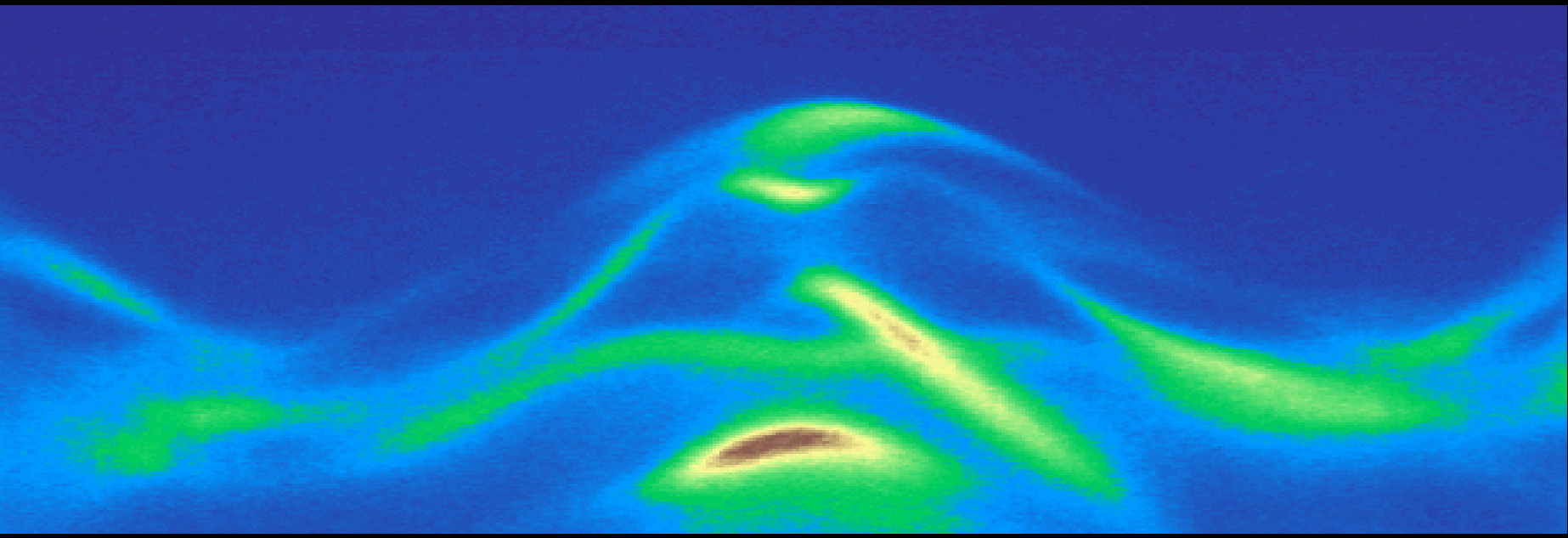
Persistent Pseudo-gap and Density Ordering in 2D Metals



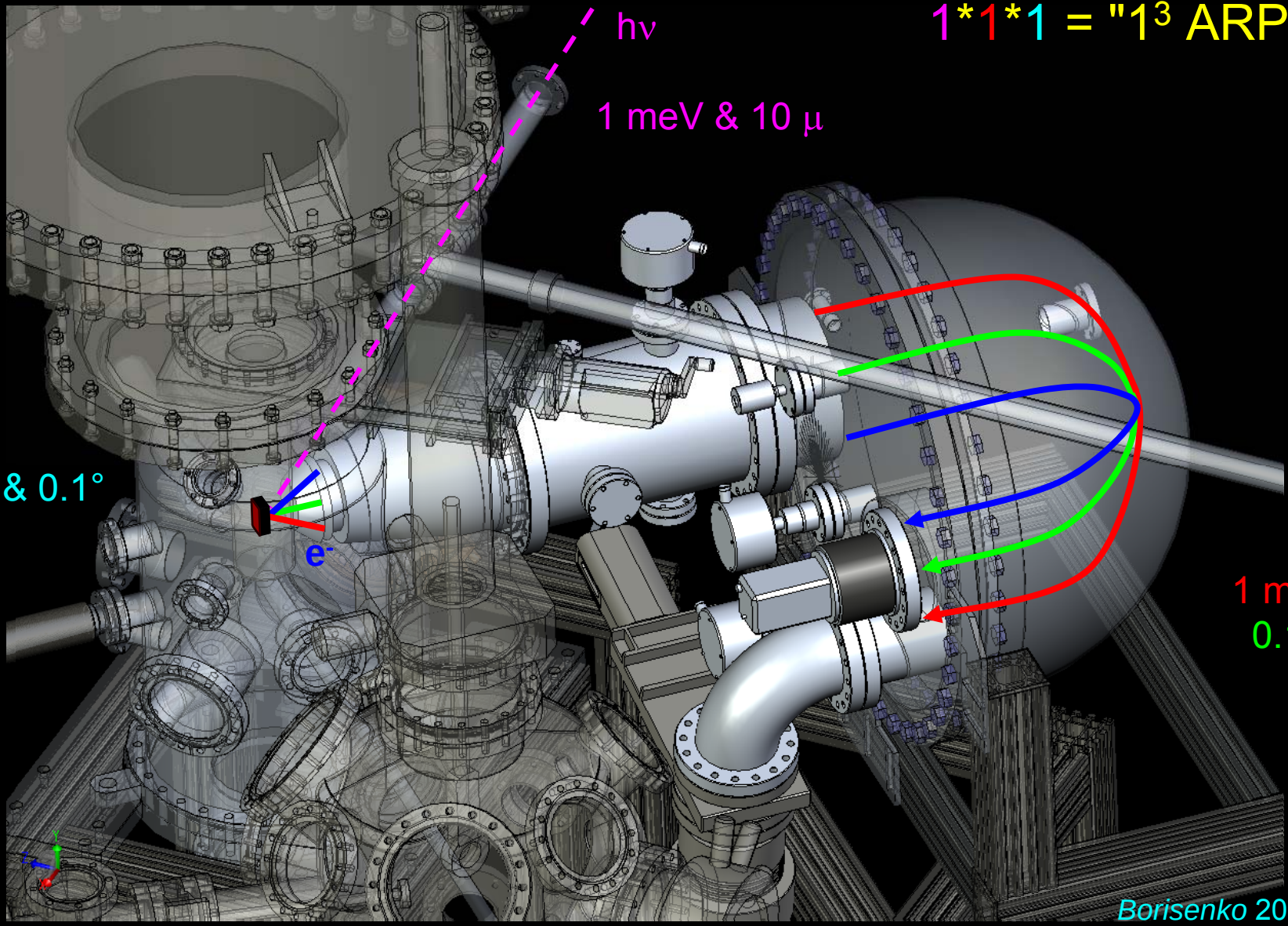
A. A. Kordyuk
IFW Dresden

Outline

I. New ARPES
   - wide acceptance angle — CARPES
   - ultimate resolution — WARPES
   - lowest temperature — TARPES

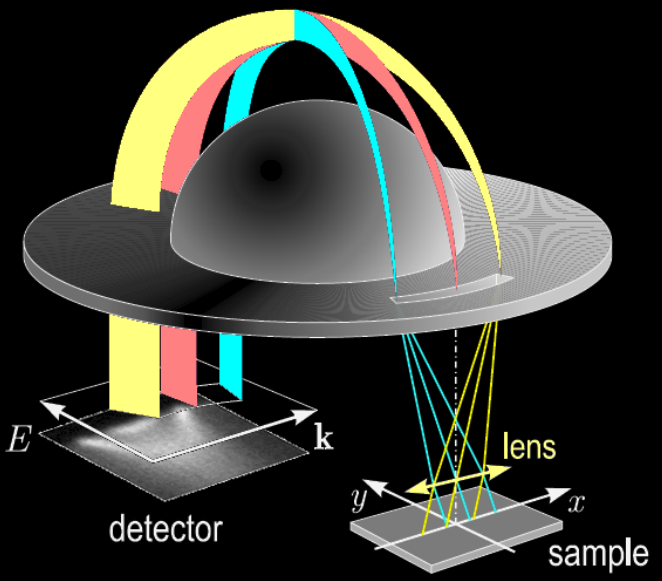
II. Pseudo-gap = Density modulation
   - CDW in dichalcogenides
   - HTSC cuprates
   - pnictides…

