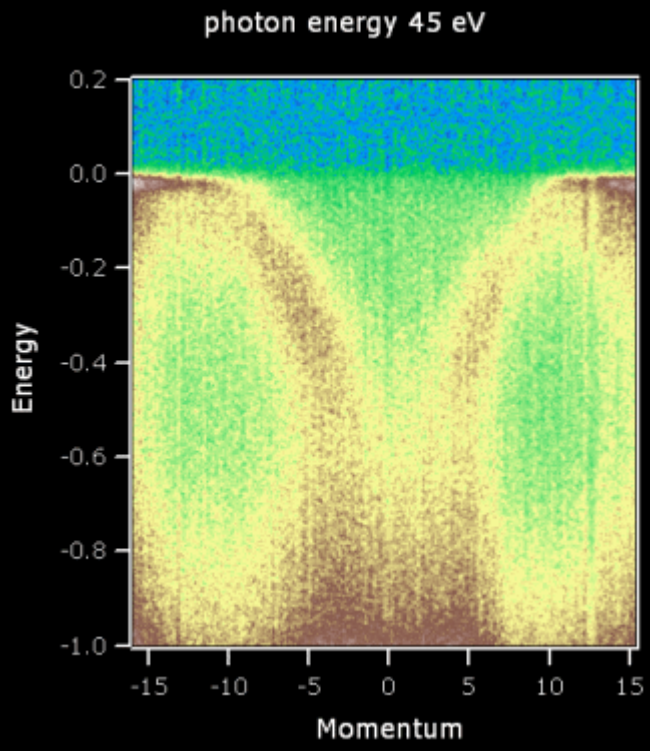

~ 0.1 eV
-15 -10 -5 0 5 10 15

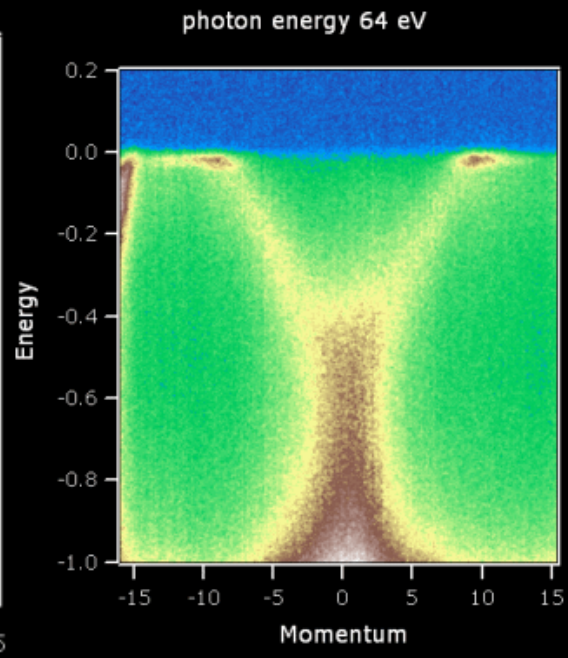

EDC
~ 0.001 eV
3 meV
15.52 15.54 15.56

Photon energy – an important parameter



„Waterfalls“

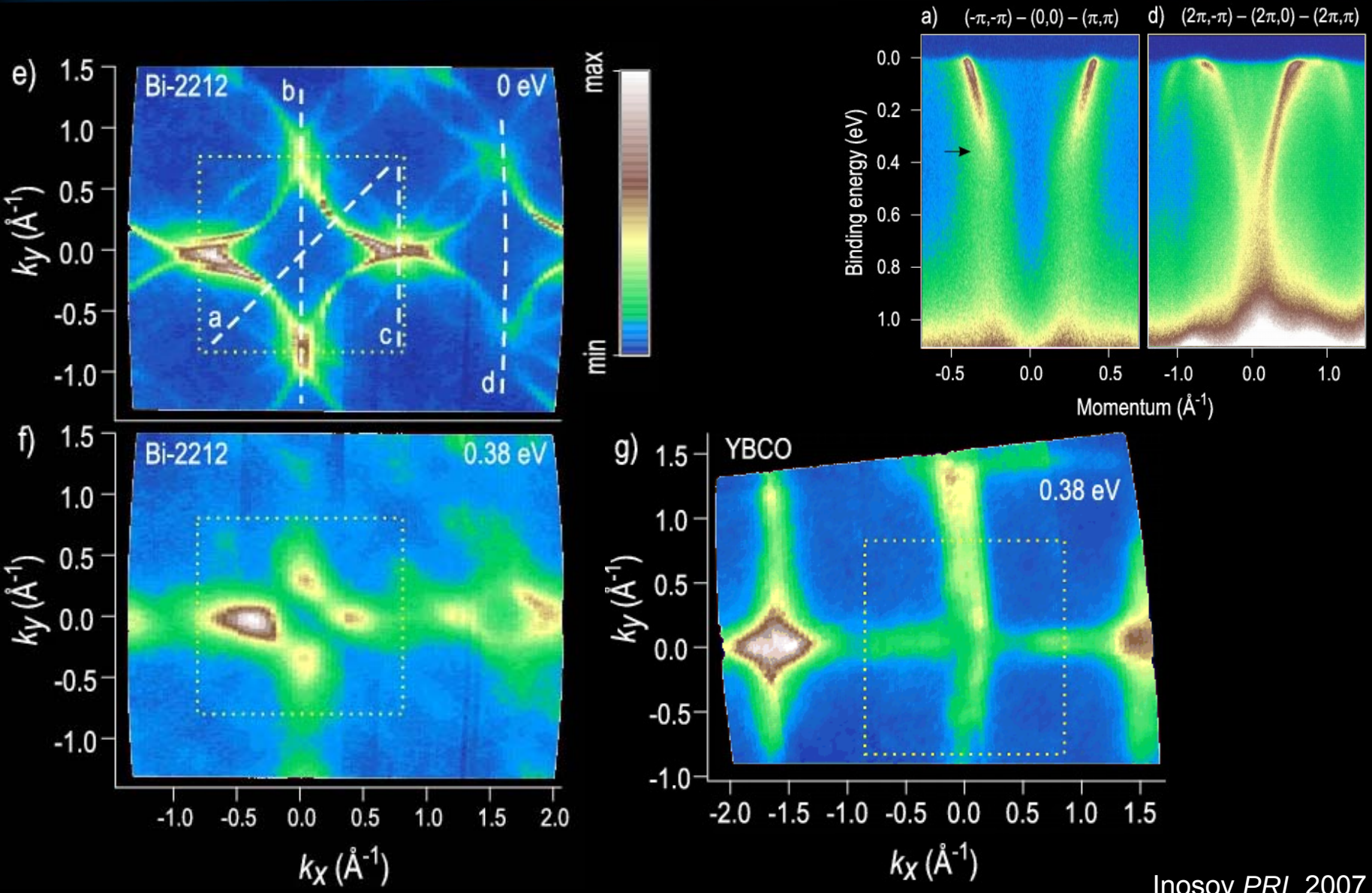




„Champagne glass“

Inosov *PRL* 2007, *PRB* 2008

Waterfalls in cuprates

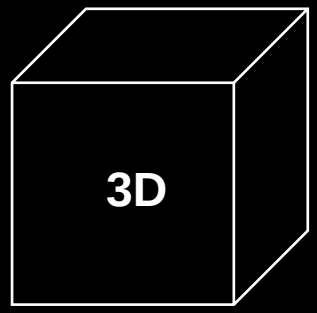


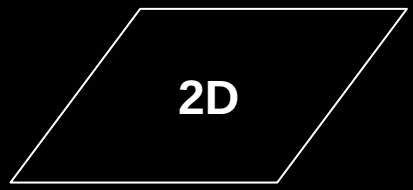
Inosov *PRL* 2007

CDW in 2D

CDW in 2D

El-ph interaction ?



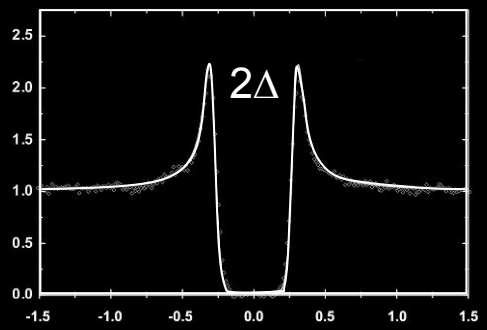


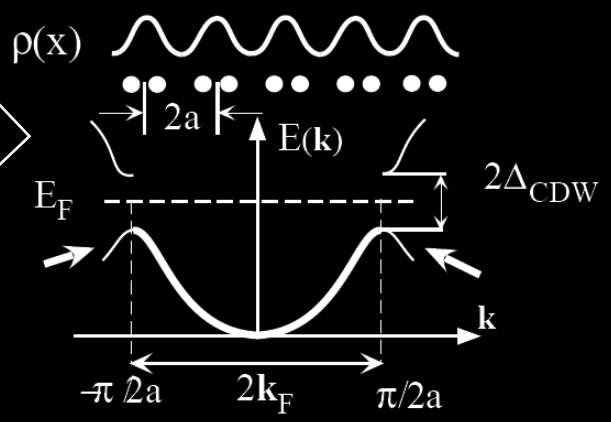
1D

both are anomalous

PG ?

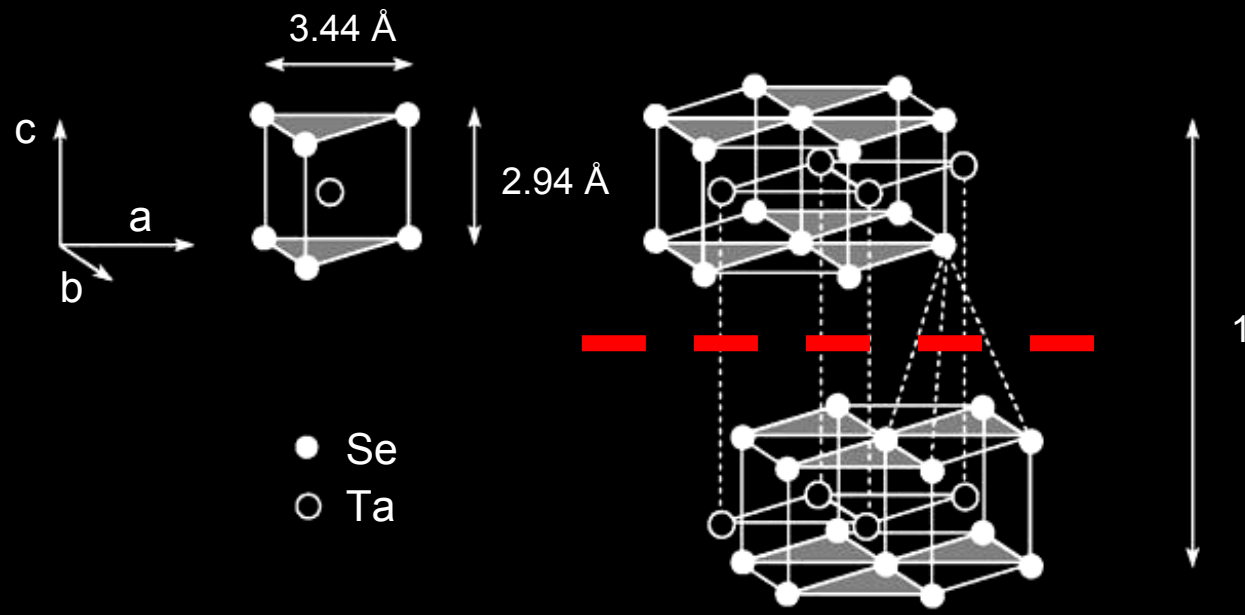
better metal ?

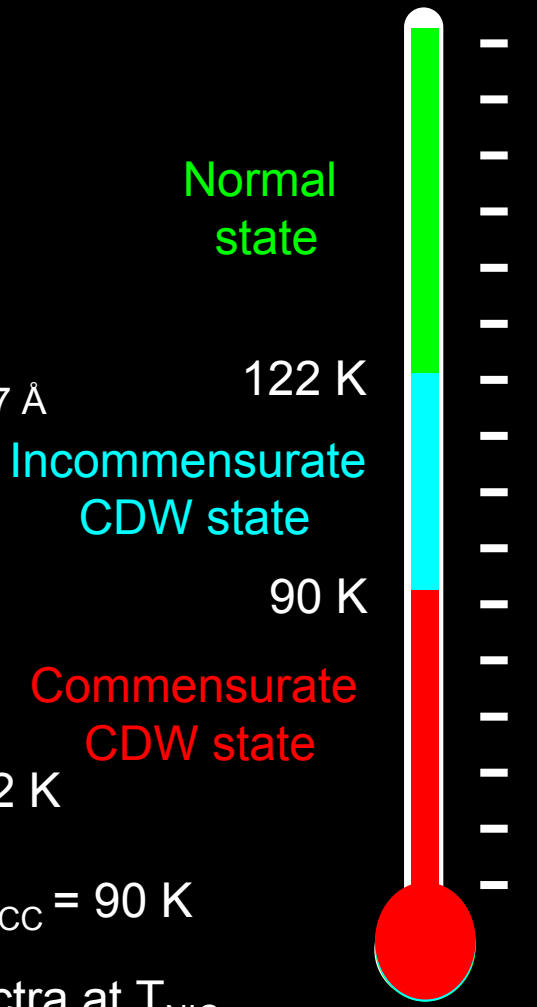




$2H\text{-}TaSe_2$

2H-$TaSe_2$ crystal structure, CDW transitions



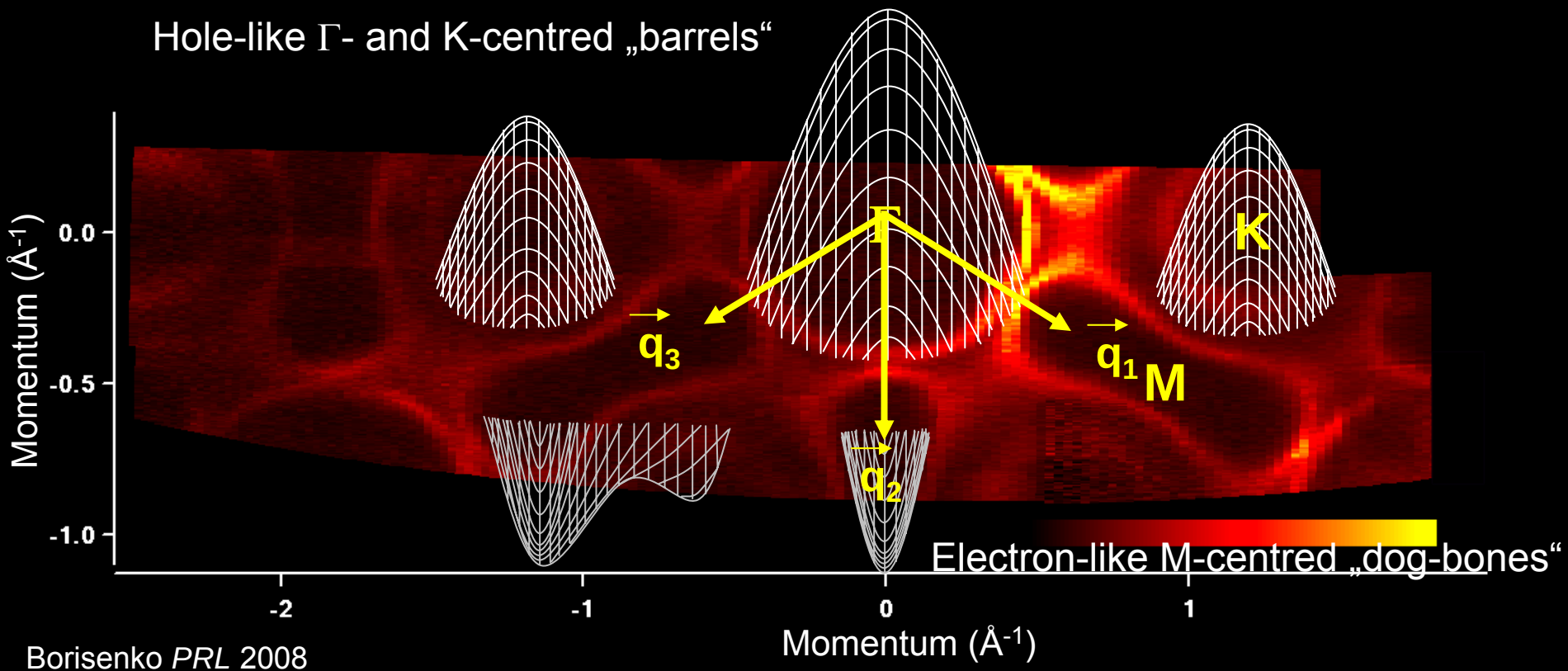


- 2nd-order transition to an incommensurate CDW at T_{NIC} = 122 K
- 1st-order lock-in transition to a 3x3 commensurate CDW at T_{ICC} = 90 K
- What was strange? No nesting. No change in ARPES spectra at T_{NIC} .
  Gap of 24-250 meV only below 90K.

Electronic structure of 2H-$TaSe_2$

Normal state

180 K

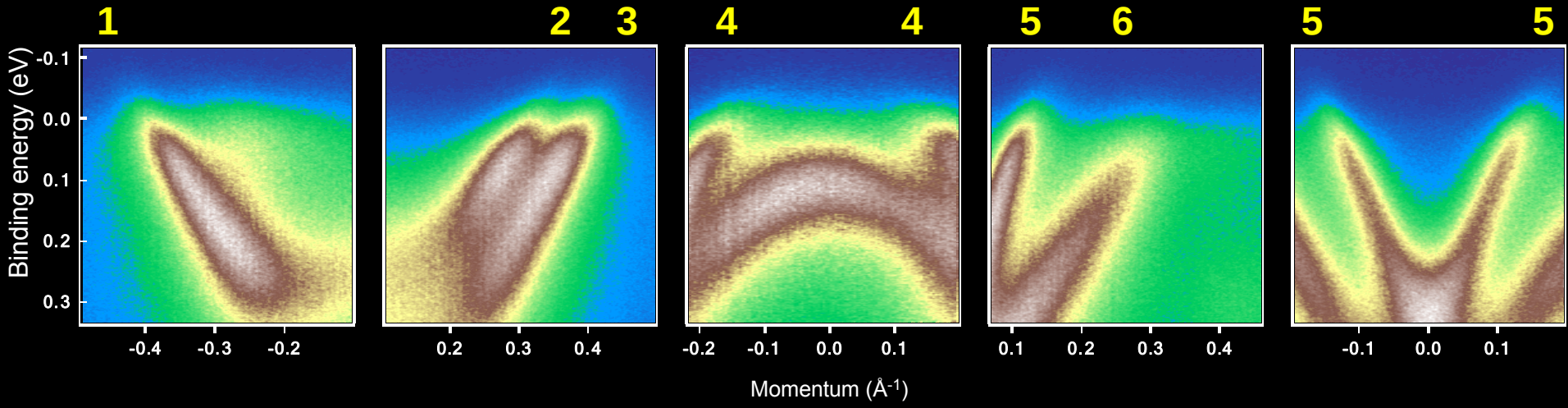


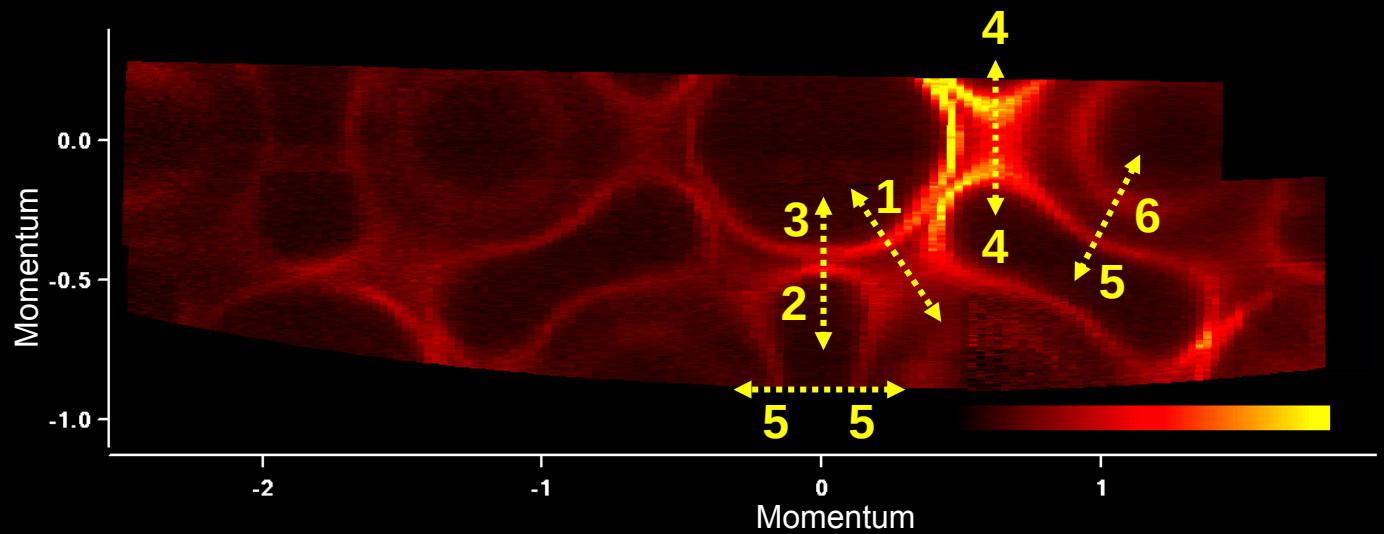
Borisenko *PRL* 2008

Normal state of 2H-$TaSe_2$

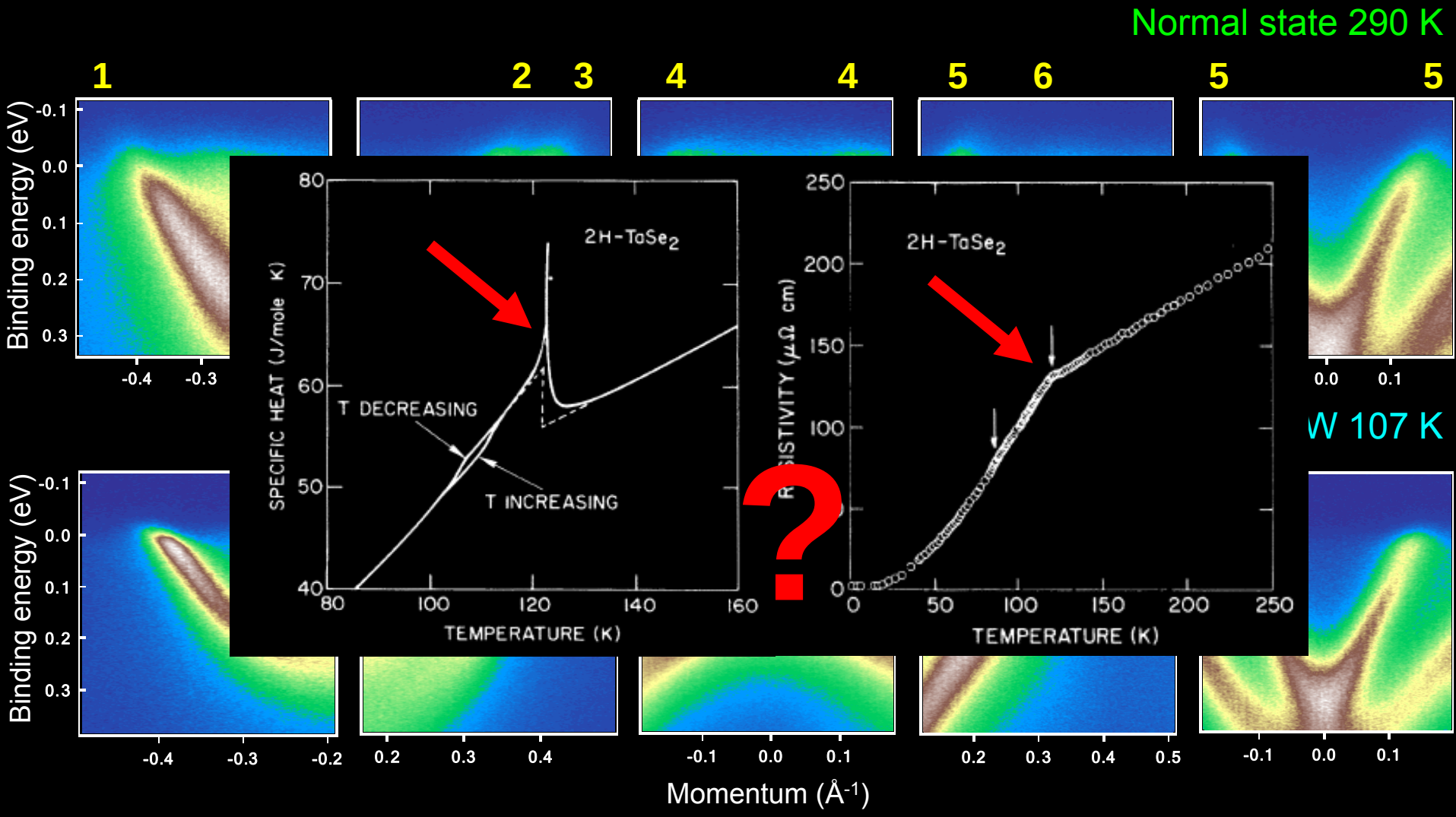
Normal state

290 K





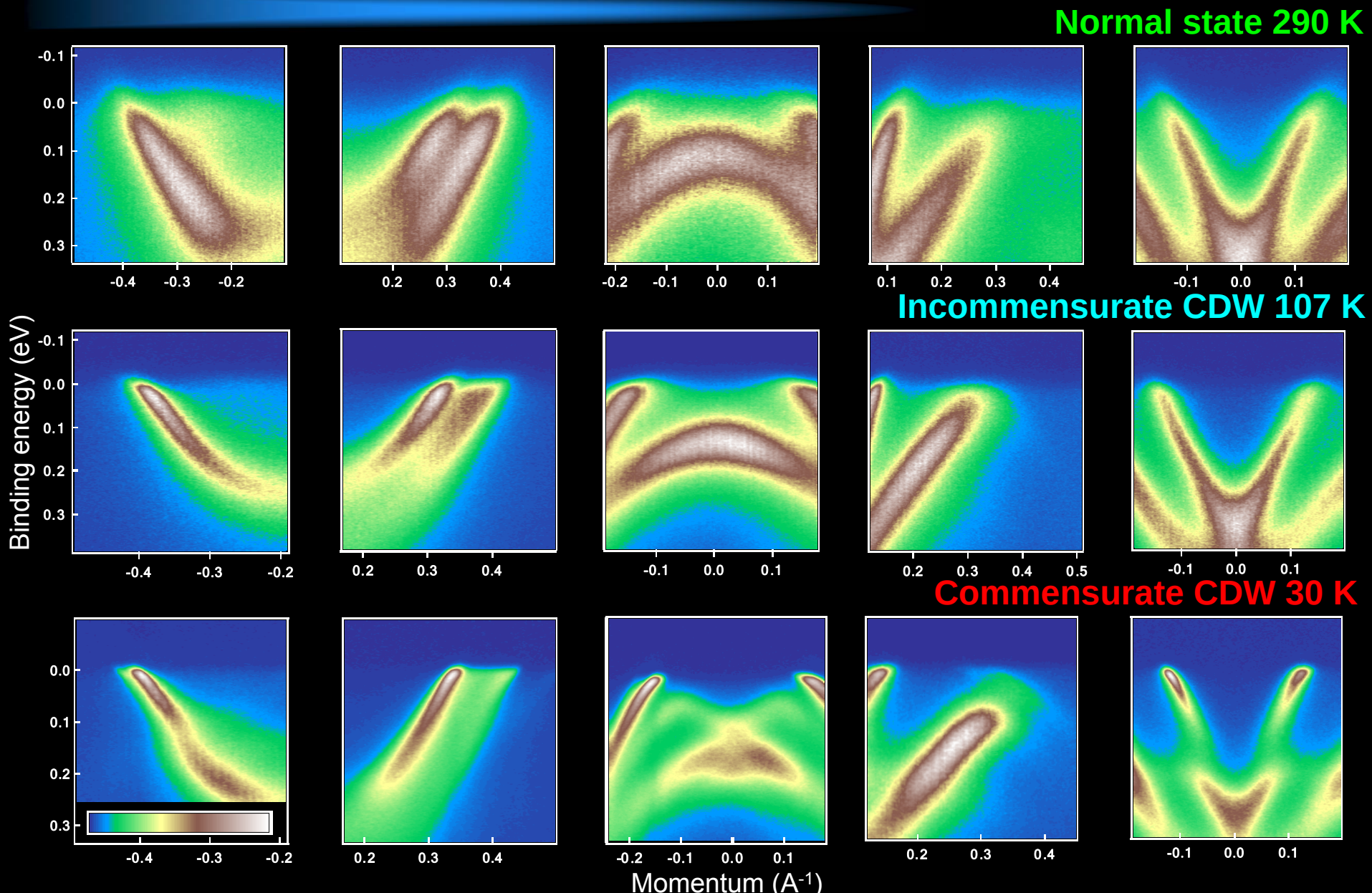
Incommensurate CDW state of $2H\text{-}TaSe_2$