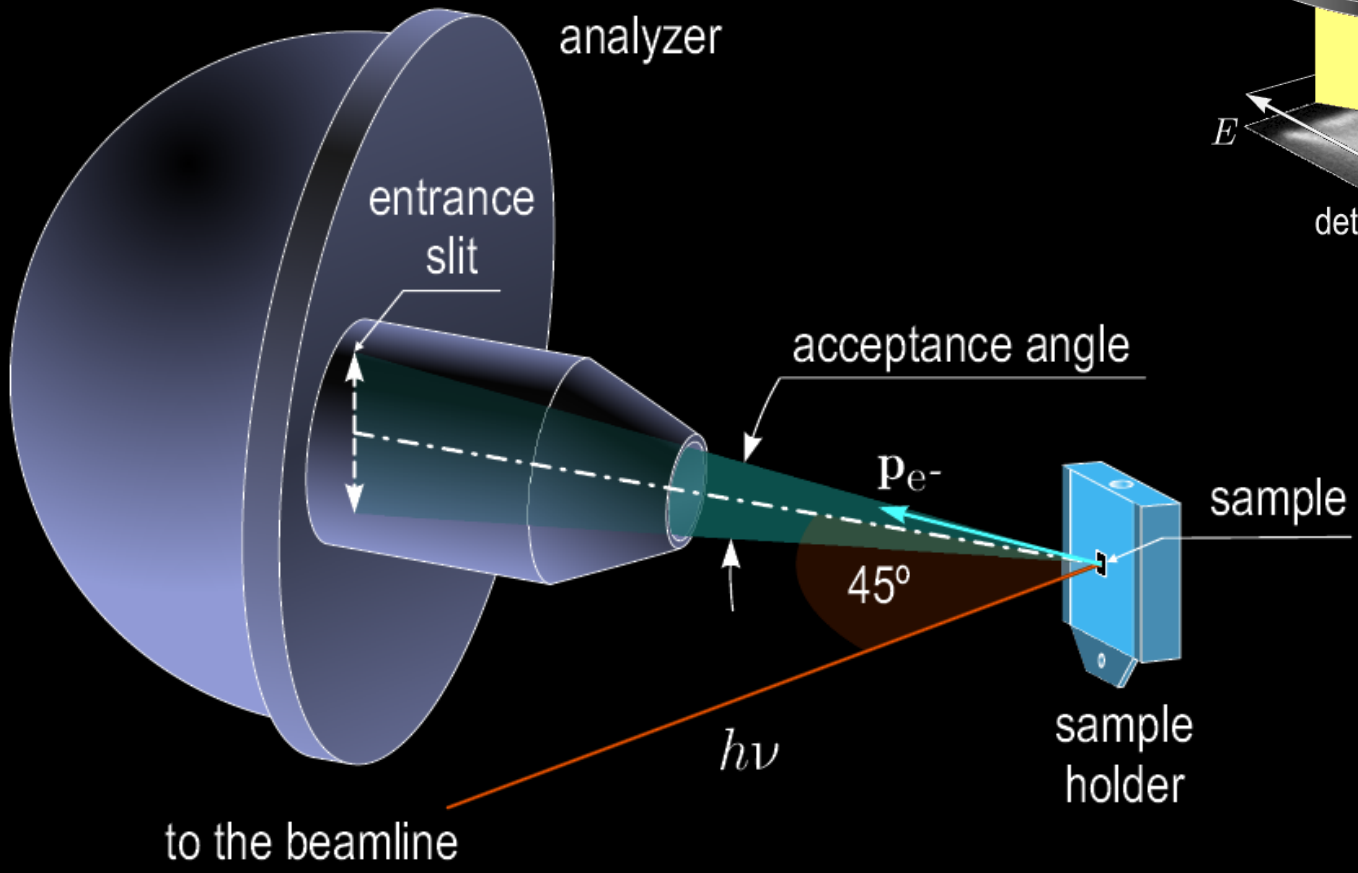
ARPES anatomy



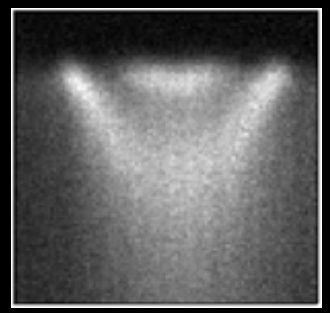
Borisenko 2008

Photoelectric effect + SES

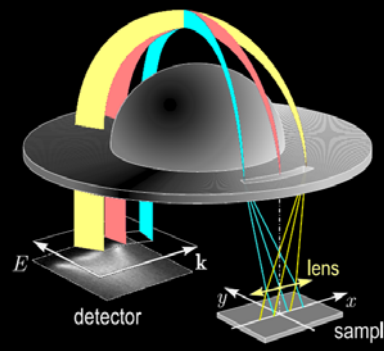


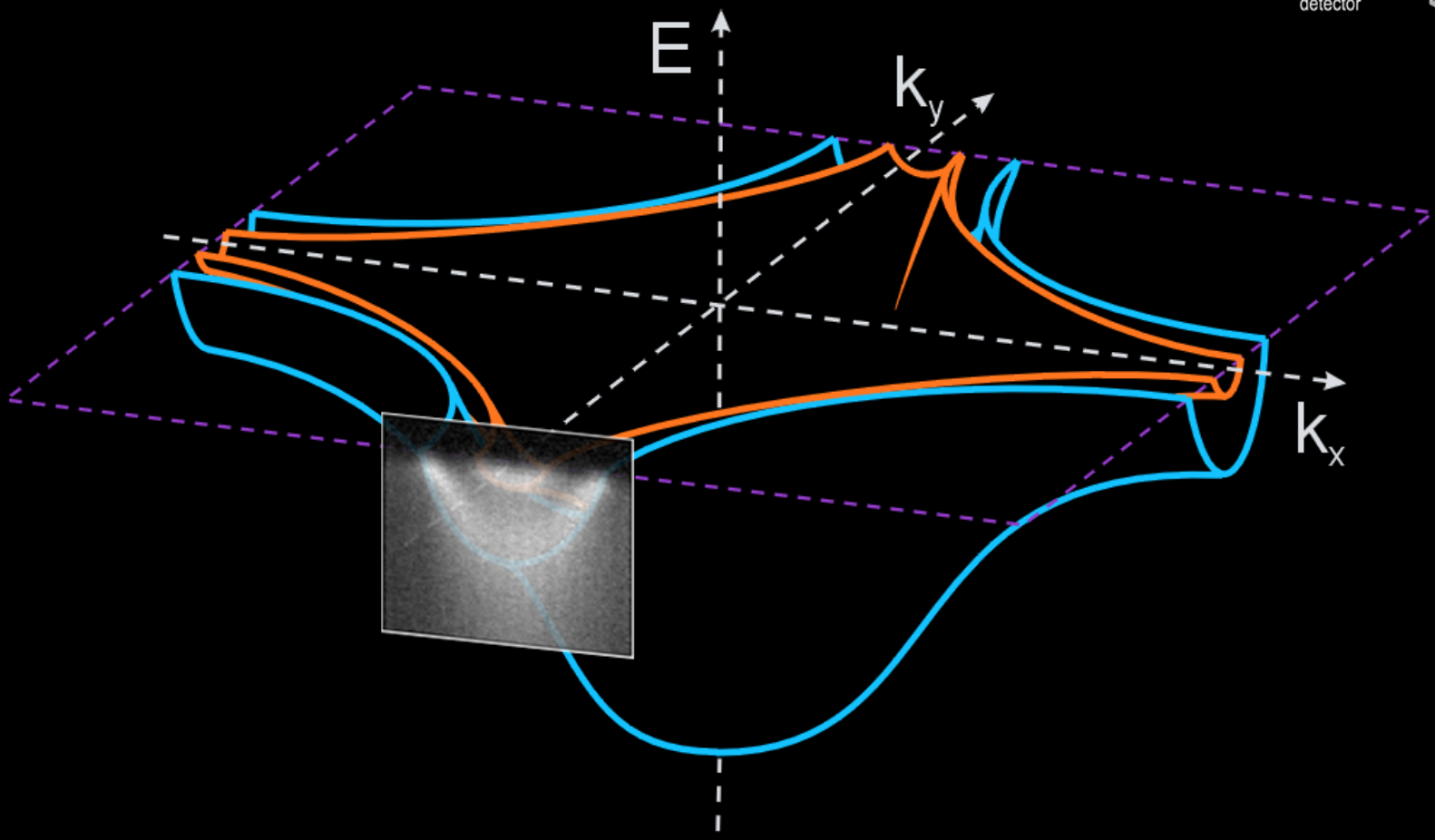


ARPES Image

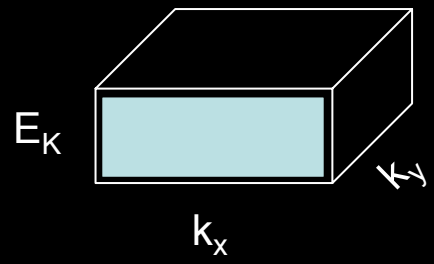


ARPES Image → ARPES Space

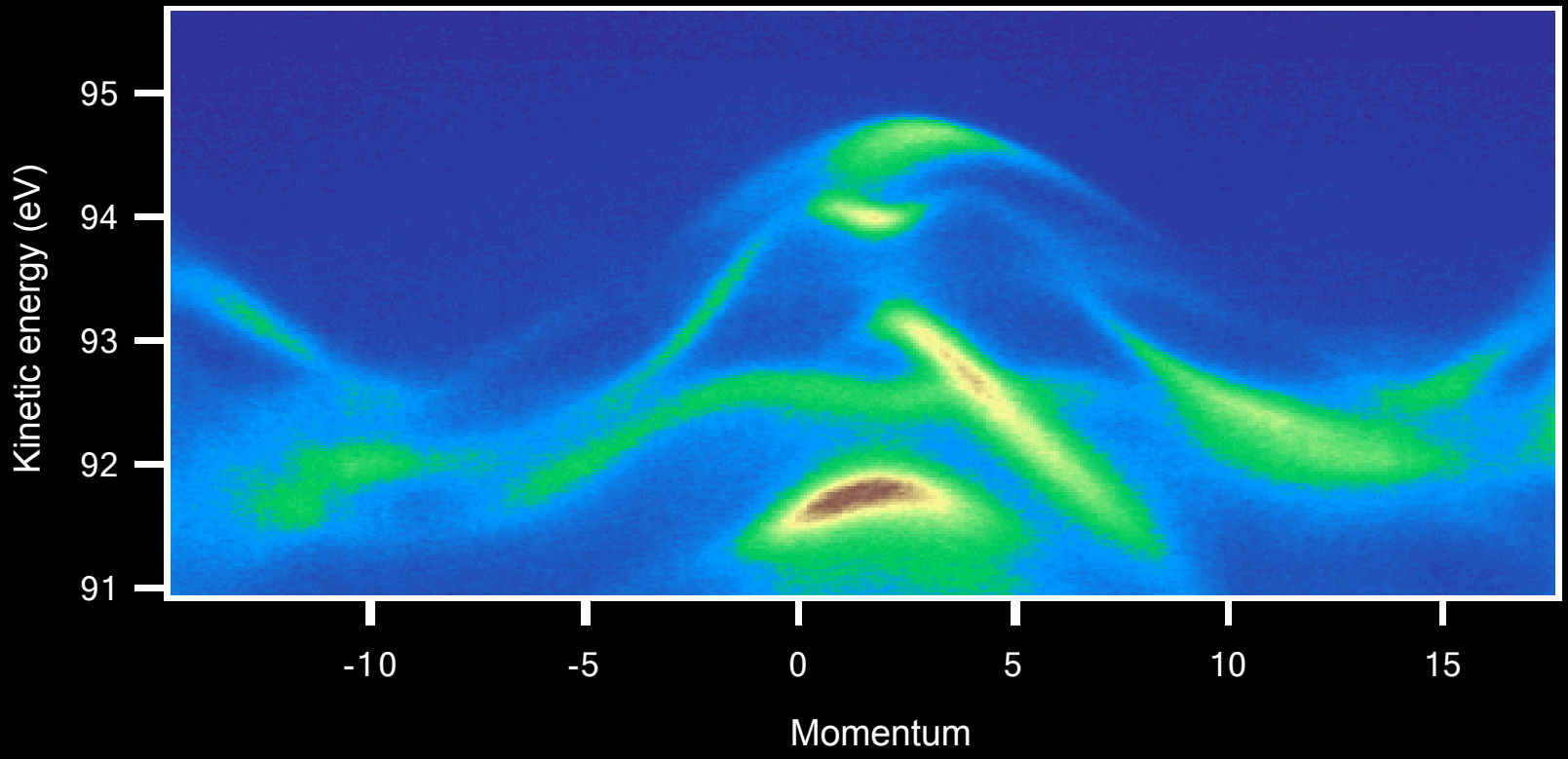




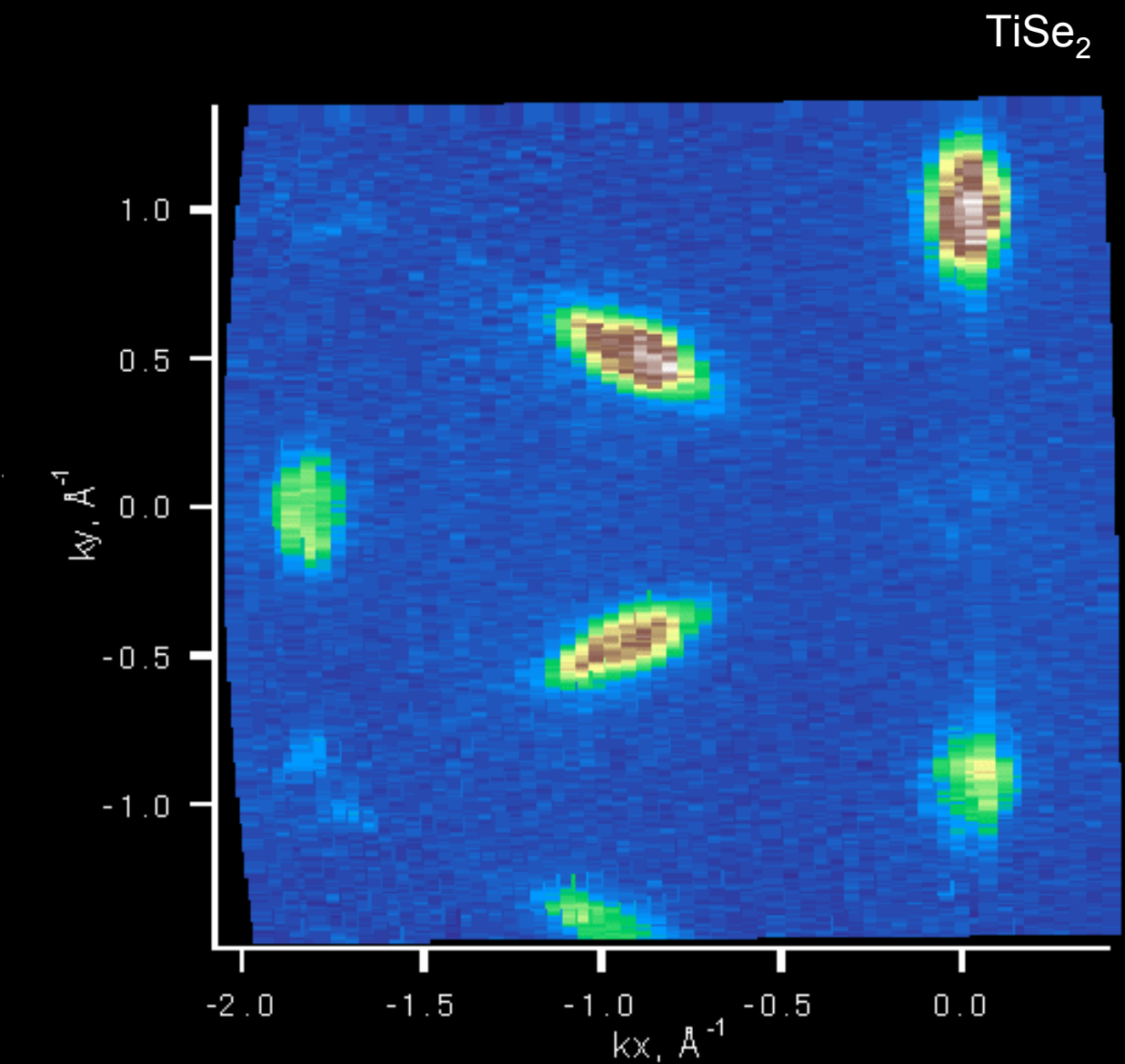
Wide - acceptance lens

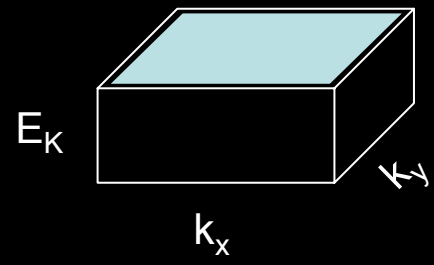


$TiSe_2$

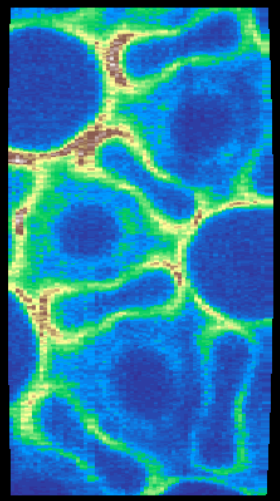


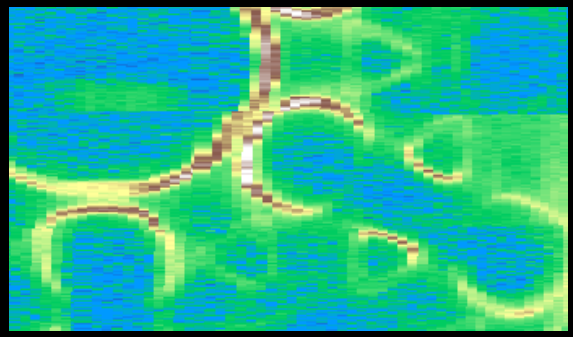
Wide acceptance lens

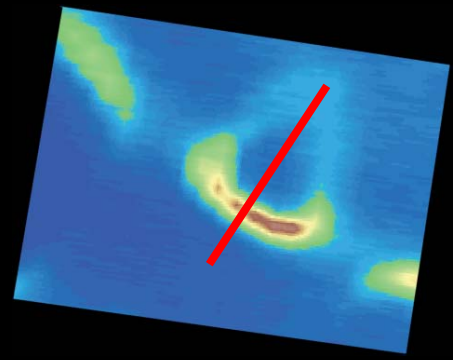


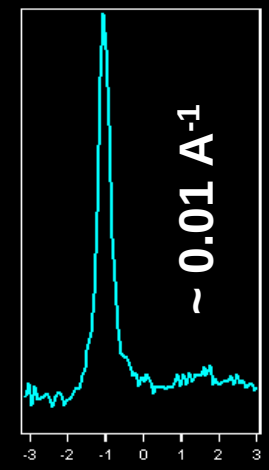


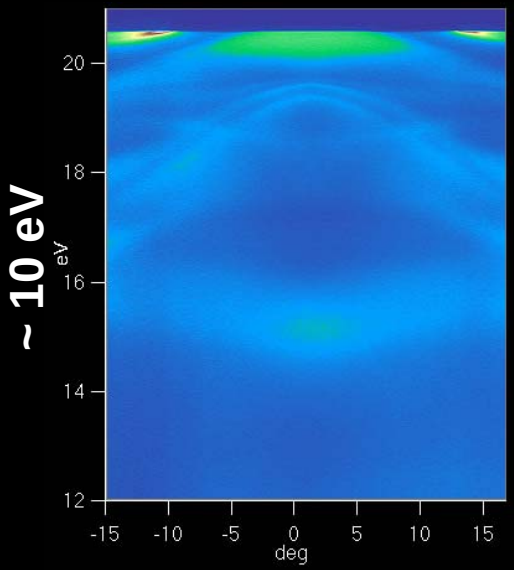
Zooming in…

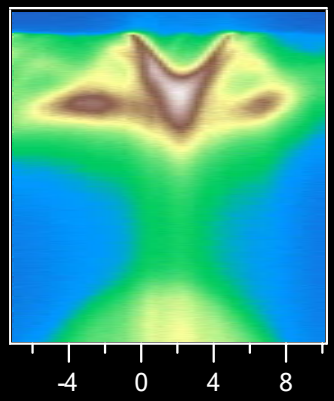

~ 10 A-1

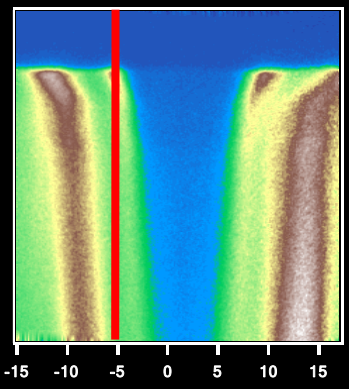

~ 1 A-1

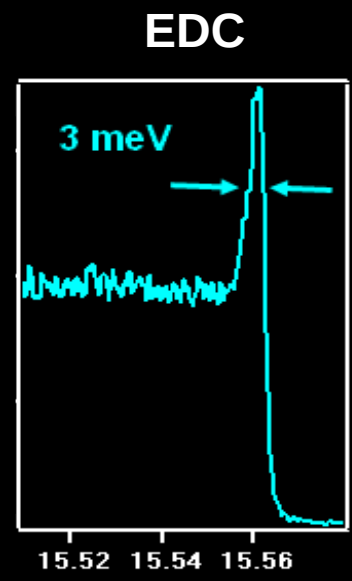

~ 0.1 A-1


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

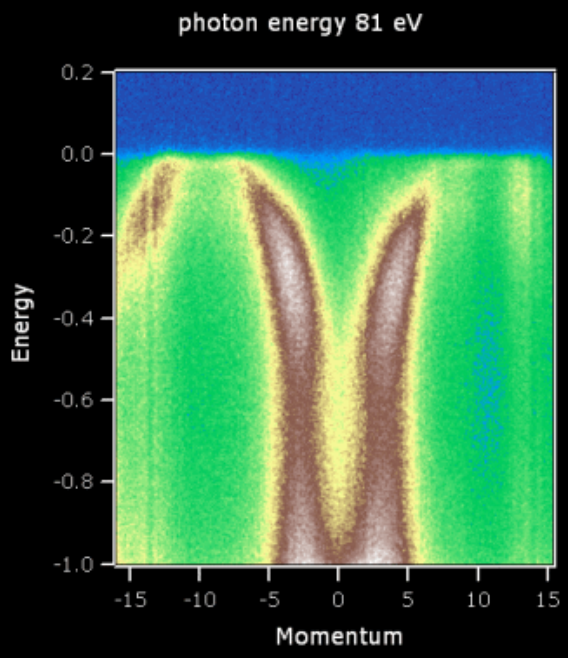

~ 10 eV
20
18
16
14
12
eV
-15 -10 -5 0 5 10 15
deg
Momentum


~ 1 eV
-4 0 4 8

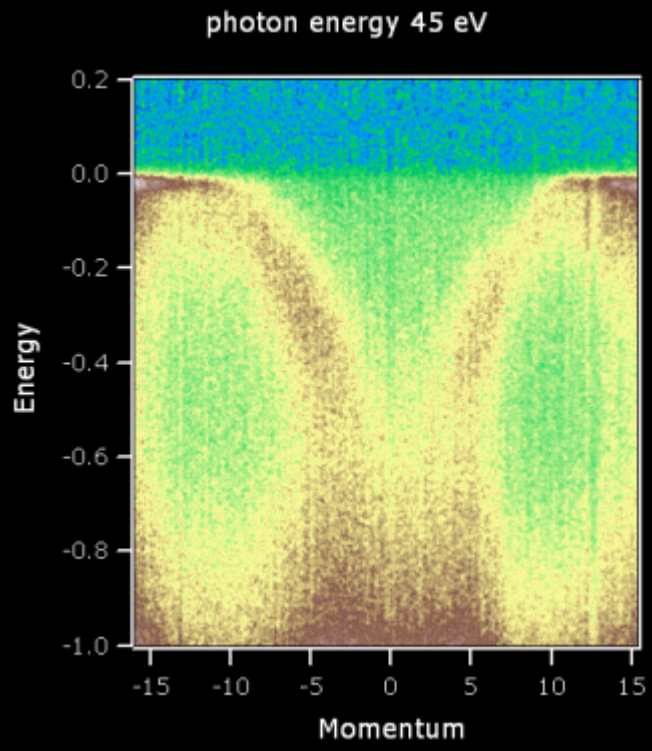

~ 0.1 eV
-15 -10 -5 0 5 10 15

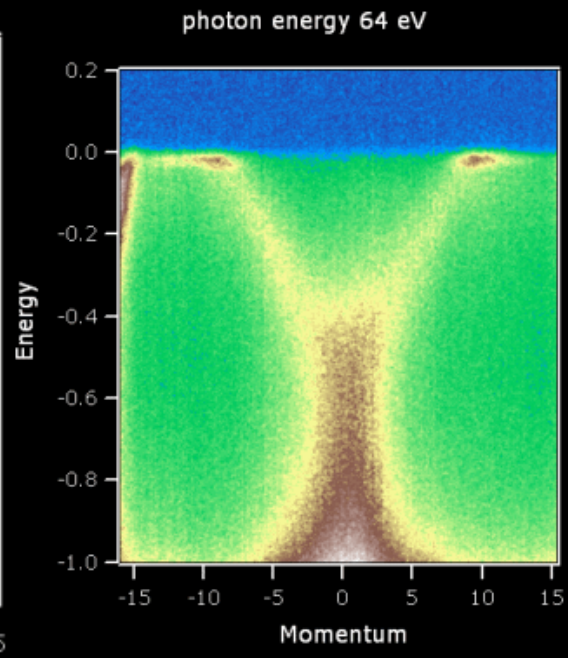

EDC
~ 0.001 eV
3 meV
15.52 15.54 15.56

Photon energy – an important parameter



„Waterfalls“

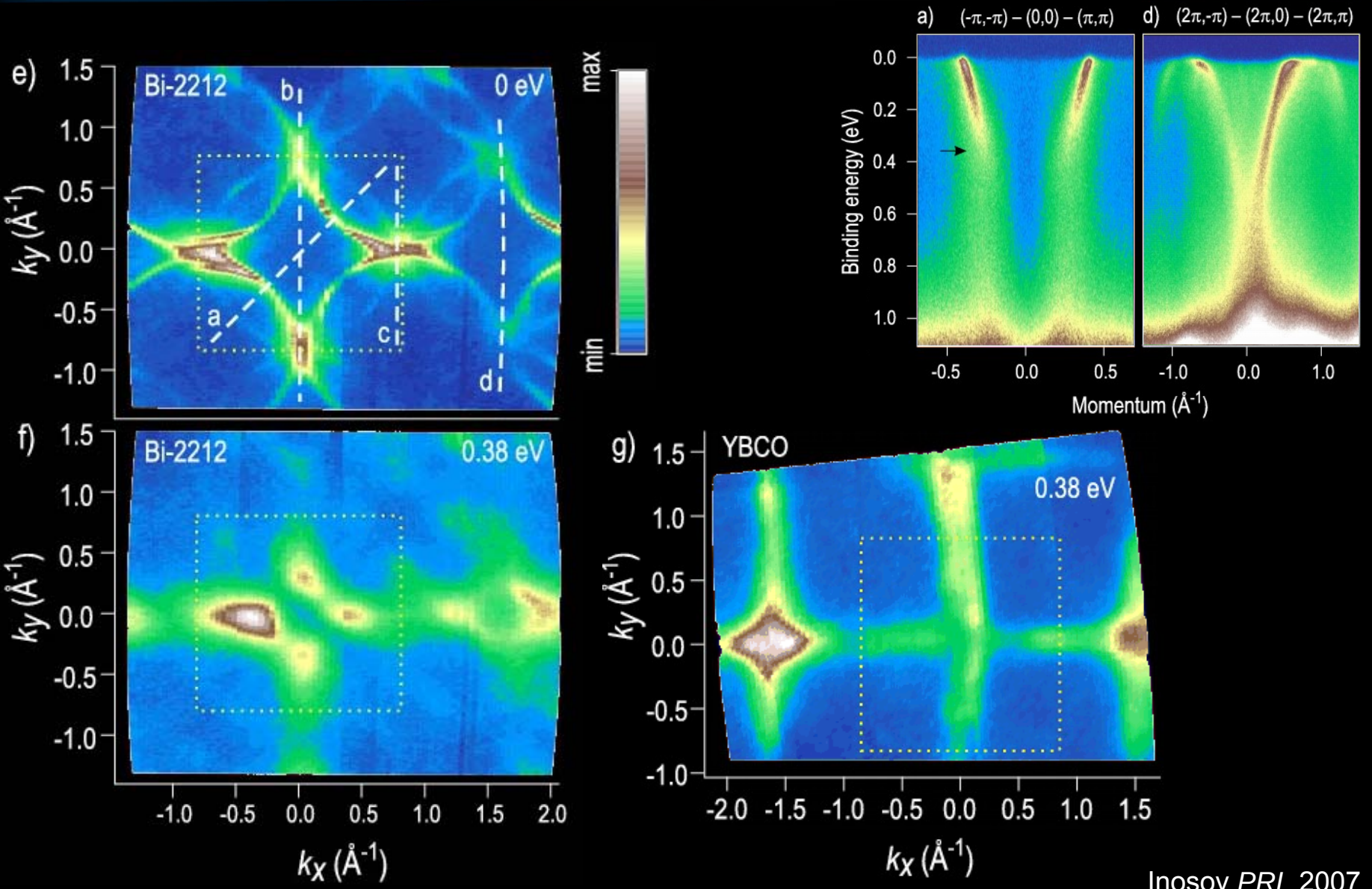




„Champagne glass“

Inosov *PRL* 2007, *PRB* 2008

Waterfalls in cuprates

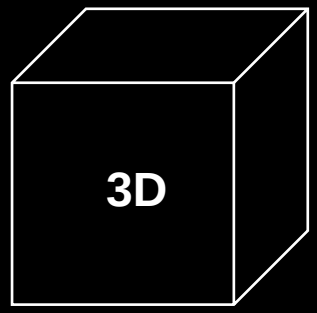


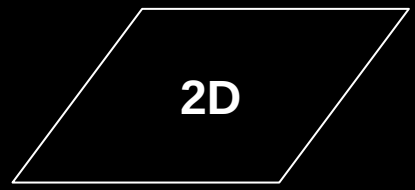
Inosov *PRL* 2007

CDW and superconductivity in 2D

CDW and superconductivity in 2D

El-ph interaction ?



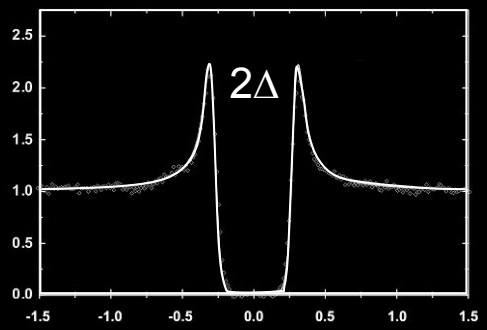


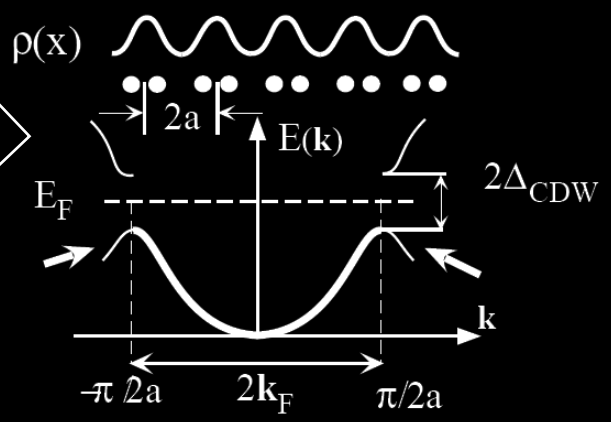
1D

both are anomalous

PG ?

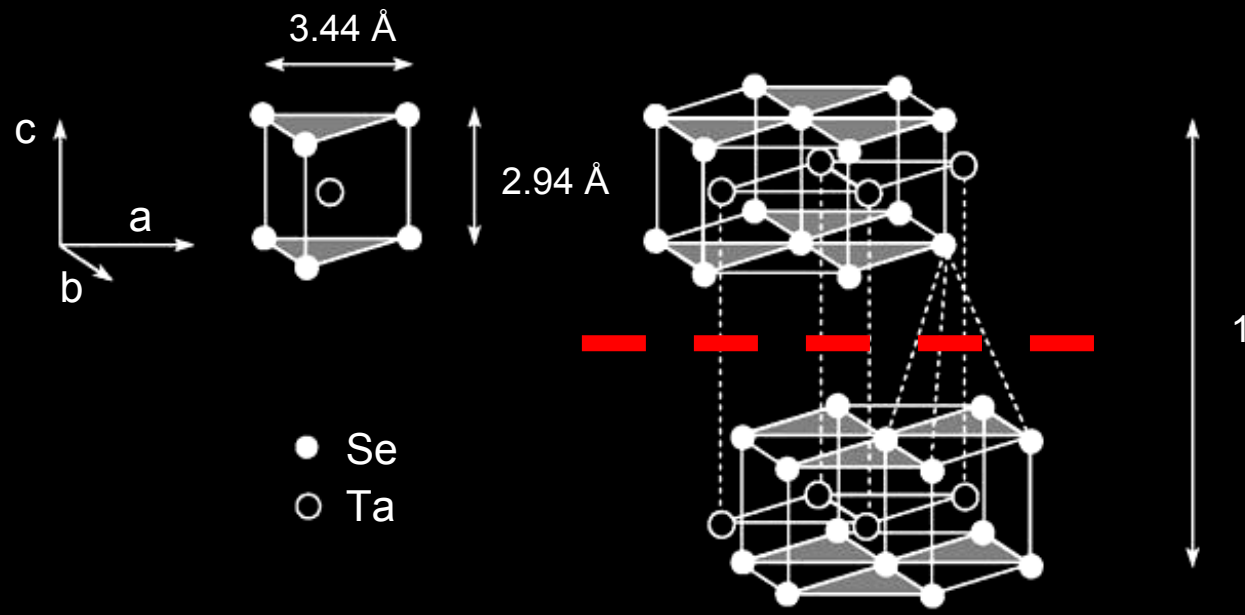
better metal ?

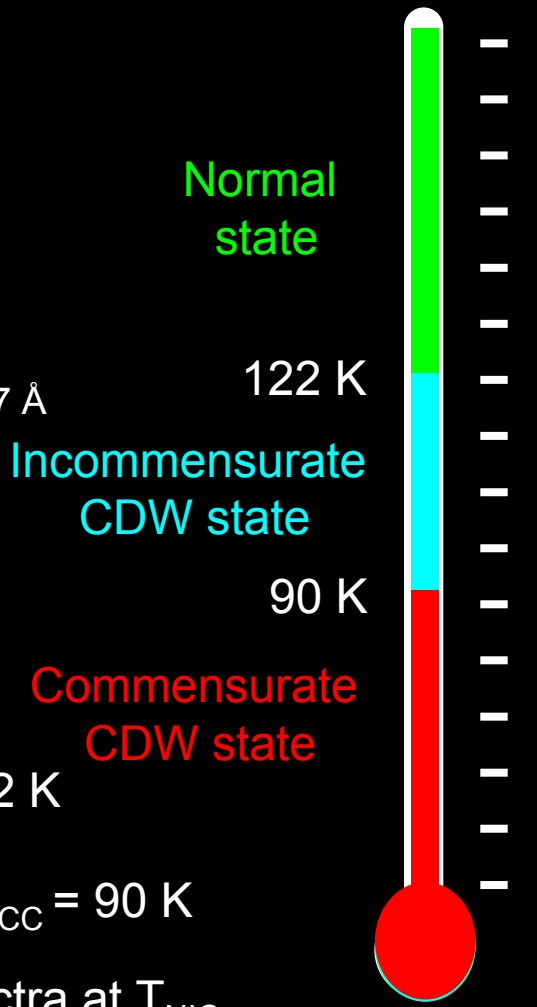




$2H\text{-}TaSe_2$

2H-$TaSe_2$ crystal structure, CDW transitions



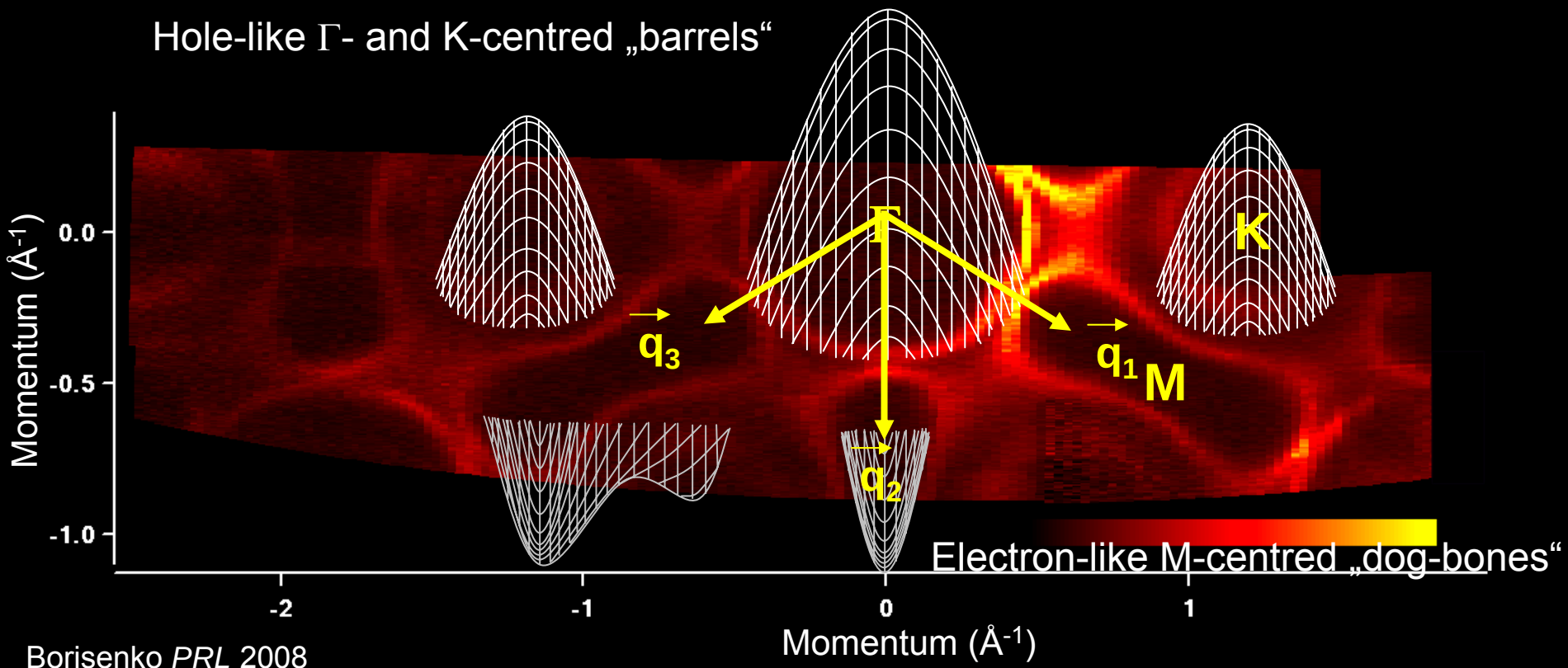


- 2nd-order transition to an incommensurate CDW at T_{NIC} = 122 K
- 1st-order lock-in transition to a 3x3 commensurate CDW at T_{ICC} = 90 K
- What was strange? No nesting. No change in ARPES spectra at T_{NIC} .
  Gap of 24-250 meV only below 90K.