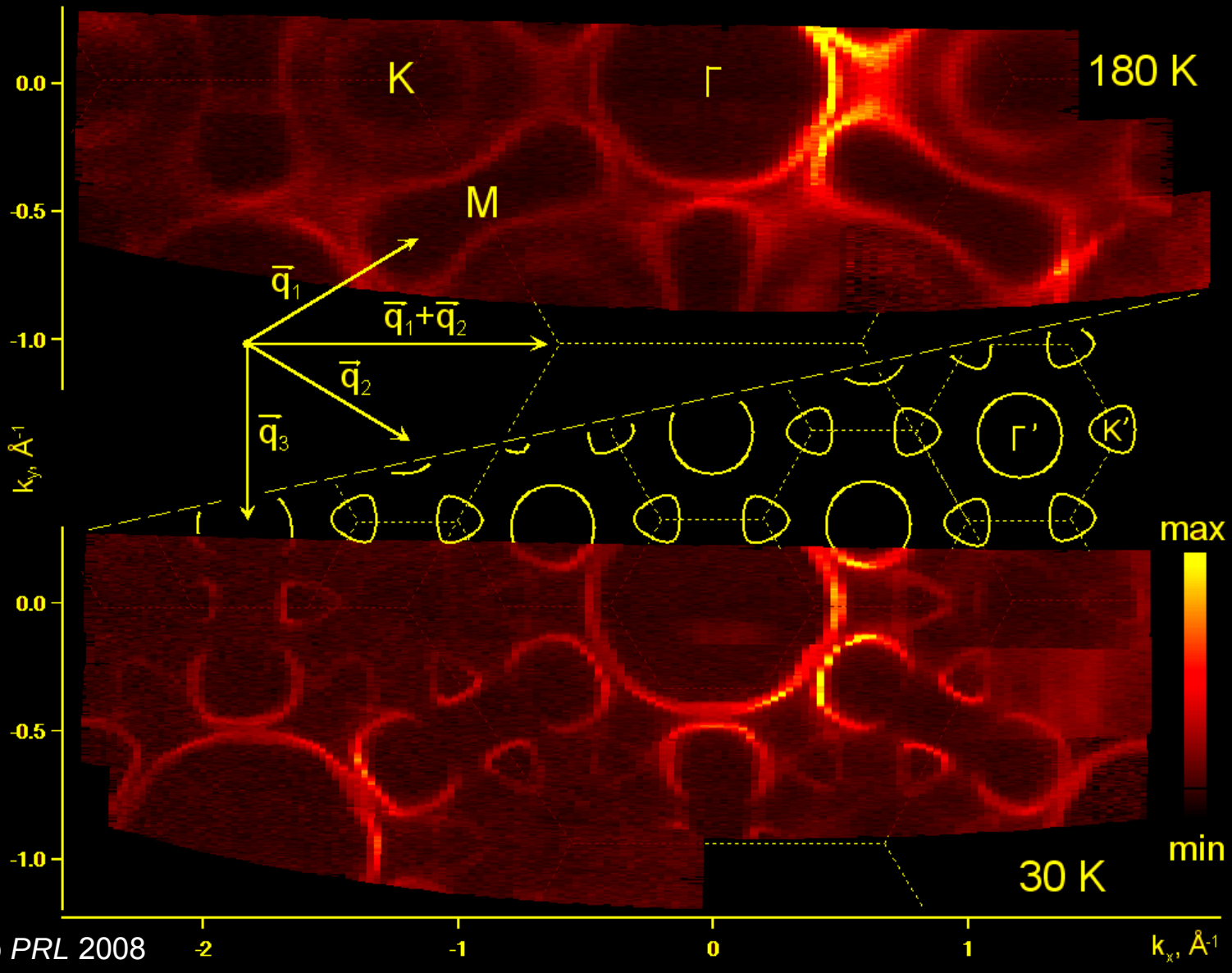
Borisenko *PRL* 2008

Craven & Meyer *PRB* 1977

Commensurate CDW state of 2H-$TaSe_2$

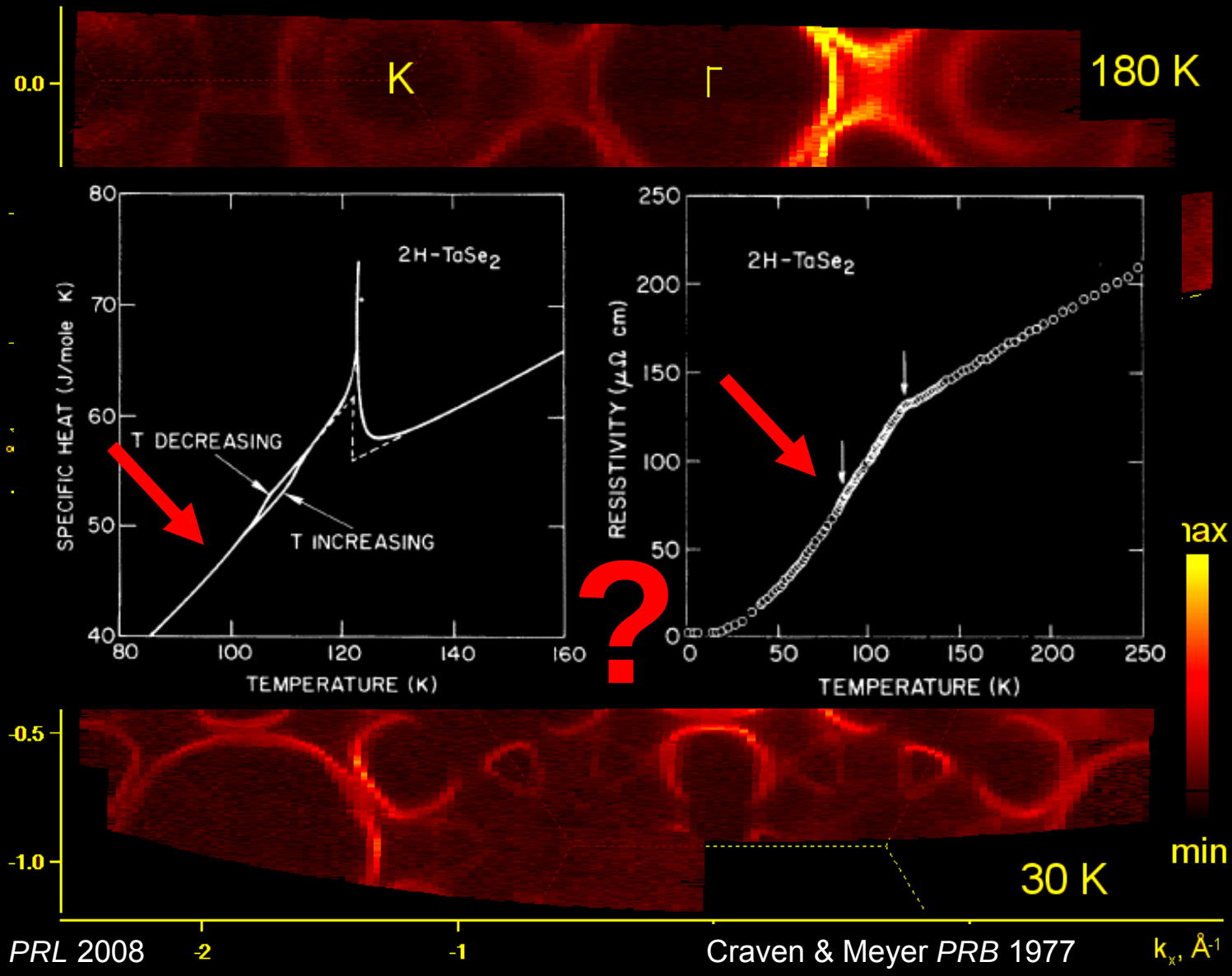


Fermi surface: commensurate CDW state

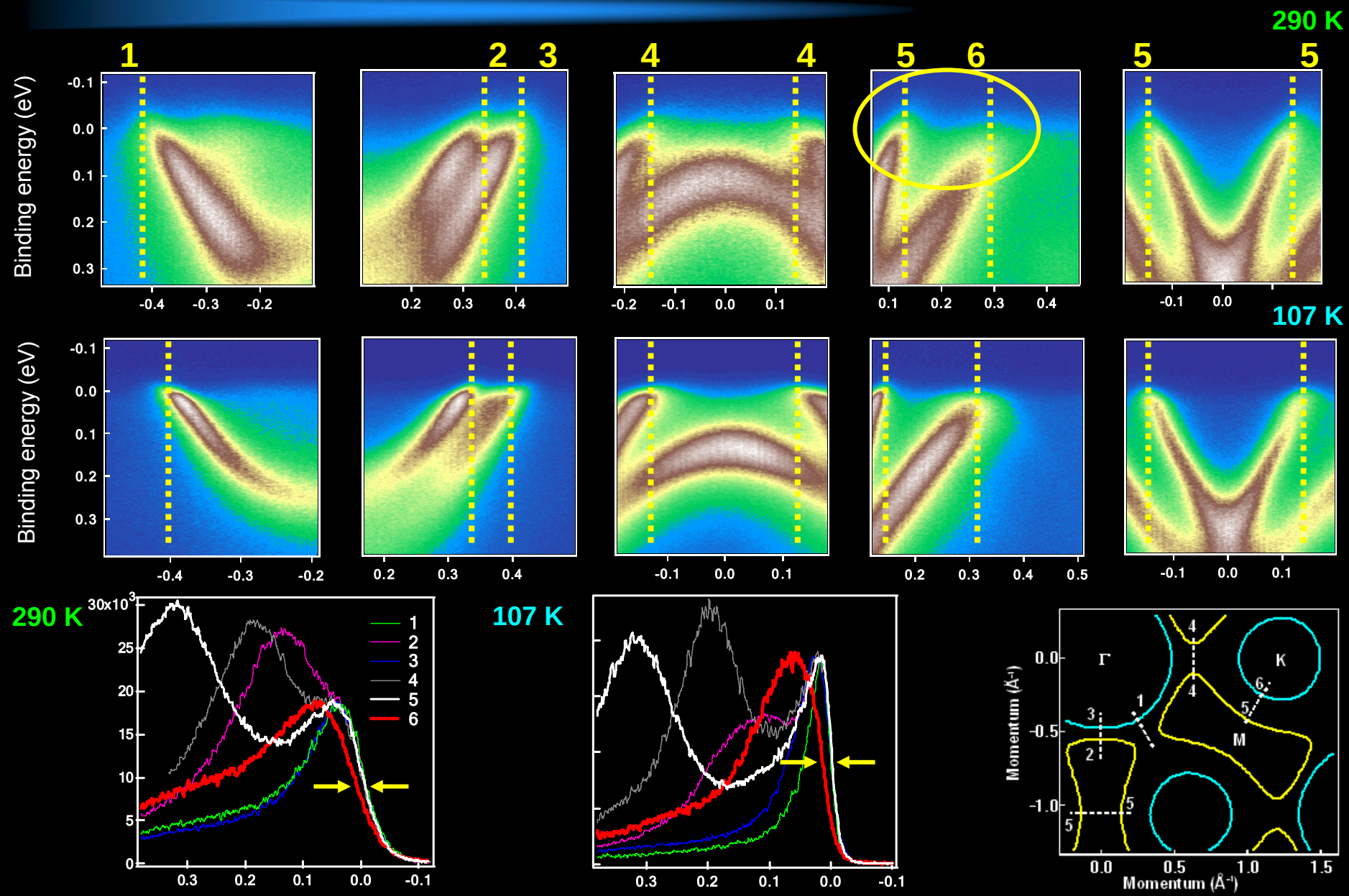


Borisenko *PRL* 2008

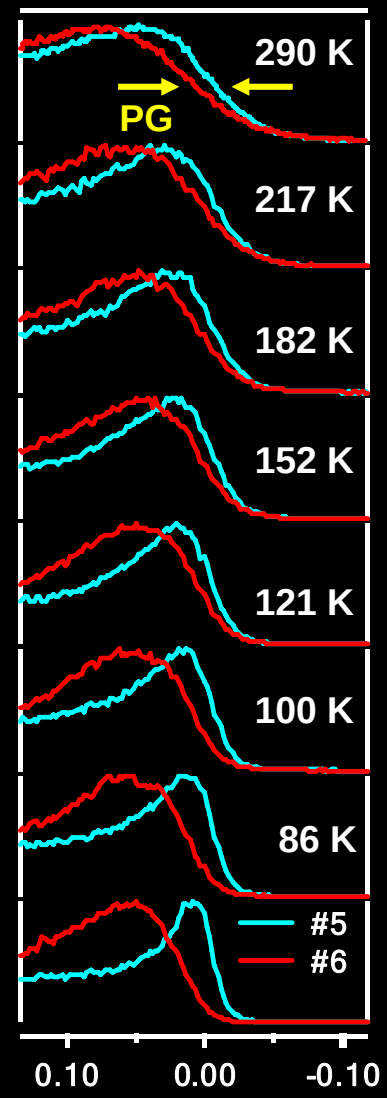
Fermi surface: commensurate CDW state

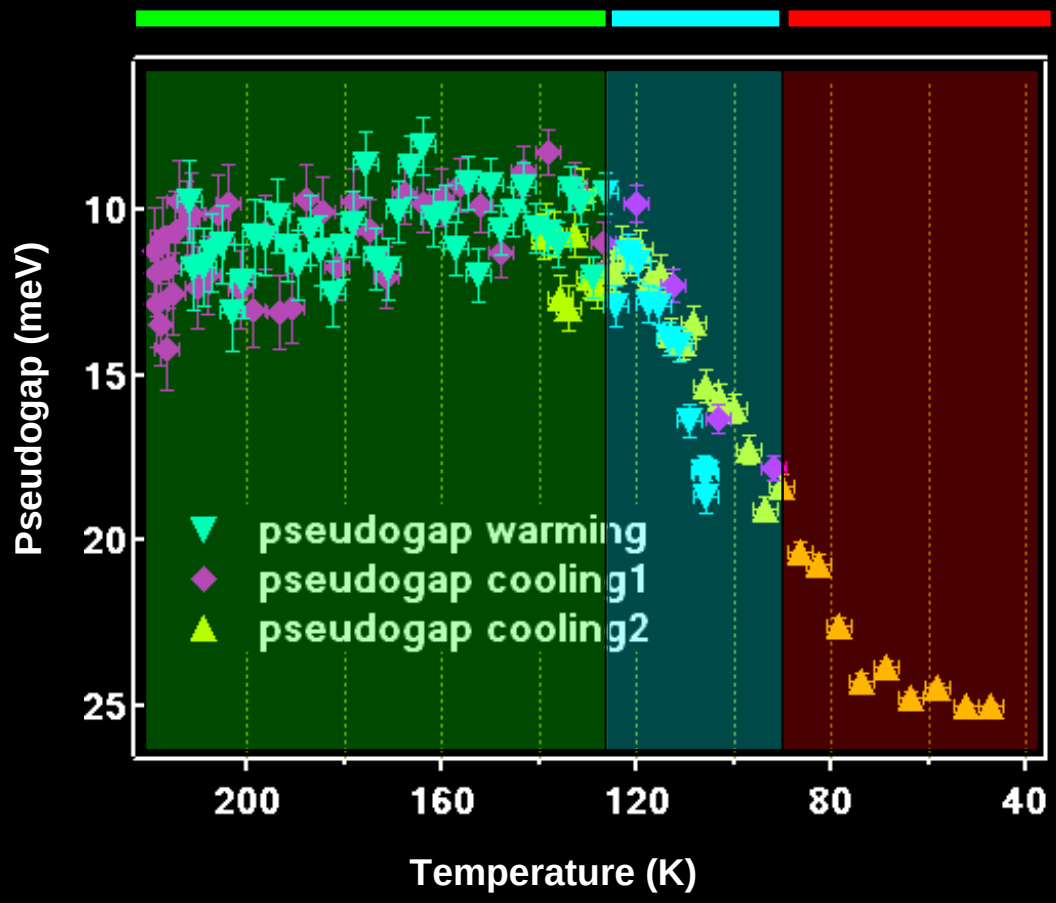


Comparison: IC-CDW and normal state



Pseudogap as a function of temperature

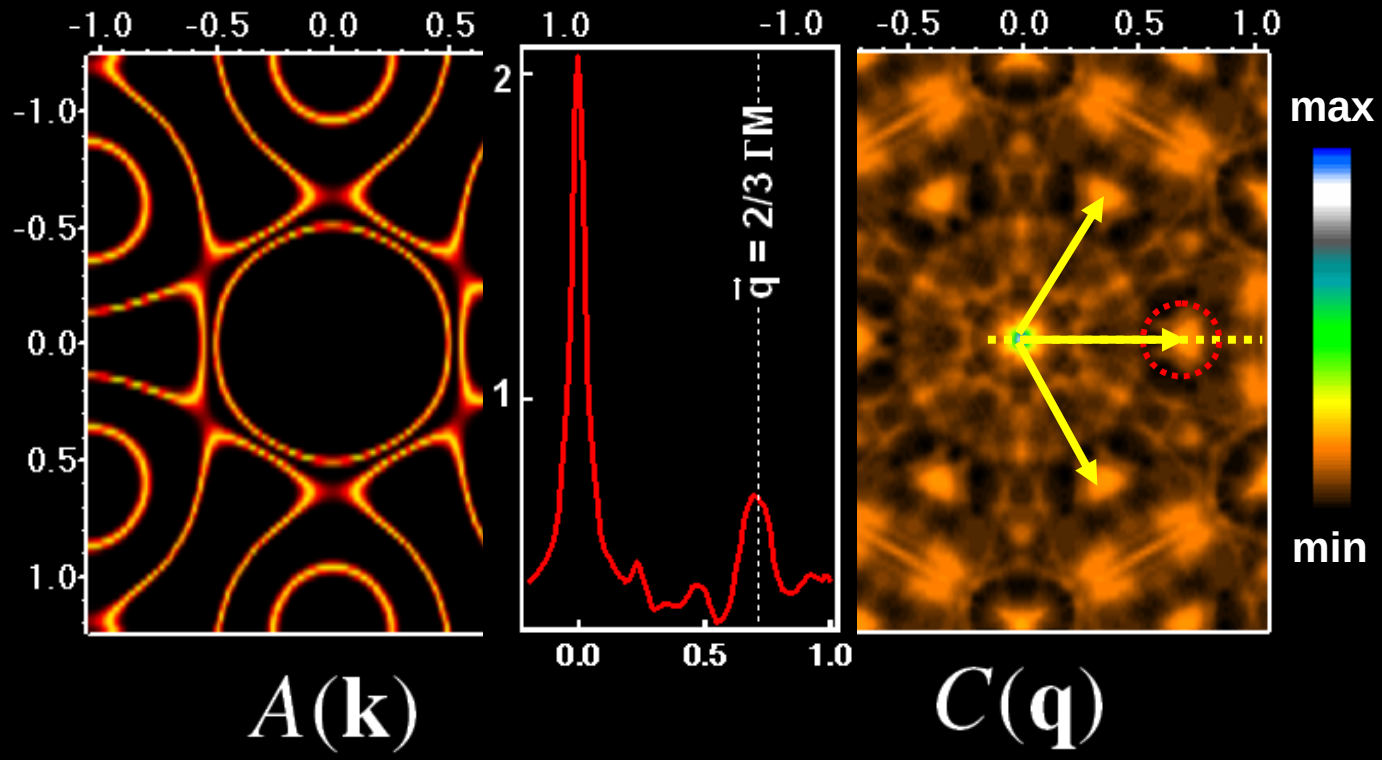




Autocorrelation – measure of nesting

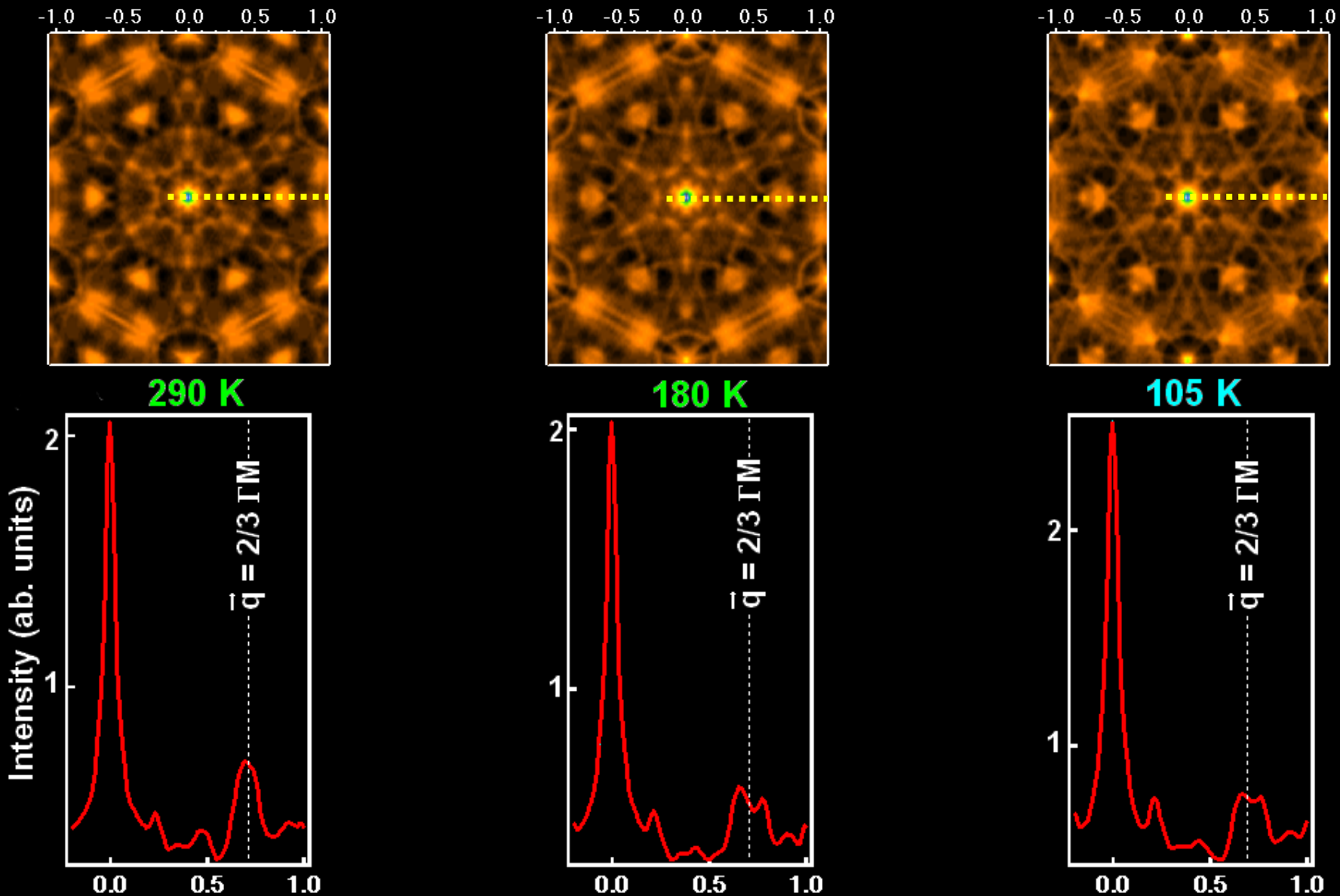
290 K

$$\mathbf{AC}\quad A(\mathbf{k}) = \int A(\mathbf{k})A(\mathbf{k}+\mathbf{q})\,d\mathbf{k} = C(\mathbf{q})$$

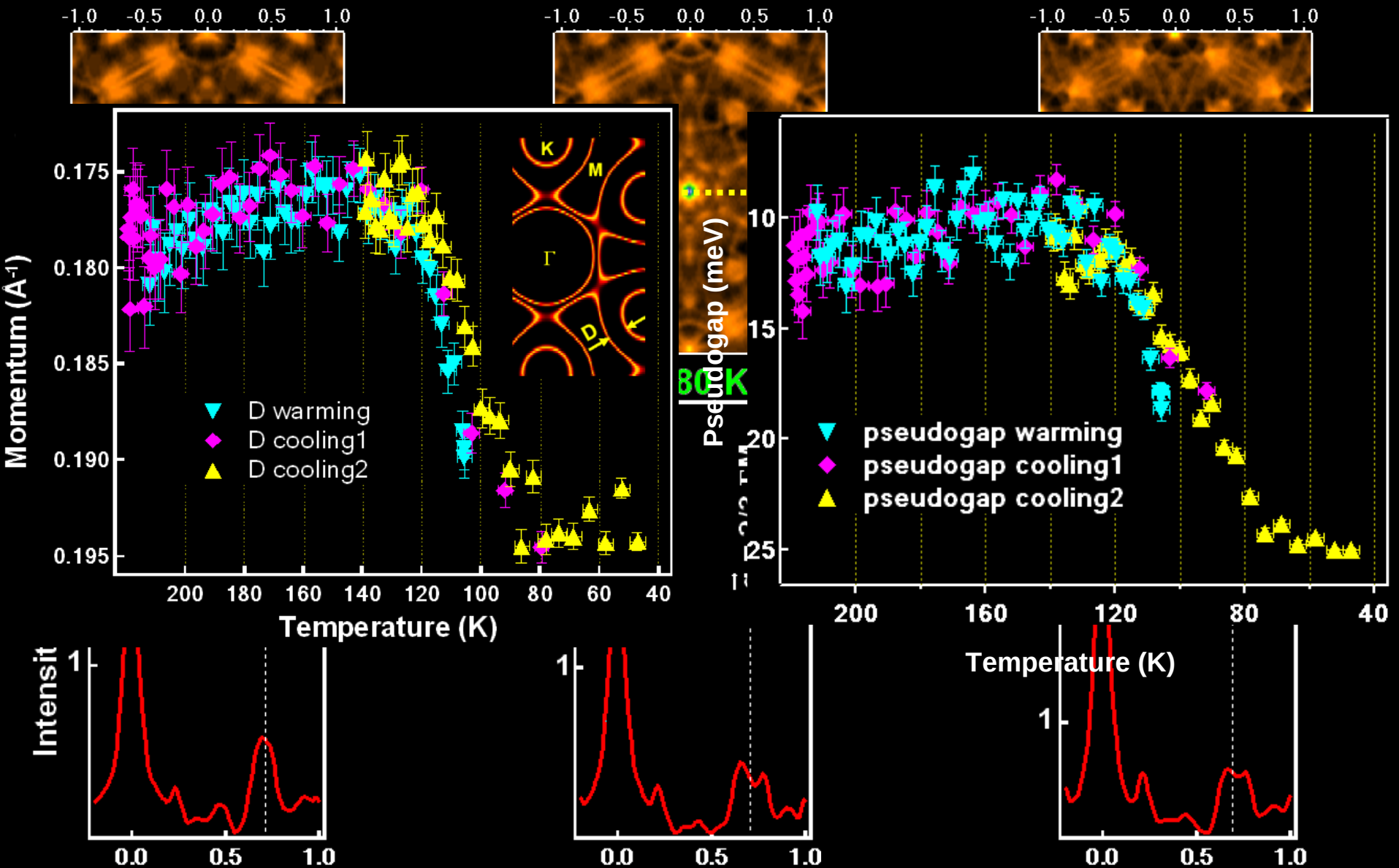


Borisenko *PRL* 2008

Nesting properties as a function of T



Nesting properties as a function of T

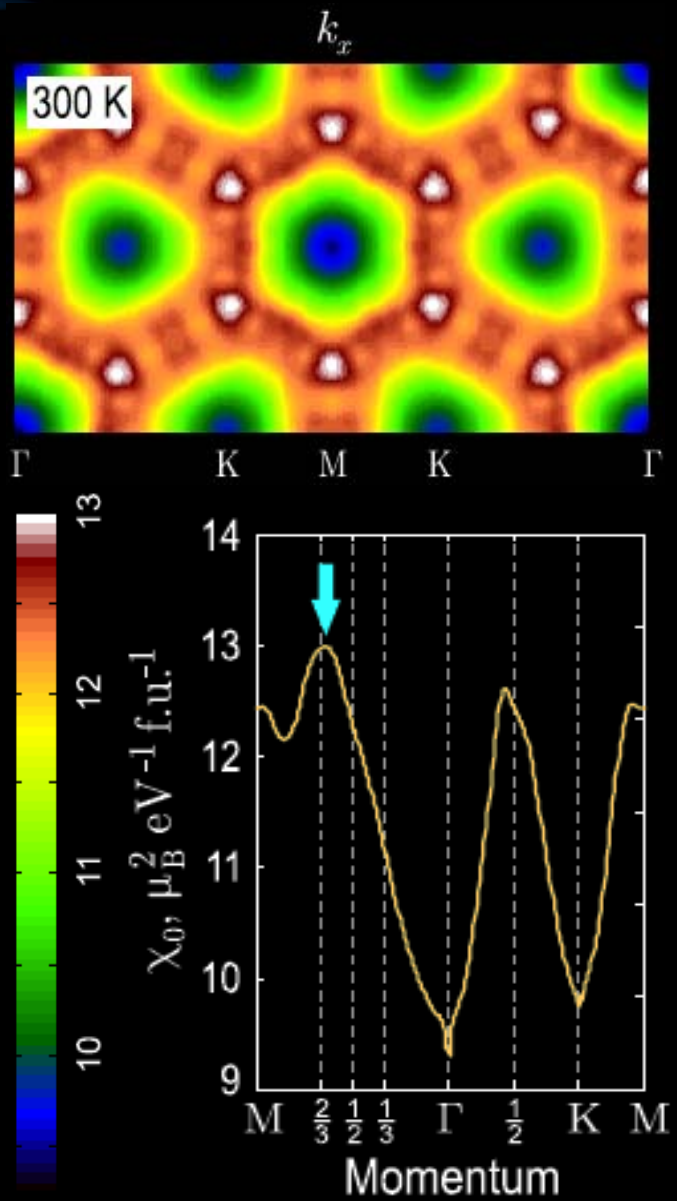


Electron susceptibility

$$\chi_0(\mathbf{q},\omega) = 2\int \frac{d\mathbf{k}}{(2\pi)^d} \frac{n_F(\epsilon_k) - n_F(\epsilon_{k+q})}{\epsilon_k - \epsilon_{k+q} + \omega + i0^+}$$

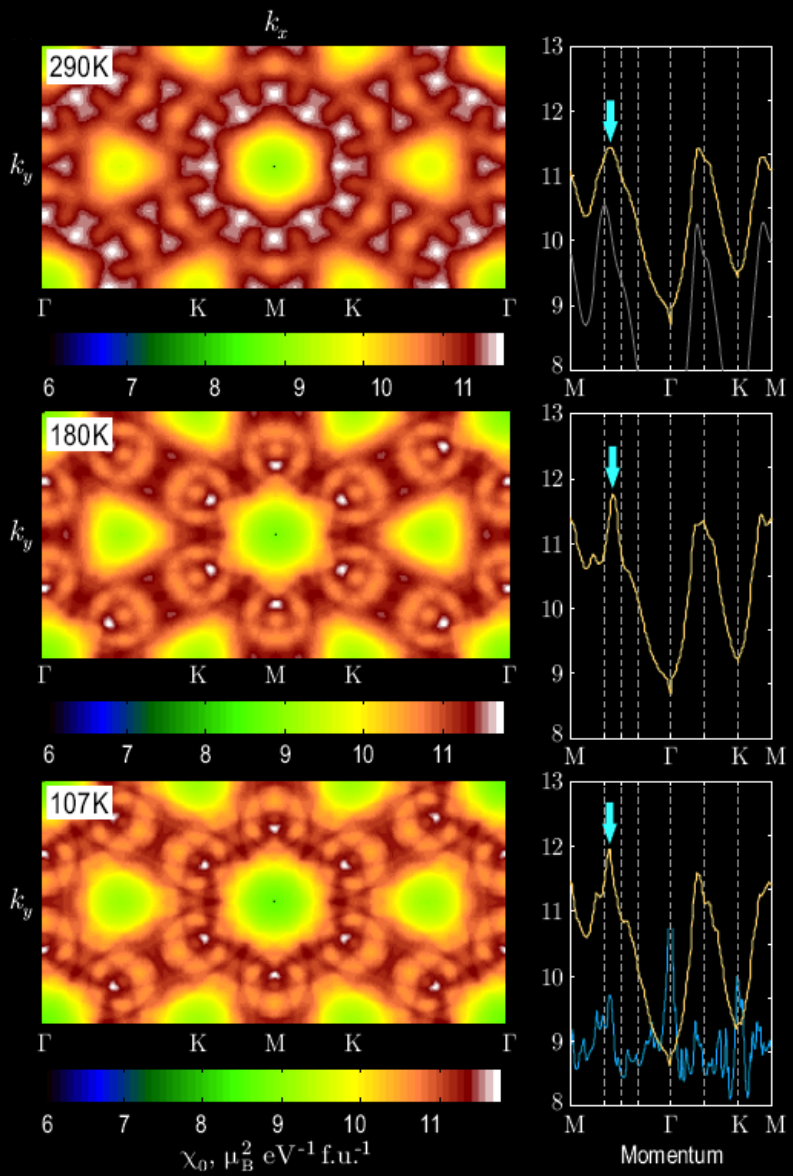
Lindhard functions at $\omega \to 0$

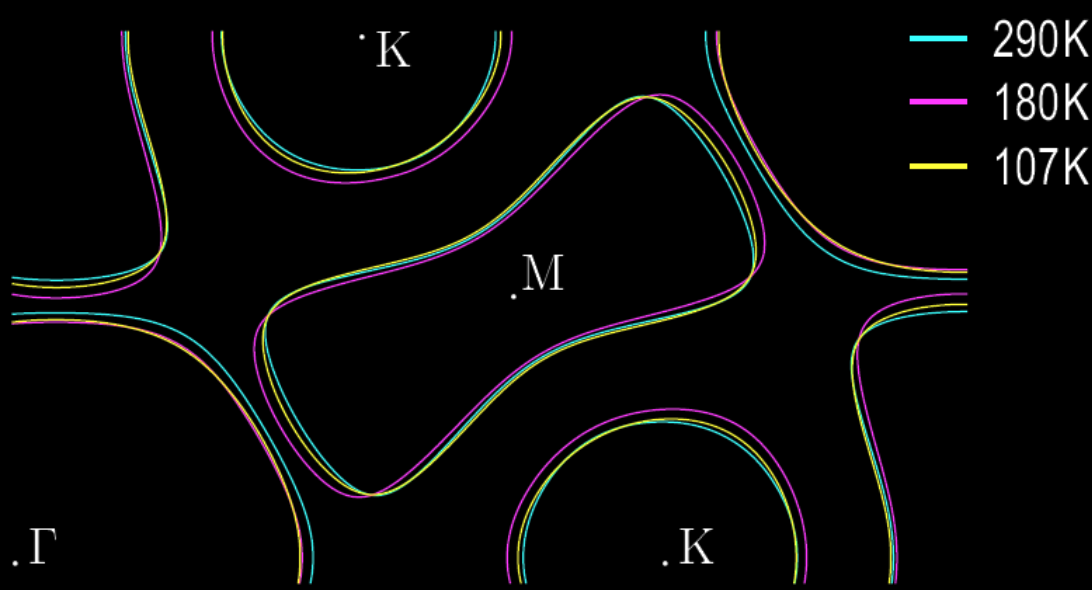
$$\chi_q = \sum_k \frac{n_F(\epsilon^a_k) - n_F(\epsilon^a_{k+q})}{\epsilon^a_k - \epsilon^a_{k+q}} + \sum_k \frac{n_F(\epsilon^a_k) - n_F(\epsilon^b_{k+q})}{\epsilon^a_k - \epsilon^b_{k+q}}$$
$$+ \sum_k \frac{n_F(\epsilon^b_k) - n_F(\epsilon^a_{k+q})}{\epsilon^b_k - \epsilon^a_{k+q}} + \sum_k \frac{n_F(\epsilon^b_k) - n_F(\epsilon^b_{k+q})}{\epsilon^b_k - \epsilon^b_{k+q}}$$