Electronic structure of 2H-$TaSe_2$

Normal state

180 K

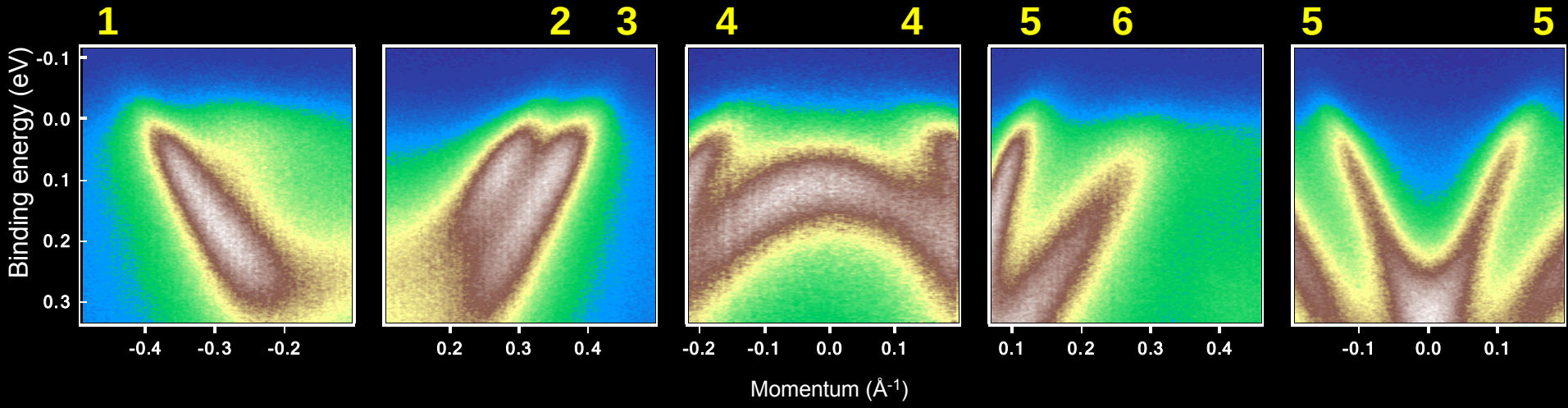


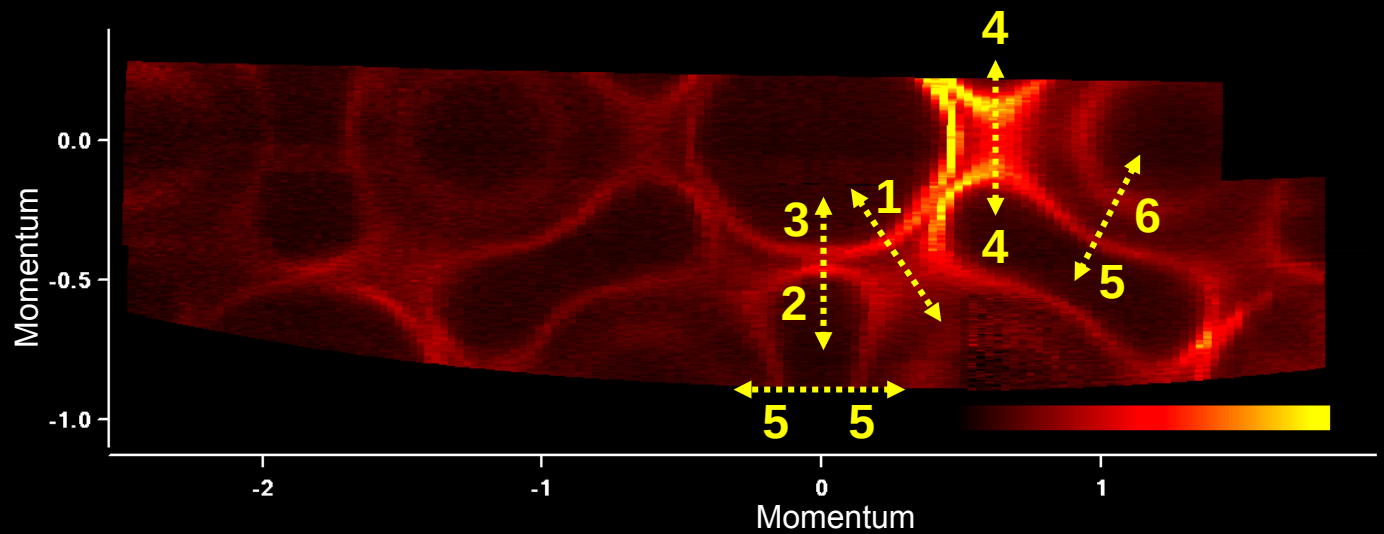
Borisenko *PRL* 2008

Normal state of 2H-$TaSe_2$

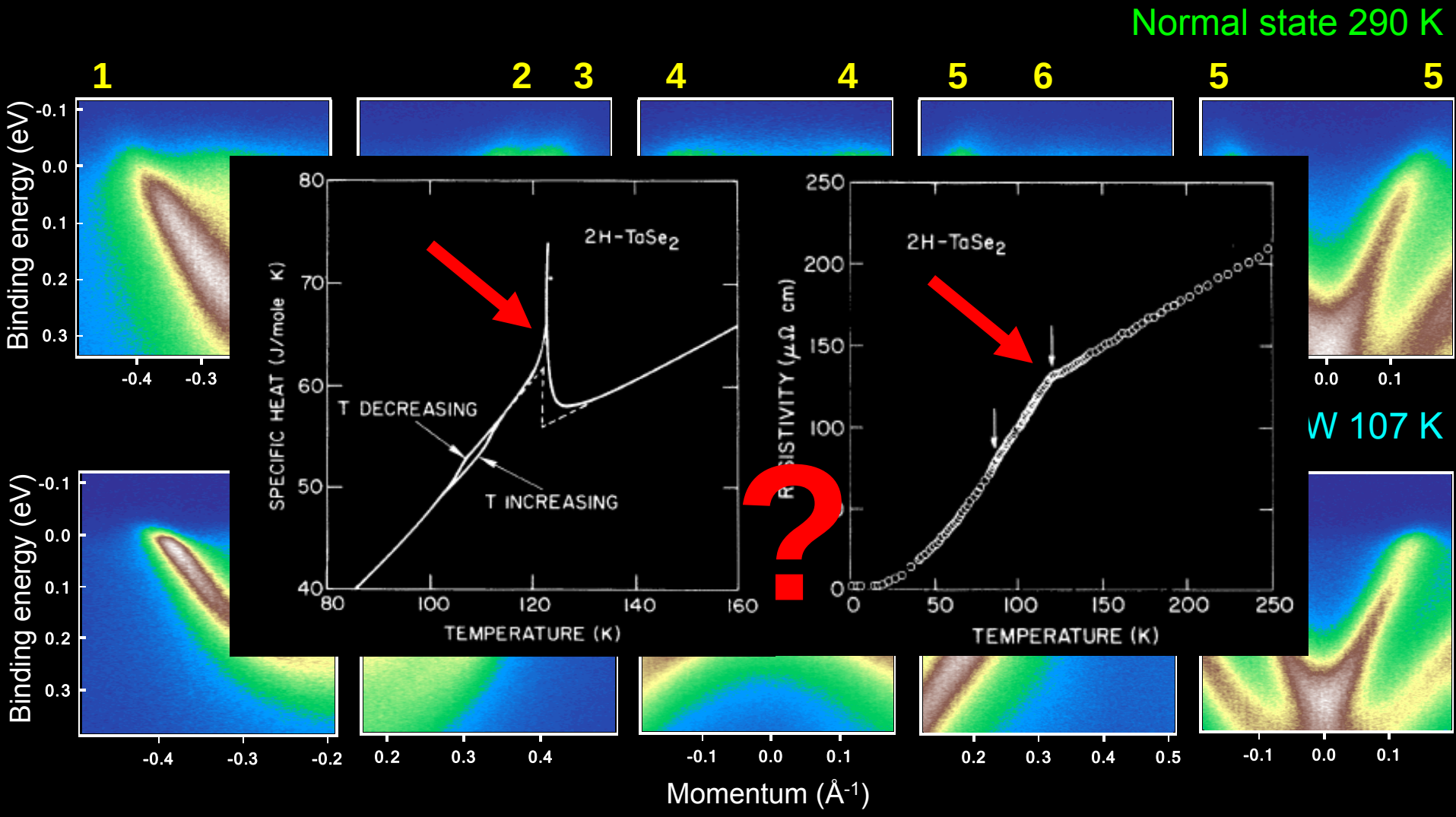
Normal state

290 K





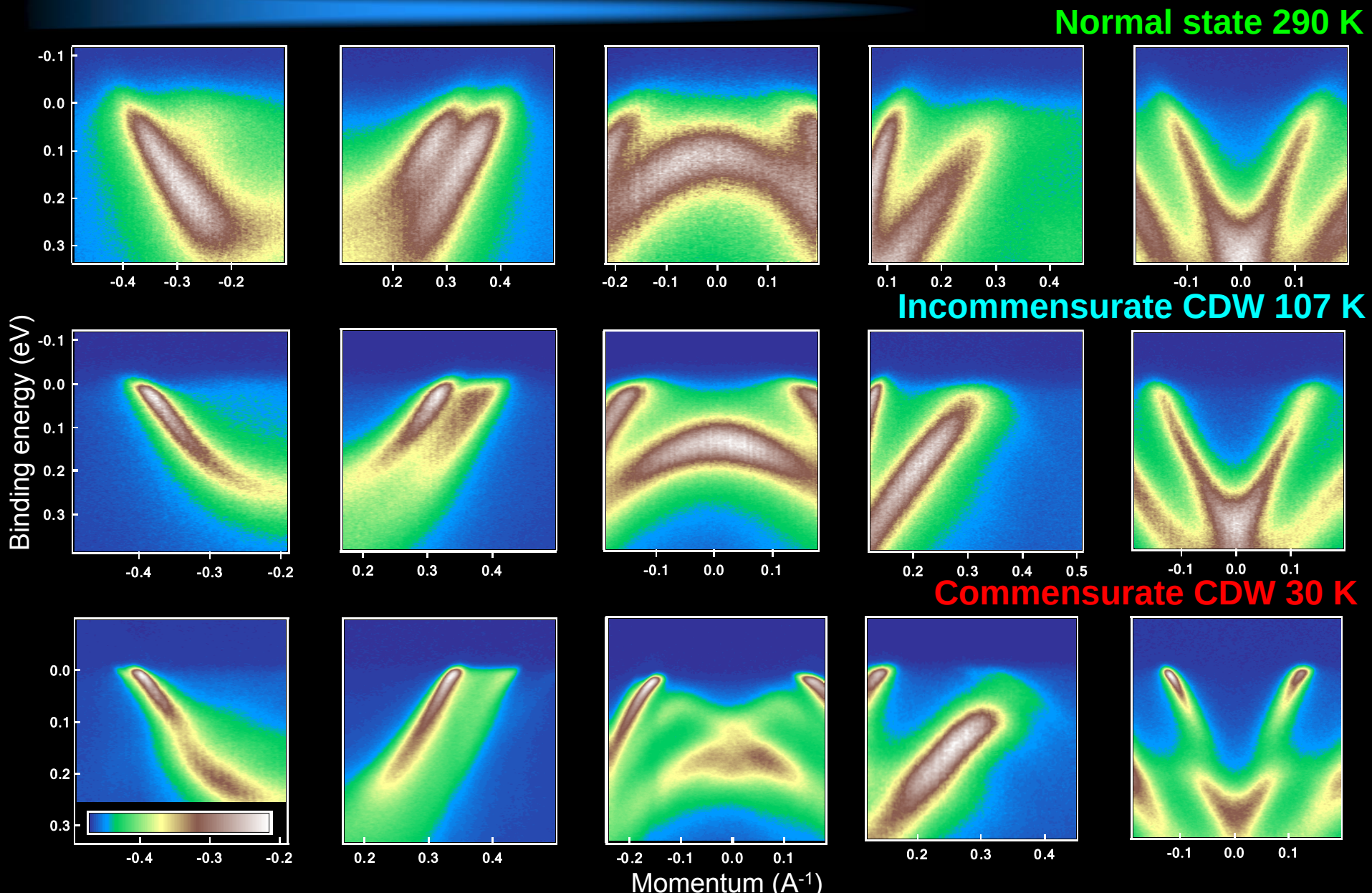
Incommensurate CDW state of 2H-$TaSe_2$



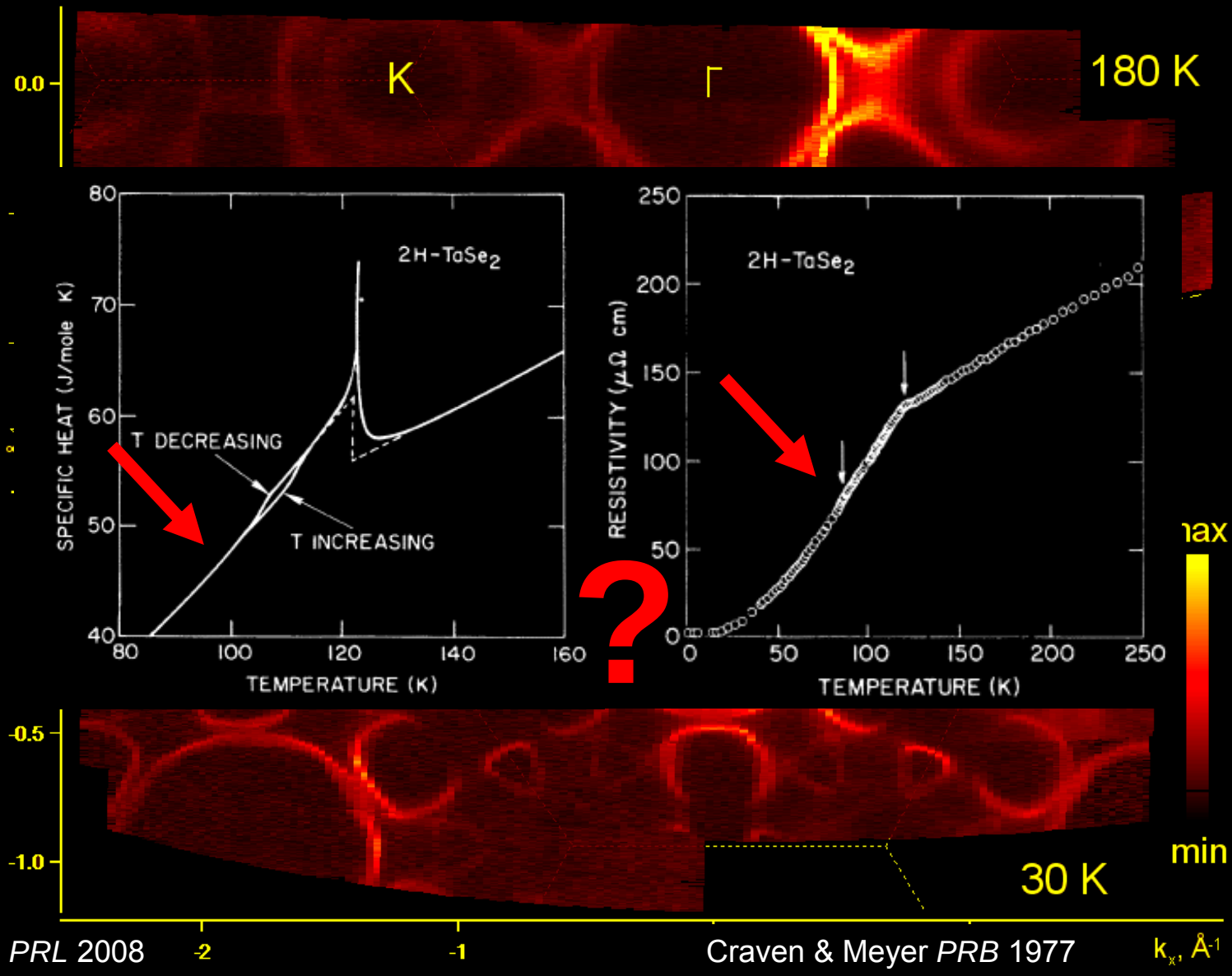
Borisenko *PRL* 2008

Craven & Meyer *PRB* 1977

Commensurate CDW state of 2H-$TaSe_2$



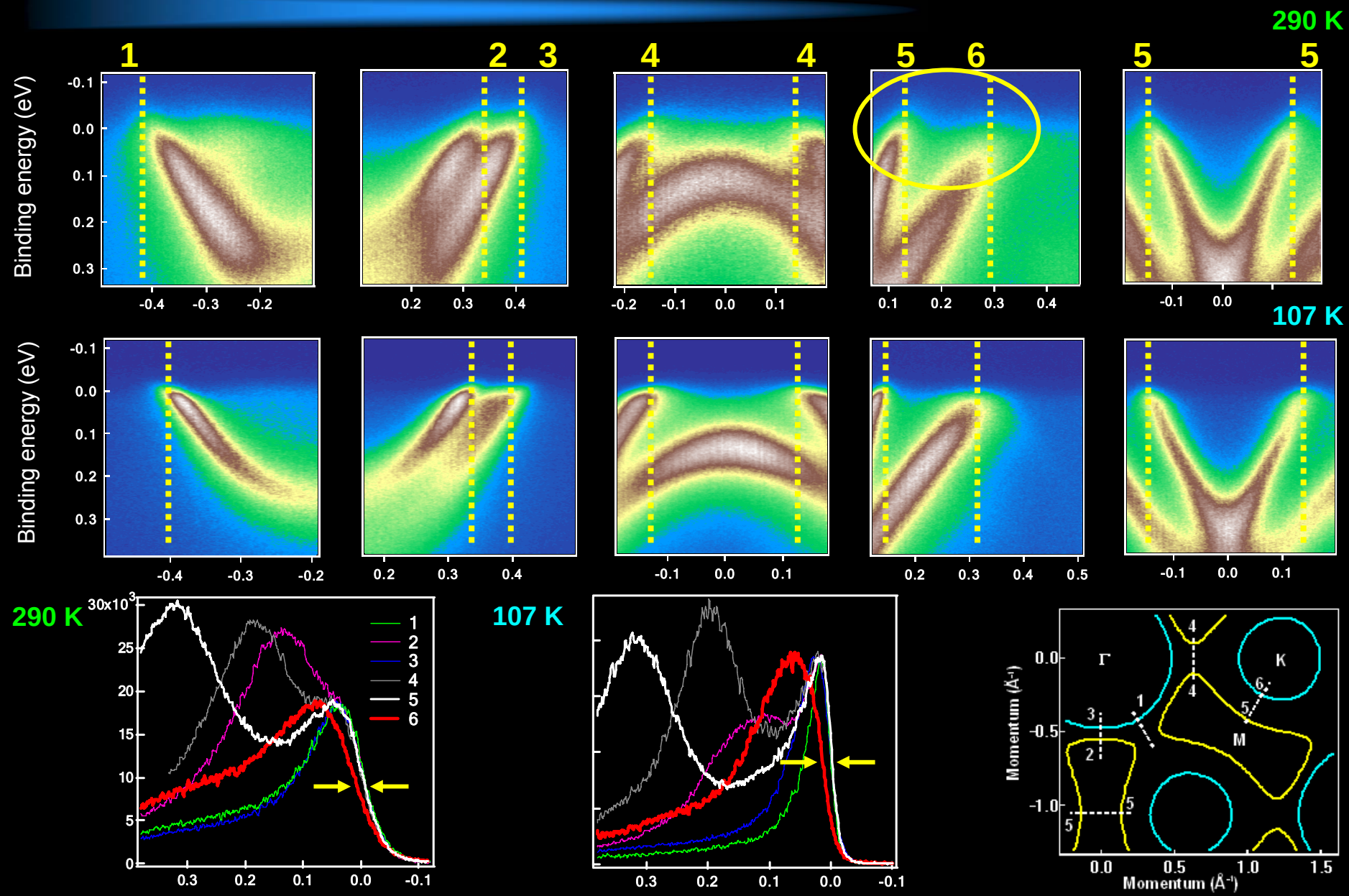
Fermi surface: commensurate CDW state



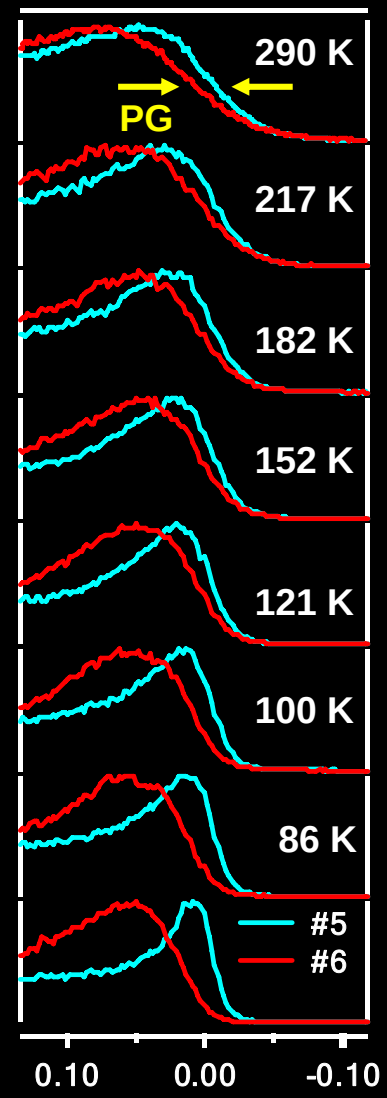
Borisenko *PRL* 2008

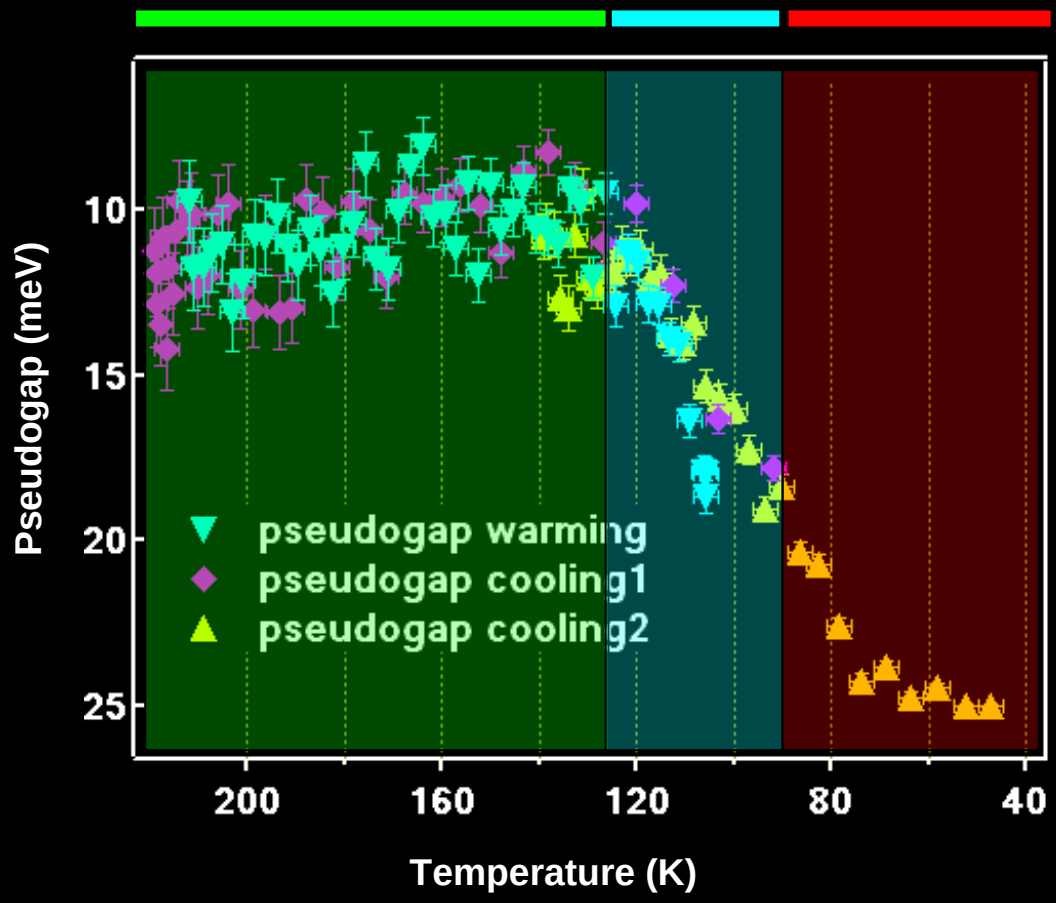
Craven & Meyer *PRB* 1977

Comparison: IC-CDW and normal state



Pseudogap as a function of temperature

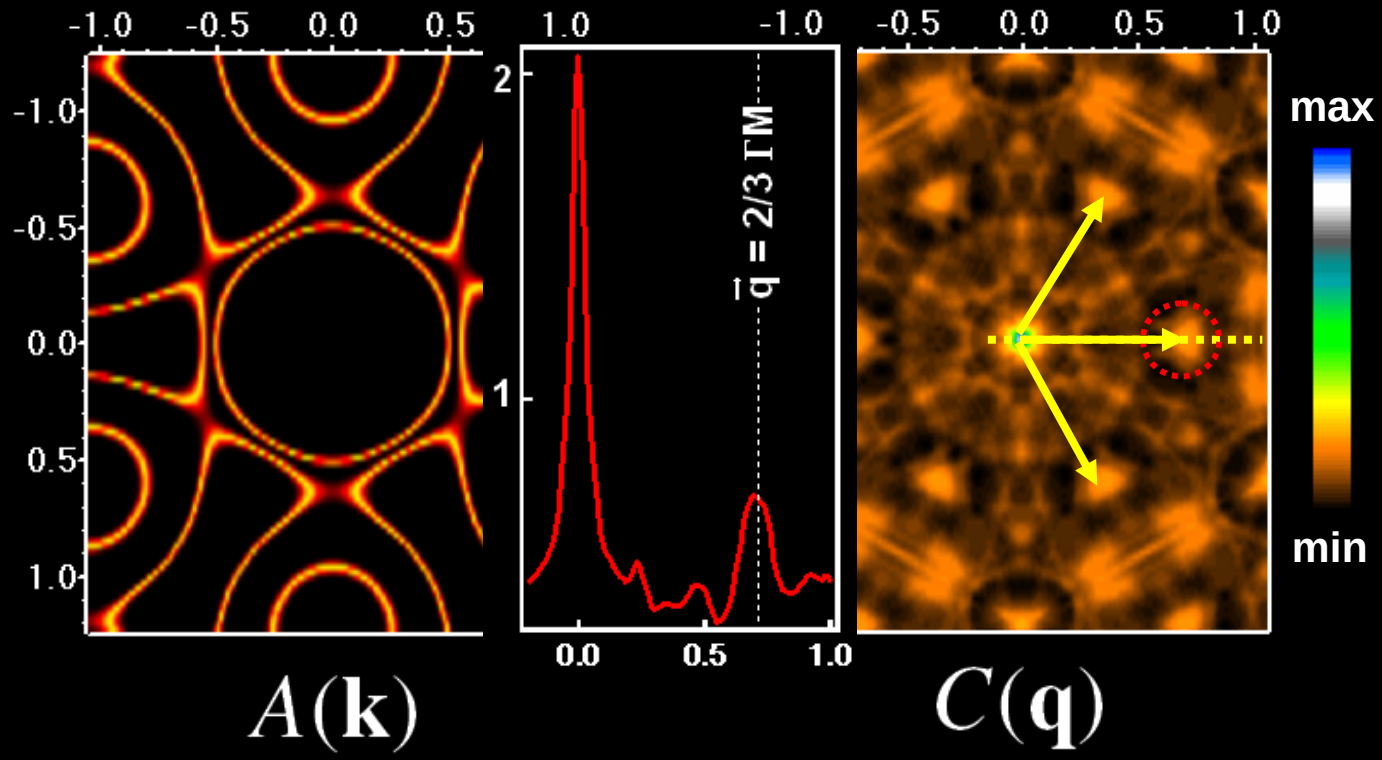




Autocorrelation – measure of nesting

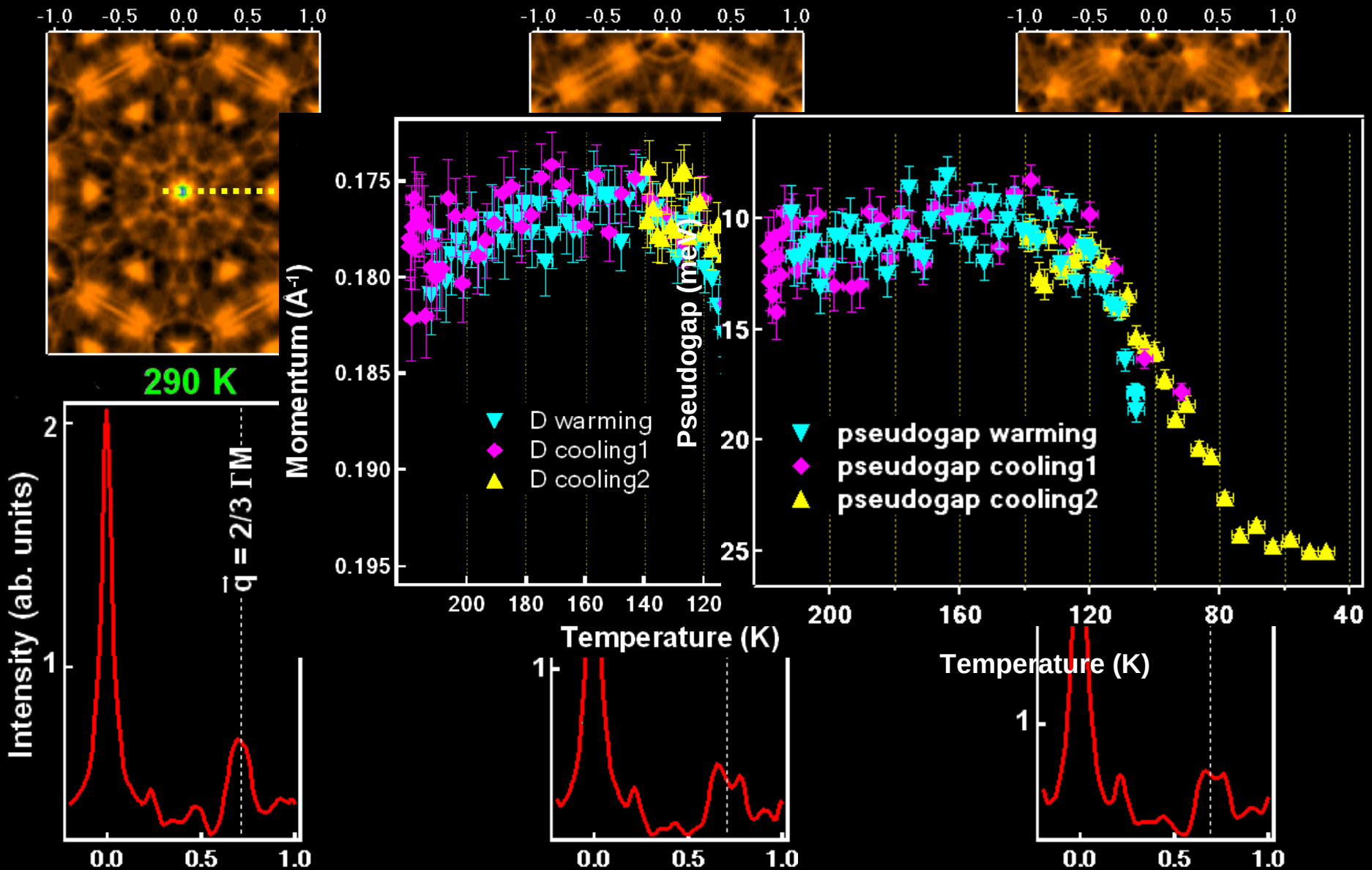
290 K

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



Borisenko *PRL* 2008

Nesting properties as a function of T

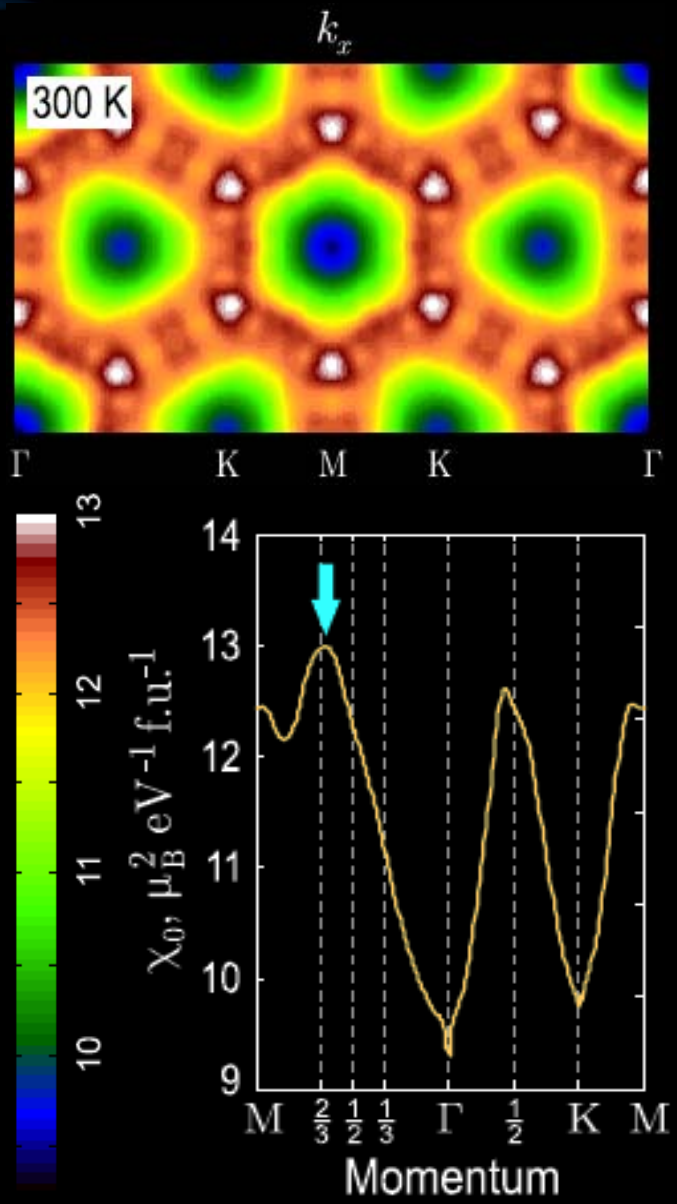


Electron susceptibility

$$\chi_0(\mathbf{q},\omega) = 2\int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^d} \frac{n_\mathrm{F}(\epsilon_\mathrm{k}) - n_\mathrm{F}(\epsilon_{\mathrm{k}+\mathrm{q}})}{\epsilon_\mathrm{k} - \epsilon_{\mathrm{k}+\mathrm{q}} + \omega + \mathrm{i}0^+}$$

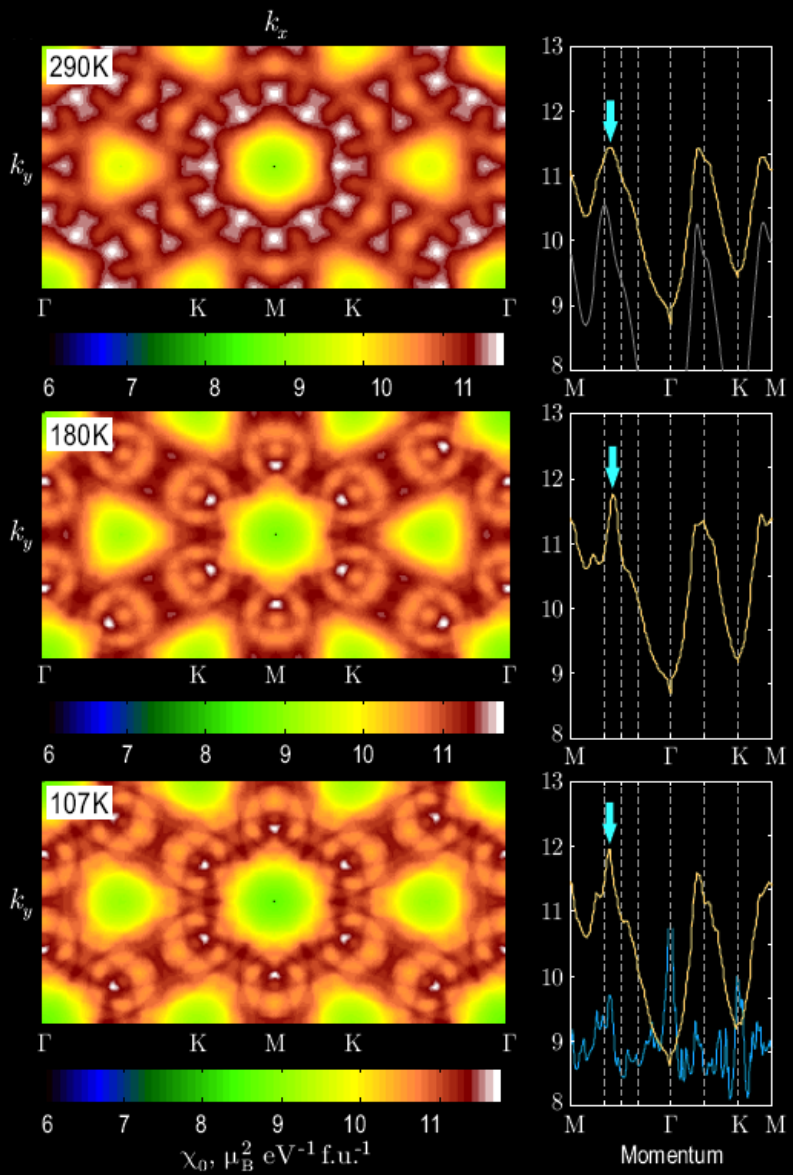
Lindhard functions at $\omega \to 0$

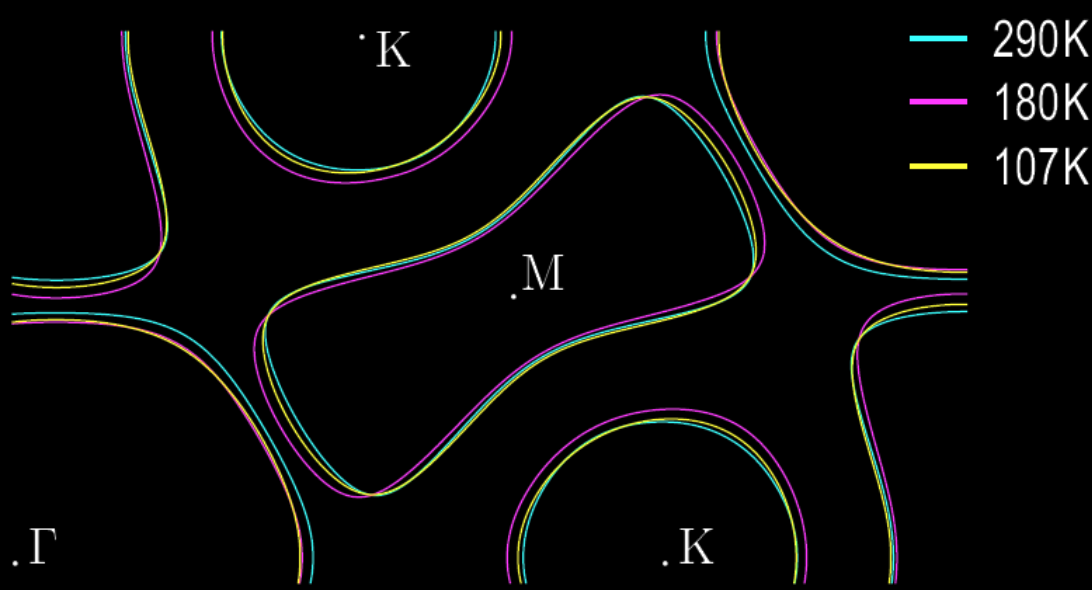
$$\chi_\mathrm{q} = \sum_\mathrm{k} \frac{n_\mathrm{F}(\epsilon^\mathrm{a}_\mathrm{k}) - n_\mathrm{F}(\epsilon^\mathrm{a}_{\mathrm{k}+\mathrm{q}})}{\epsilon^\mathrm{a}_\mathrm{k} - \epsilon^\mathrm{a}_{\mathrm{k}+\mathrm{q}}} + \sum_\mathrm{k} \frac{n_\mathrm{F}(\epsilon^\mathrm{a}_\mathrm{k}) - n_\mathrm{F}(\epsilon^\mathrm{b}_{\mathrm{k}+\mathrm{q}})}{\epsilon^\mathrm{a}_\mathrm{k} - \epsilon^\mathrm{b}_{\mathrm{k}+\mathrm{q}}}$$
$$+ \sum_\mathrm{k} \frac{n_\mathrm{F}(\epsilon^\mathrm{b}_\mathrm{k}) - n_\mathrm{F}(\epsilon^\mathrm{a}_{\mathrm{k}+\mathrm{q}})}{\epsilon^\mathrm{b}_\mathrm{k} - \epsilon^\mathrm{a}_{\mathrm{k}+\mathrm{q}}} + \sum_\mathrm{k} \frac{n_\mathrm{F}(\epsilon^\mathrm{b}_\mathrm{k}) - n_\mathrm{F}(\epsilon^\mathrm{b}_{\mathrm{k}+\mathrm{q}})}{\epsilon^\mathrm{b}_\mathrm{k} - \epsilon^\mathrm{b}_{\mathrm{k}+\mathrm{q}}}$$



Inosov arXiv:0805.4105, arXiv:0807.3929

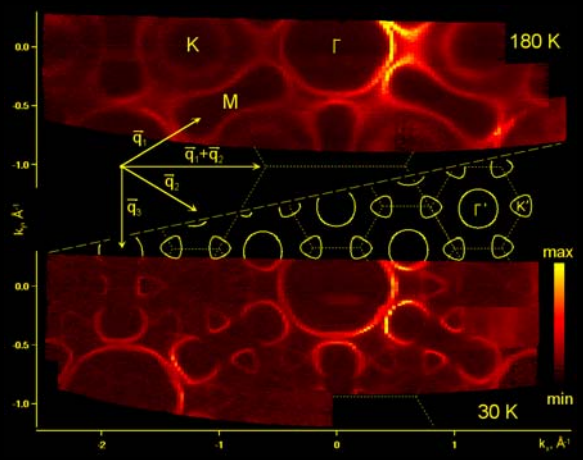
Electron susceptibility

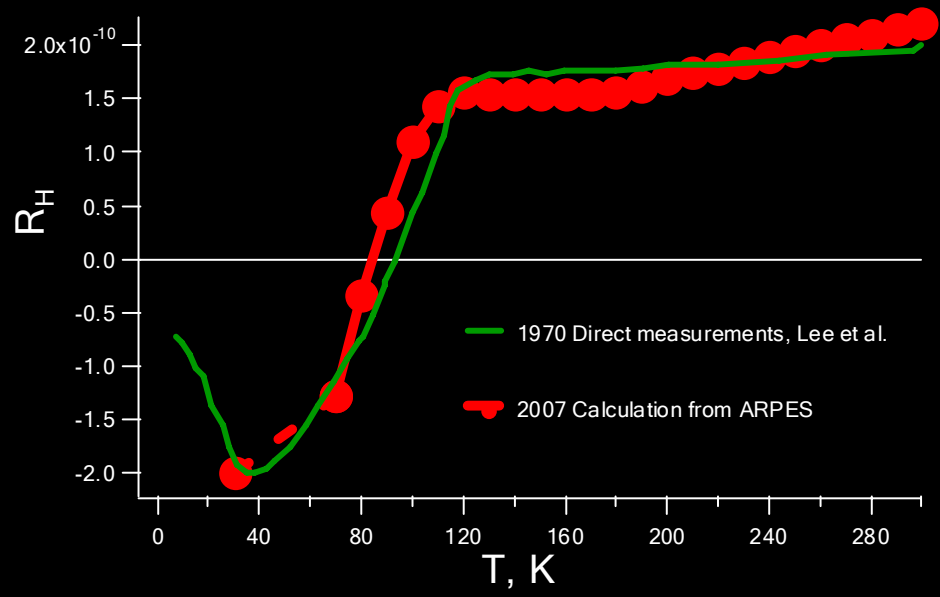




Inosov arXiv:0805.4105, arXiv:0807.3929

Hall coefficient of 2H-$TaSe_2$ from ARPES



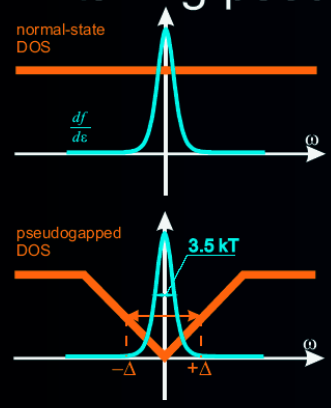


Hall coefficient from electronic structure

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

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

taking pseudogap into account

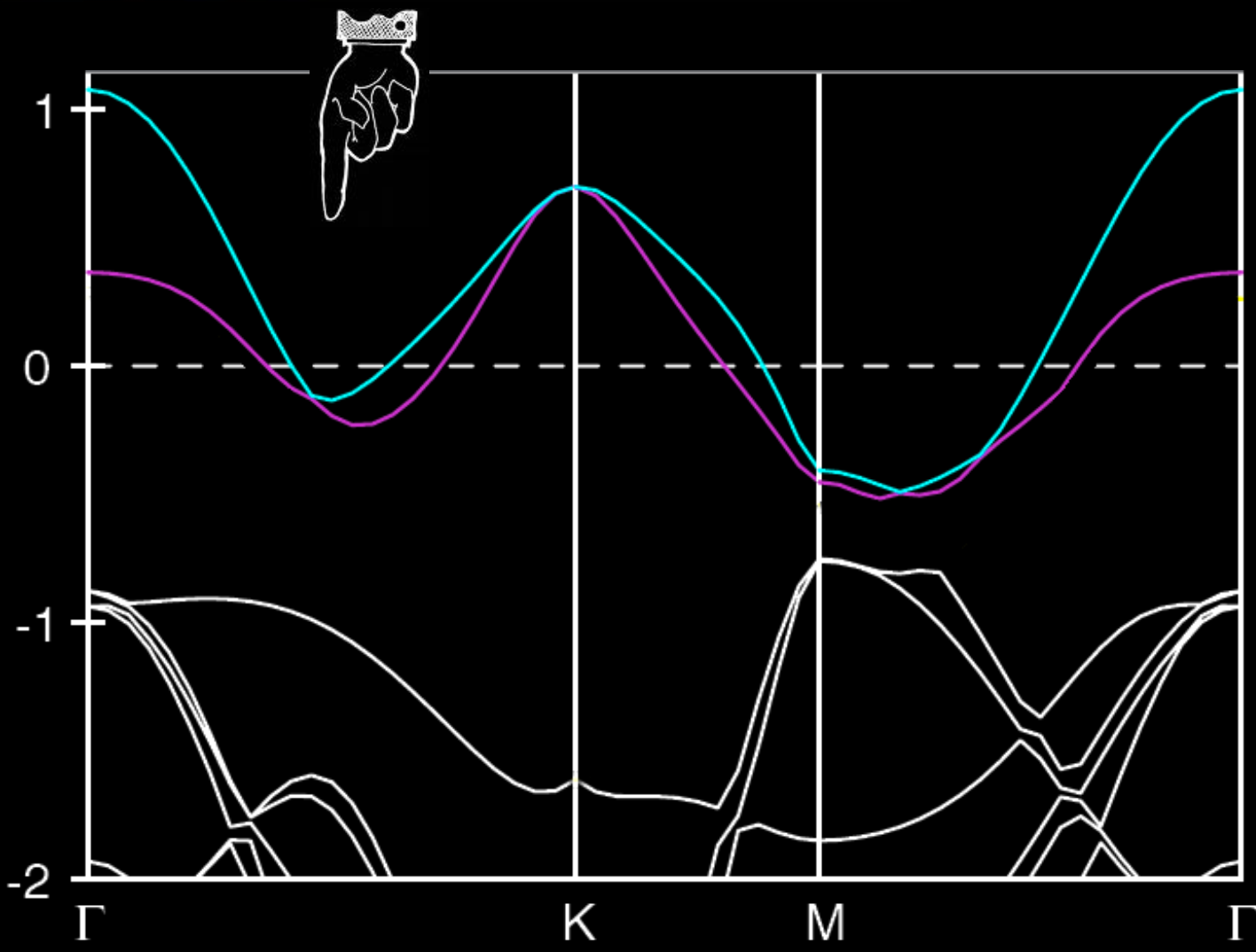


$$D(\mathbf{k}) = -\int_{-\infty}^{\infty} \frac{df}{d\varepsilon} \cdot A(\varepsilon, \mathbf{k}) \cdot d\varepsilon \le 1$$