Inosov arXiv:0805.4105, arXiv:0807.3929

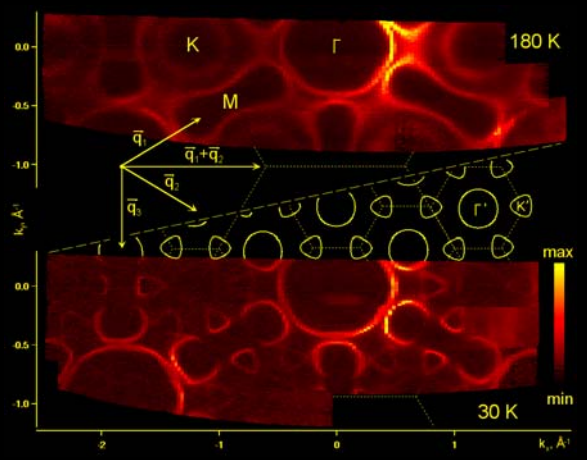
Electron susceptibility

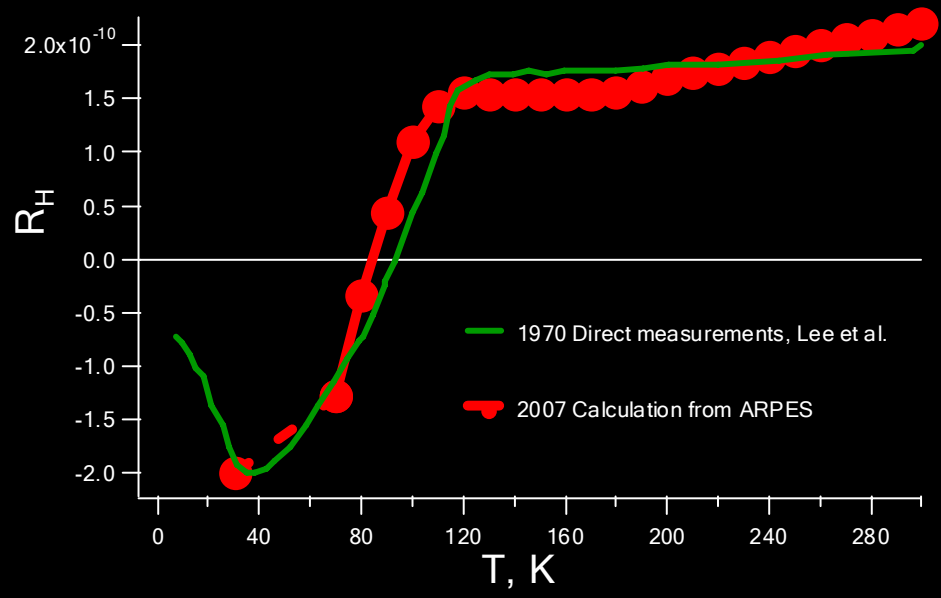




Inosov arXiv:0805.4105, arXiv:0807.3929

Hall coefficient of 2H-$TaSe_2$ from ARPES



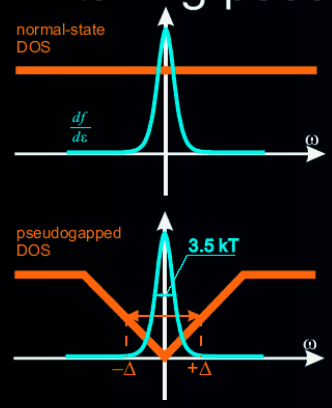


Hall coefficient from electronic structure

$$\tau(\mathbf{k}) = \text{const}$$

$$R_H = \frac{\sigma_{xy}}{H \cdot \sigma_{xx}^2} = \frac{\int \tau(\mathbf{k})^2 \cdot \frac{v_F^2(\mathbf{k})}{\rho(\mathbf{k})} \cdot dk}{\left(\int \tau(\mathbf{k}) \cdot v_F(\mathbf{k}) \cdot dk\right)^2} = \frac{\int \frac{v_F^2(\mathbf{k})}{\rho(\mathbf{k})} \cdot dk}{\left(\int v_F(\mathbf{k}) \cdot dk\right)^2}$$

taking pseudogap into account

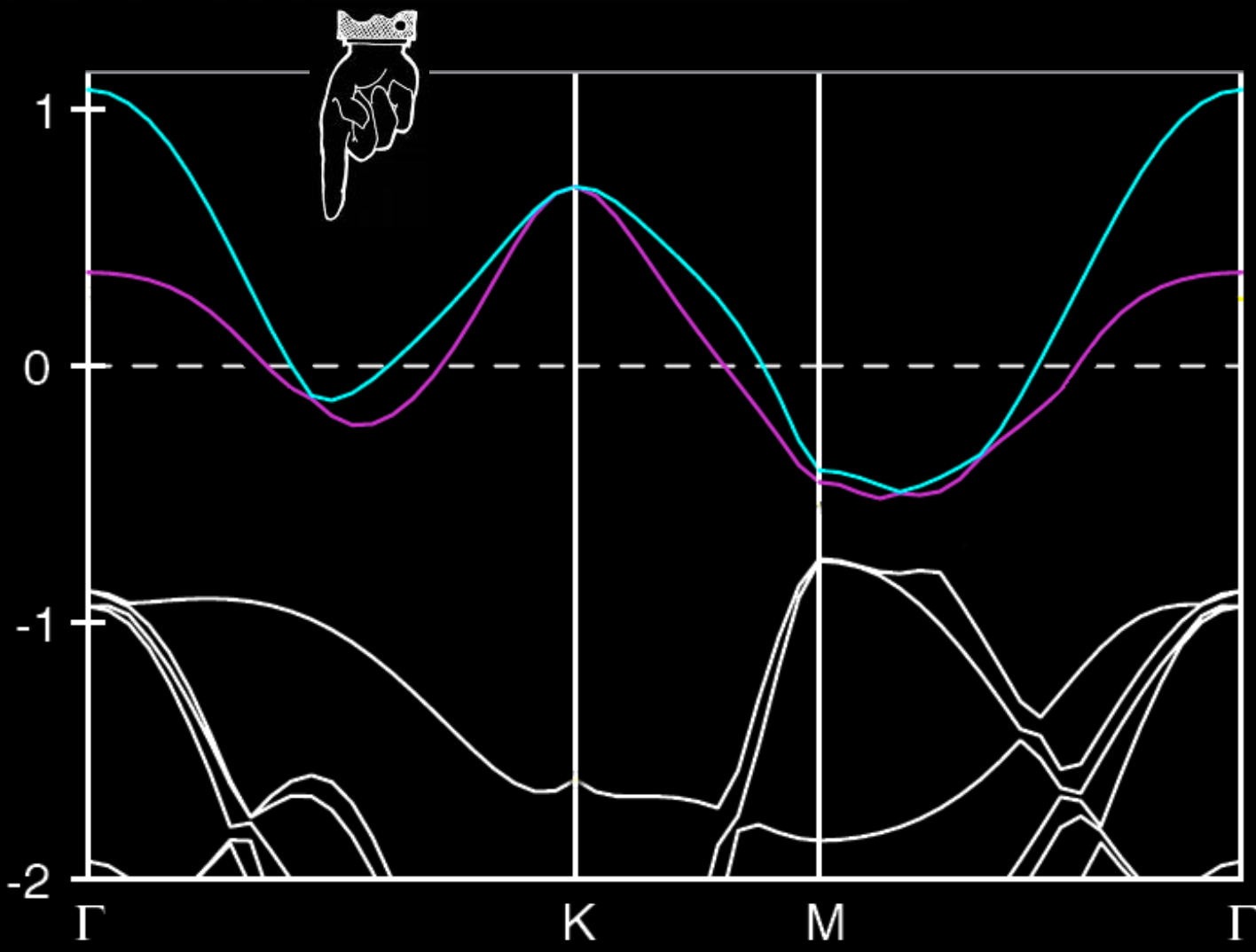


$$D(\mathbf{k}) = -\int_{-\infty}^{\infty} \frac{df}{d\varepsilon} \cdot A(\varepsilon, \mathbf{k}) \cdot d\varepsilon \le 1$$

$$\sigma_{xy} \propto \int D(\mathbf{k}) \cdot \frac{\tau^2(\mathbf{k}) \cdot v_F^2(\mathbf{k})}{\rho(\mathbf{k})} \cdot dk$$

Evtushinsky *PRL* 2008

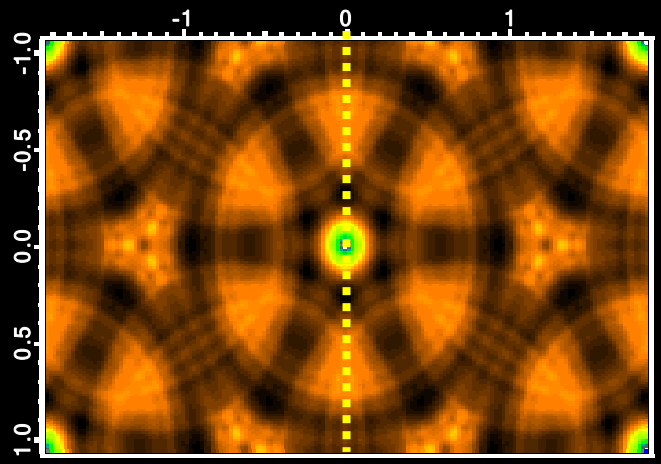
Band structure of 2H- $NbSe_2$



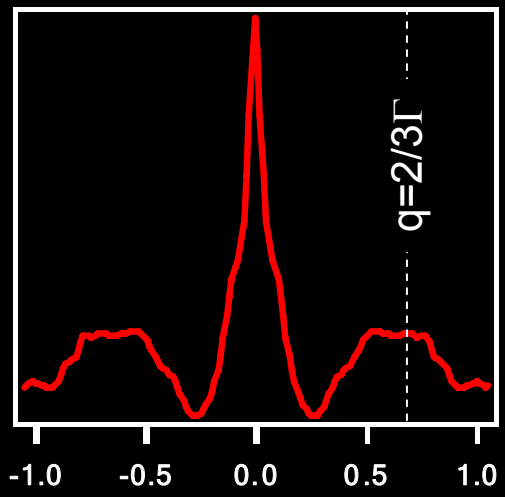
M
„dogbones“

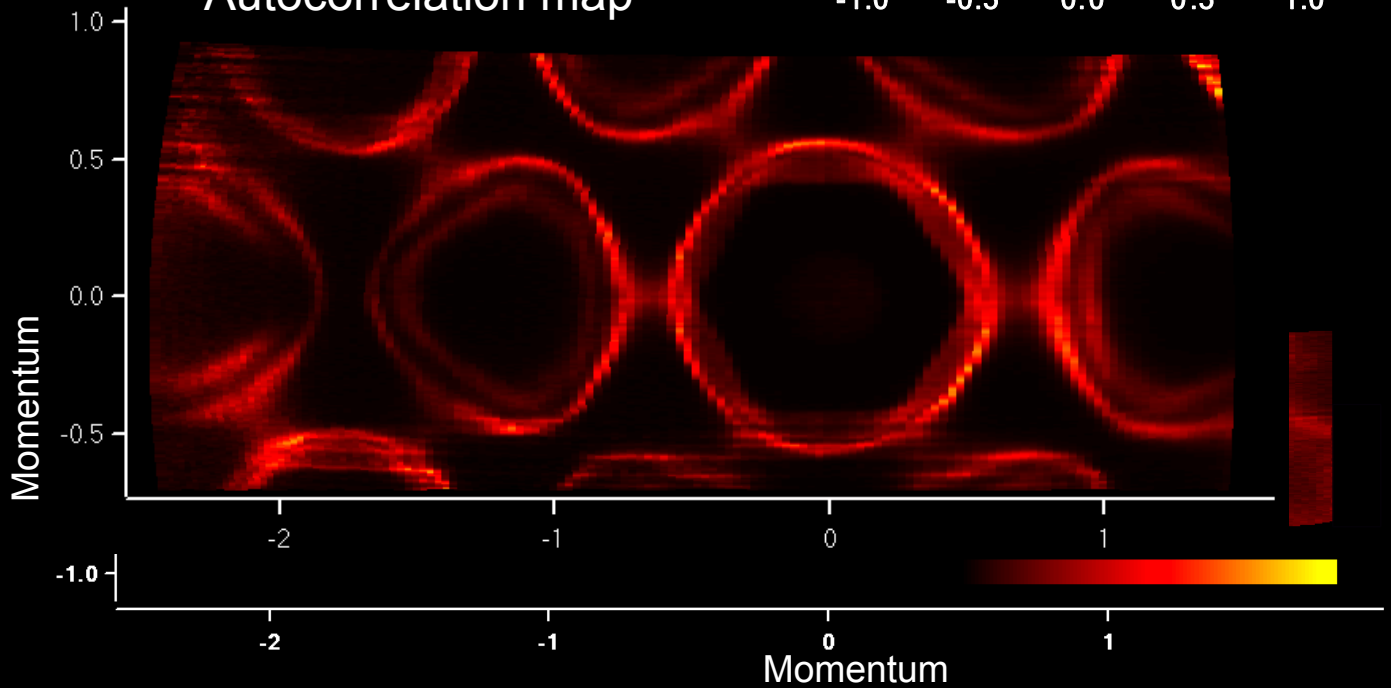
Γ, K
„barrels“

Modification of the nesting properties



Autocorrelation map



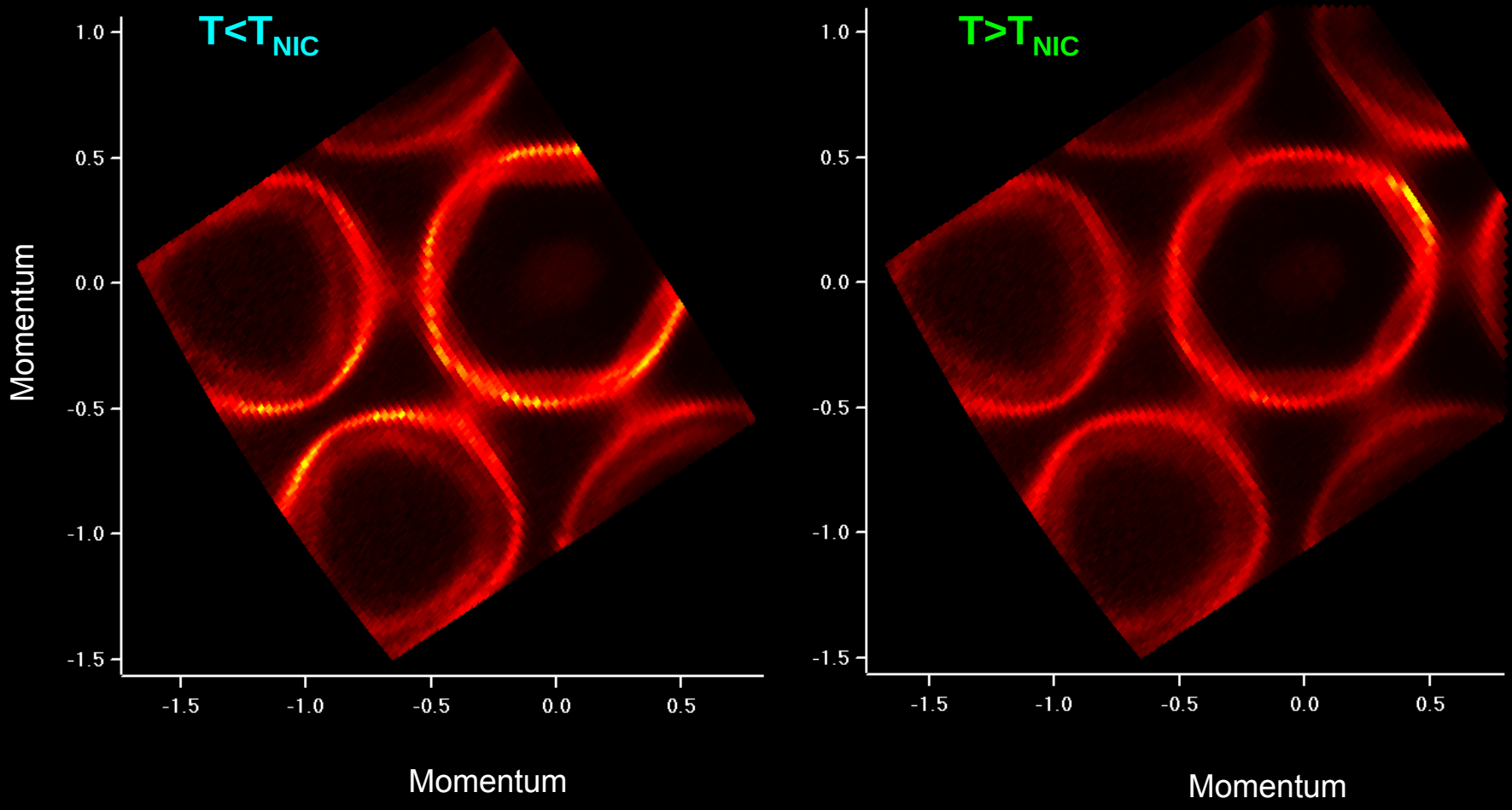


2H-$NbSe_2$

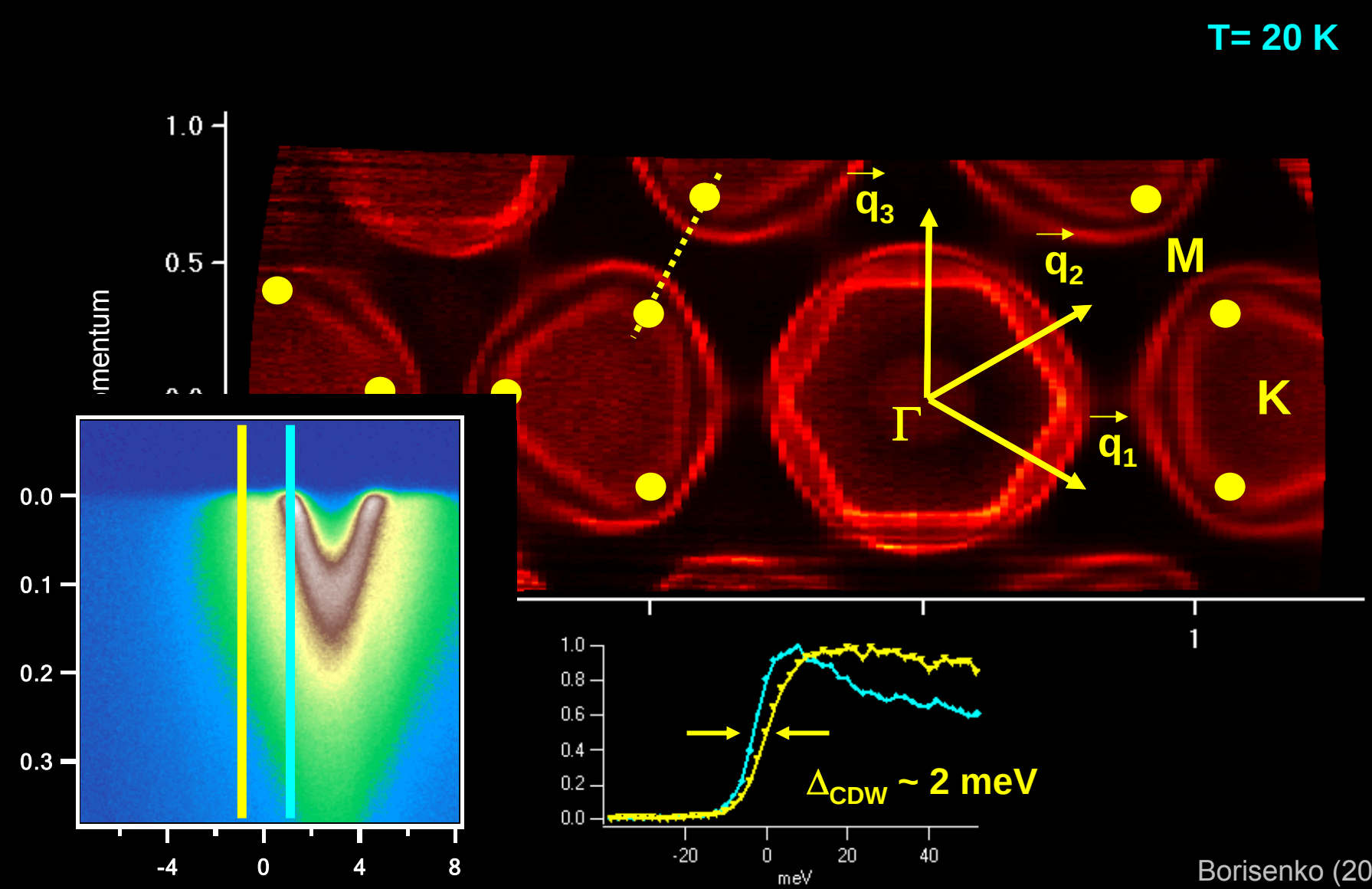
T_{NIC}~ 33 K

T_C= 7.2 K

Fermi surface of 2H-$NbSe_2$

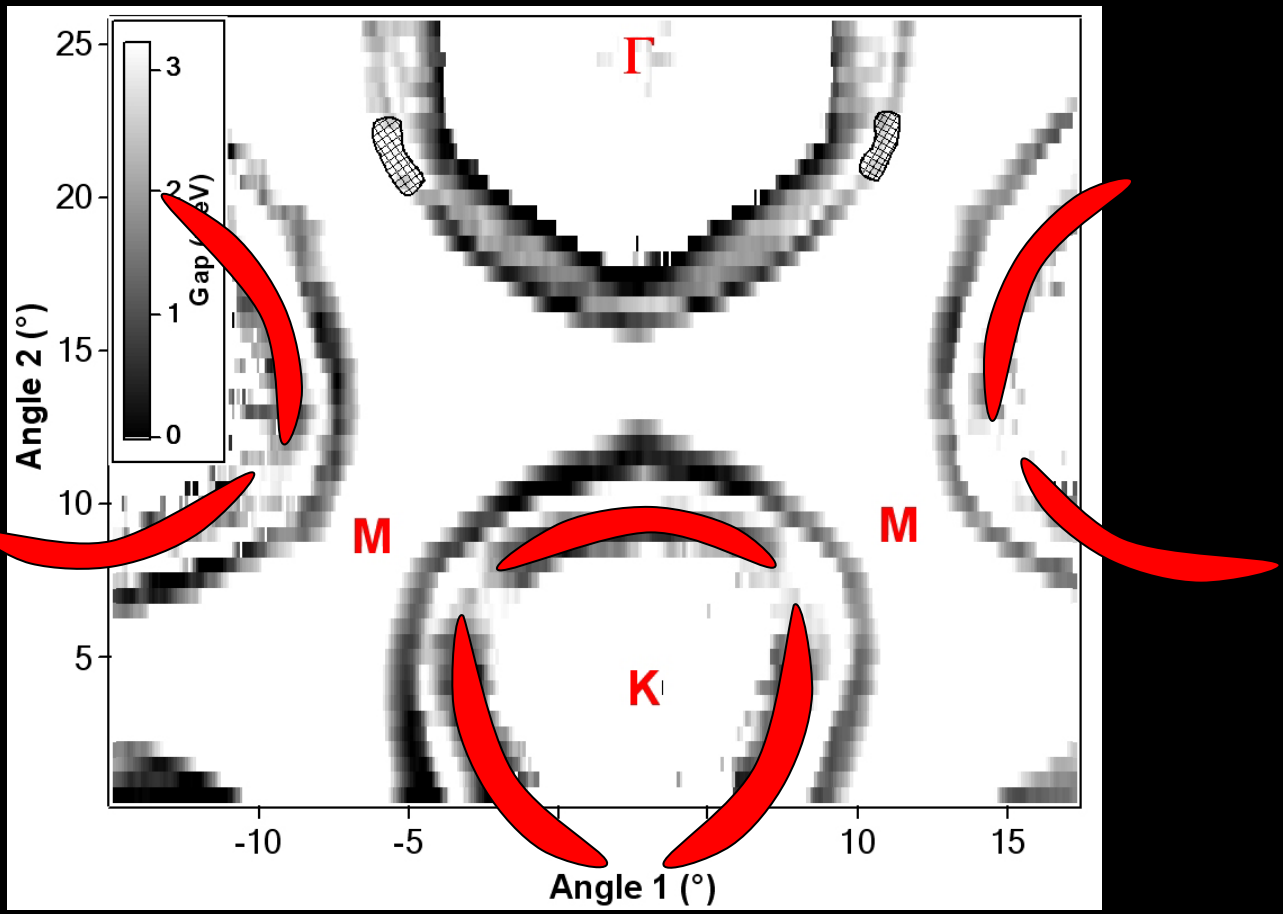


Incommensurate CDW state in 2H-$NbSe_2$



Borisenko (2008)

Fermi surface "arcs" in $NbSe_2$



Map of gaps, 20 K

Charge Density Waves compounds

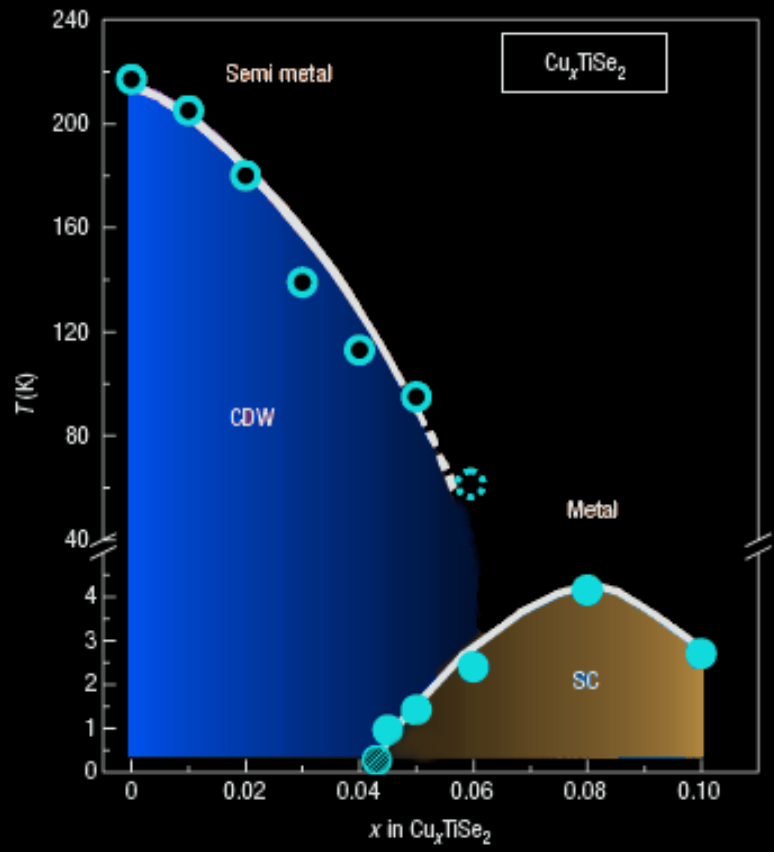
1T-TaS_2, T_0= 550 K

$TiSe_2$, T_0= 200 K

2H-$TaSe_2$, T_0= 122 K

2H-$NbSe_2$, T_0= 33 K

1T-$TaSe_2$, T_0= 473 K



Morosan et al. Nature Phys. 06

Pseudogap in dichalcogenides

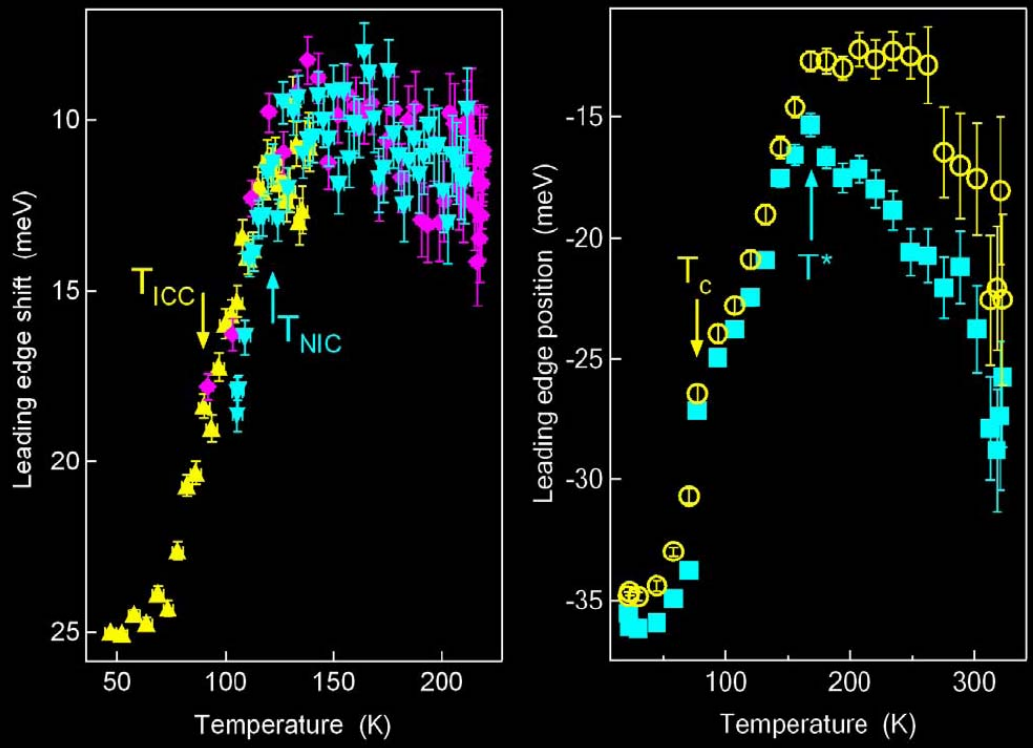
- ✓ Incommensurate CDW causes a PG in one-particle excitation spectrum
- ✓ CDW formation depends crucially on electronic band structure
- ✓ CDW and SC compete for the phase space

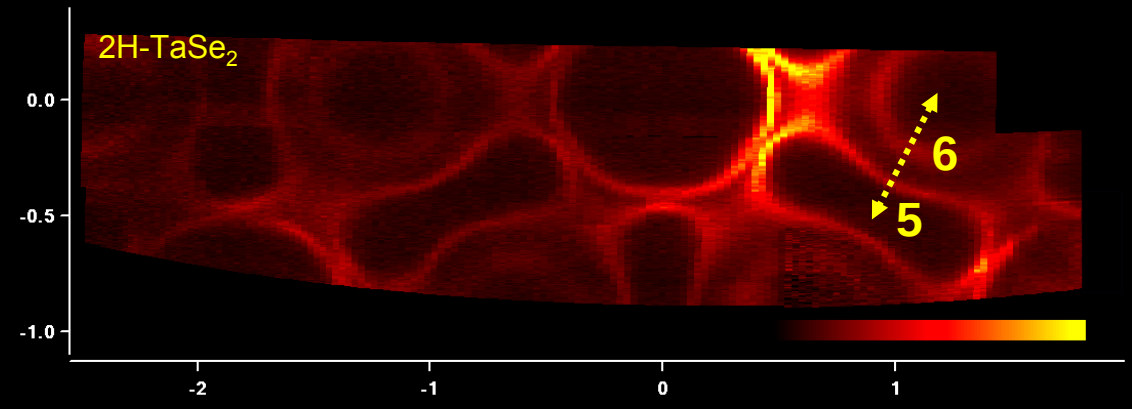
2D electronic structure of dichalcogenides is unstable to a density wave formation.