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

Evtushinsky *PRL* 2008

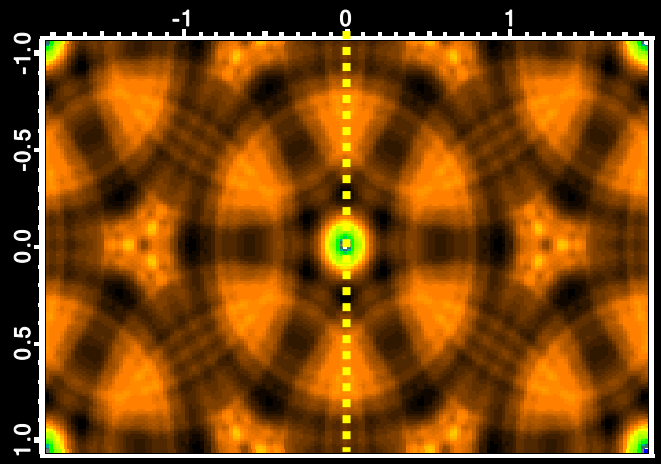
Band structure of 2H- $NbSe_2$



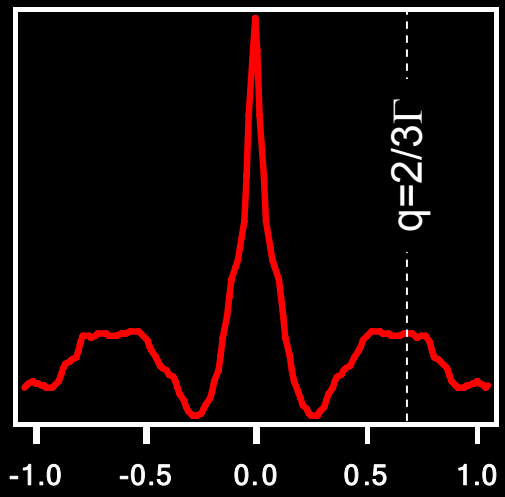
M
„dogbones“

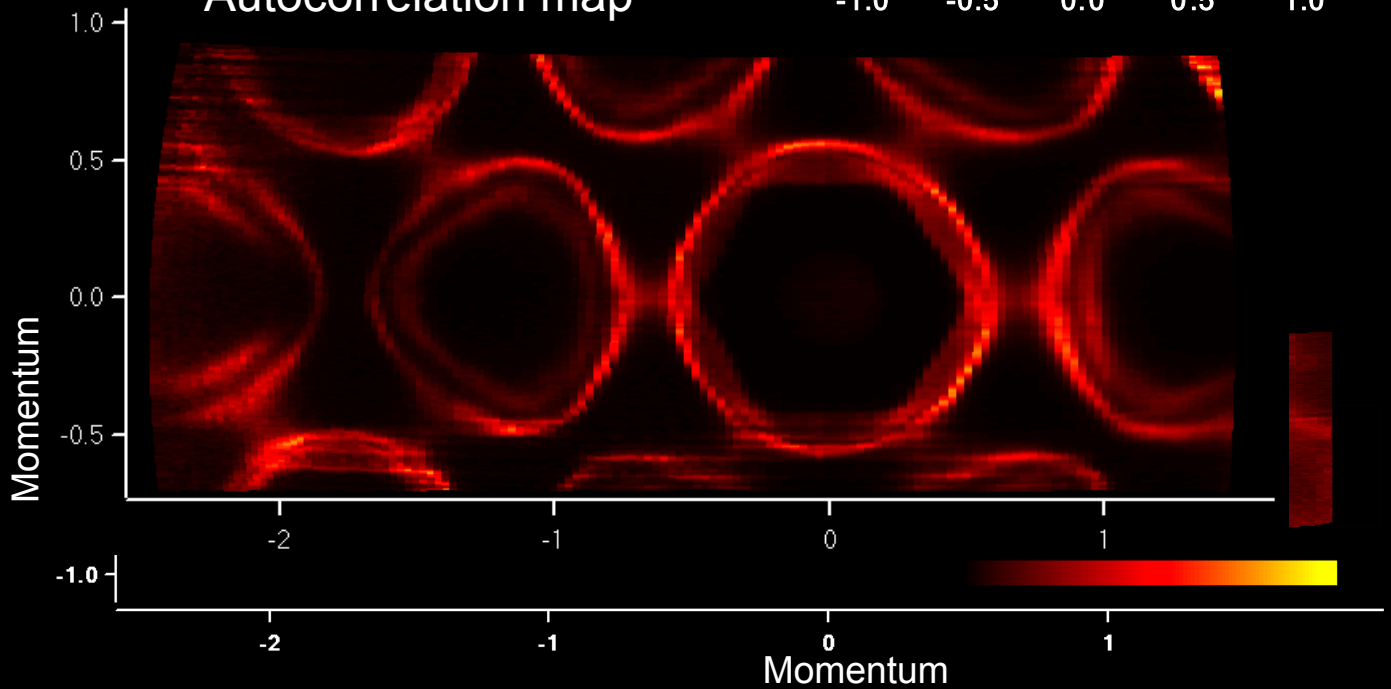
Γ, K
„barrels“

Modification of the nesting properties



Autocorrelation map



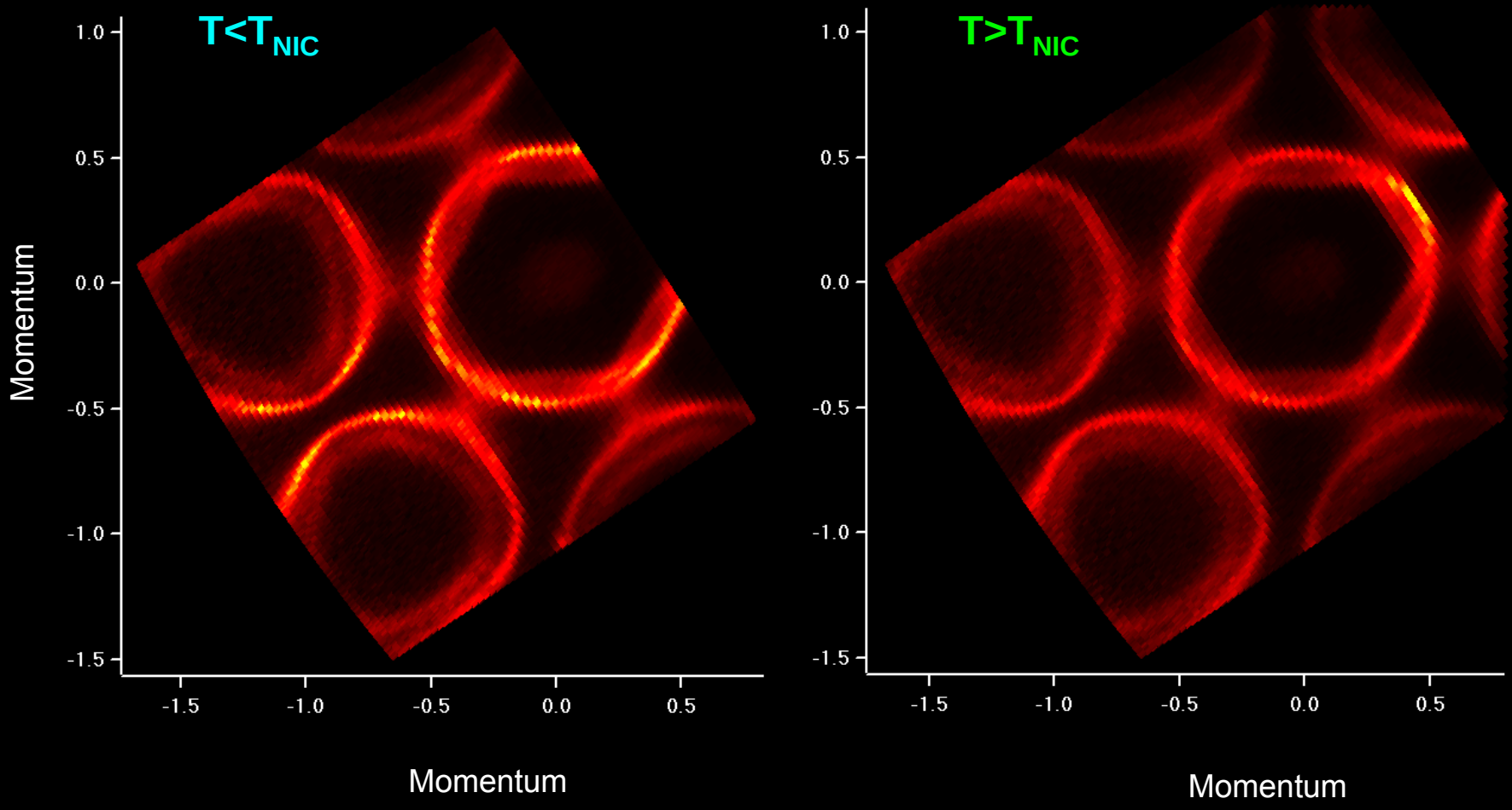


2H-$NbSe_2$

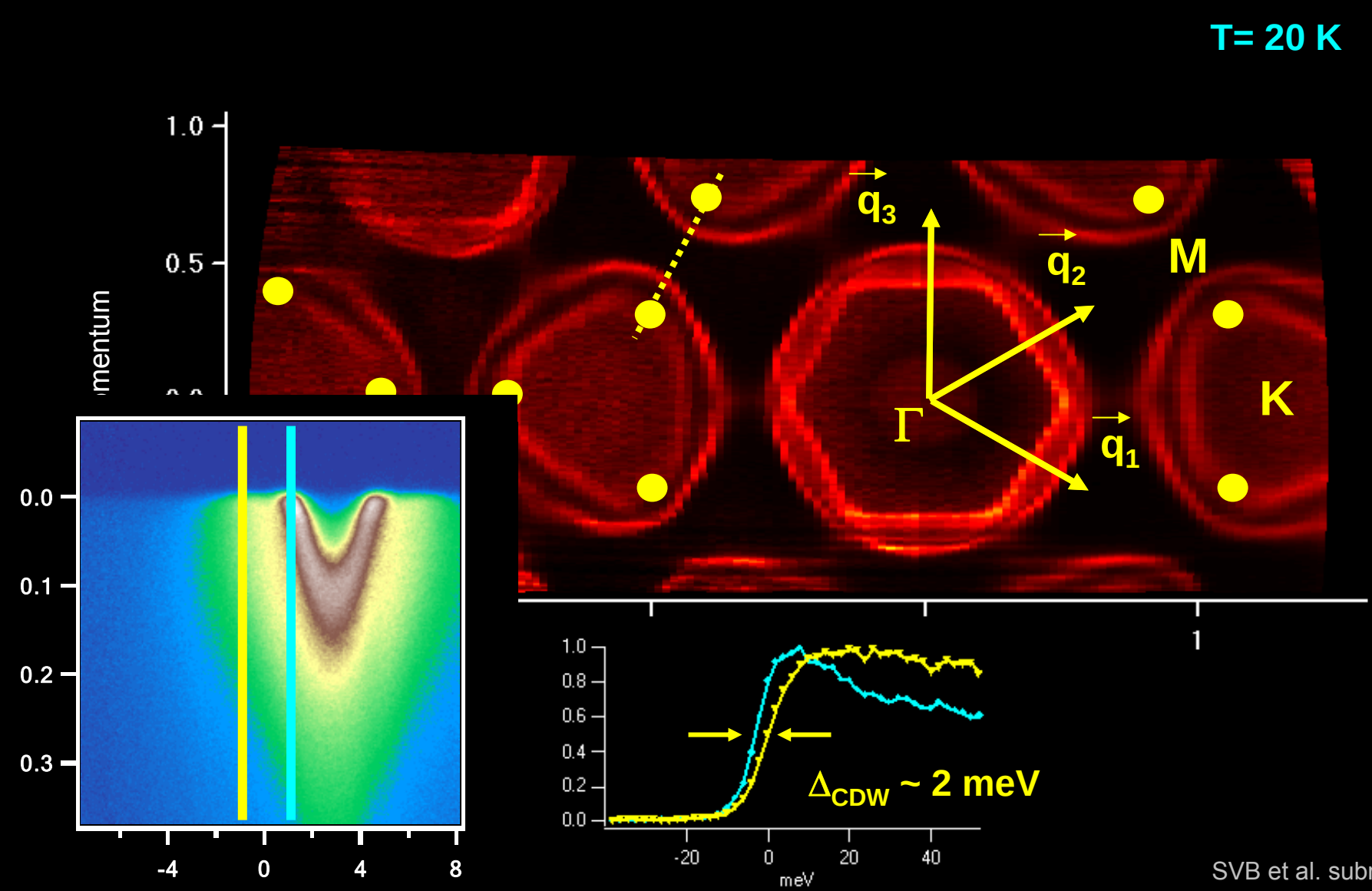
T_{NIC}~ 33 K

T_C= 7.2 K

Fermi surface of 2H-$NbSe_2$

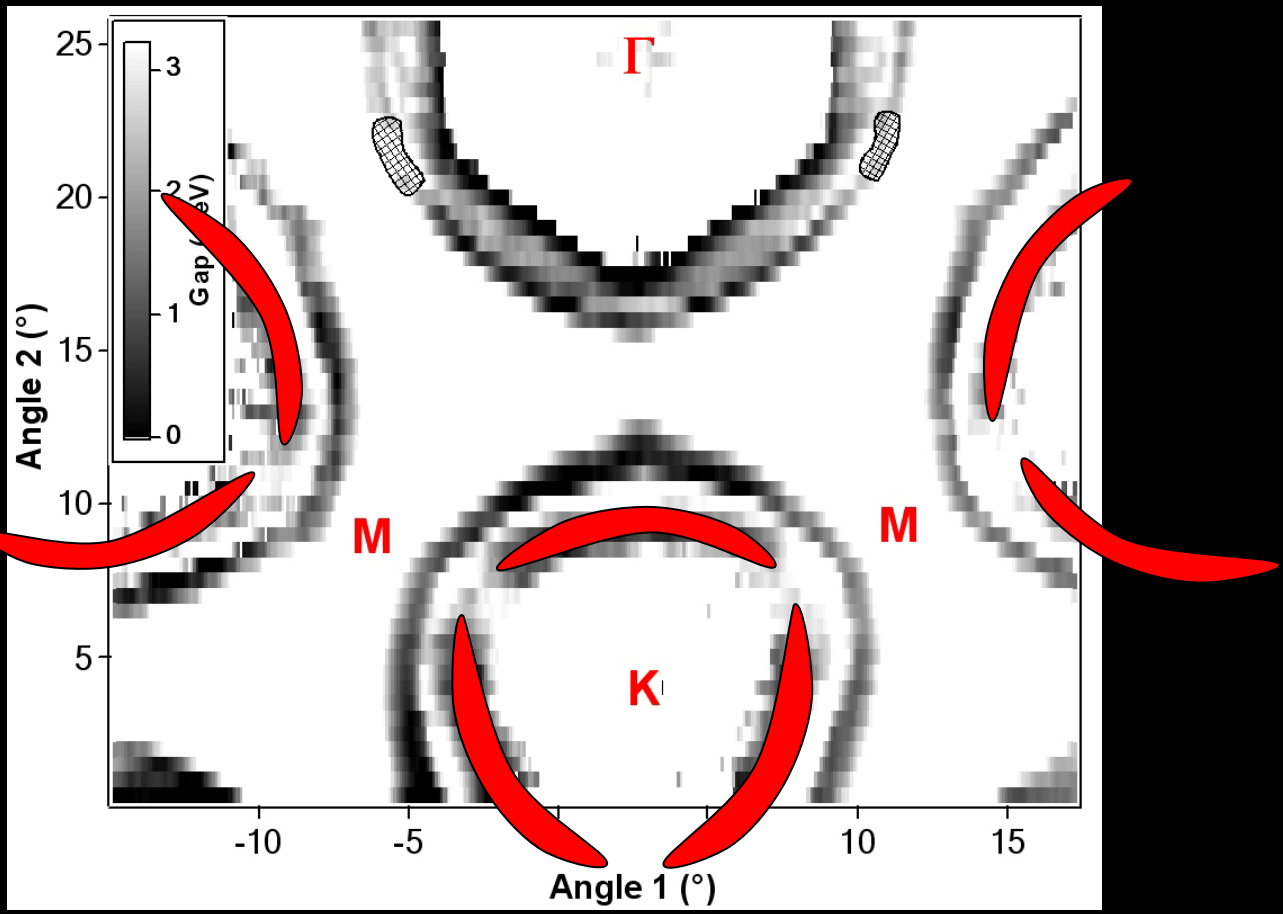


Incommensurate CDW state in 2H-$NbSe_2$



SVB et al. submitted

Fermi surface "arcs" in $NbSe_2$



Map of gaps, 20 K

Charge Density Waves compounds

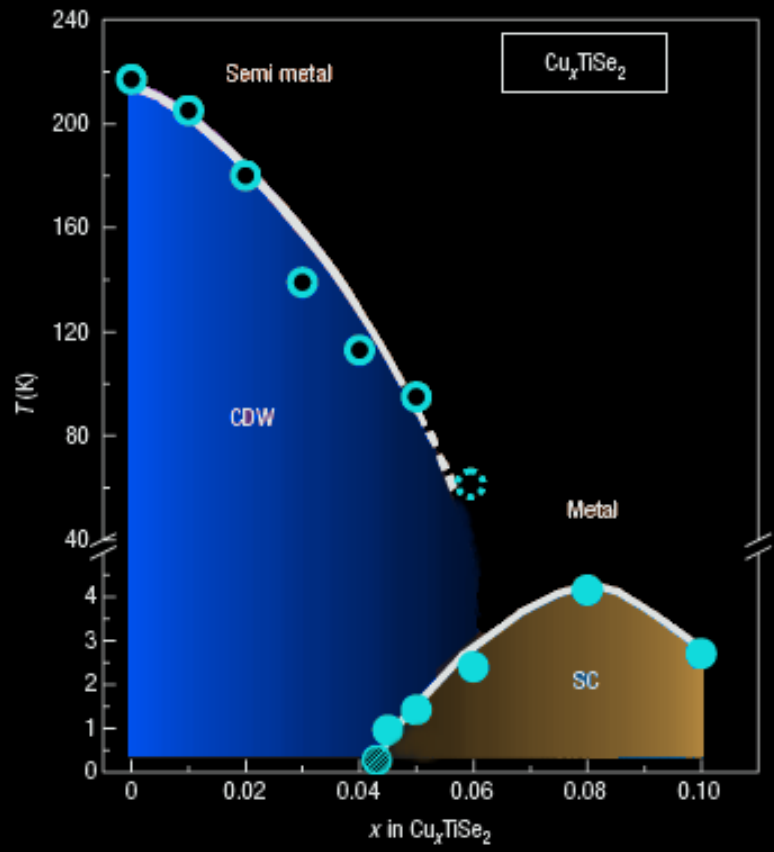
1T-TaS_2, T_0= 550 K

$TiSe_2$, 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?

Hall coefficient in cuprates and 2D-CDWs

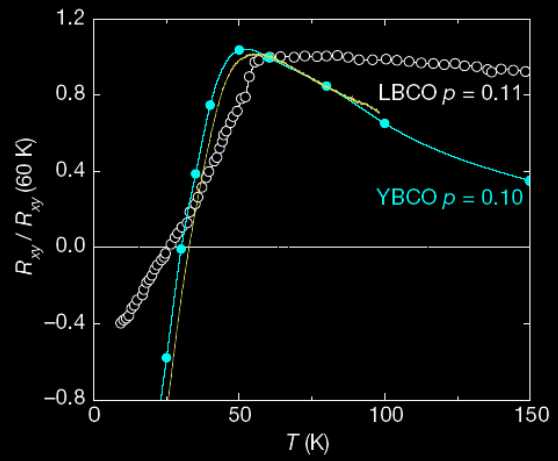


Figure 1 | Hall resistance of LBCO and YBCO. Hall resistance R_{xy} versus T,

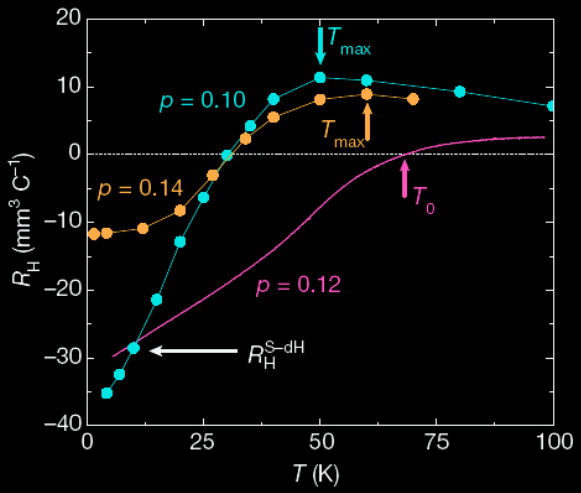


Figure 3 | Normal-state Hall coefficient versus temperature. Hall coefficient R_H versus T for Y123-II, Y123-VIII and Y124 (data multiplied by ten), at

D. Le Boeuf et al. , Nature (2007)

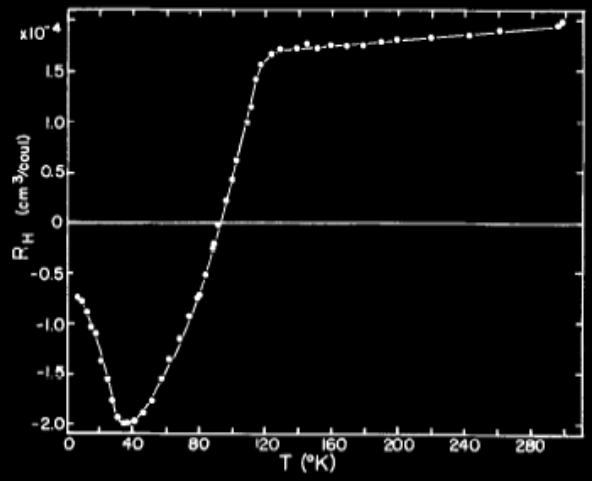


FIG. 4. The Hall coefficient vs. temperature for $TaSe_2$.

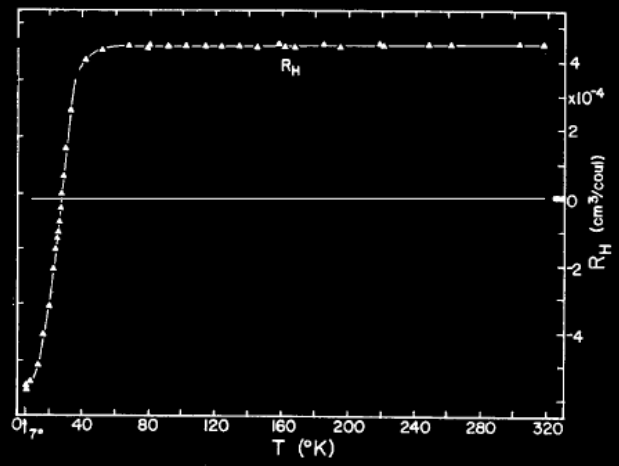


FIG. 1. The resistivity and Hall coefficient of $NbSe_2$ as a function of temperature.

Lee et al. , J. Solid State Chem. (1970)

High-Temperature Superconductors

$HgBa_2Ca_2Cu_3O_{8+x}$, T_C= 138 K

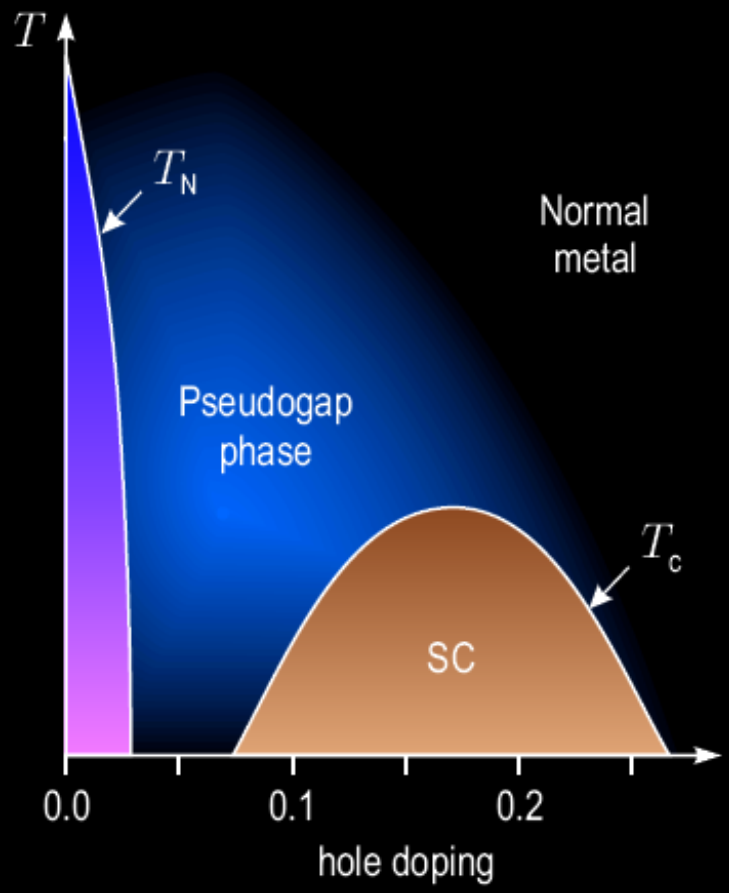
$Tl_2Ca_2Ba_2Cu_3O_{10}$, T_C= 125 K

$YBa_2Cu_3O_7$, T_C= 92 K

$Bi_2Sr_2CaCu_2O_{8+x}$, T_C= 91 K

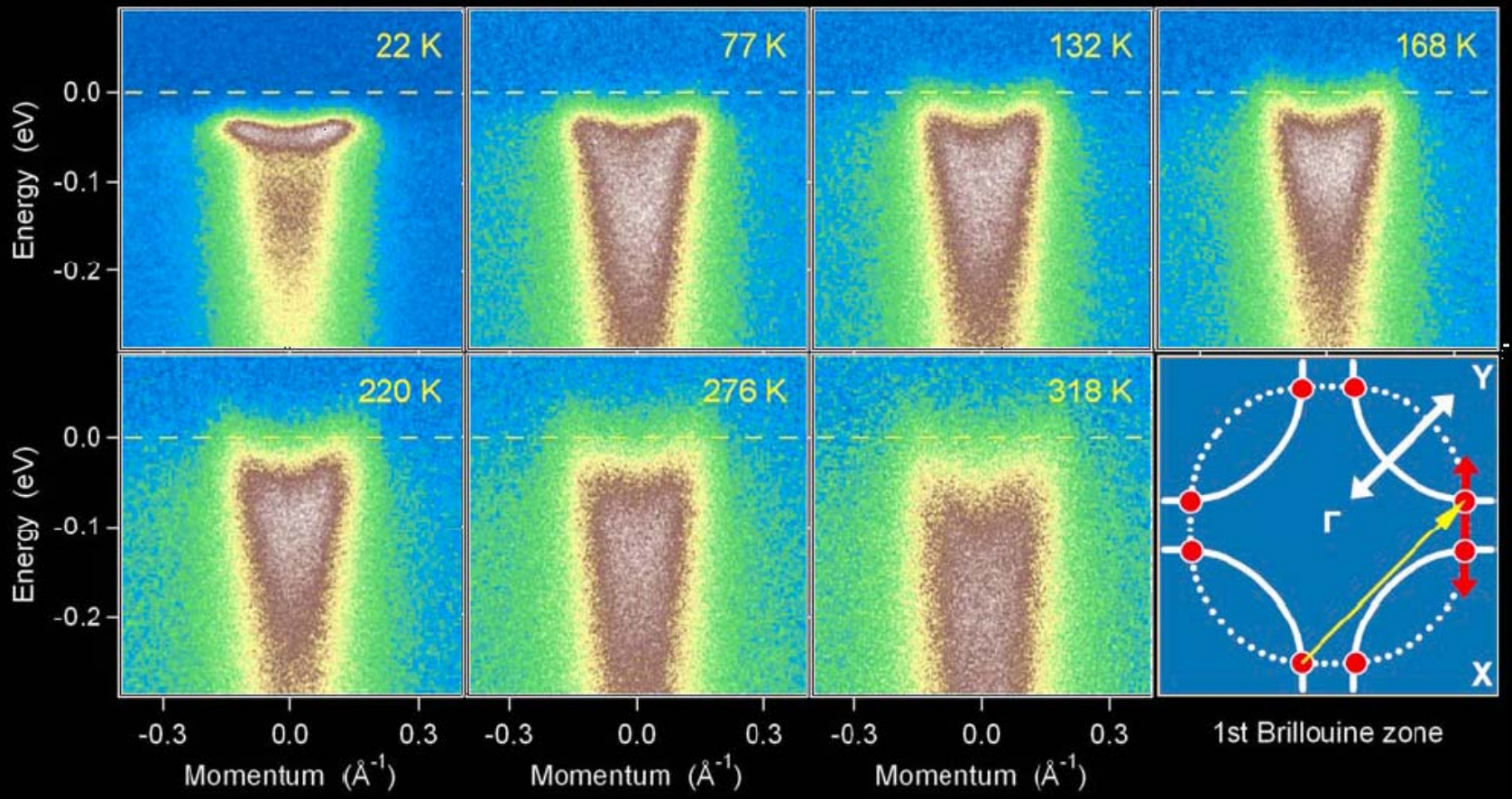
$La_{1.85}Sr_{0.15}CuO_4$, T_C= 39 K

$Nd_{1.85}Ce_{0.15}CuO_4$, T_C= 24 K



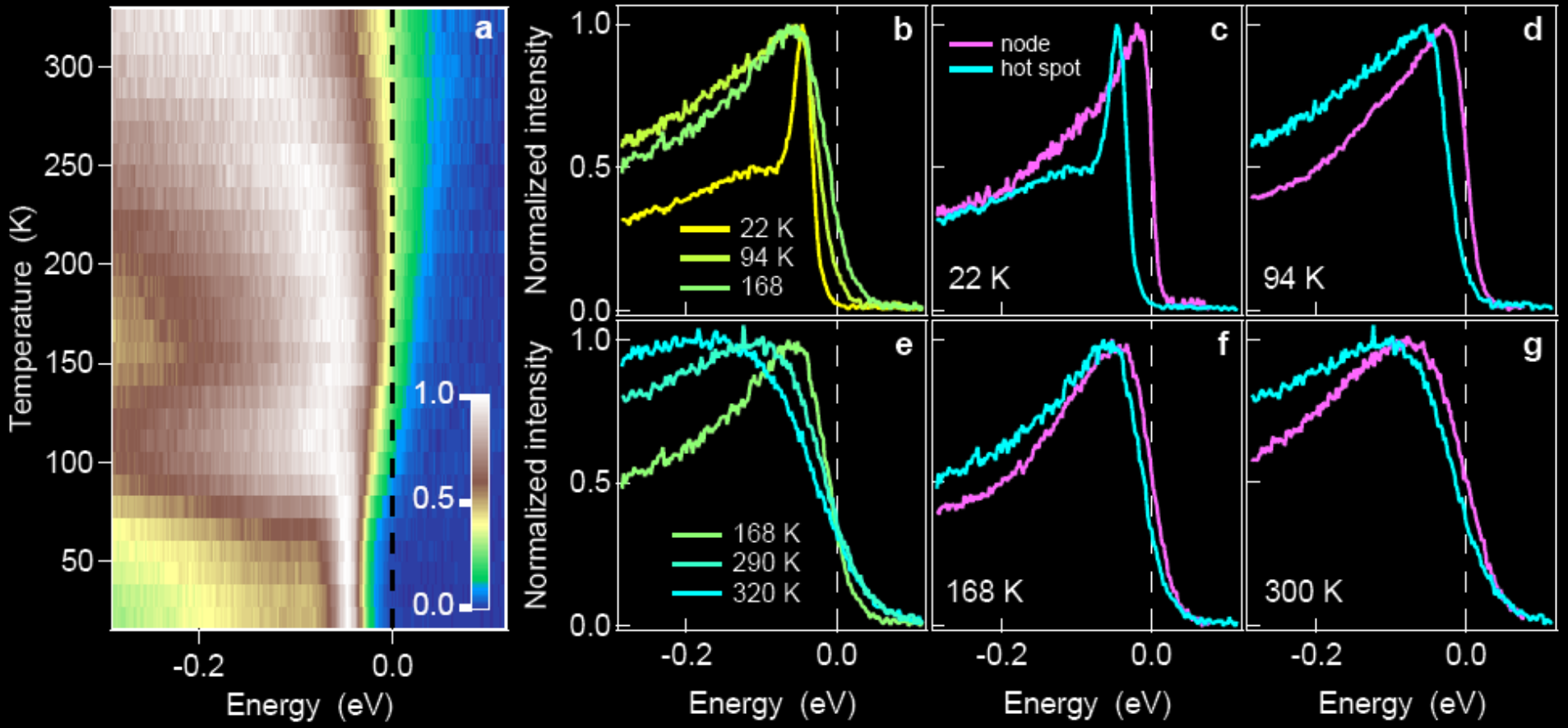
BSCCO

Non-monotonic pseudo-gap in BSCCO



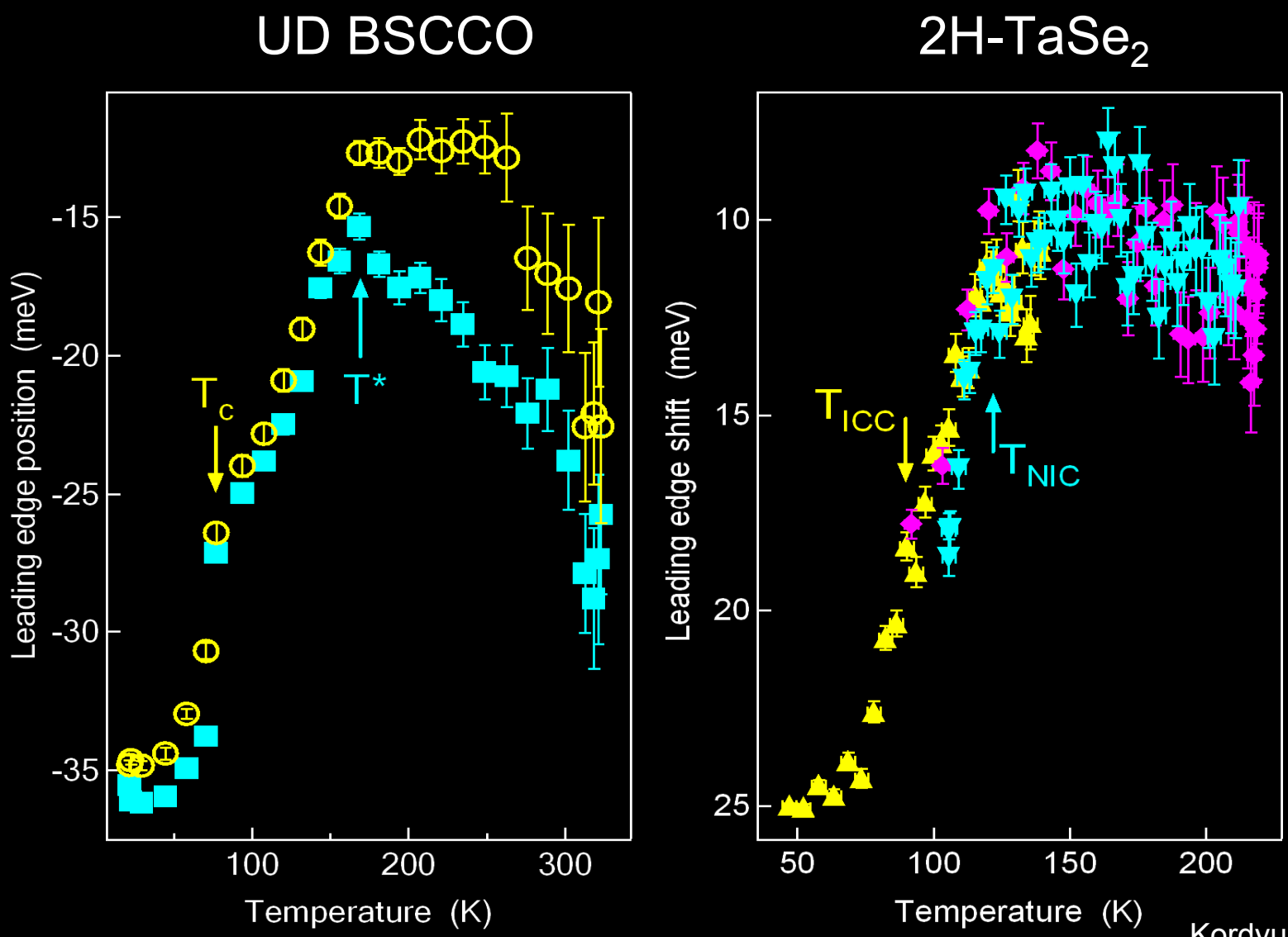
Kordyuk arXiv:0801.2546

Non-monotonic pseudo-gap in BSCCO



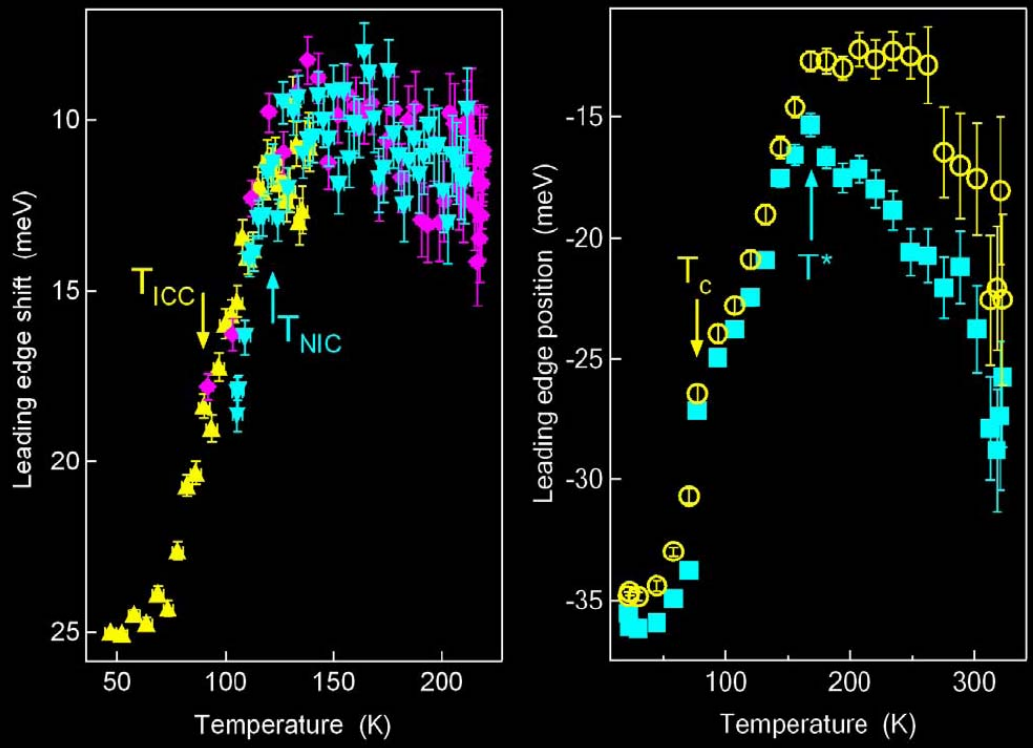
Kordyuk arXiv:0801.2546

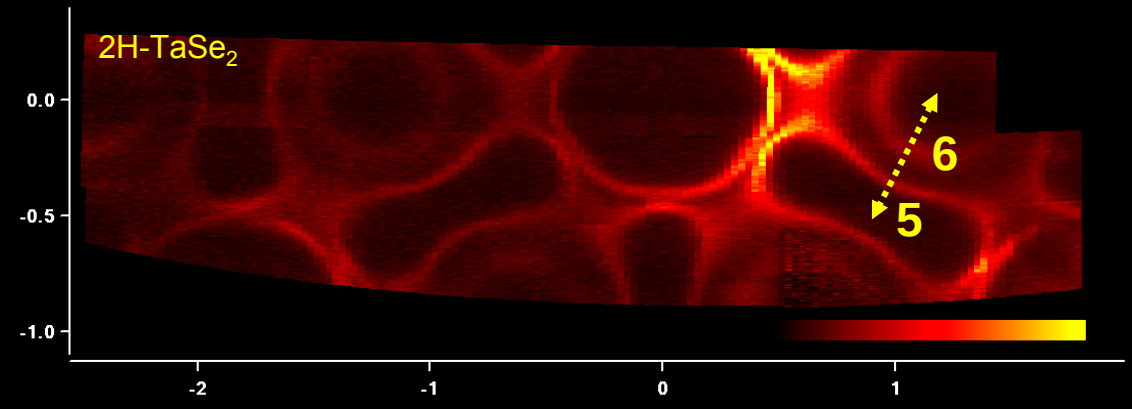
Non-monotonic pseudo-gap in BSCCO

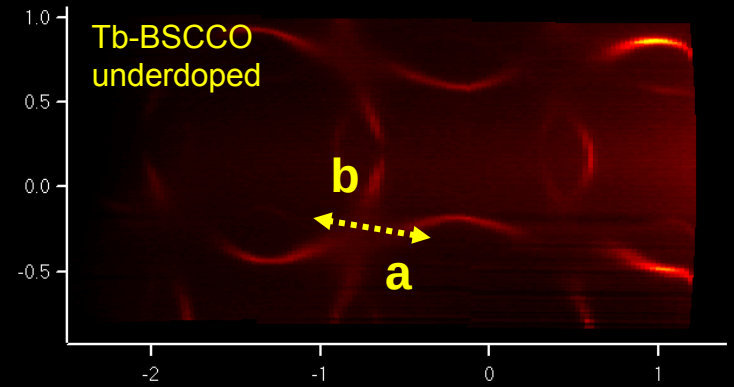


Kordyuk arXiv:0801.2546

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







Pseudogap in cuprates?

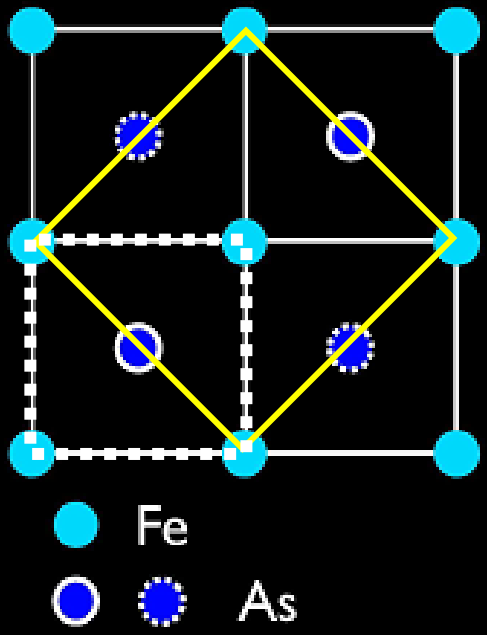
- ✓ PG and SG are two different gaps
- ✓ Pseudo-gap = Density modulation (incommensurate SDW)
- ✓ PG and SG compete for the phase space but both depend on electronic band structure

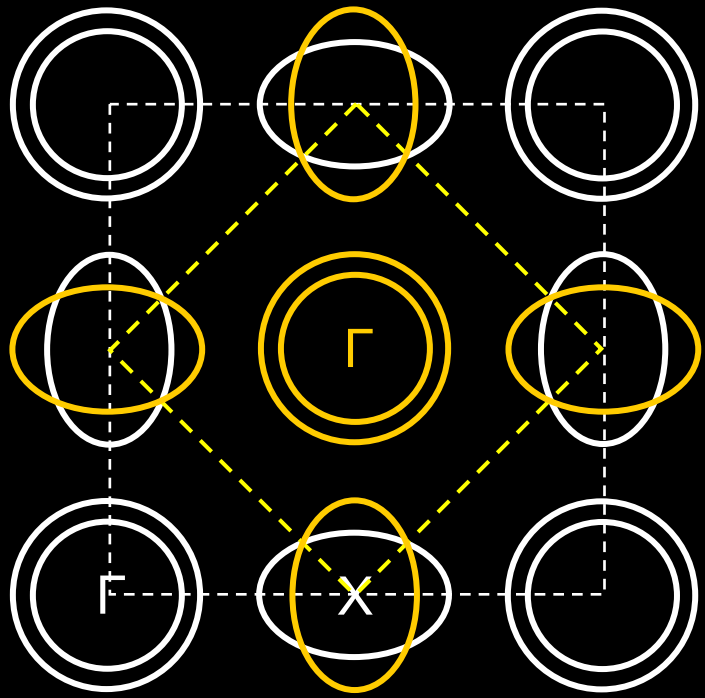
It seems that the electronic structure of both cuprates and dichalcogenides is unstable to a density wave formation.

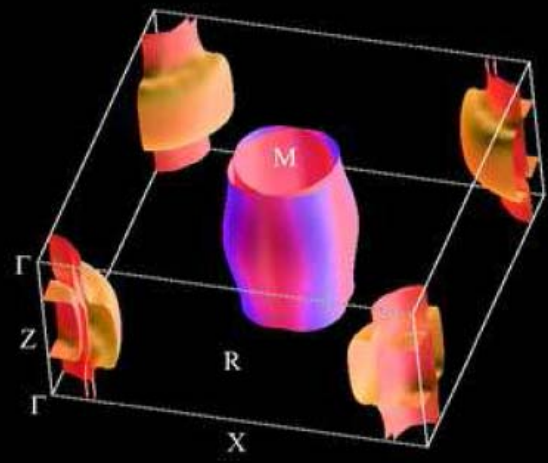
Are the cuprates and dichalcogenides unique in this sence?

Superconducting pnictides (BKFA)

Fermi surface of pnictides (calculated)

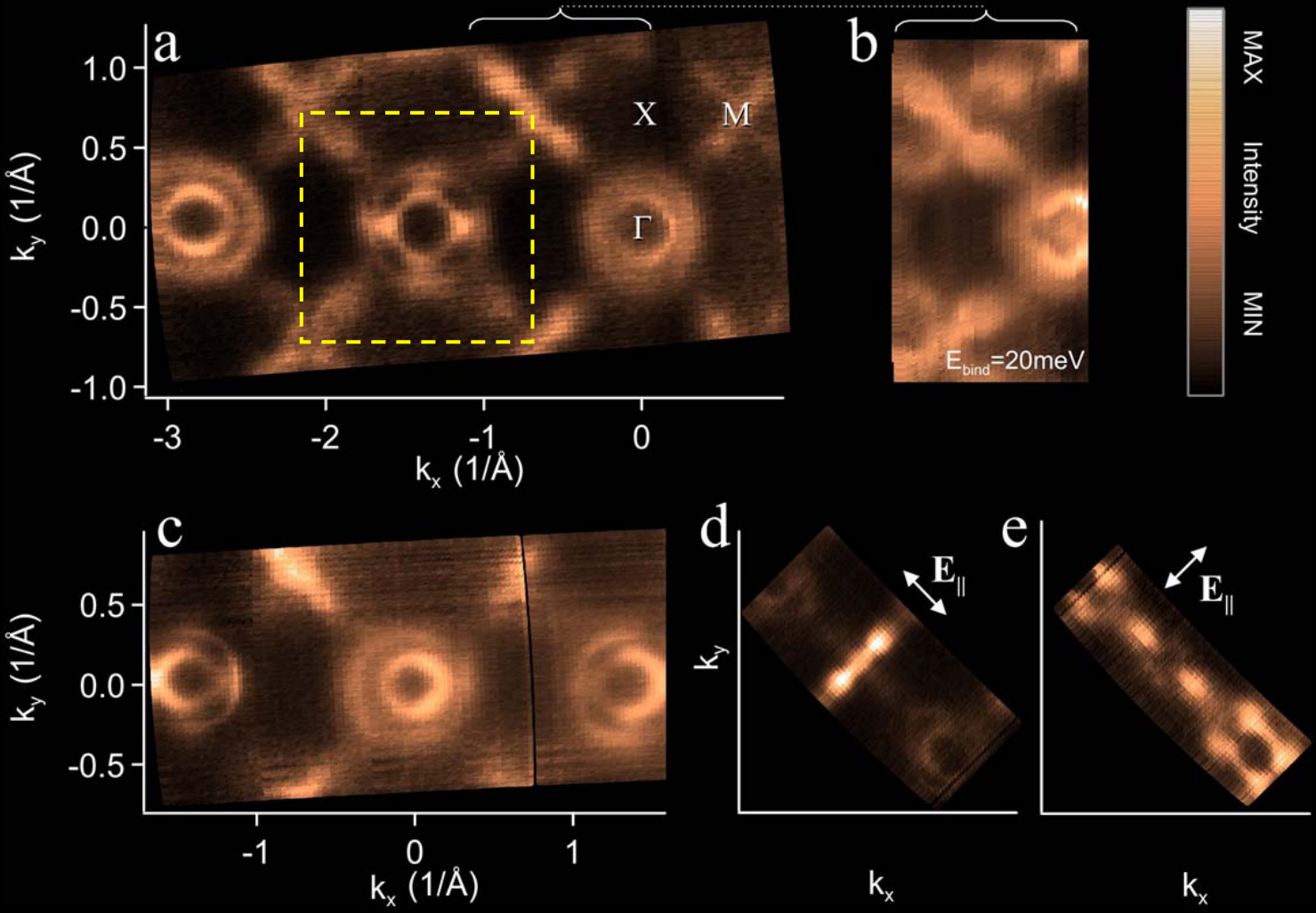






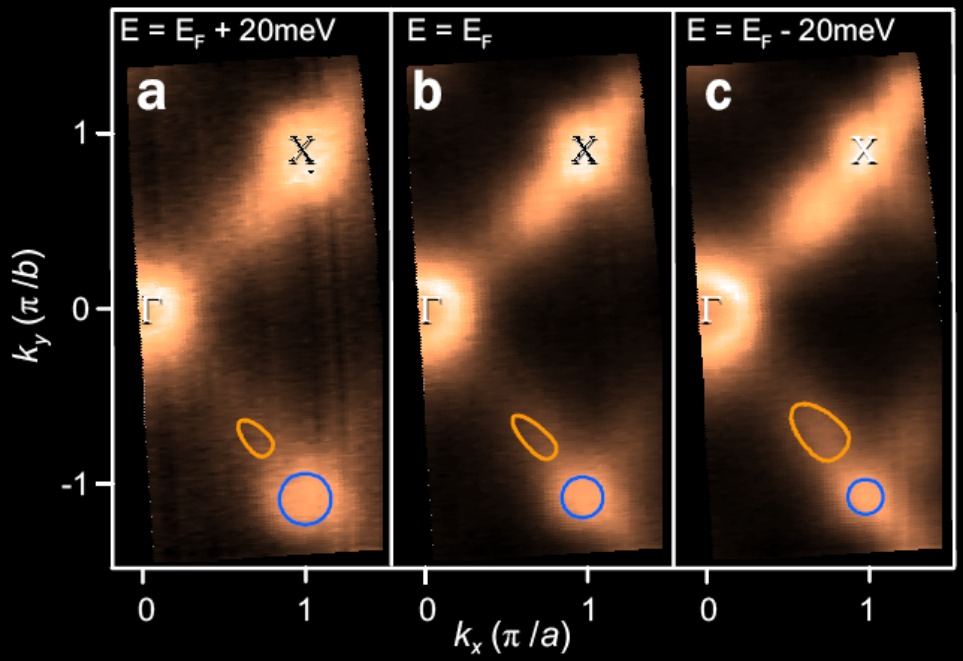
Korshunov & Eremin MPI 2008
Singh arXiv:0803.0429
Mazin arXiv:0803.2740

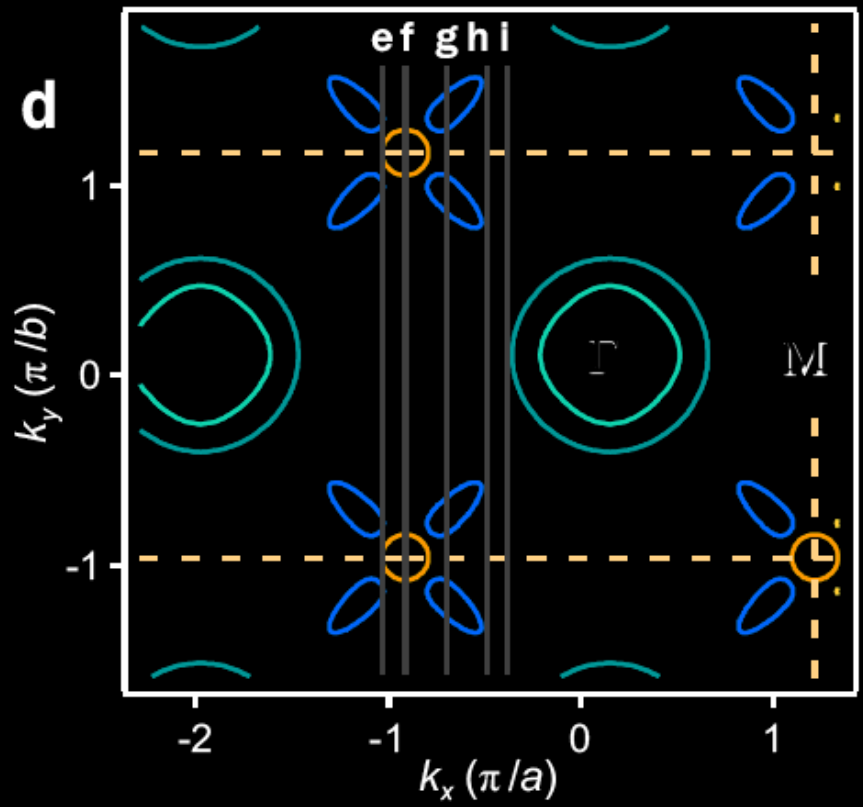
Fermi surface of BKFA (our experiment)