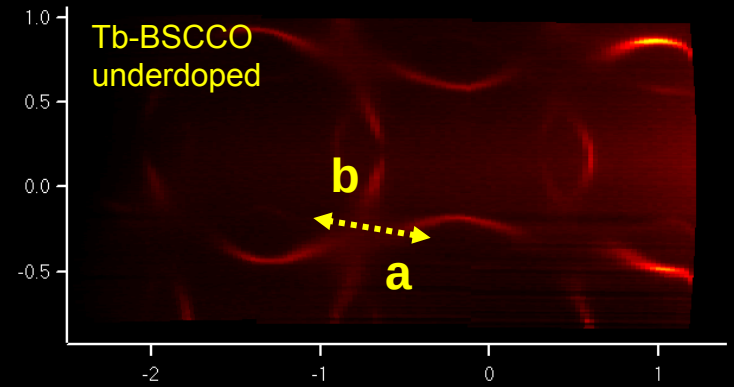
Are the dichalcogenides unique?

Ordering in cuprates

Pseudogap in 2H-$TaSe_2$ and Tb-BSCCO



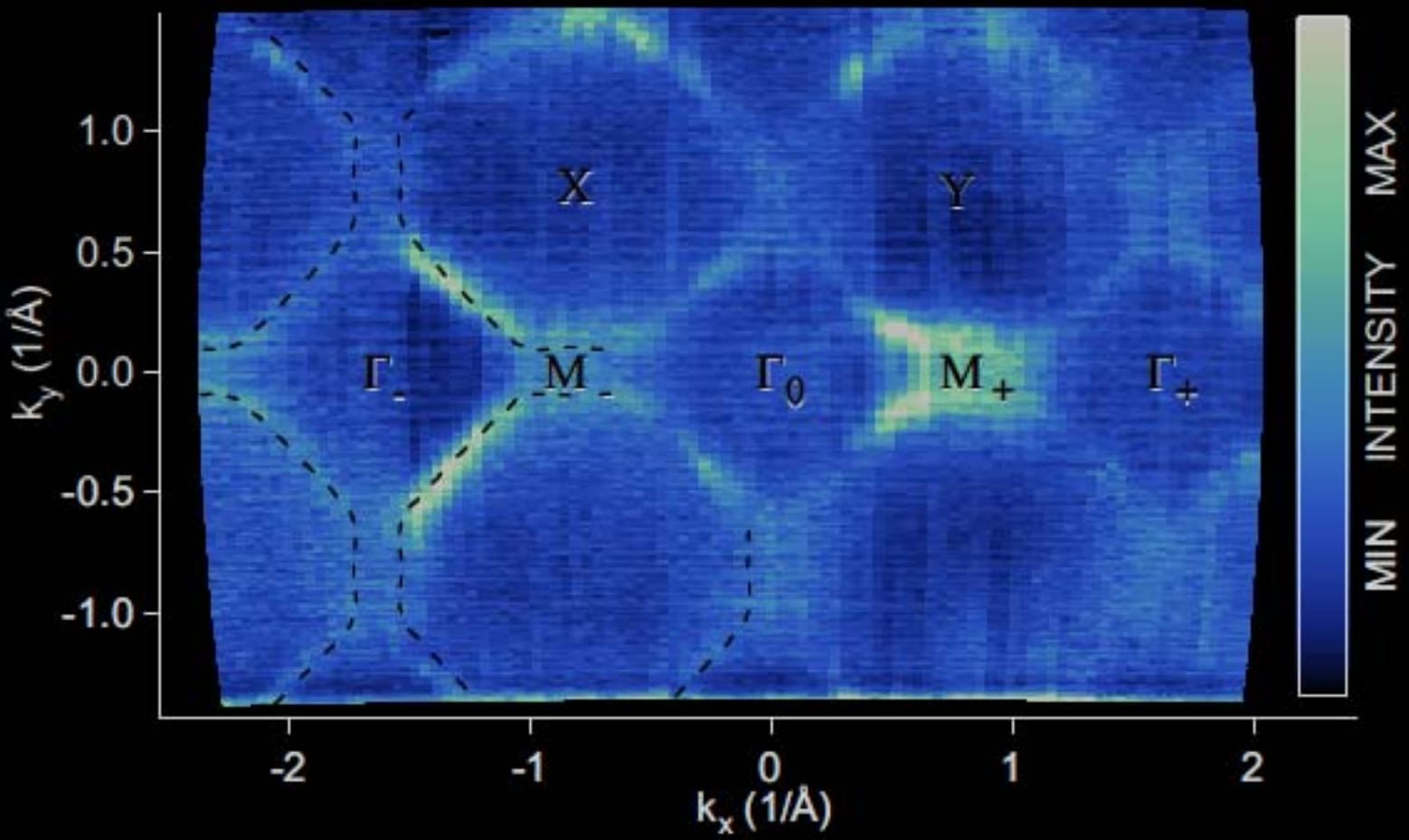




Pseudogap in cuprates?

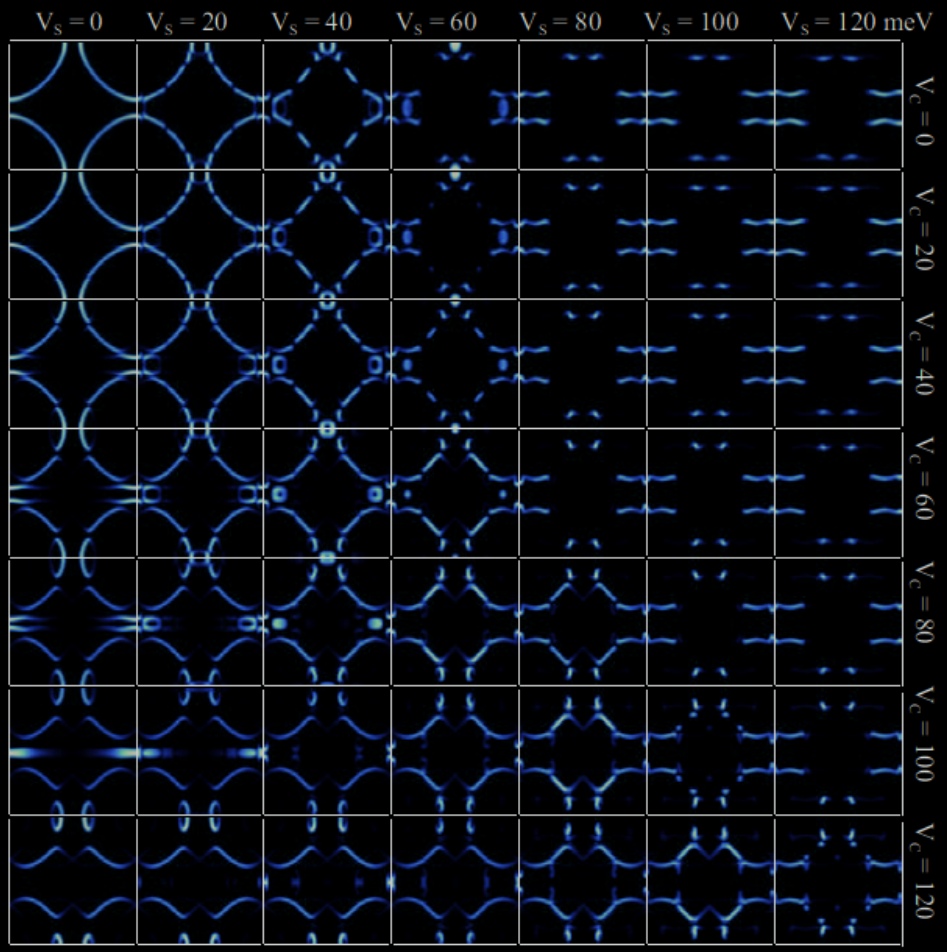
- ✓ PG and SG are two different gaps
- ✓ Pseudo-gap = Density modulation (incommensurate SDW)
- ✓ PG and SG compete for the phase space but both depend on electronic band structure

Ordering in La(Eu)SrCuO 1/8



Zabolotnyy arXiv:0809.2237

Ordering in La(Eu)SrCuO 1/8



$$V_s = \langle \mathbf{k}|\hat{V}_s(\mathbf{r})|\mathbf{k} \pm \mathbf{Q}_s\rangle, \text{with } \mathbf{Q}_s = (3\pi/4;\pi), \text{ and}$$
$$V_c = \langle \mathbf{k}|\hat{V}_c(\mathbf{r})|\mathbf{k} \pm \mathbf{Q}_c\rangle, \text{with } \mathbf{Q}_c = (\pi/4;0).$$

$$\hat{H} = \sum_{\substack{\mathbf{q}\in \mathrm{RBZ} \\ m,n=0,\ldots,7}} (\delta_{m,n}\varepsilon_{\mathbf{q}+\mathbf{g}_m} + V_{m,n})\hat{c}^{\dagger}_{\mathbf{q}+\mathbf{g}_m}\hat{c}_{\mathbf{q}+\mathbf{g}_n}, \text{with}$$

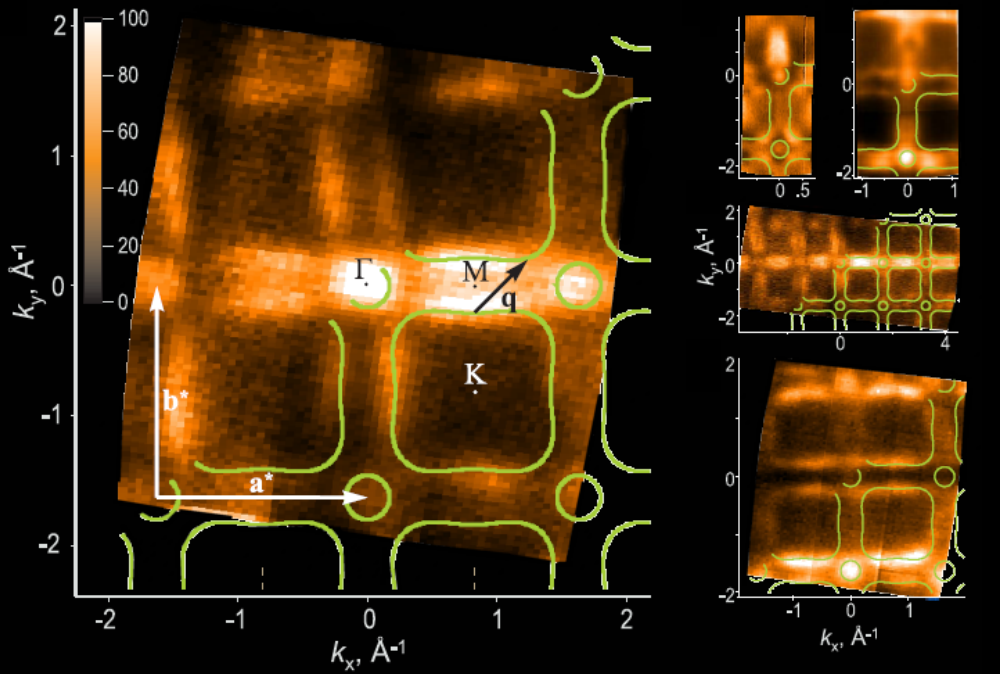
$$V_{m,n}(\mathbf{q}) = \begin{pmatrix} 0 & V_c & 0 & V_c & 0 & V_s & V_s & 0 \\ V_c & 0 & V_c & 0 & 0 & 0 & V_s & V_s \\ 0 & V_c & 0 & V_c & V_s & 0 & 0 & V_s \\ V_c & 0 & V_c & 0 & V_s & V_s & 0 & 0 \\ 0 & 0 & V_s & V_s & 0 & V_c & 0 & V_c \\ V_s & 0 & 0 & V_s & V_c & 0 & V_c & 0 \\ V_s & V_s & 0 & 0 & 0 & V_c & 0 & V_c \\ 0 & V_s & V_s & 0 & V_c & 0 & V_c & 0 \end{pmatrix}$$

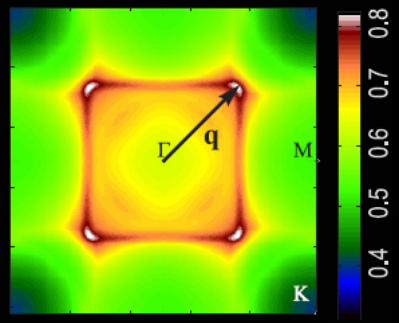
Zabolotnyy arXiv:0809.2237

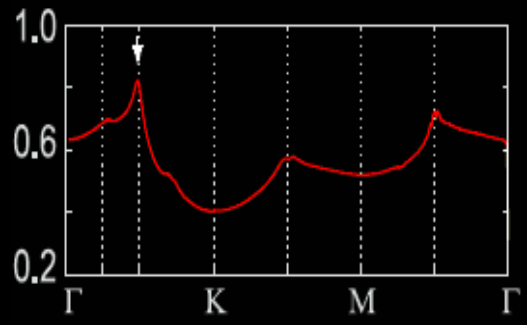
It seems that the electronic structure of both cuprates and dichalcogenides is unstable to a density wave formation.

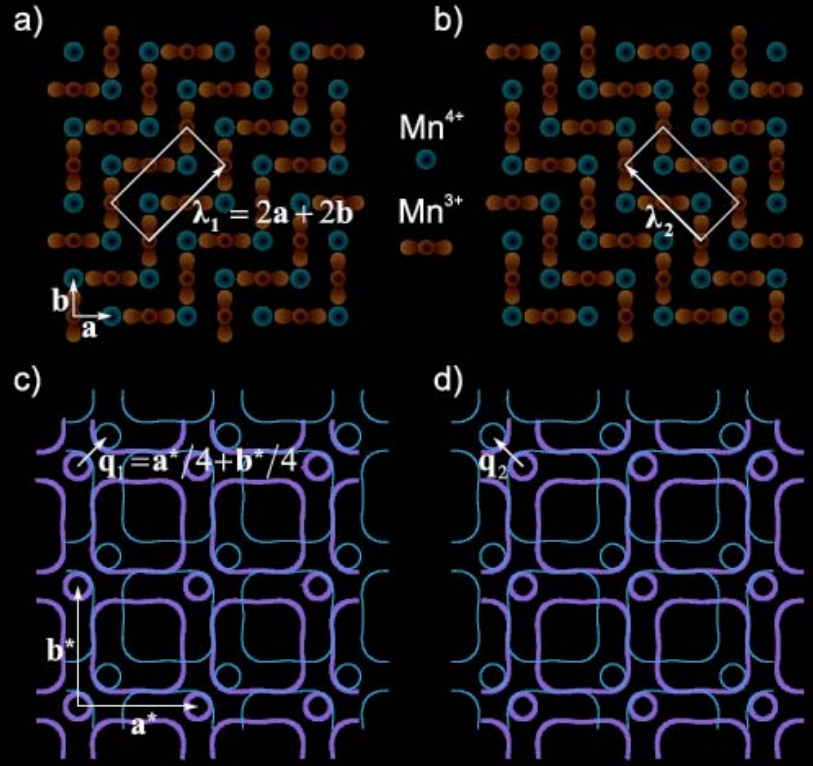
Are the cuprates and dichalcogenides unique in this sence?

Charge-orbital ordering and Fermi surface instabilities in $La_{0.5}Sr_{1.5}MnO_4$



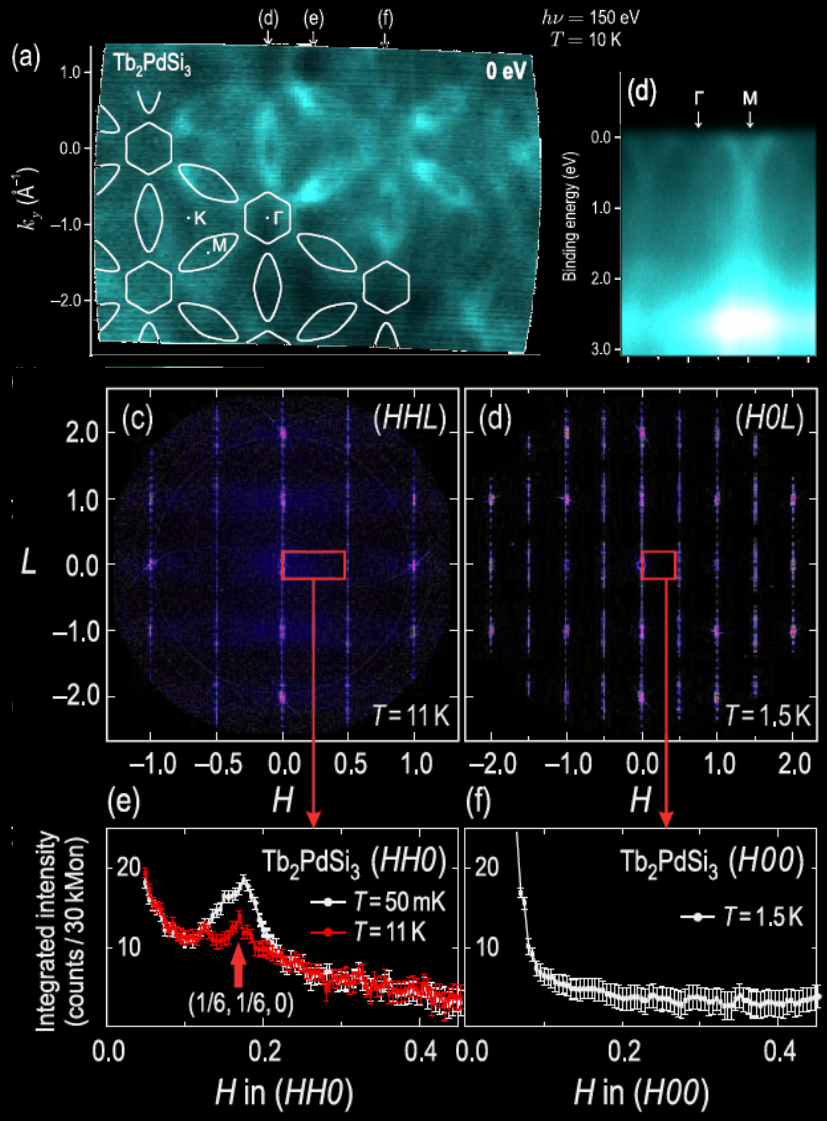


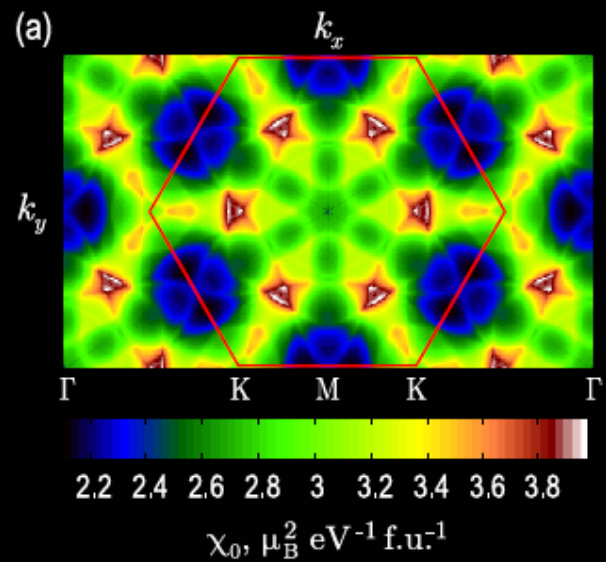


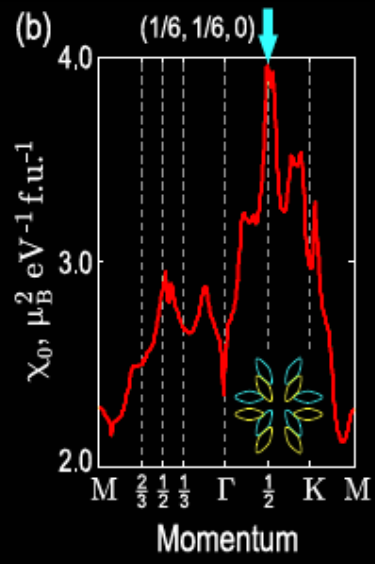


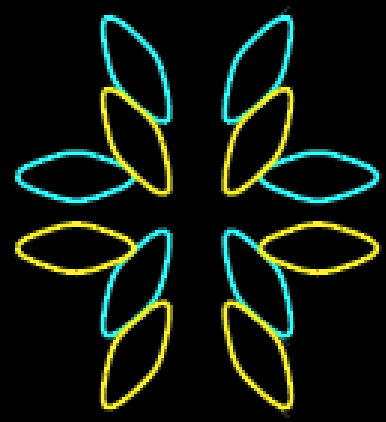
Evtushinsky 2008

Nesting-driven enhancement of the RKKY interaction in Gd_2PdSi_3 and Tb_2PdSi_3



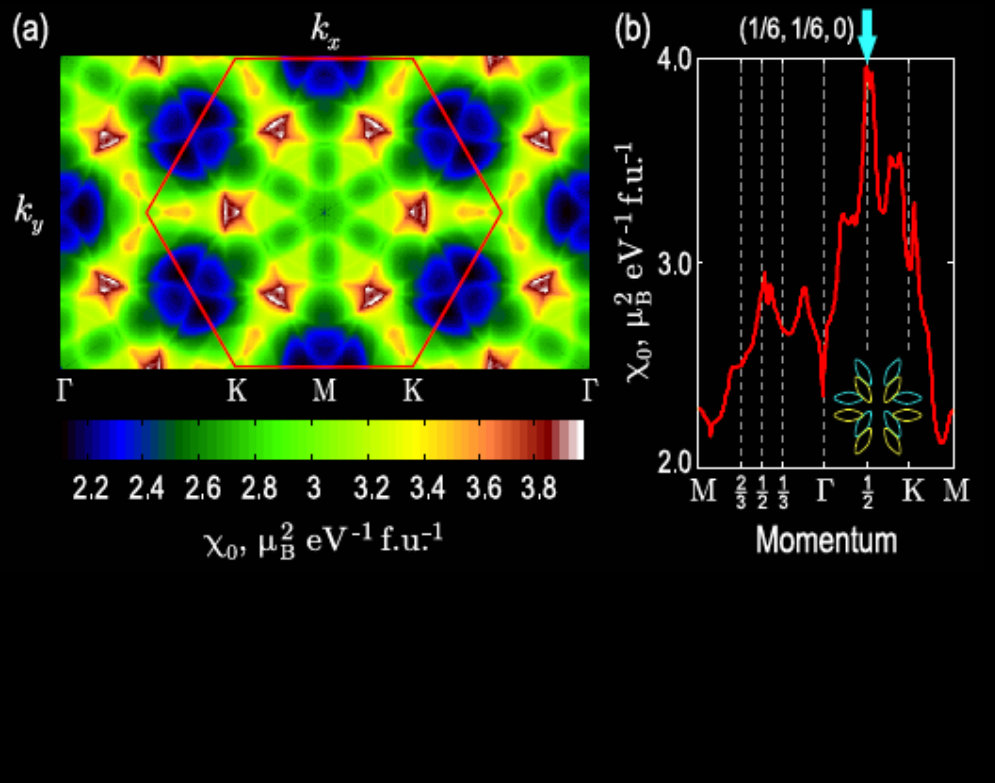


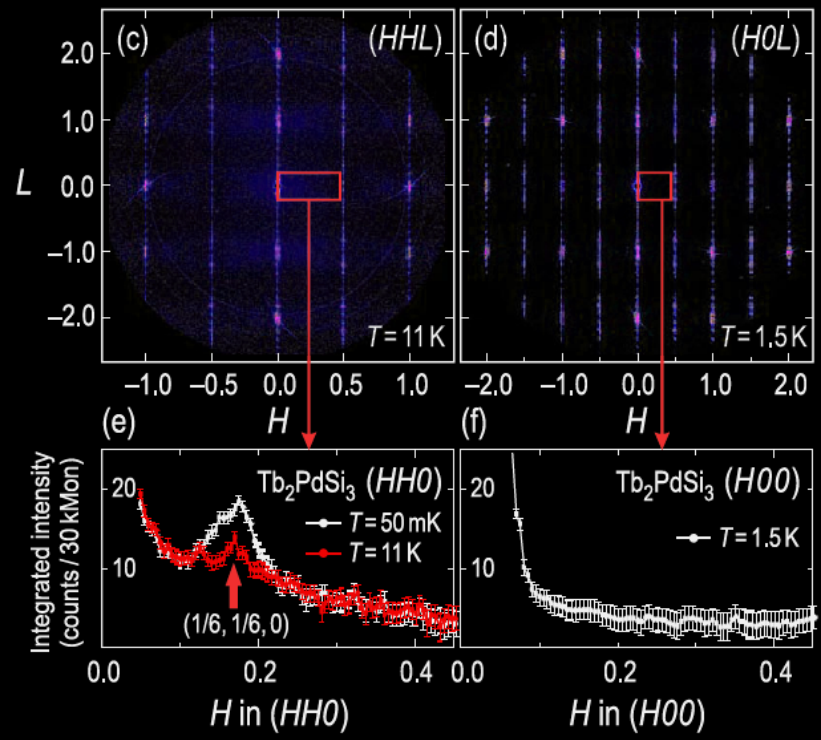




Inosov *PRL* 2009

Nesting-driven enhancement of the RKKY interaction in Gd_2PdSi_3 and Tb_2PdSi_3

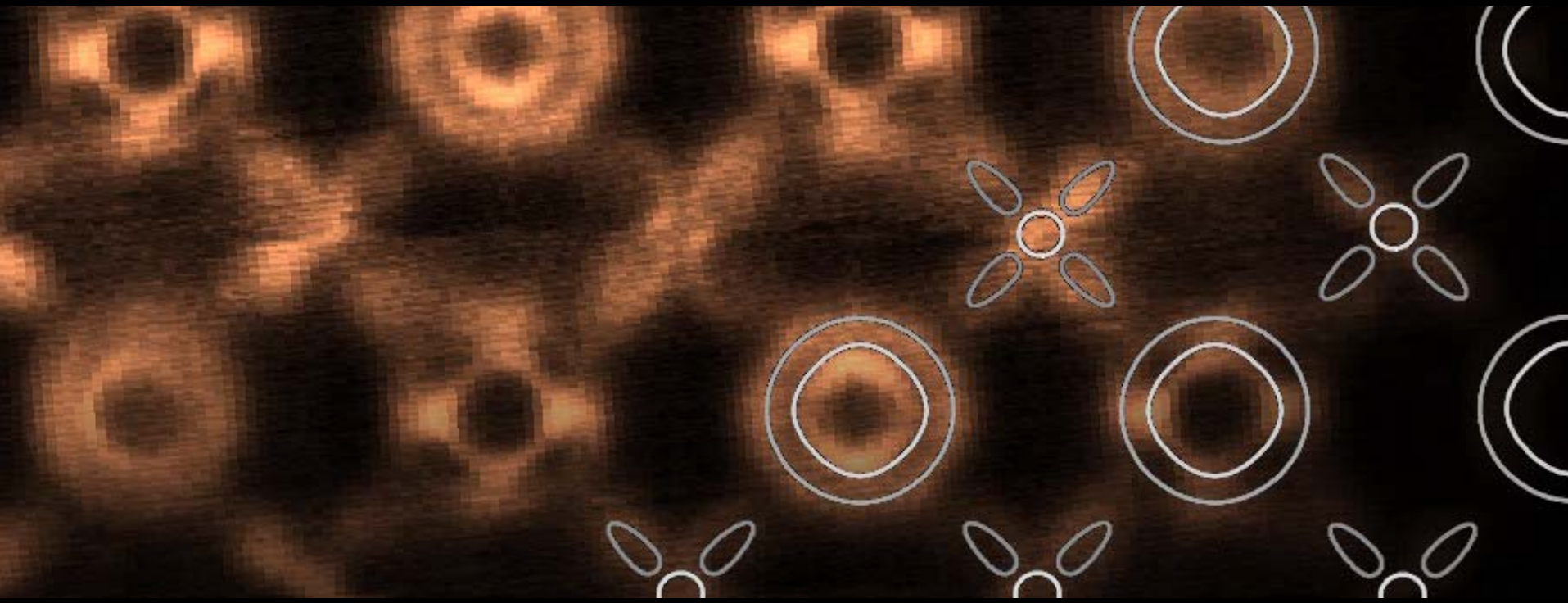




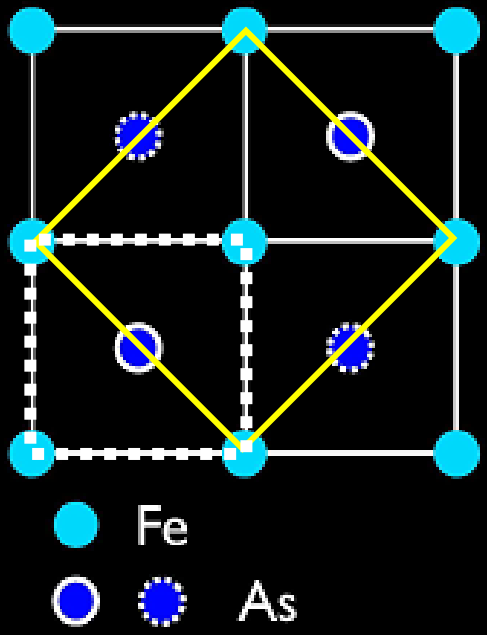
Inosov *PRL* 2009

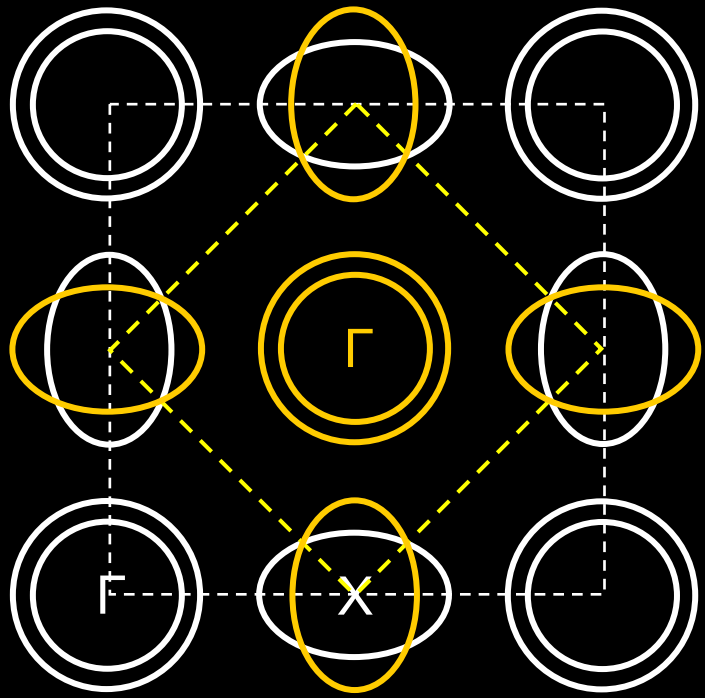
Ordering in pnictides (BKFA)