Zabolotnyy arXiv:0808.2454

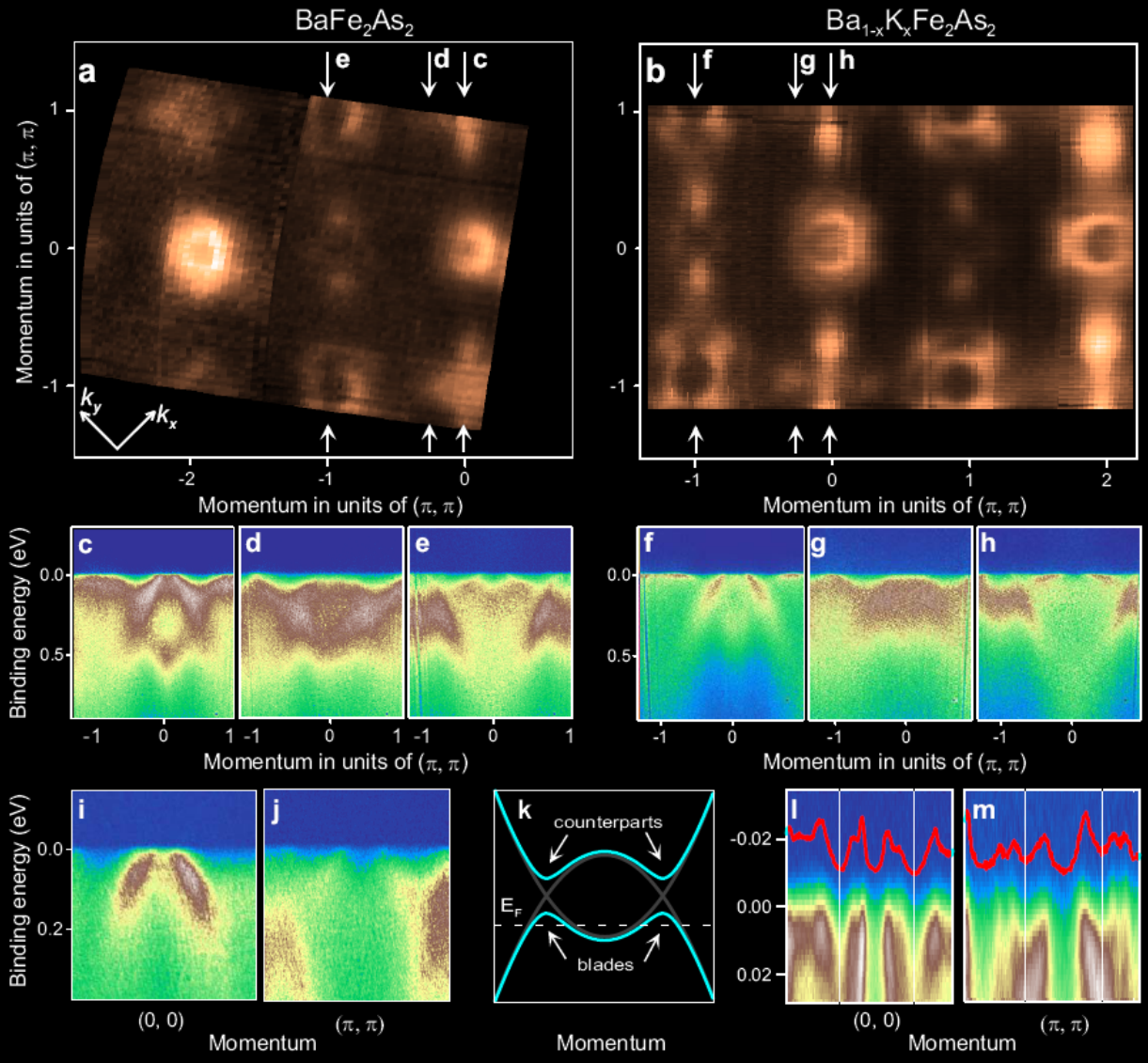
Fermi surface of BKFA (our experiment)



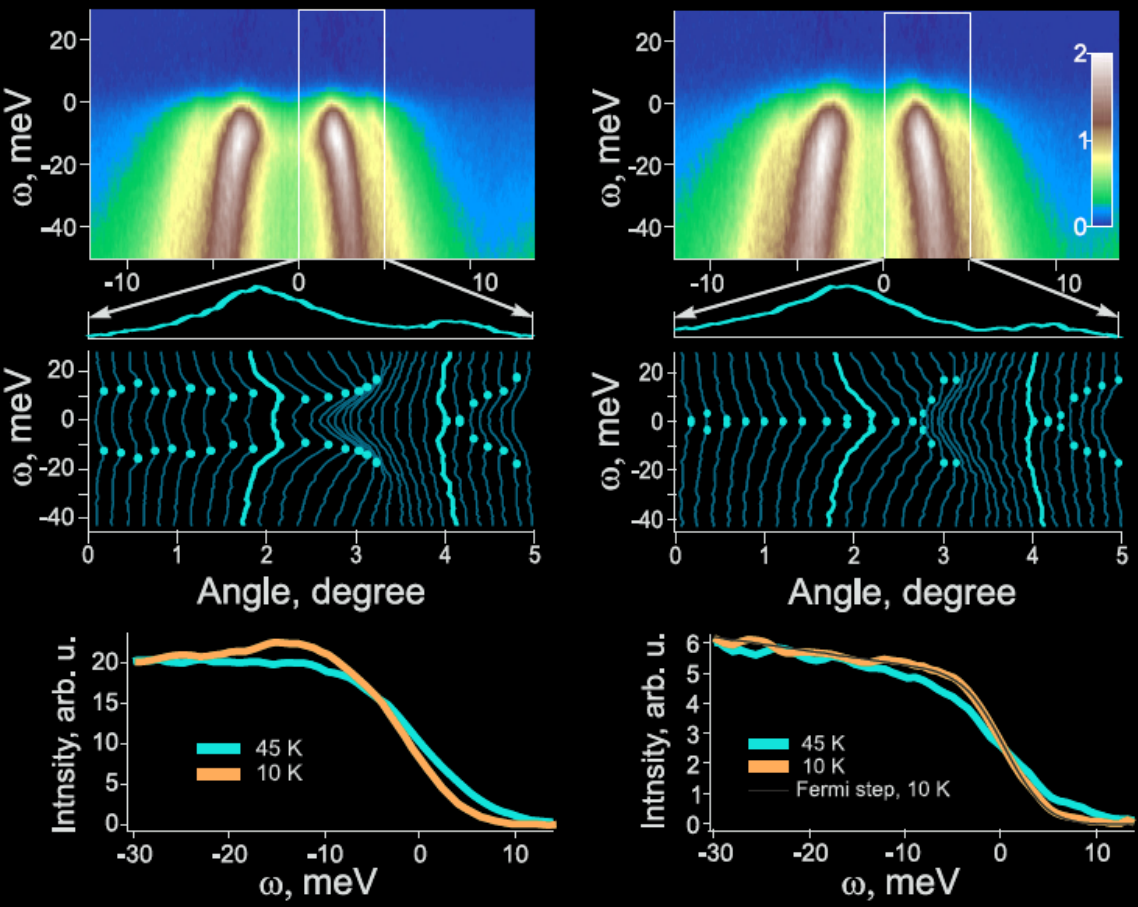


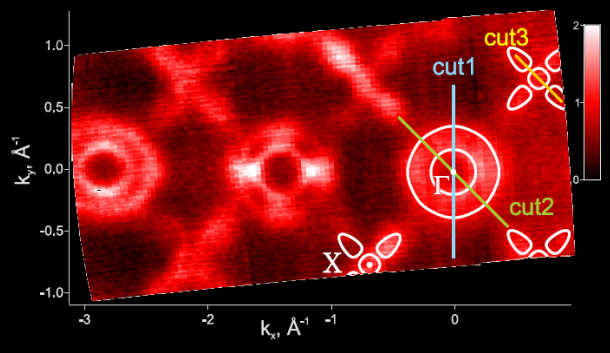
Zabolotnyy arXiv:0808.2454

Fermi surface of BKFA (our experiment)



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

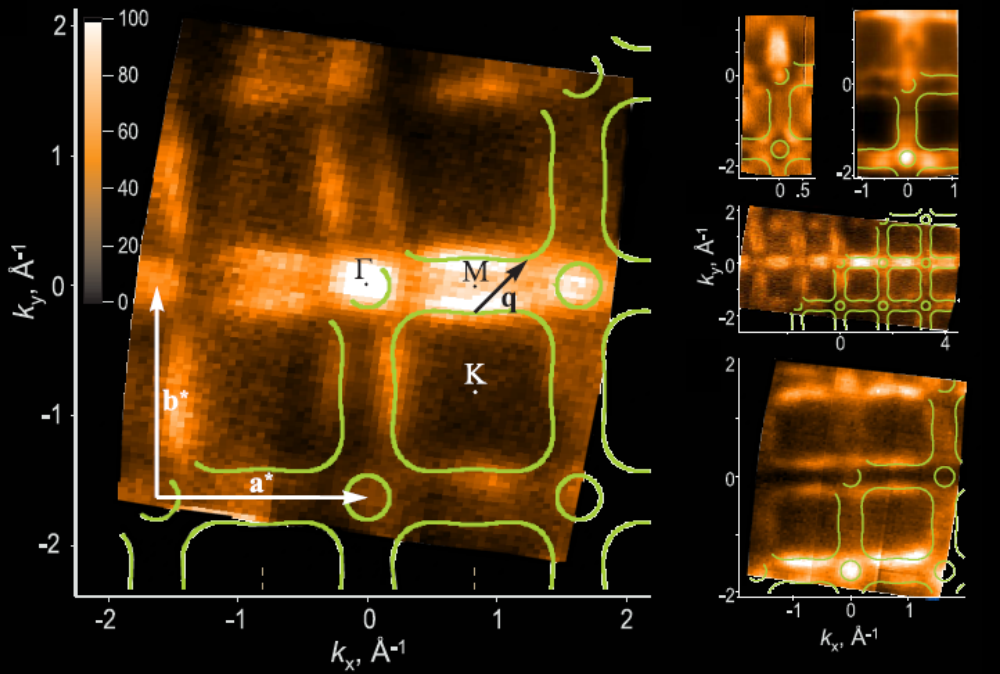
Evtushinsky arXiv:0809.4455

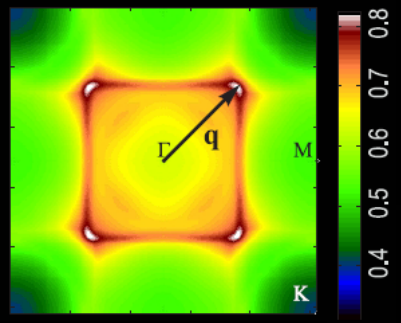
Ordering in pnictides?

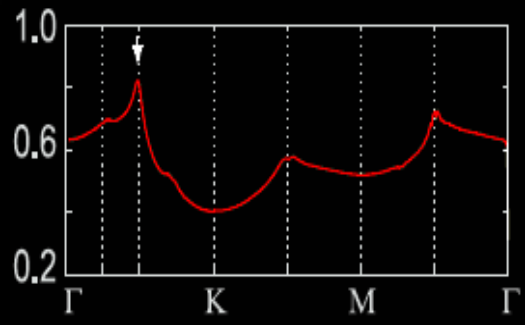
- ✓ Electron density in pnictides shows (π, π) ordering already in the normal state

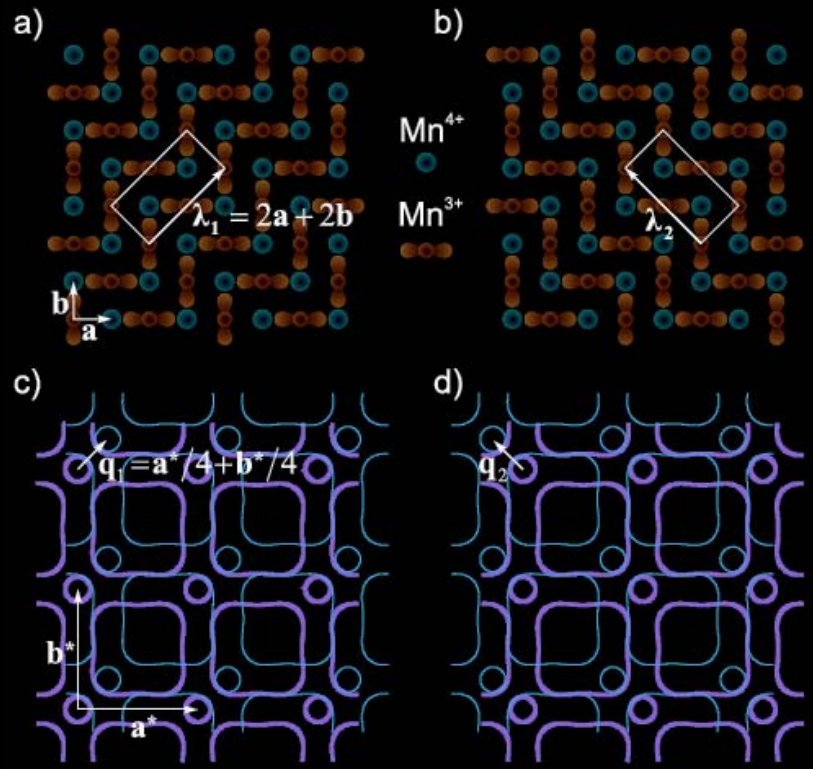
- ? Isn't a general property of 2D metals?

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



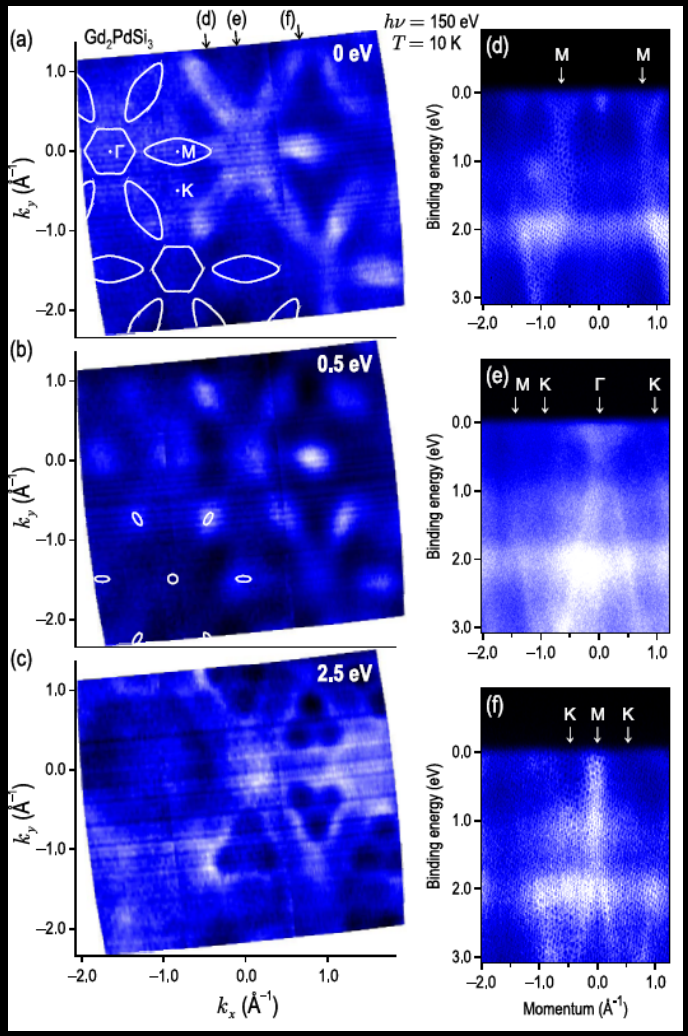


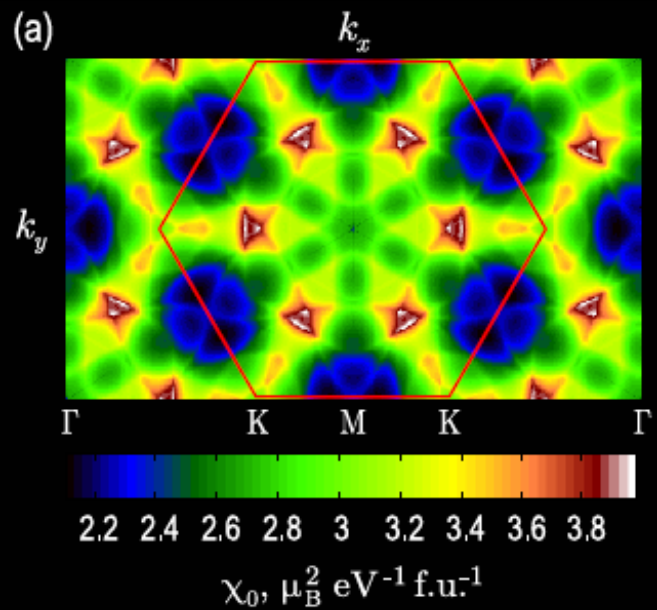


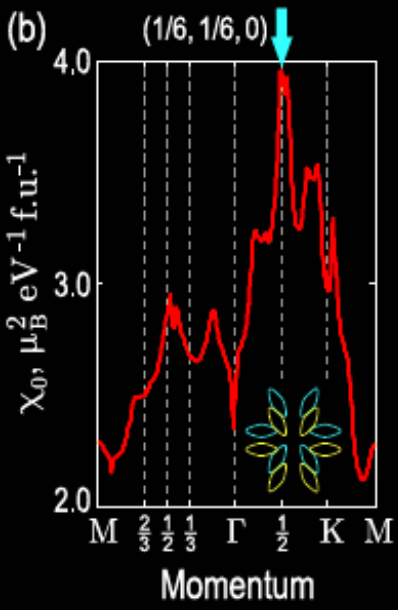


Evtushinsky 2008

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







Inosov arXiv:0808.2898

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

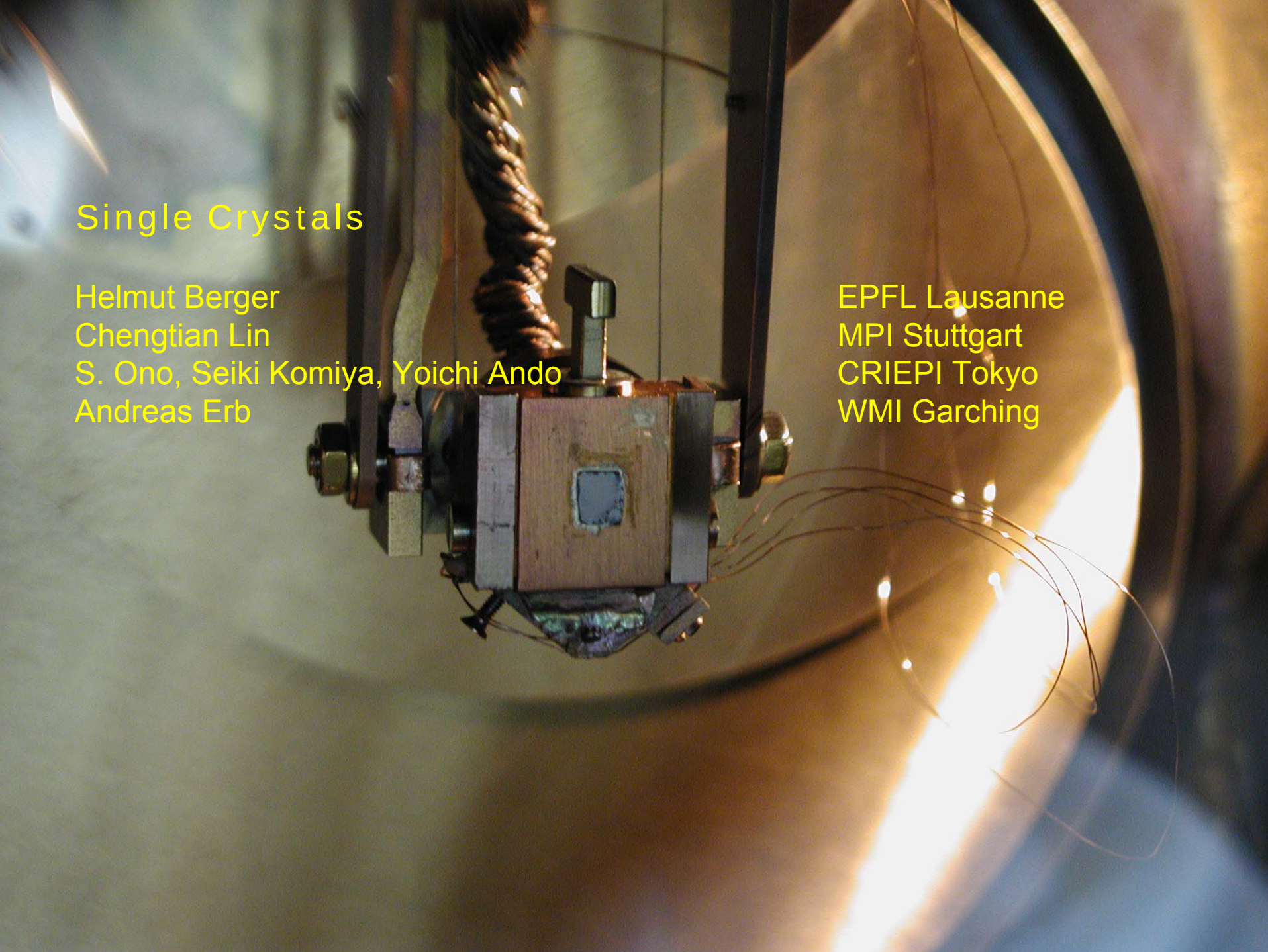
Thanks to:

Spectroscopy Group IFF, IFW Dresden

Sergey Borisenko,
Volodya Zabolotny, Dima Inosov, Daniil Evtushinskiy, Roman Schuster
Roland Hübel, Martin Knupfer, Jörg Fink, Bernd Büchner

Neutrons:
Vladimir Hinkov, Bernhard Keimer (Stuttgart)

Theory:
Alexander Yaresko, Iliya Eremin (Dresden),
Thomas Dahm (Tübingen), Doug Scalapino (Santa Barbara)



Single Crystals

Helmut Berger	EPFL Lausanne
Chengtian Lin	MPI Stuttgart
S. Ono, Seiki Komiya, Yoichi Ando	CRIEPI Tokyo
Andreas Erb	WMI Garching

Synchrotron Light

Rolf Follath, Andrei Varykhalov — BESSY Berlin
Stefano Turchini, Cesare Grazioli — ELETTRA Trieste
Ming Shi, Luc Patthey — SLS Villigen