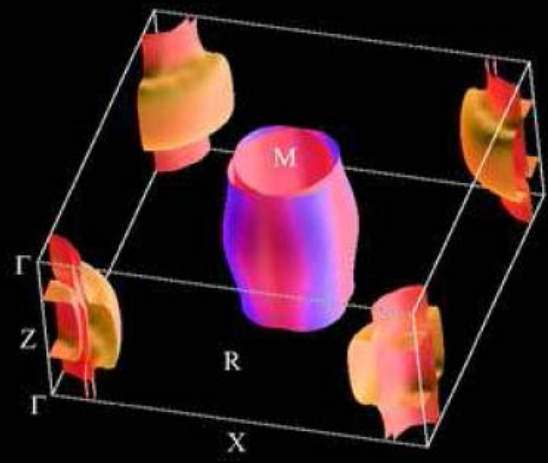
(π, π) electronic order in pnictides



Fermi surface of pnictides (calculated)



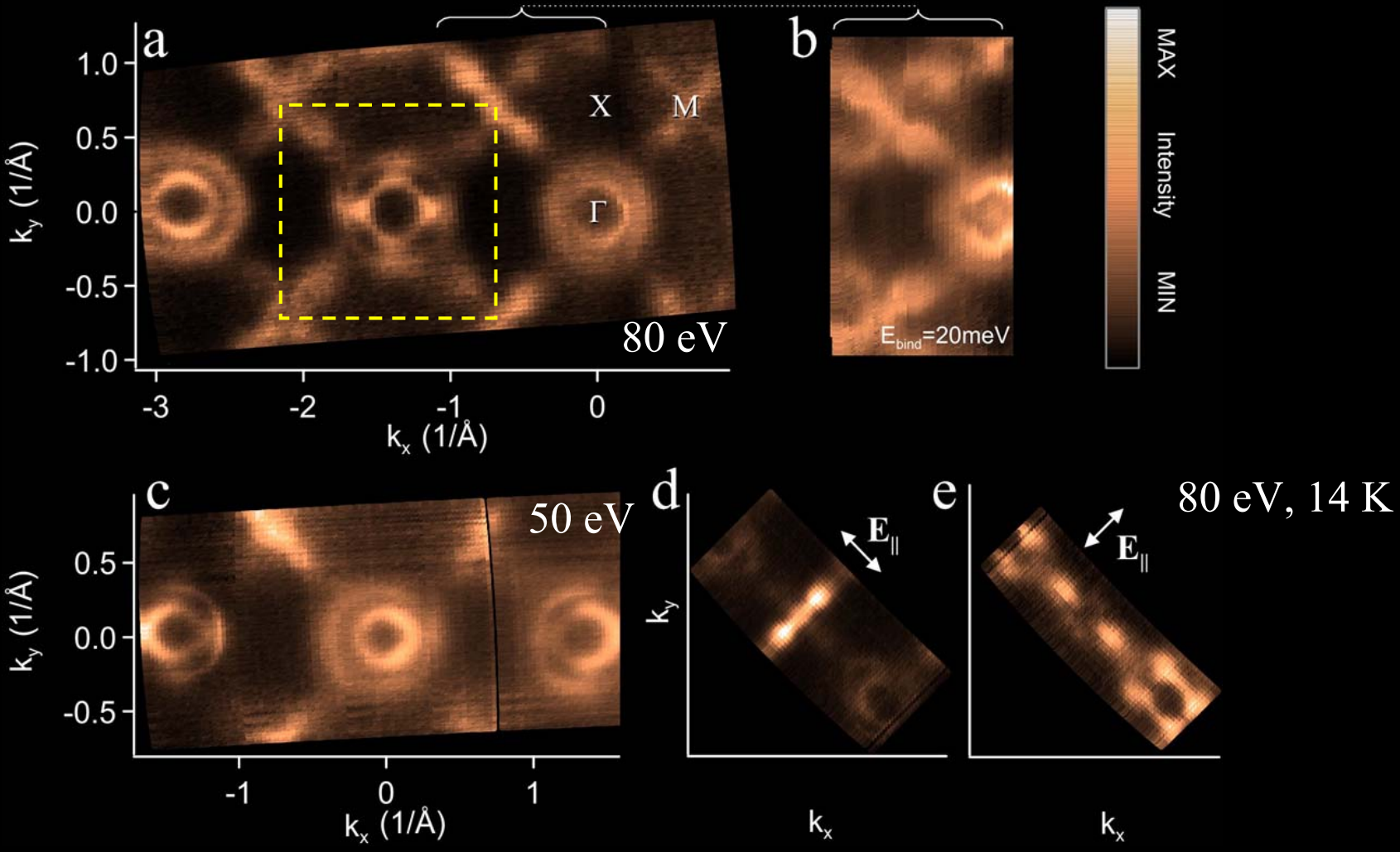




Korshunov & Eremin MPI 2008
Singh arXiv:0803.0429
Mazin arXiv:0803.2740

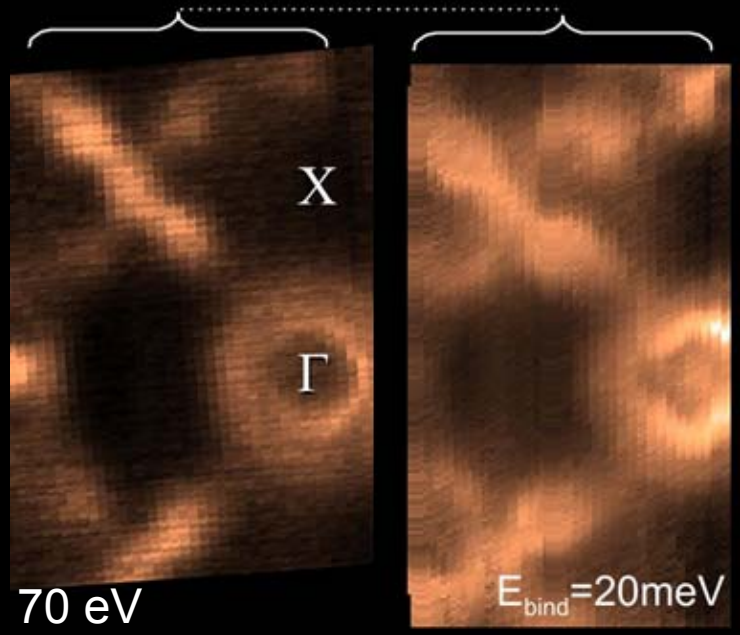
Fermi surface topology

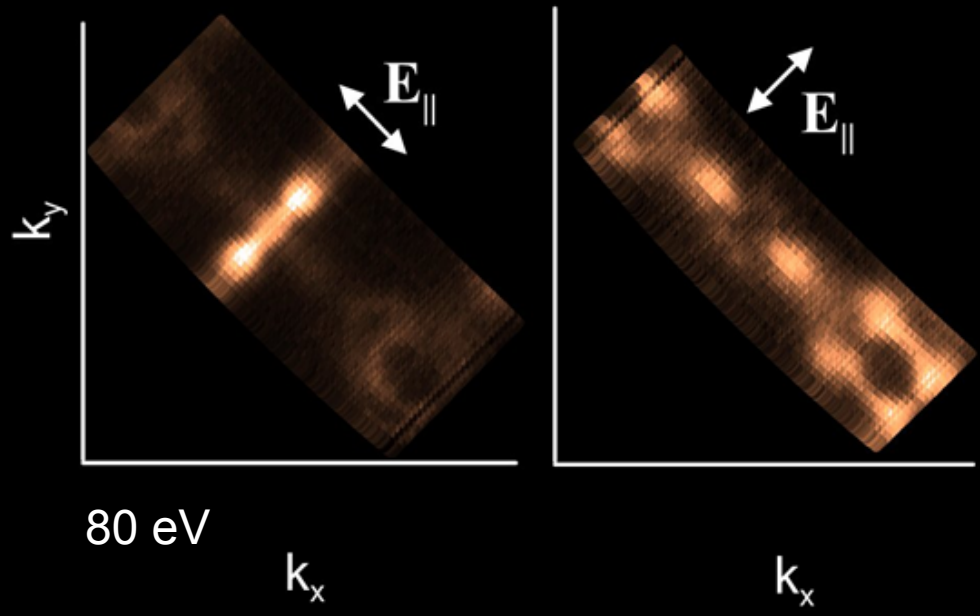
$Ba_{1-x}K_xFe_2As_2$

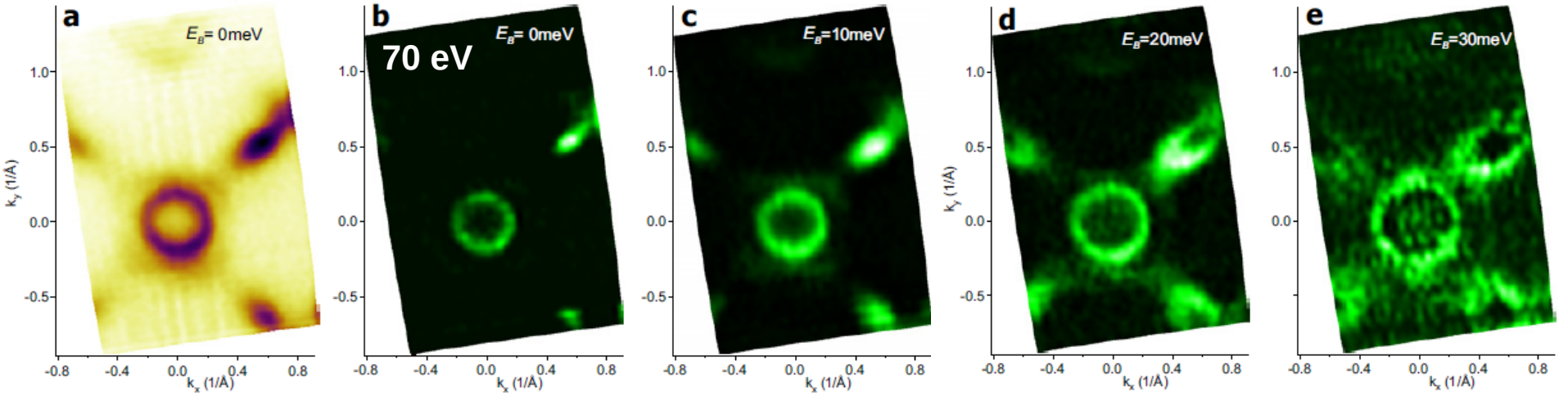


Zabolotnyy *Nature* 2009

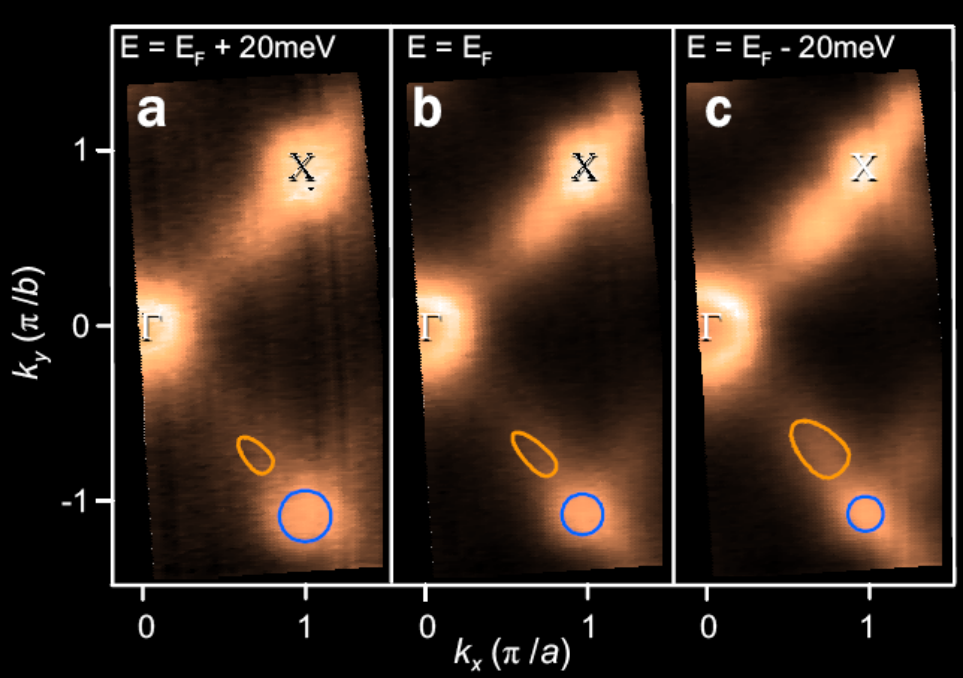
Fermi surface topology

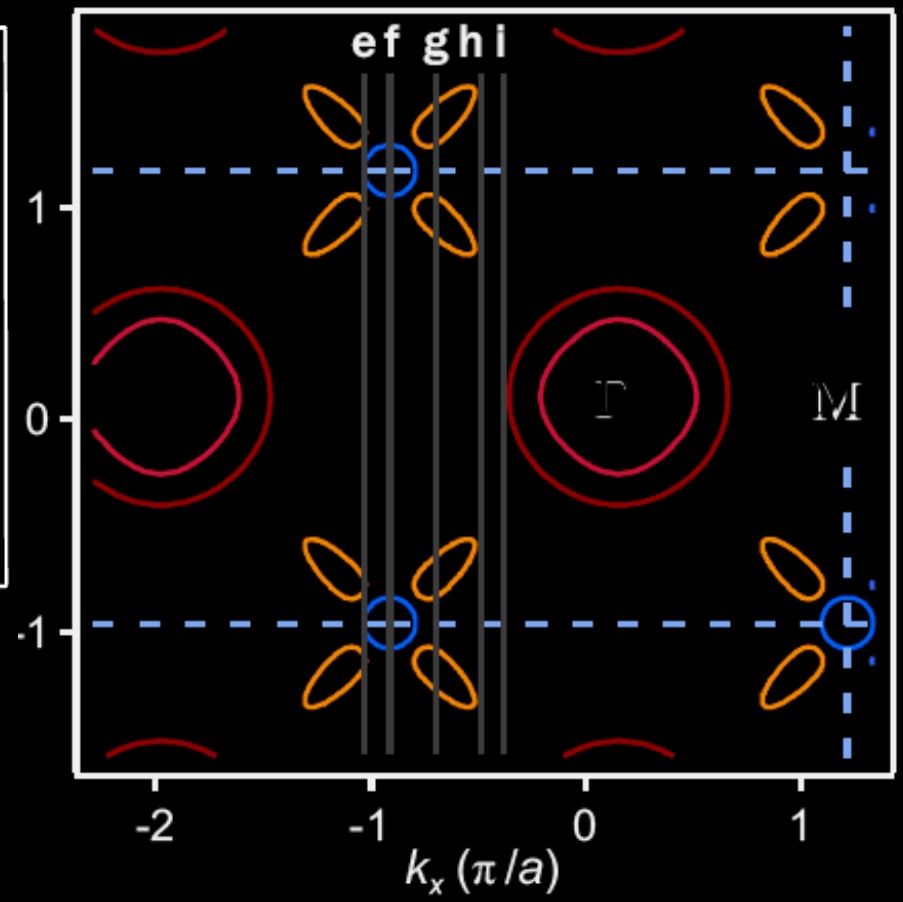






Fermi surface topology





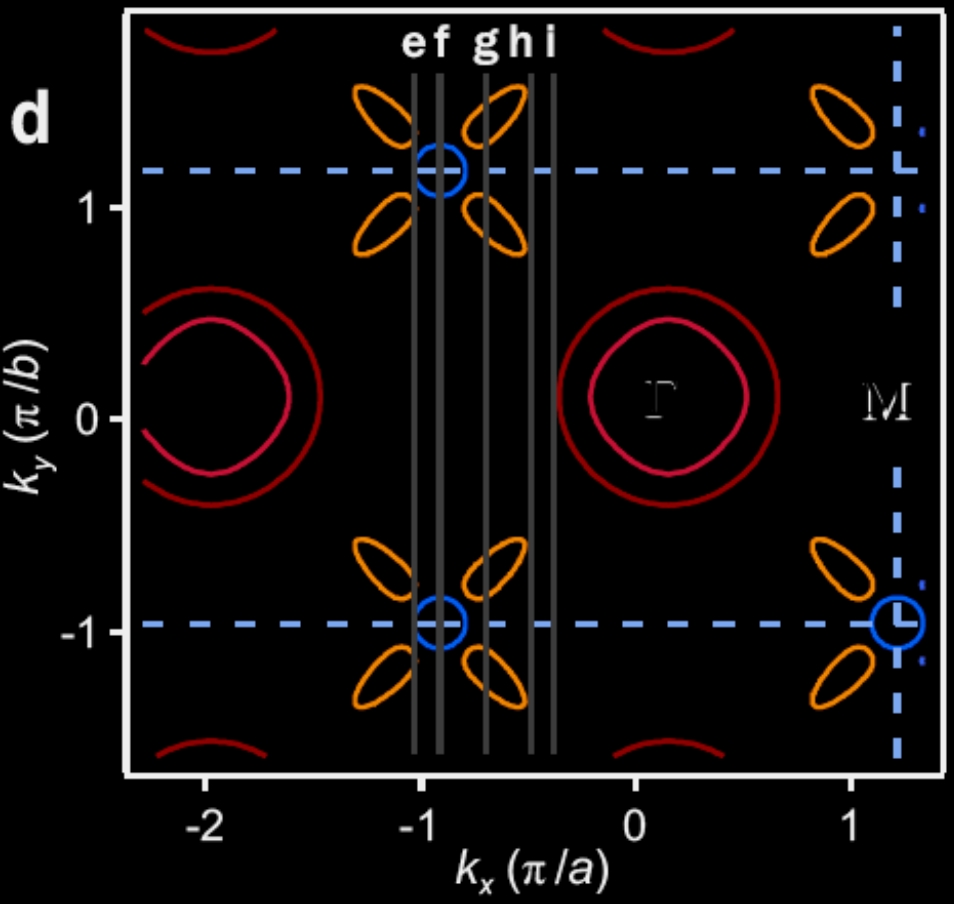
hv = 70 eV
T = 150 K

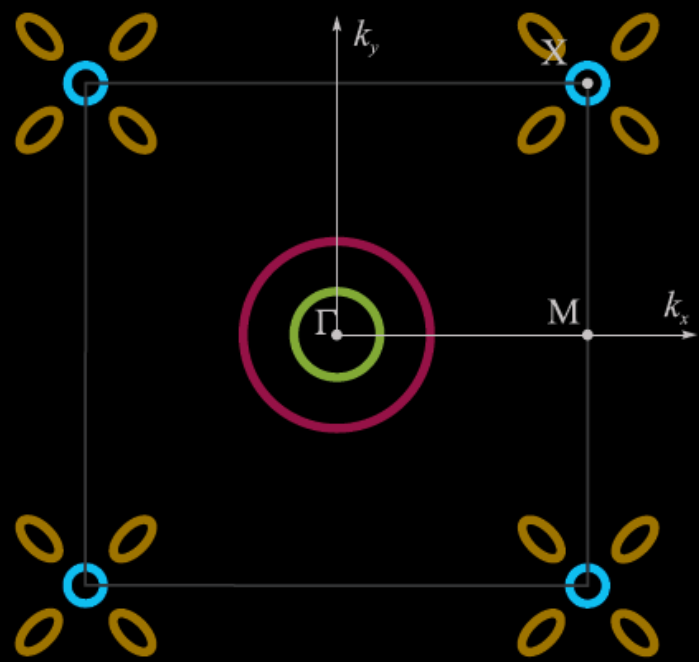
$Ba_{1-x}K_xFe_2As_2$

Zabolotnyy *Nature* 2009

Fermi surface topology

$Ba_{1-x}K_xFe_2As_2$



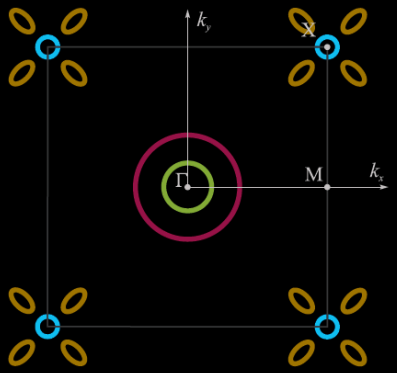


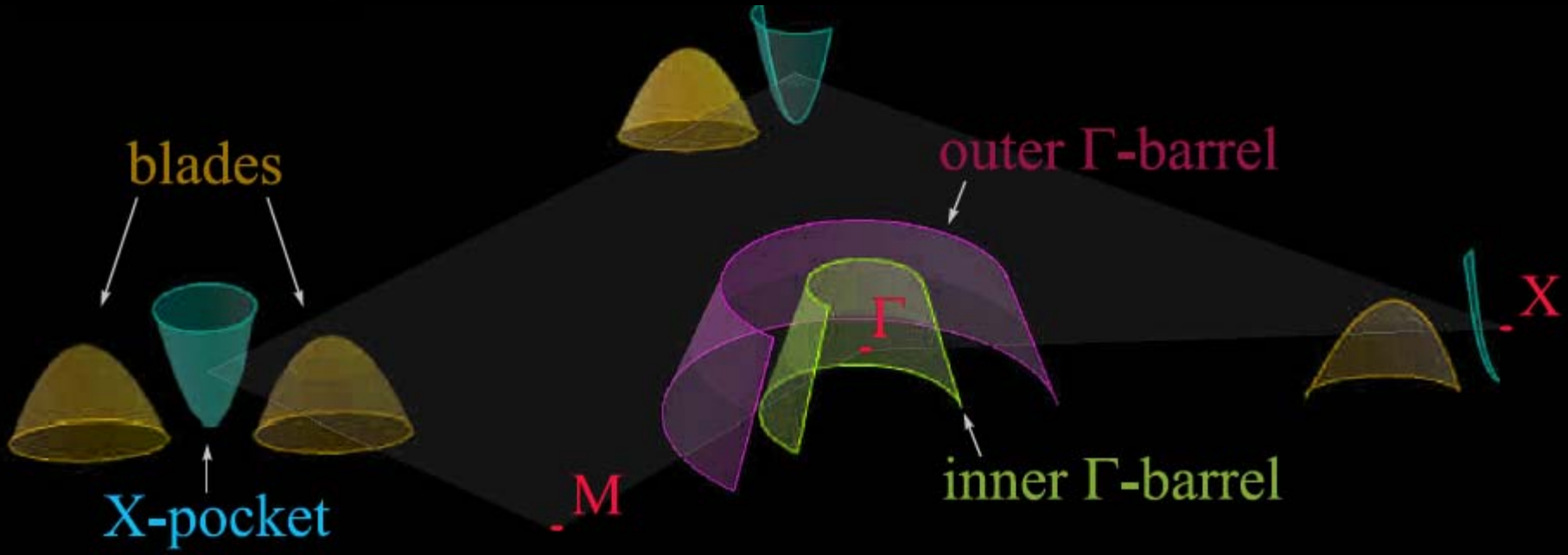
Zabolotnyy *Nature* 2009

Evtushinsky *NJP* 2009

Fermi surface topology

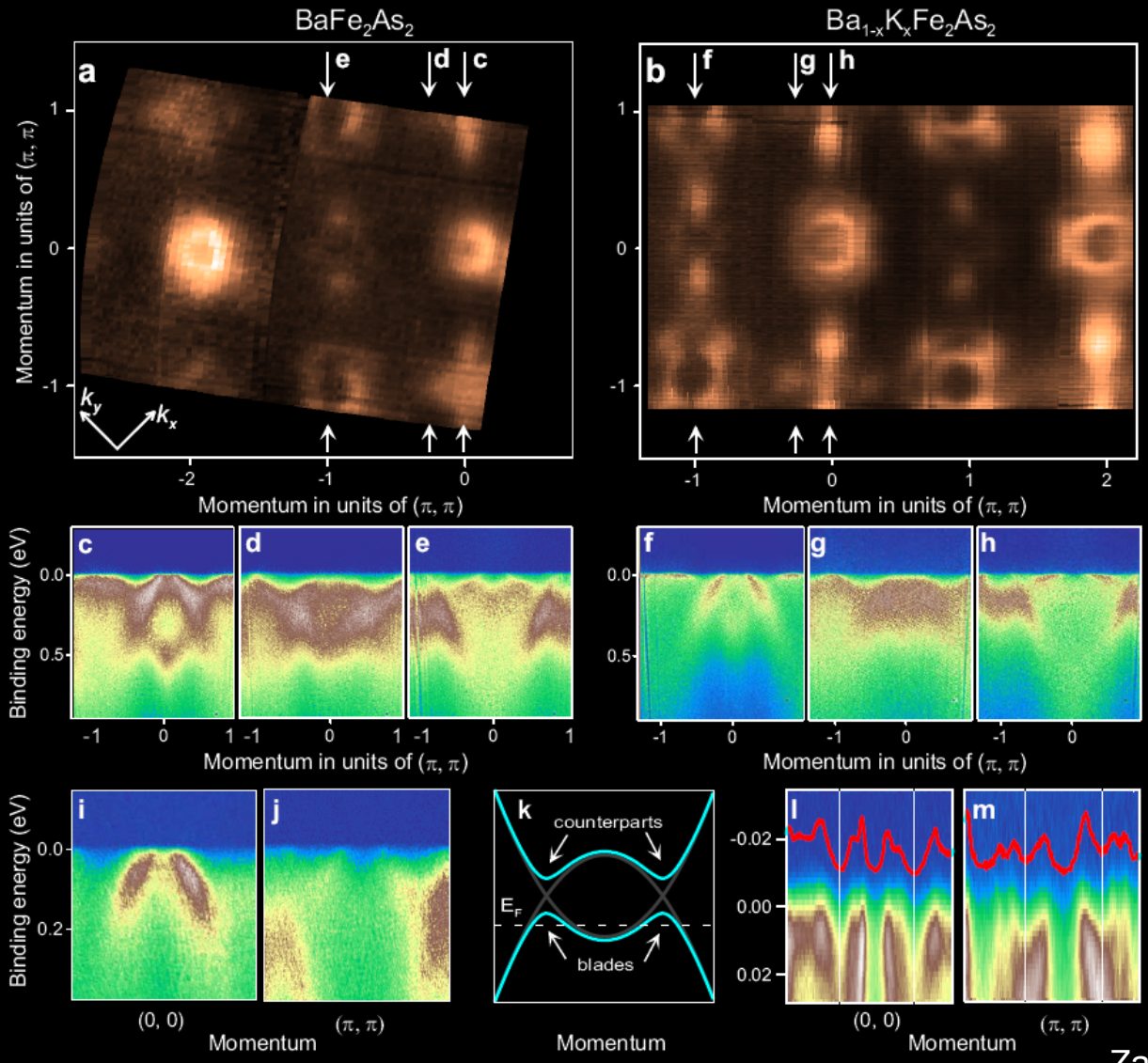
$Ba_{1-x}K_xFe_2As_2$





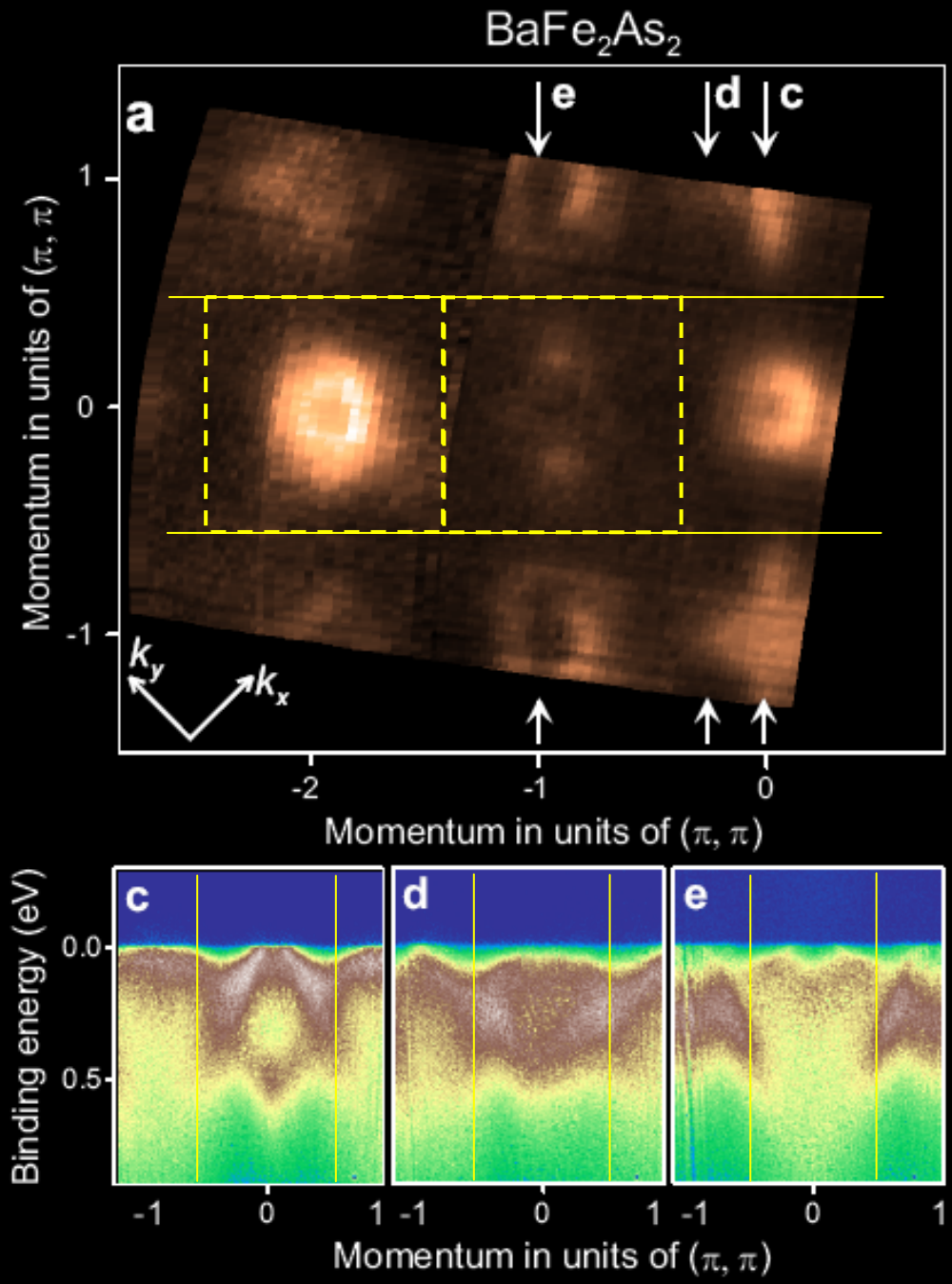
Evtushinsky *NJP* 2009

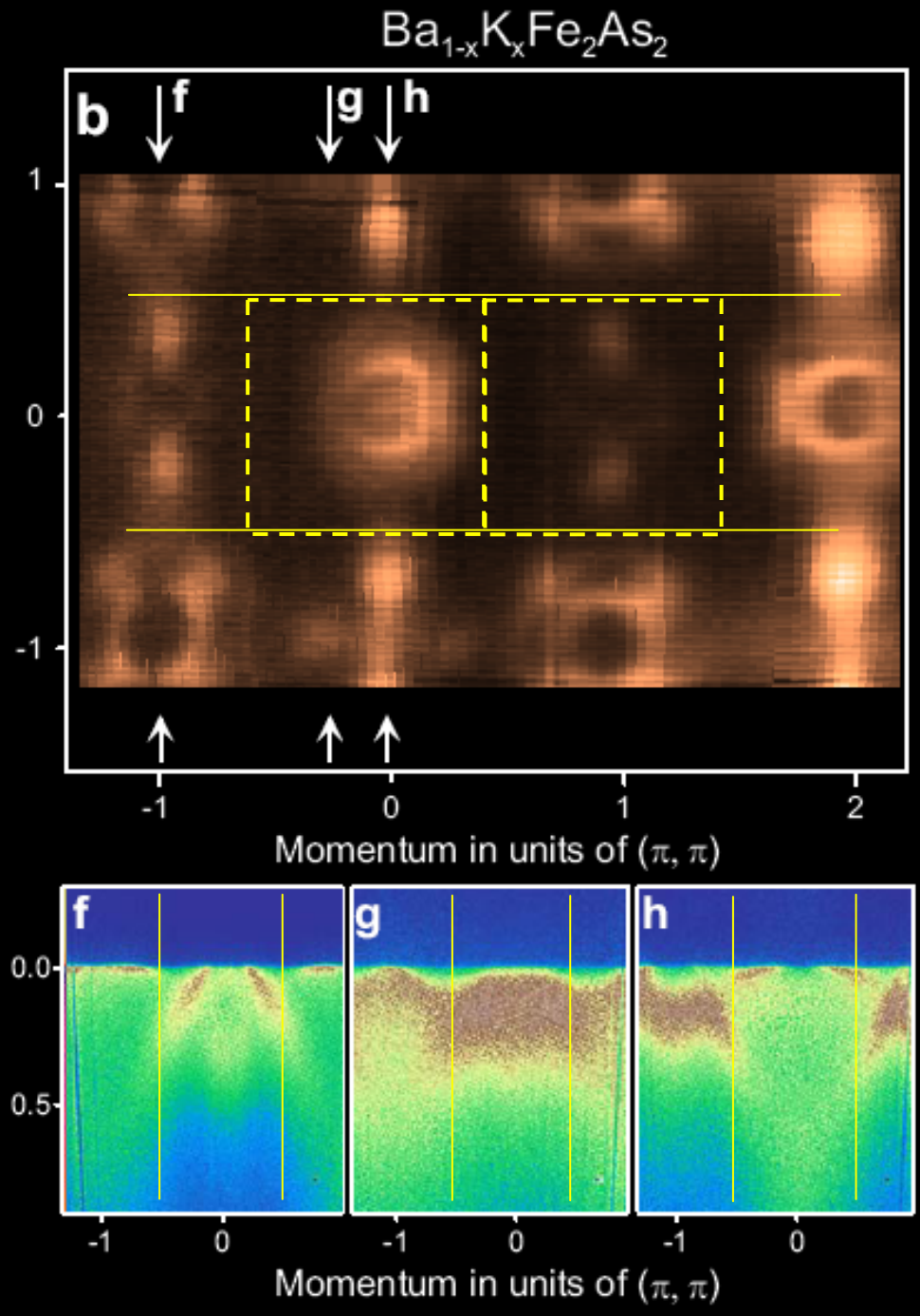
(π, π) electronic order

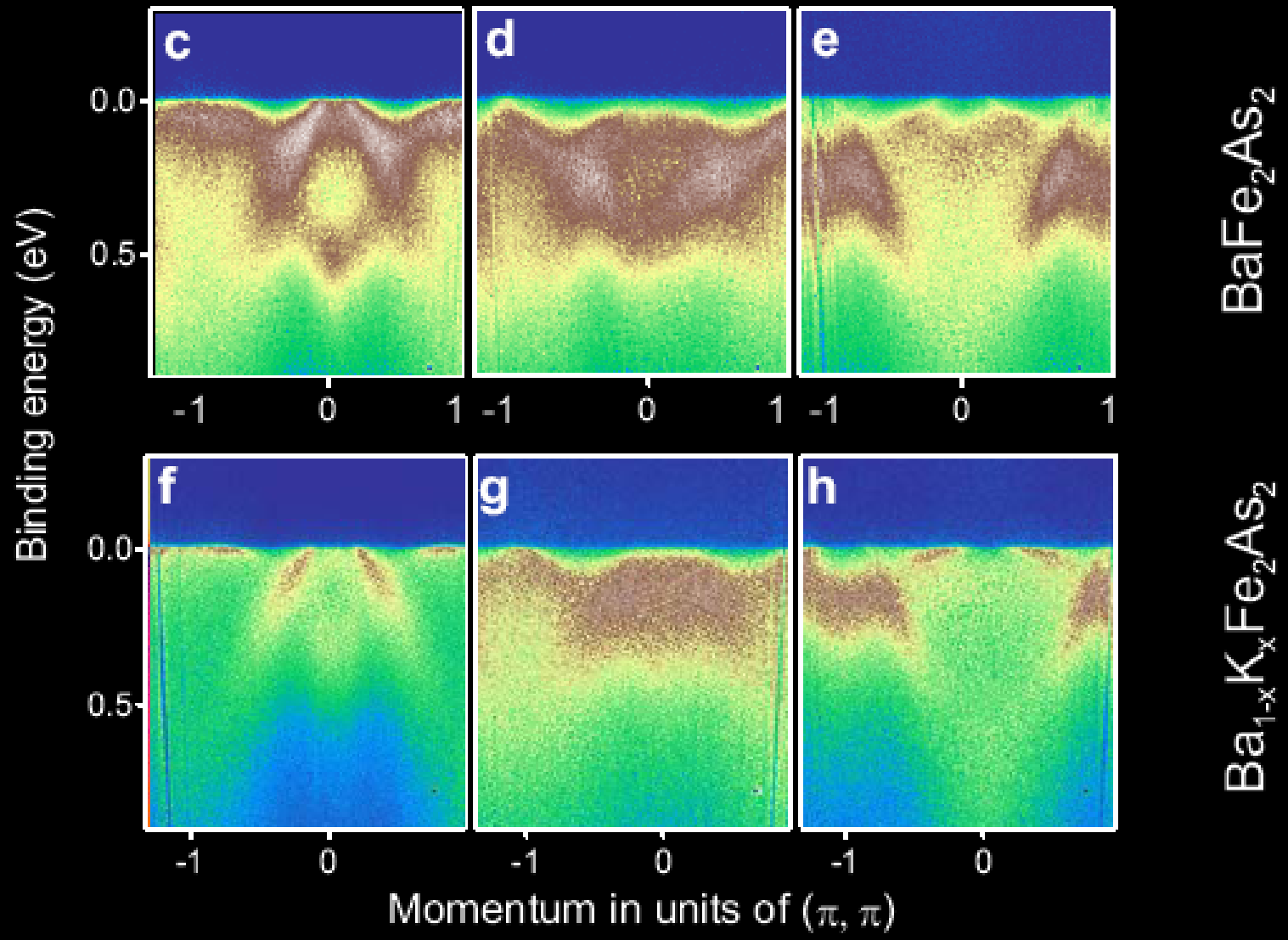


$h\nu = 80$ eV

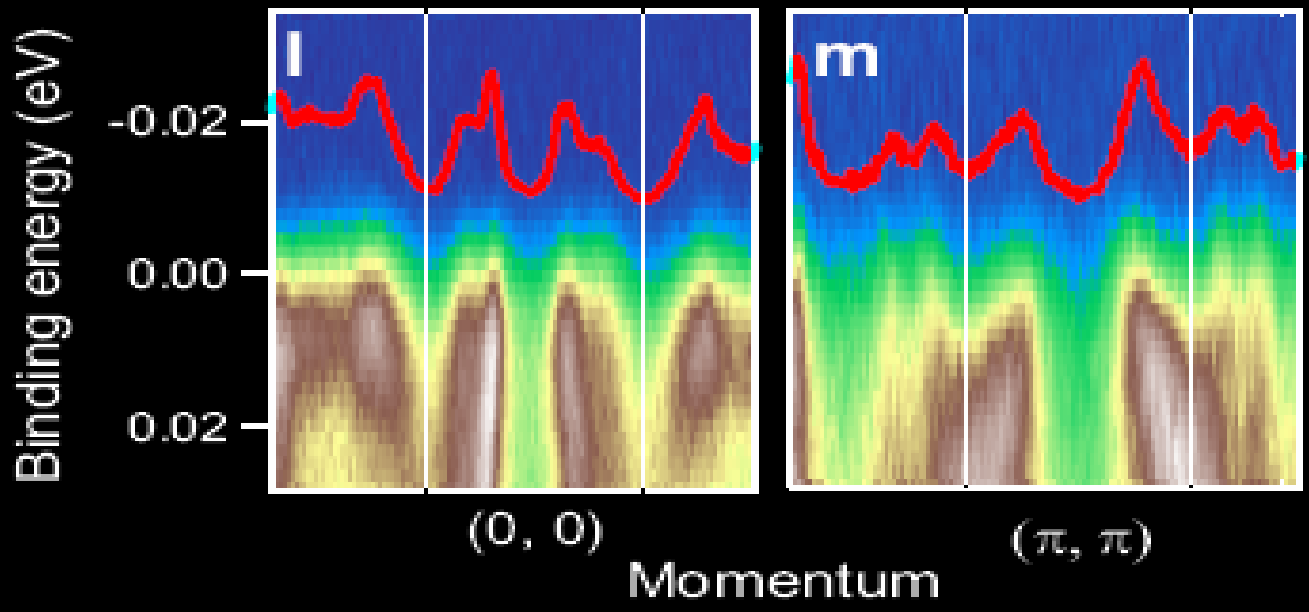
Zabolotnyy *Nature* 2009


BaFe2As2
a
e
d
c
1
0
-1
Momentum in units of (π, π)
ky
kx
-2
-1
0
Momentum in units of (π, π)
c
d
e
Binding energy (eV)
0.0
0.5
-1
0
1
-1
0
1
-1
0
1
Momentum in units of (π, π)

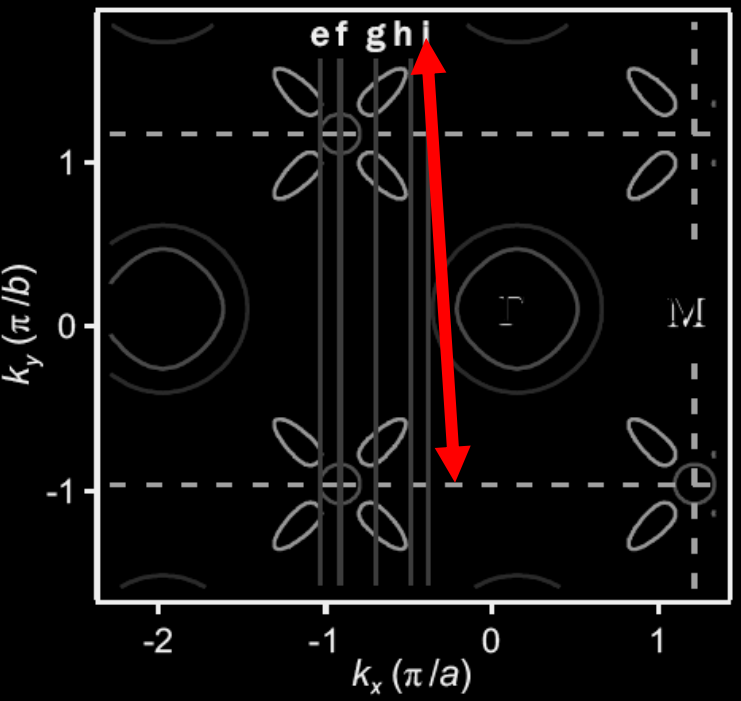

Ba1-xKxFe2As2
b
f
g
h
1
0
-1
-1
0
1
2
Momentum in units of (π, π)
f
g
h
0.0
0.5
-1
0
-1
0
-1
0
Momentum in units of (π, π)

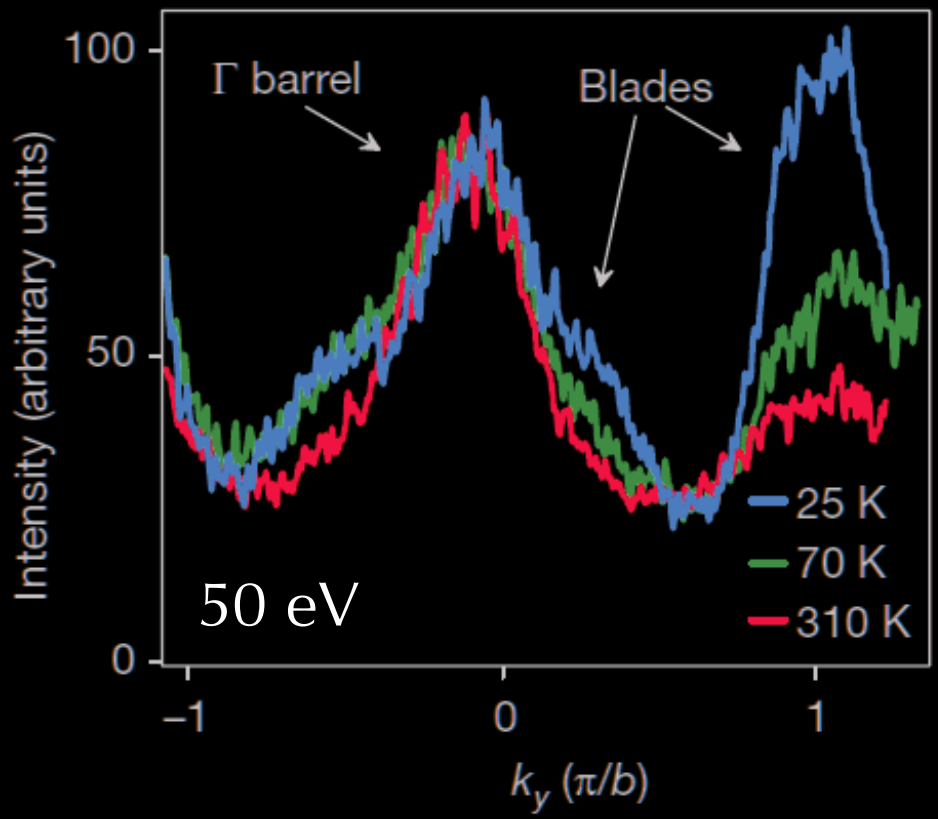

c
d
e
f
g
h
0.0
0.5
Binding energy (eV)
-1
0
1
Momentum in units of (π, π)
BaFe2As2
Ba1-xKxFe2As2

$Ba_{1-x}K_xFe_2As_2$



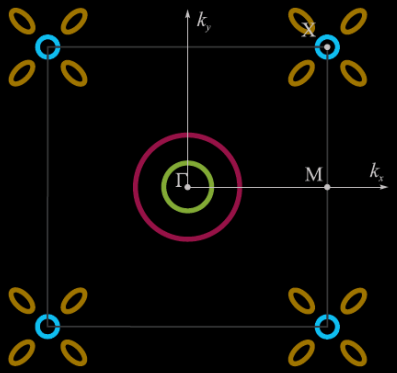
(π, π) electronic order: *T*- dependence

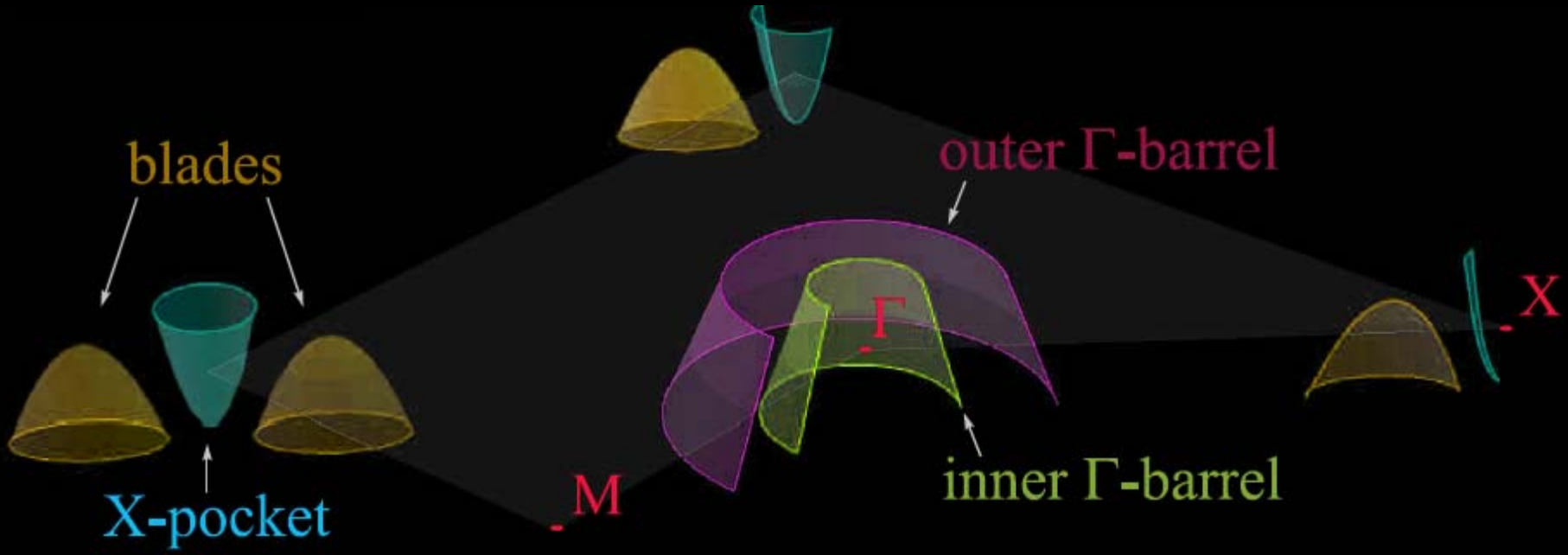




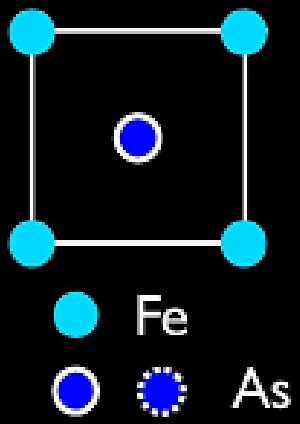
Fermi surface topology

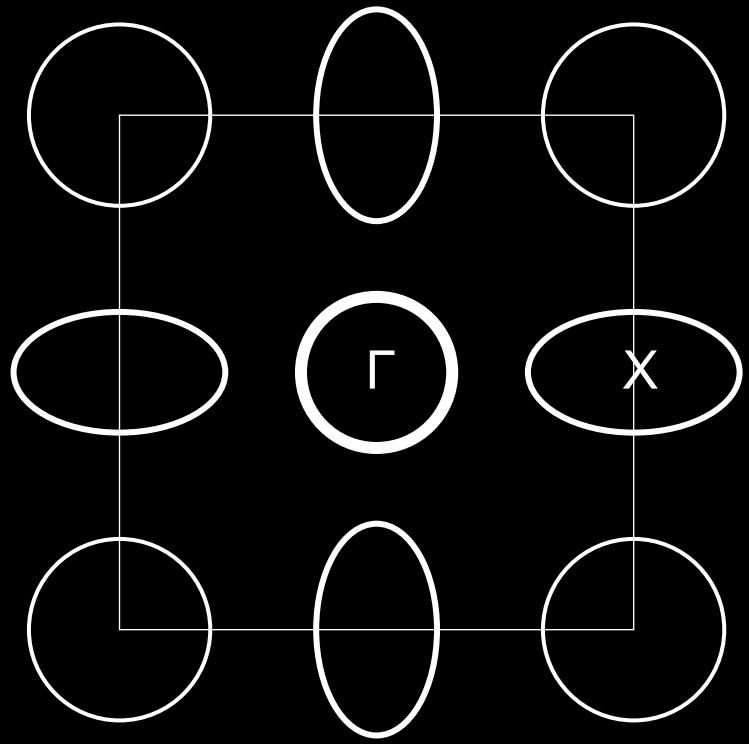
$Ba_{1-x}K_xFe_2As_2$

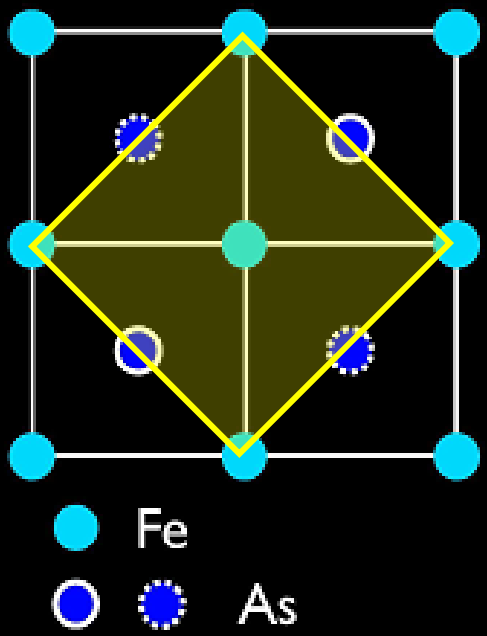


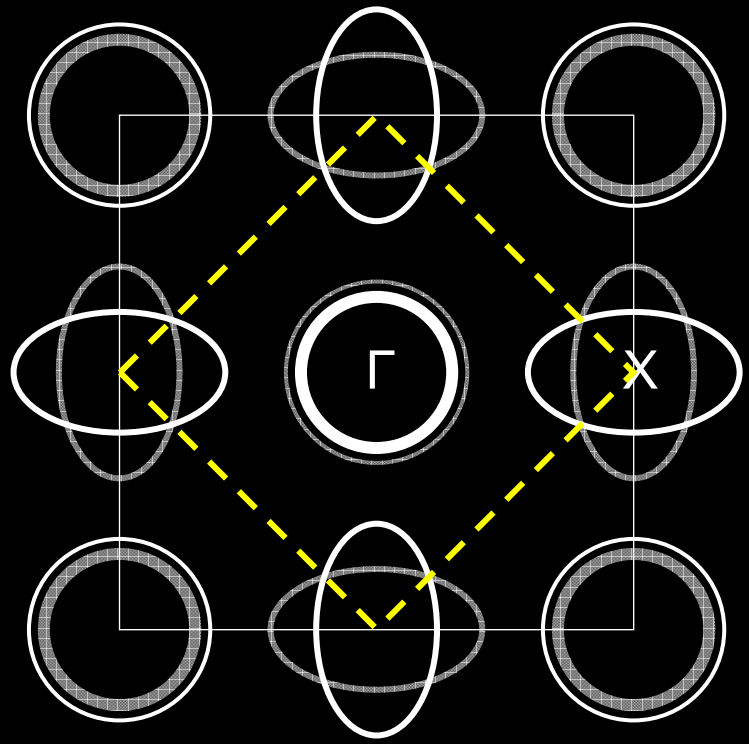


Evtushinsky *NJP* 2009

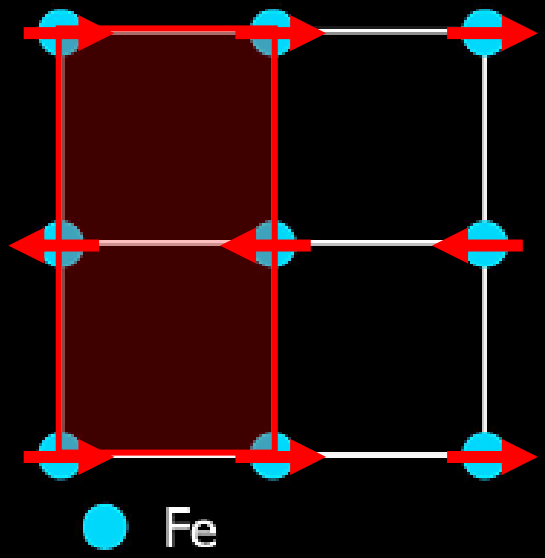

Fe
As

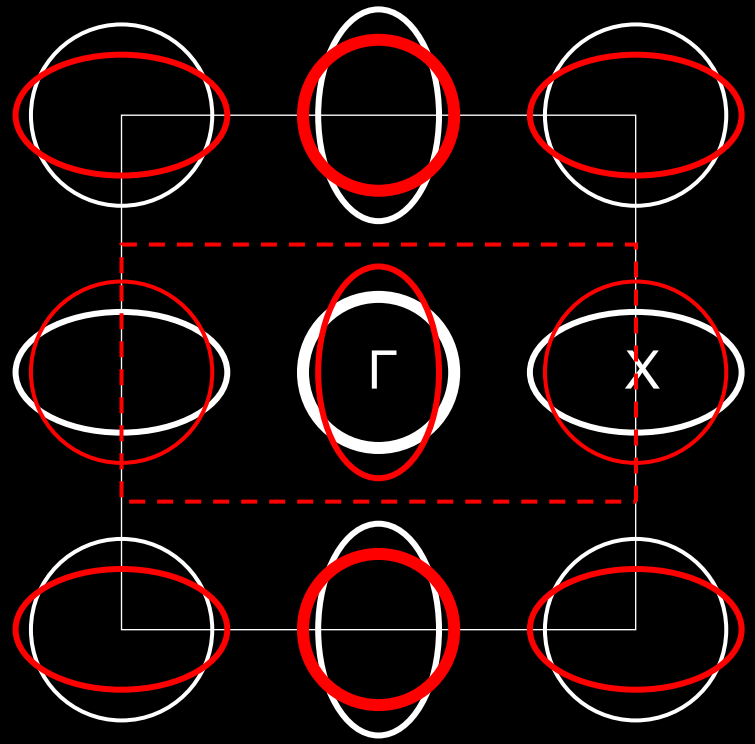

Γ
X



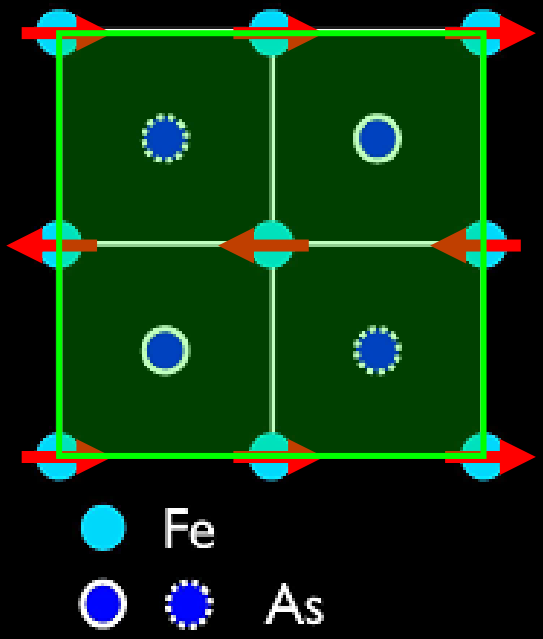


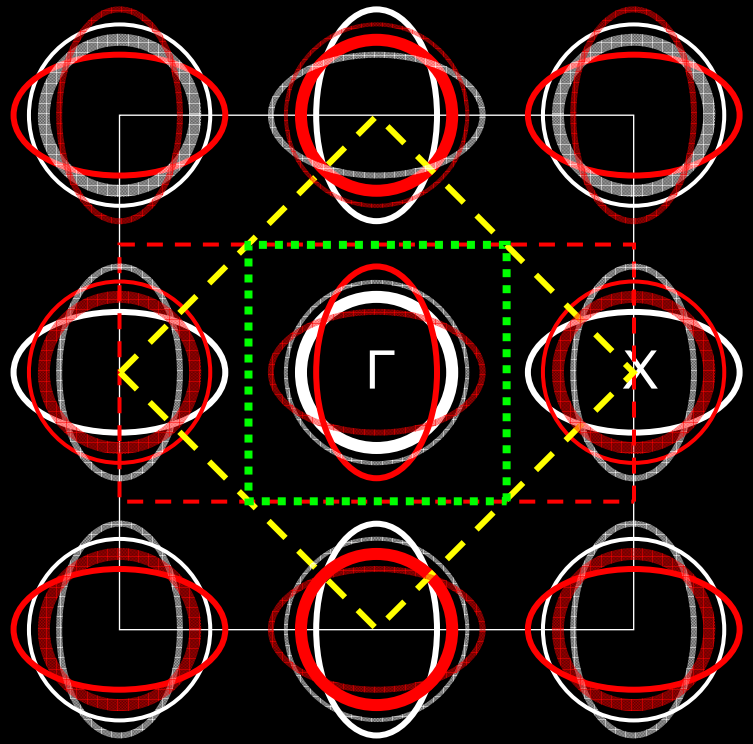
Fe BZ: (π, π)

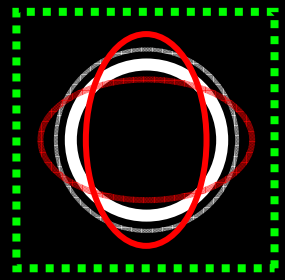




Fe BZ: $(0, \pi)$

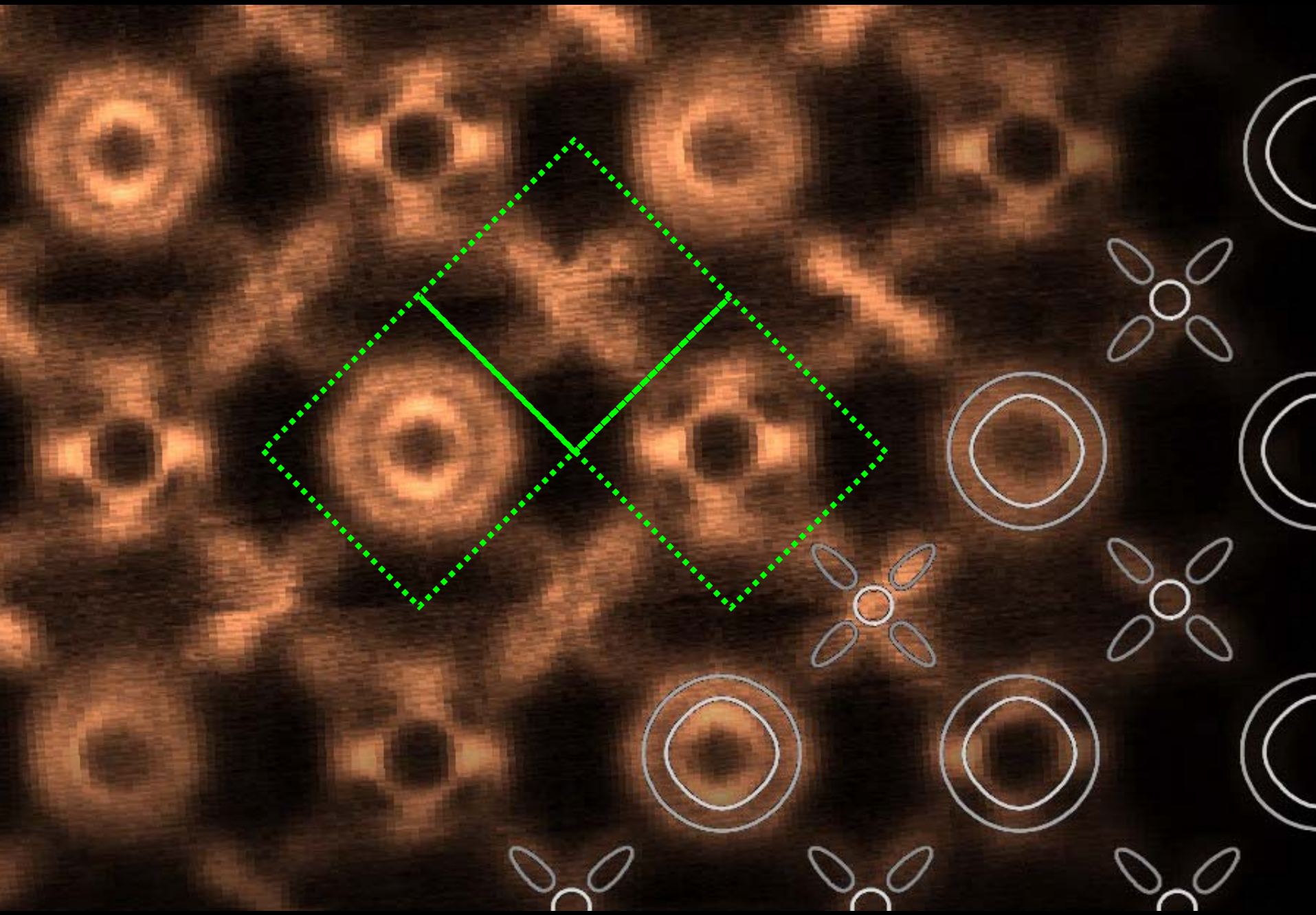


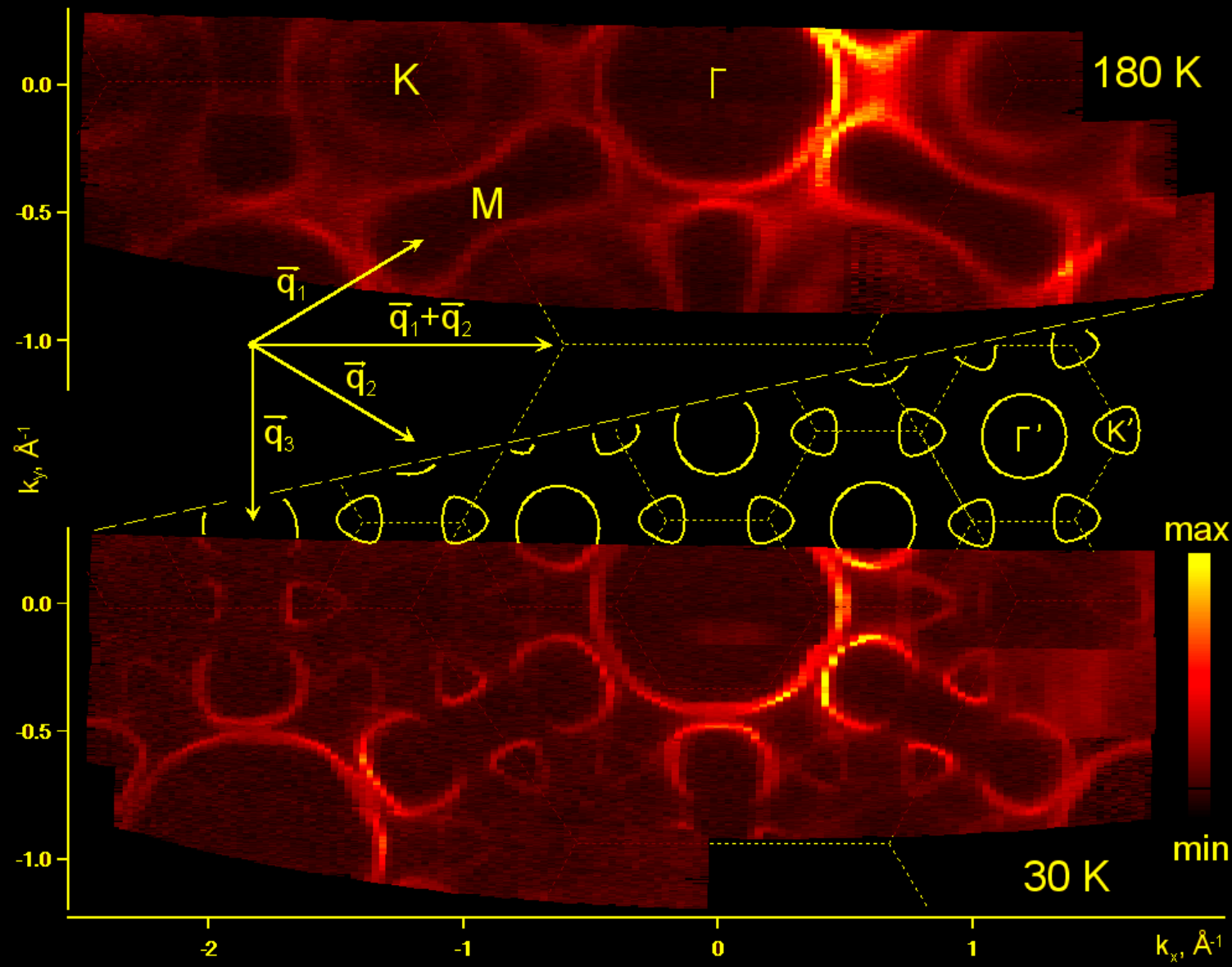


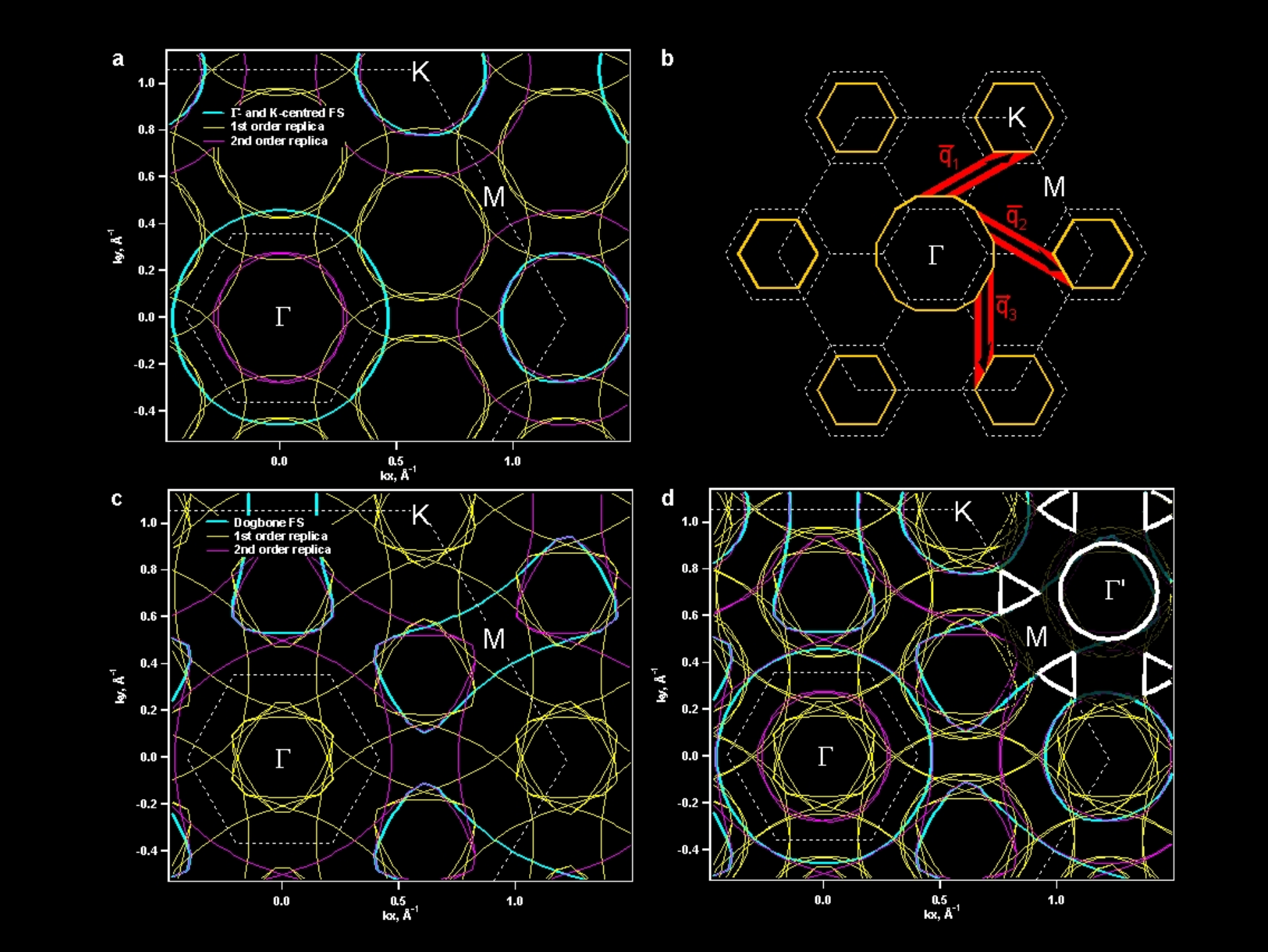


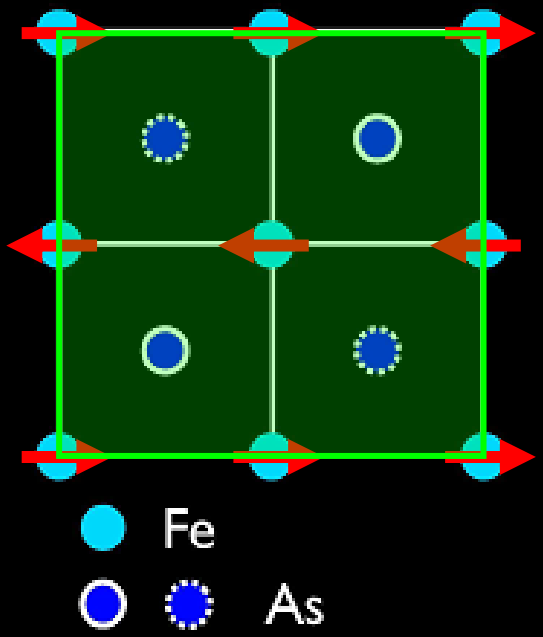
Fe BZ: $(0, \pi) + (\pi, \pi)$

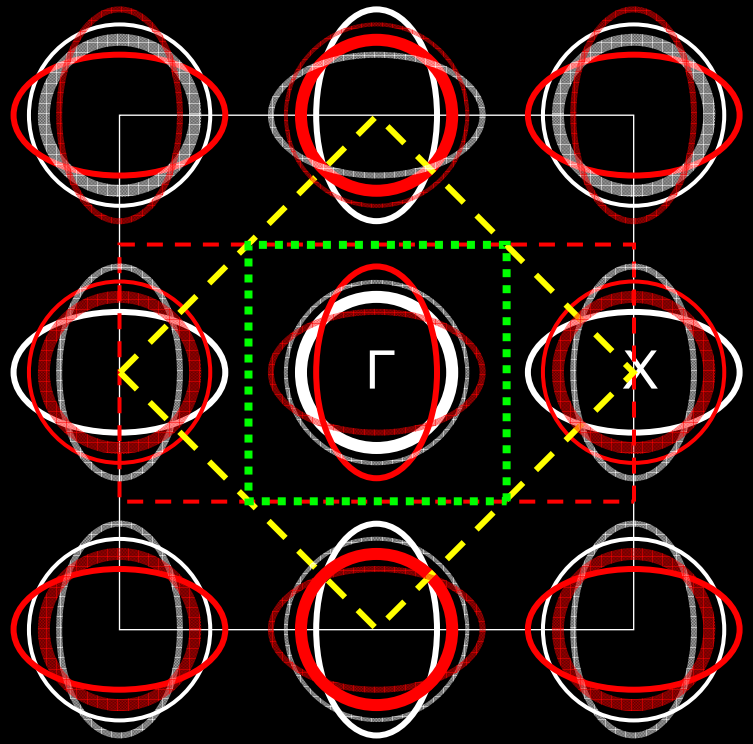
$= (\pi, \pi)$ in As BZ

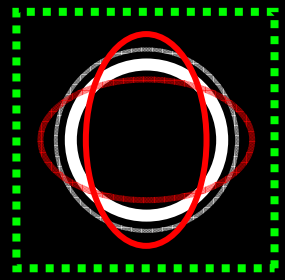



K
Γ
M
180 K
$\bar{q}_1$
$\bar{q}_1+\bar{q}_2$
$\bar{q}_2$
$\bar{q}_3$
Γ'
K'
max
min
30 K
0.0
-0.5
-1.0
k_y, Å^{-1}
-2
-1
0
1
k_x, Å^{-1}


a
K
M
Γ
Γ- and K-centred FS
1st order replica
2nd order replica
ky, Å-1
kx, Å-1
b
K
M
Γ
q1
q2
q3
c
K
M
Γ
Dogbone FS
1st order replica
2nd order replica
ky, Å-1
kx, Å-1
d
K
M
Γ
Γ'
ky, Å-1
kx, Å-1

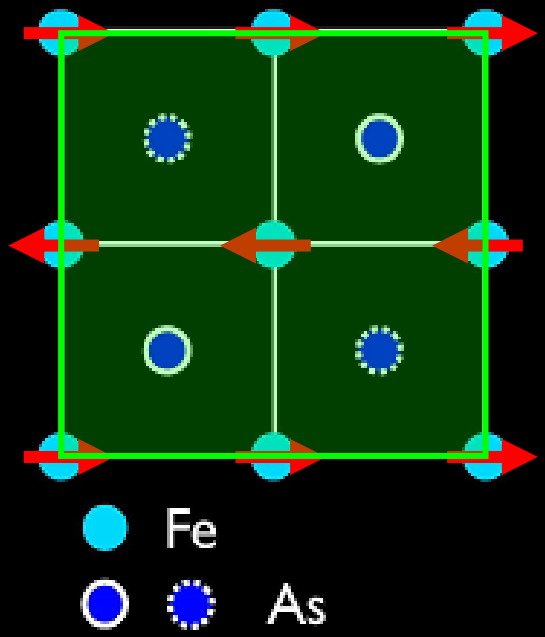


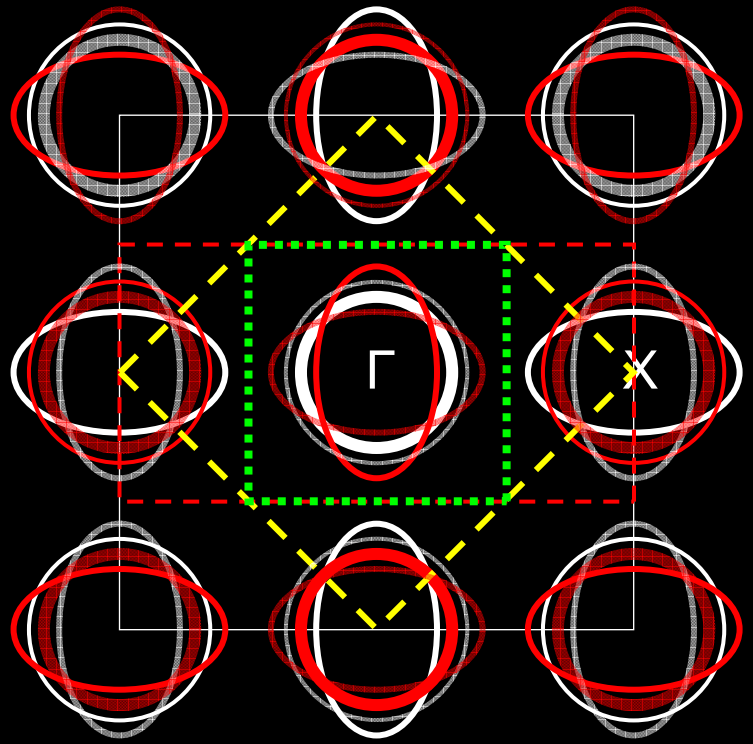


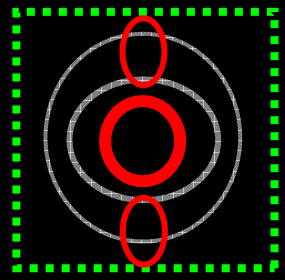


Fe BZ: $(0, \pi) + (\pi, \pi)$

$= (\pi, \pi)$ in As BZ



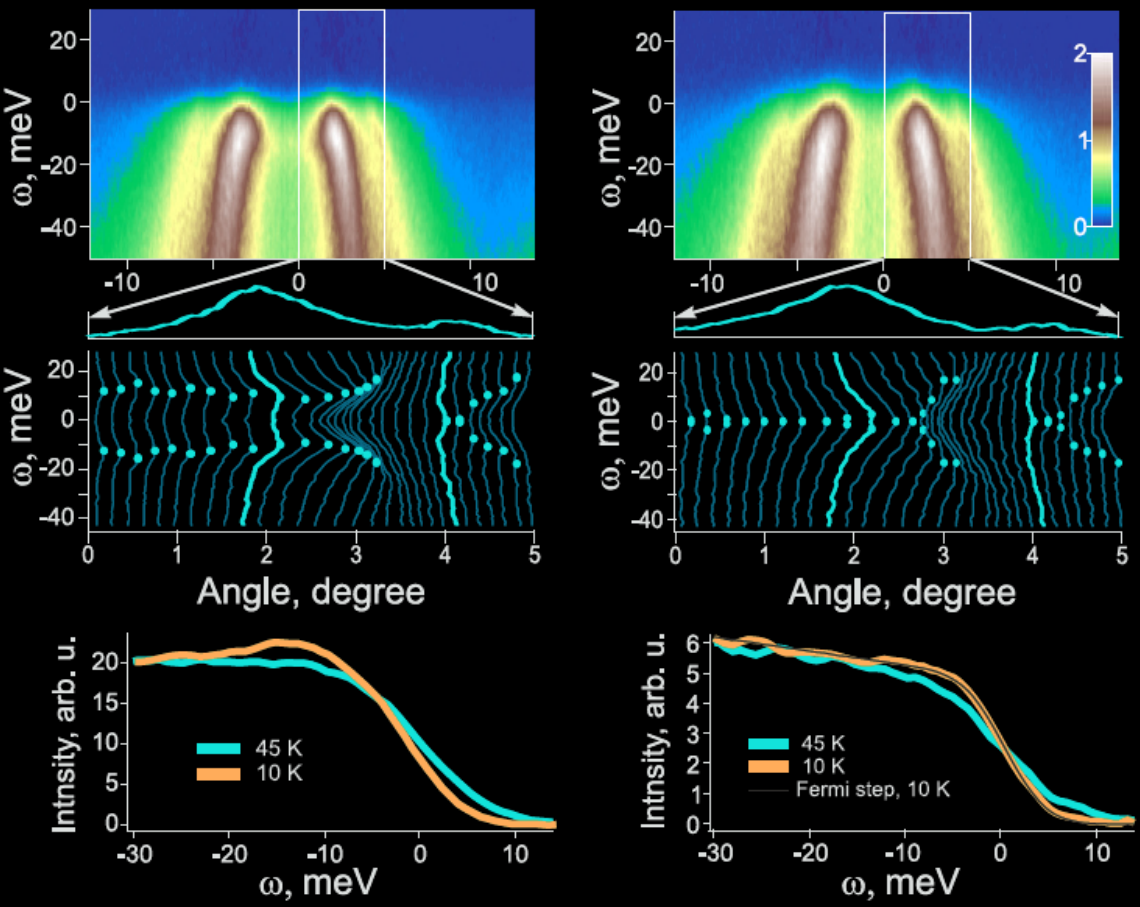


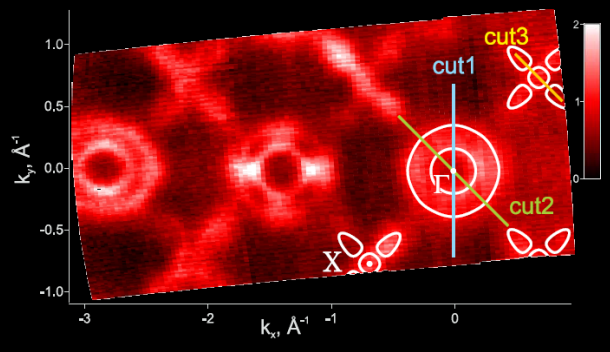


Fe BZ: $(0, \pi) + (\pi, \pi)$

$= (\pi, \pi)$ in As BZ

Superconducting gap in BKFA





Gap values (meV)

Inner Γ-barrel	9 ± 1
Outer Γ-barrel	<4
X-pocket	9 ± 2
Blades	~ 9
Gap anisotropy	<1.5

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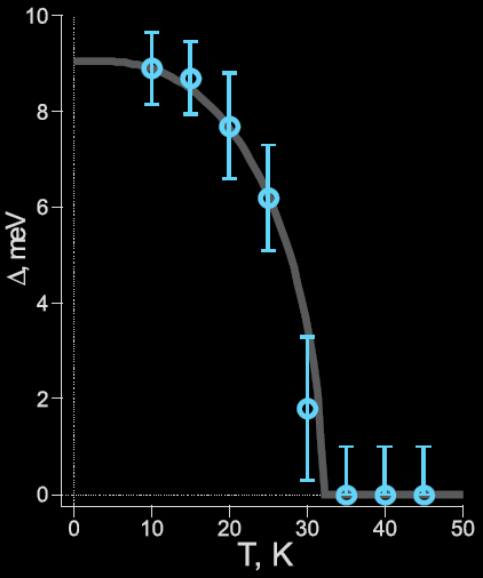
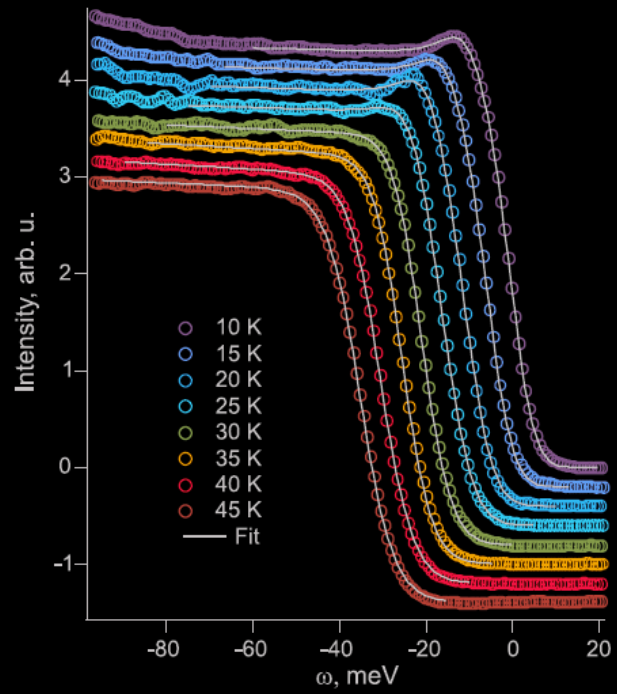
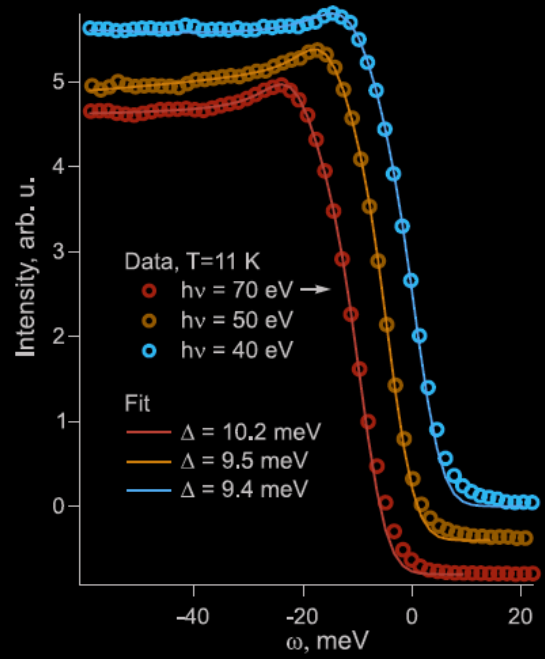
Superconducting gap in BKFA







$$\mathrm{IEDC}(\omega) = \left[f(\omega, T) \cdot \left| \mathrm{Re} \frac{\omega - i\Sigma''}{E} \right| \right] \otimes R_\omega(\delta E)$$

$$E = \sqrt{(\omega - i\Sigma'')^2 - \Delta_k^2}$$

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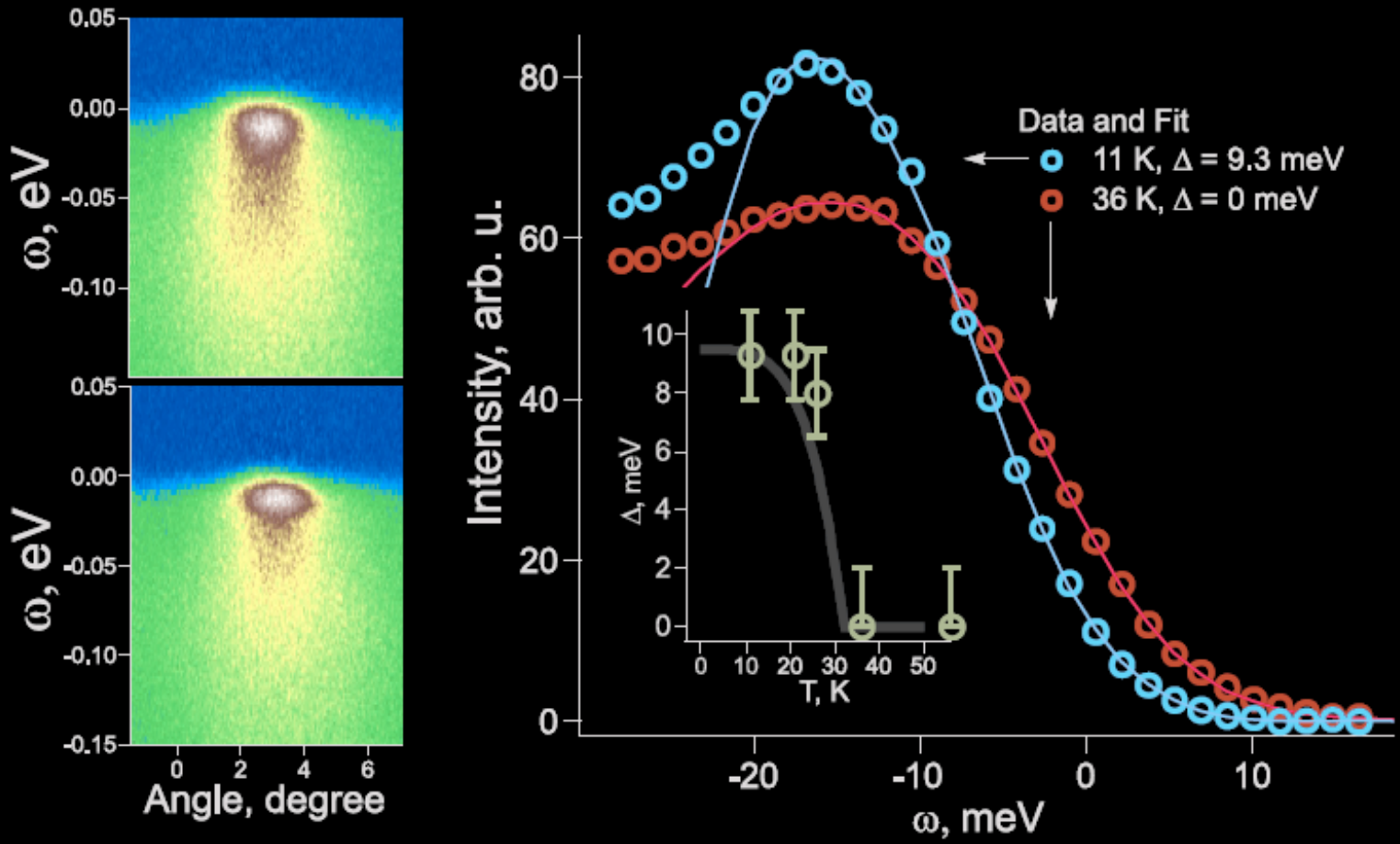
Superconducting gap in BKFA



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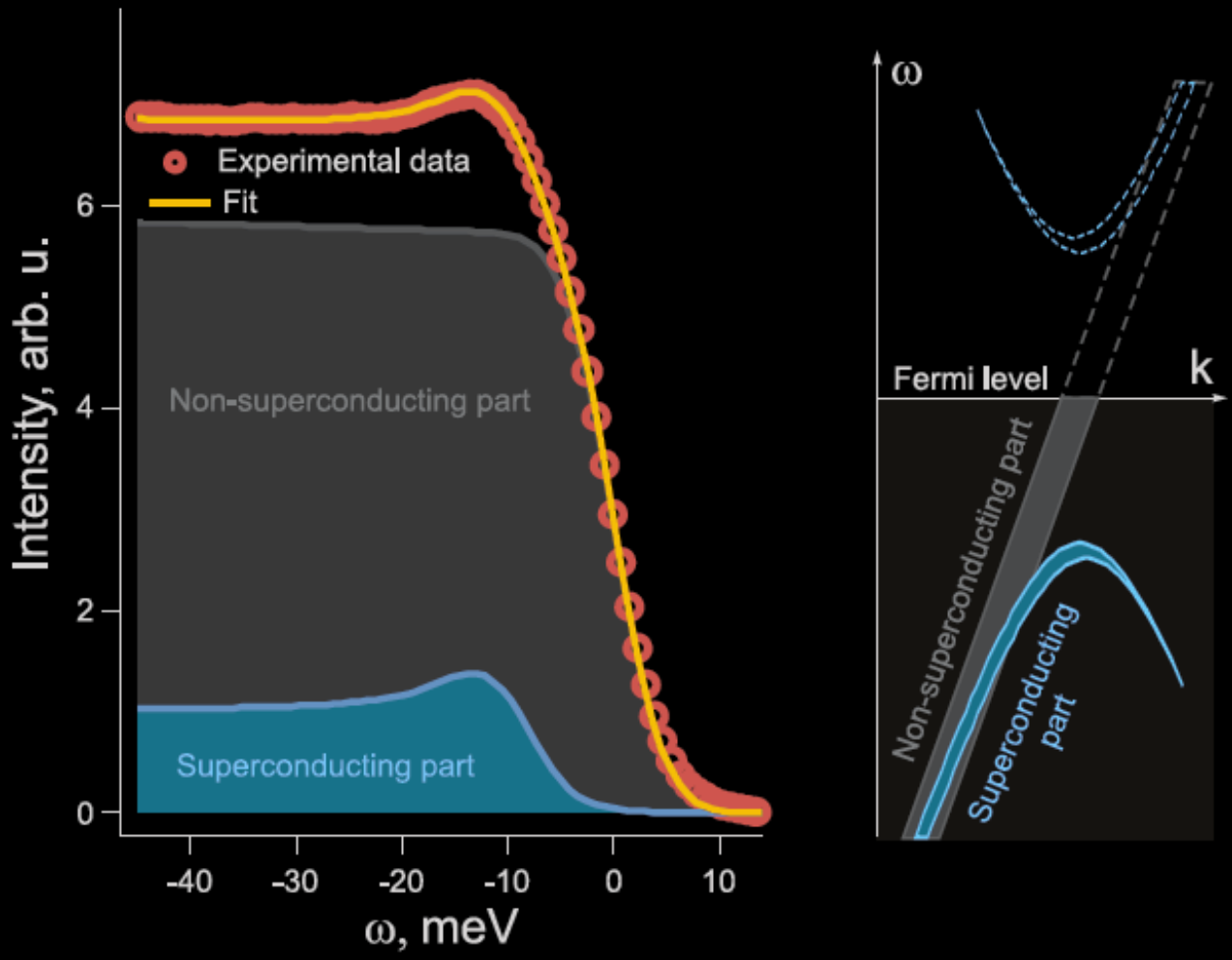
Superconducting gap in BKFA



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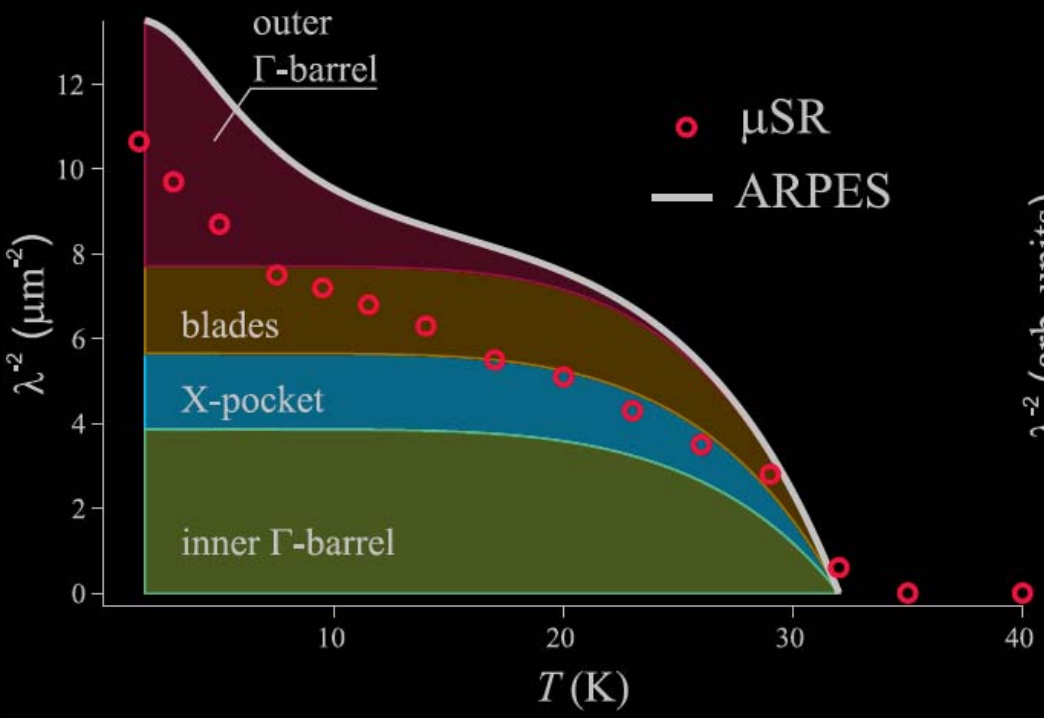
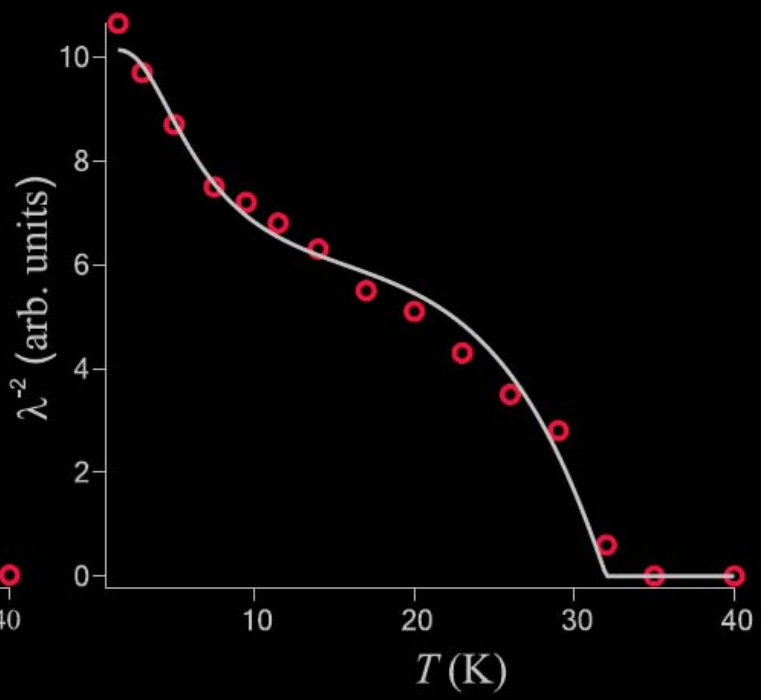
Evtushinsky *PRB* 2009

Superconducting gap from ARPES & μSR

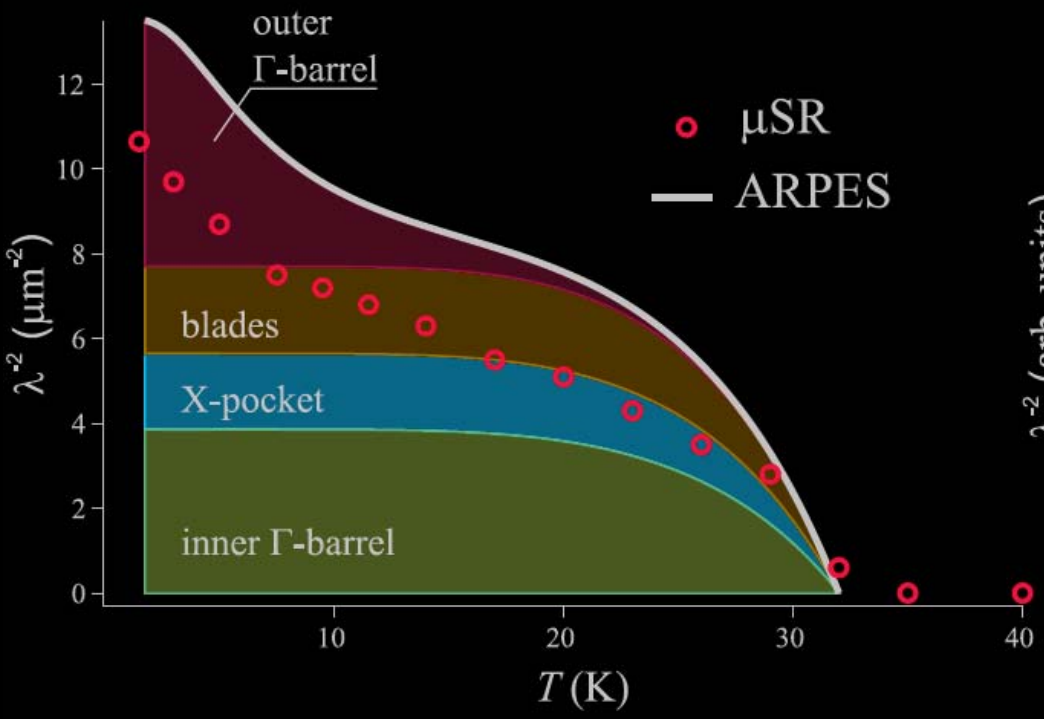


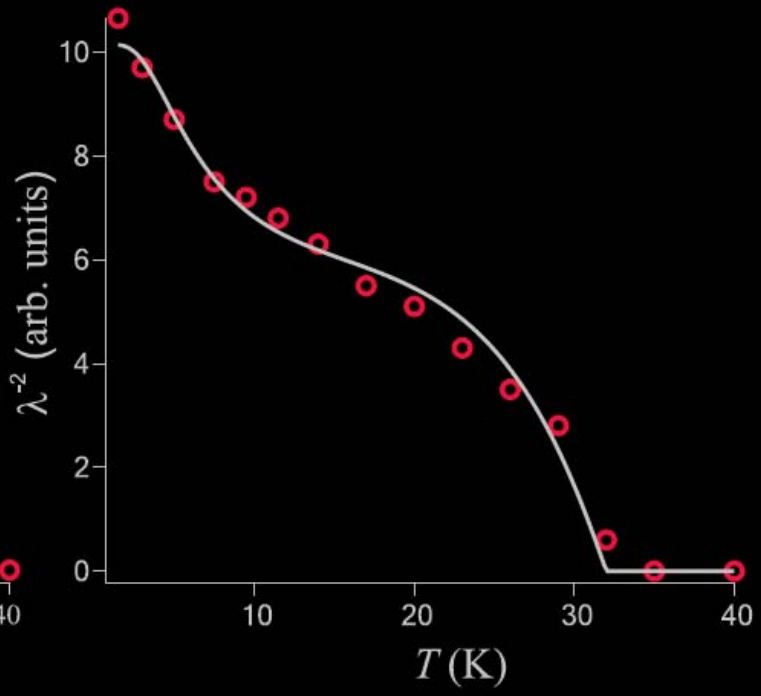


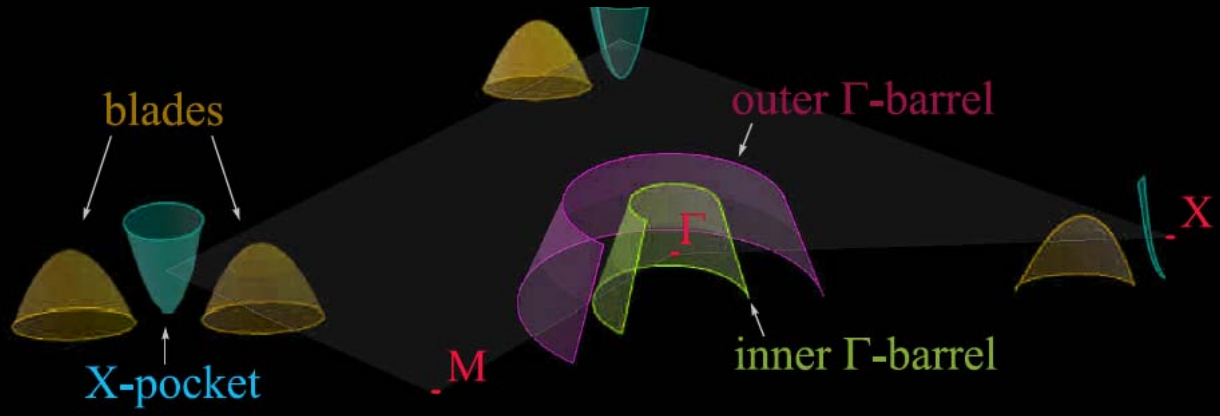
$$\frac{1}{\lambda^2(T)} = \frac{e^2}{2\pi\varepsilon_0 c^2 h L_c} \cdot \int_{\mathrm{FS}} v_{\mathrm{F}}(\mathbf{k}) \left[1 - \int_{-\infty}^{+\infty} \left(-\frac{\partial f_T(\omega)}{\partial \omega} \right) \left| \mathrm{Re} \frac{\omega + i\Sigma''}{\sqrt{(\omega + i\Sigma'')^2 - \Delta_{\mathbf{k}}^2(T)}} \right| \mathrm{d}\,\omega \right] \mathrm{d}\,k$$

Evtushinsky *NJP* 2009

Superconducting gap from ARPES & μSR

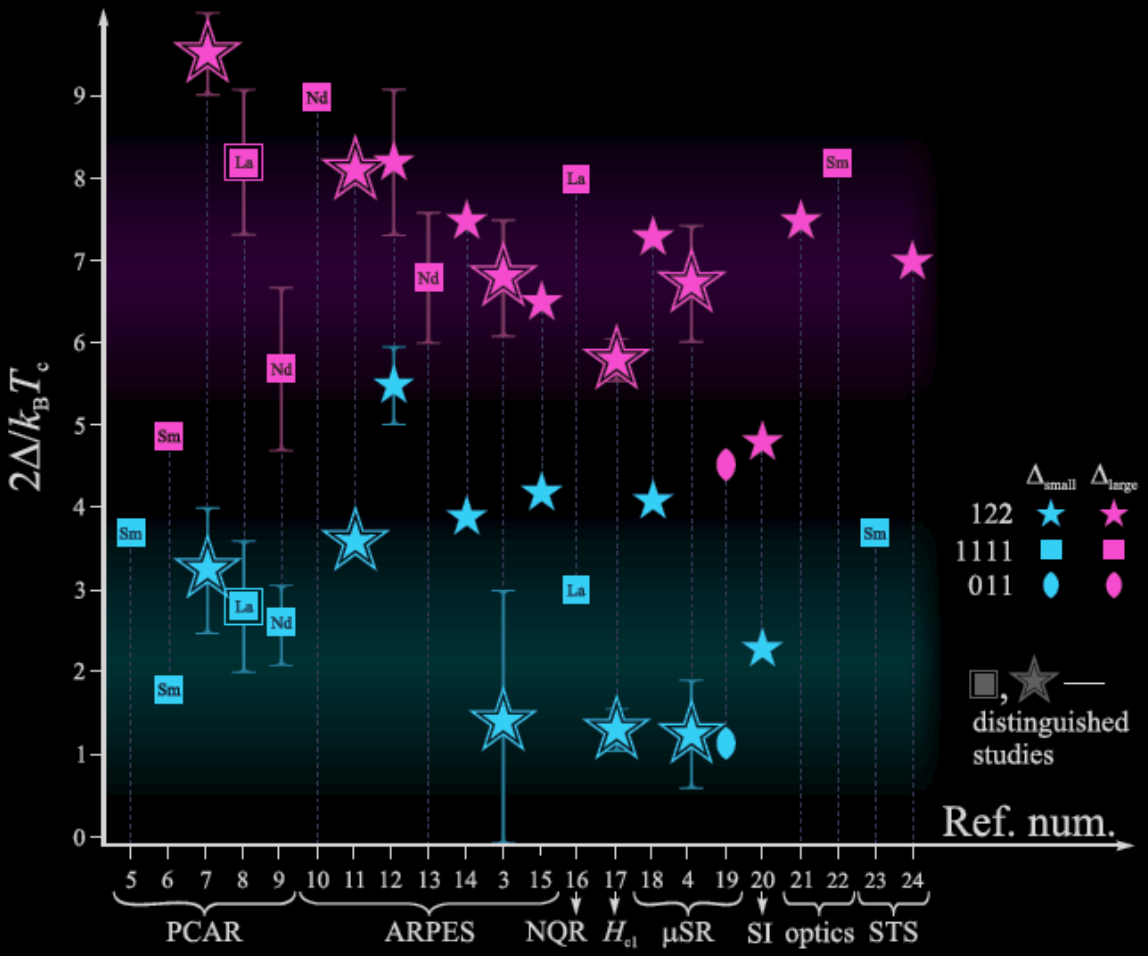






Evtushinsky *NJP* 2009

Superconducting gap in BKFA



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Ordering in pnictides?

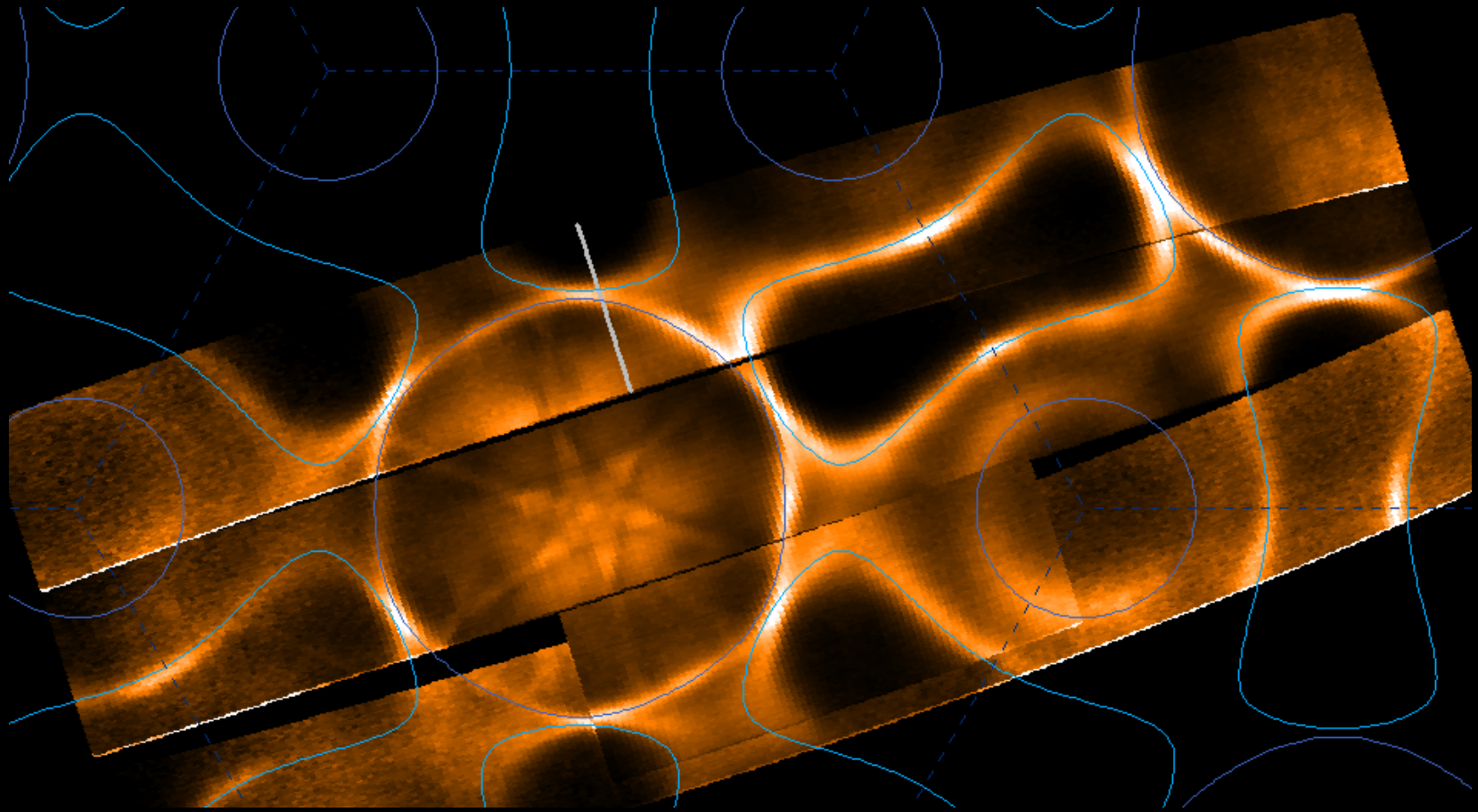
- ✓ Electron density in pnictides shows (π, π) ordering already in the normal state

- ? Isn't a general property of 2D metals?

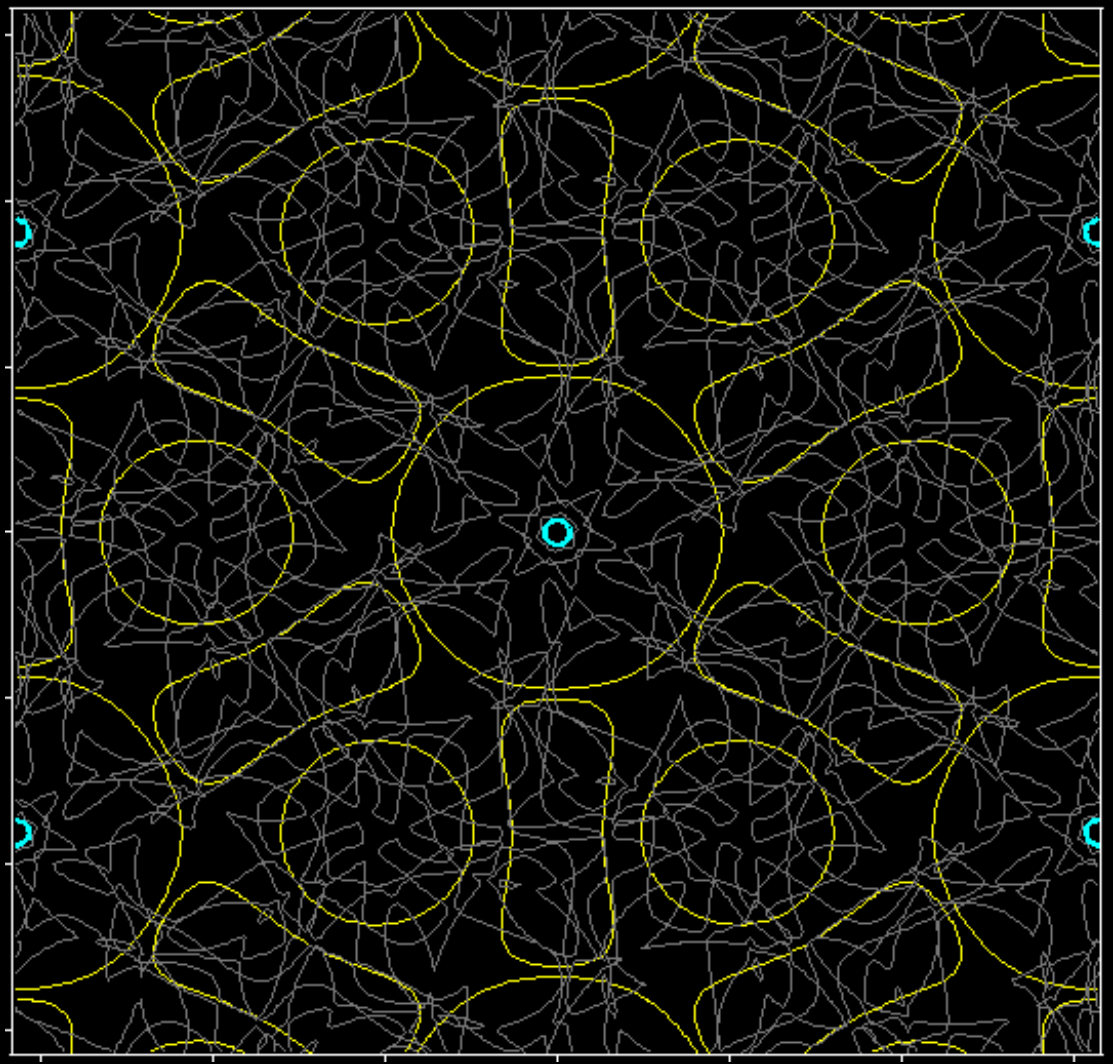
Pseudo-gap and Density Ordering in 2D Metals

- ✓ Uniform distribution of the electron density in 2D metal is usually unstable
- ✓ PG is a consequence of additional electronic ordering / propensity to ordering
- ✓ The parameters of this instability depends crucially on electronic band structure

Just an example: 2H-Cu_xTaSe_2



Just an example: 2H-Cu_xTaSe_2



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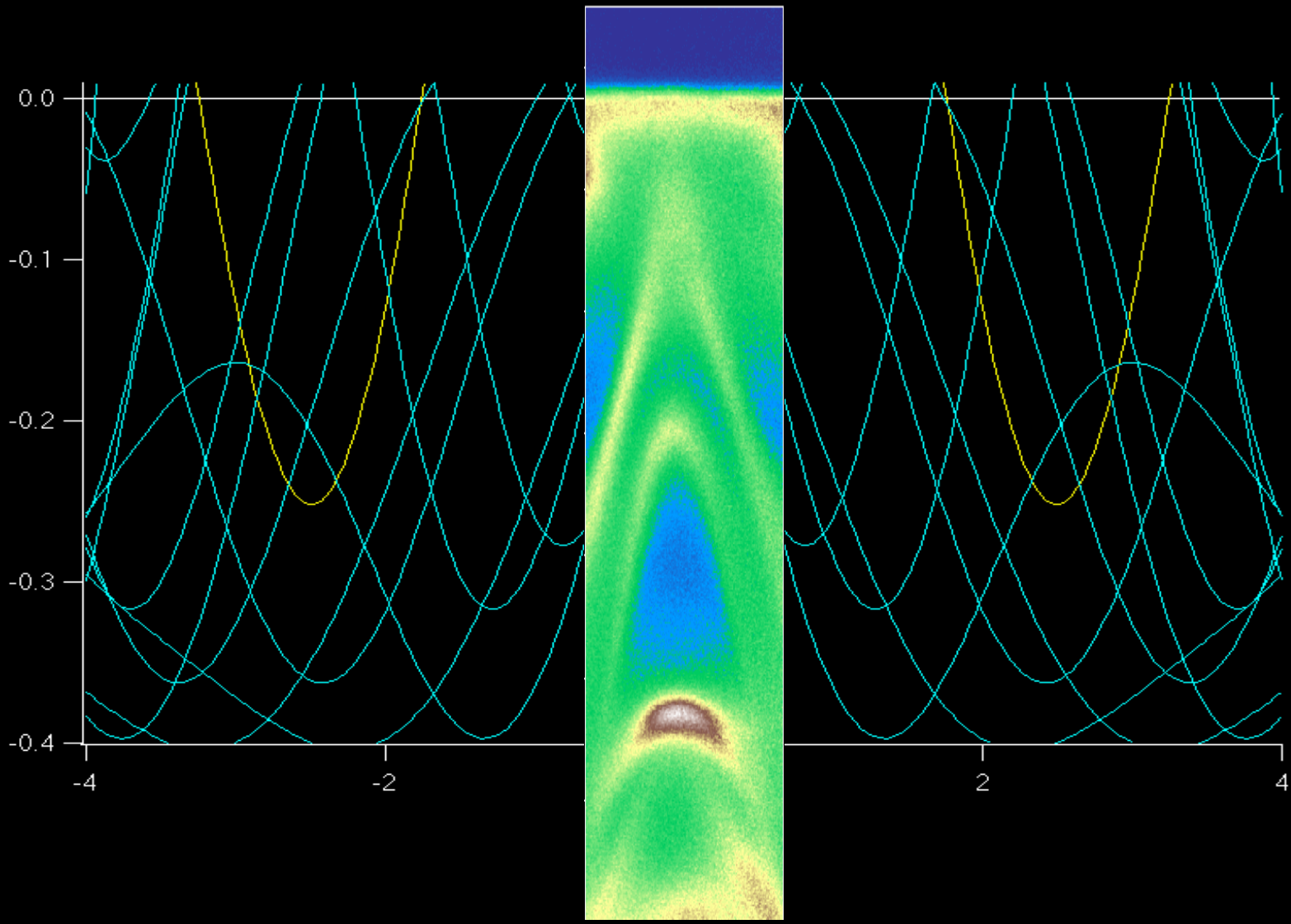

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Theory:
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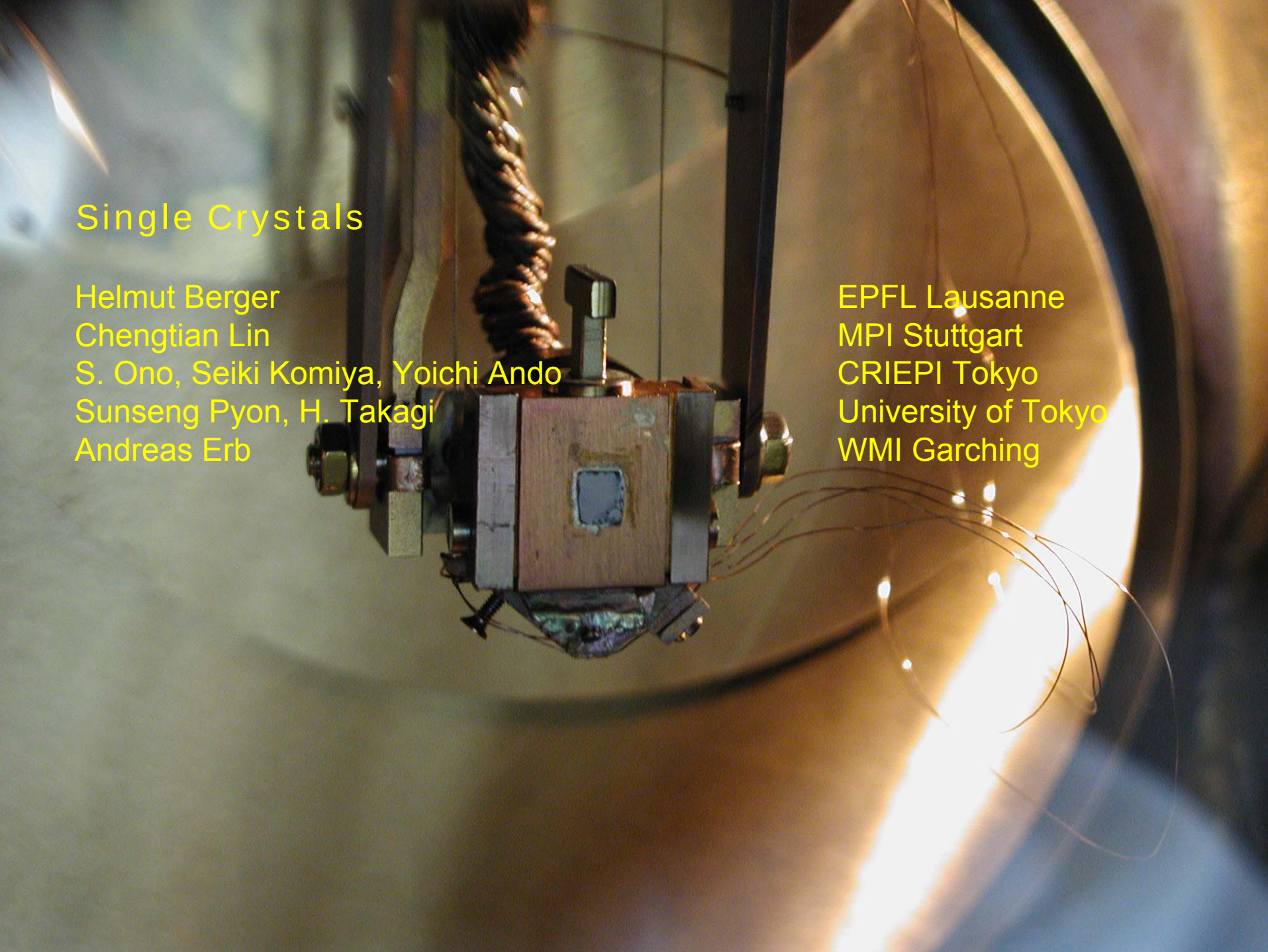
Thomas Dahm (Tübingen), Doug Scalapino (Santa Barbara)



Single Crystals

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Sunseng Pyon, H. Takagi	University of Tokyo
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