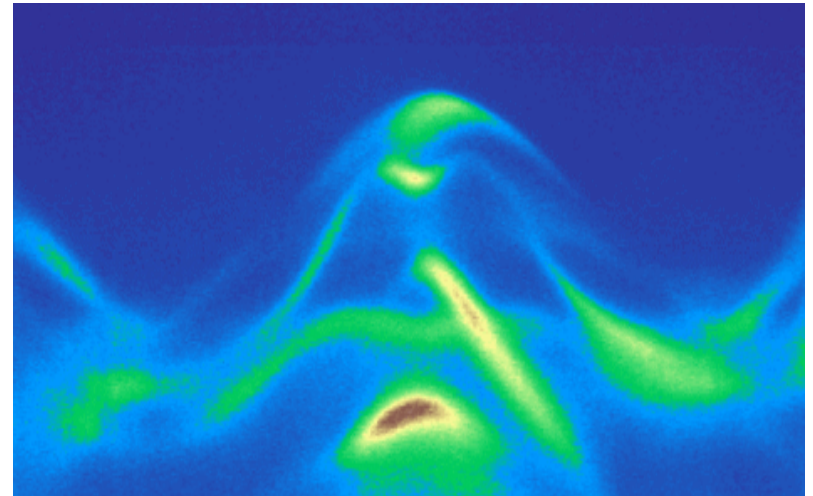
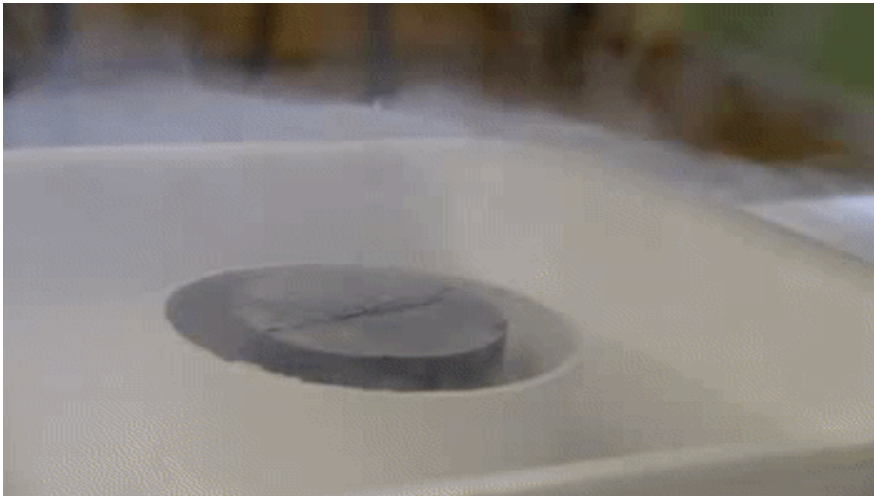


Superconductivity and Electronic Structure

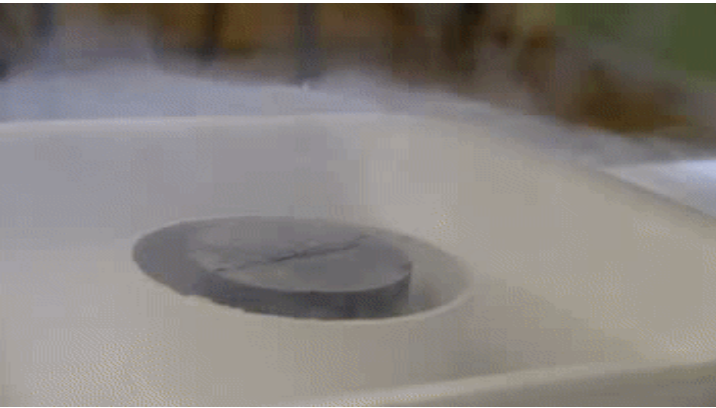


[Alexander Kordyuk](#)

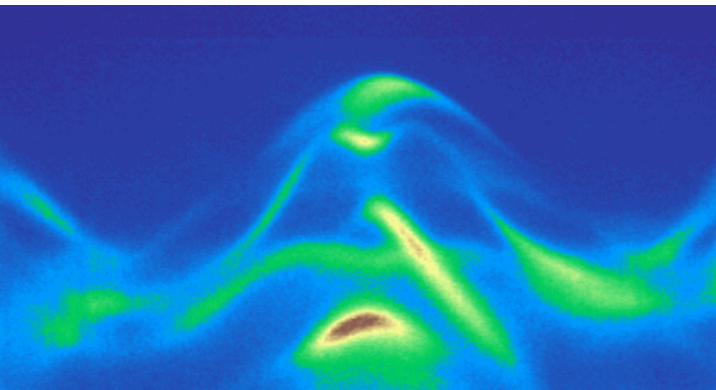
[Kyiv Academic University](#) & Institute for Metal Physics, NAS of Ukraine

kordyuk@gmail.com

Plan



- Introduction to superconductivity



- Electronic band structure and high temperature superconductivity

Introduction to superconductivity

- The phenomenon, models and properties (history)
- Vortex matter
- Microscopic theory, T_c and Δ
- Application of superconductors
- Cuprates and theory of HTSC
- Iron-based superconductors
- Towards RTSC

The story of superconductivity started from LHe

1908

He \longrightarrow LHe



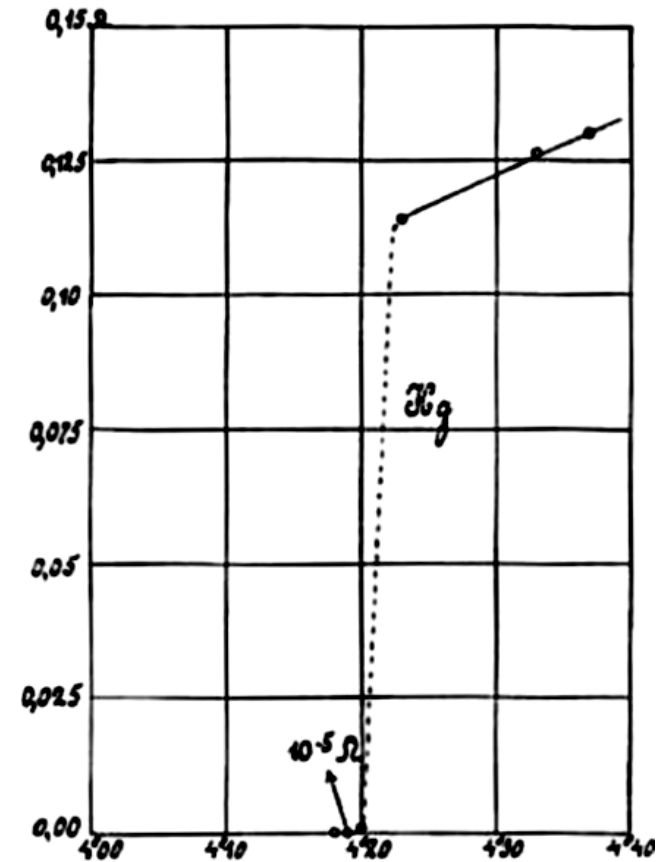
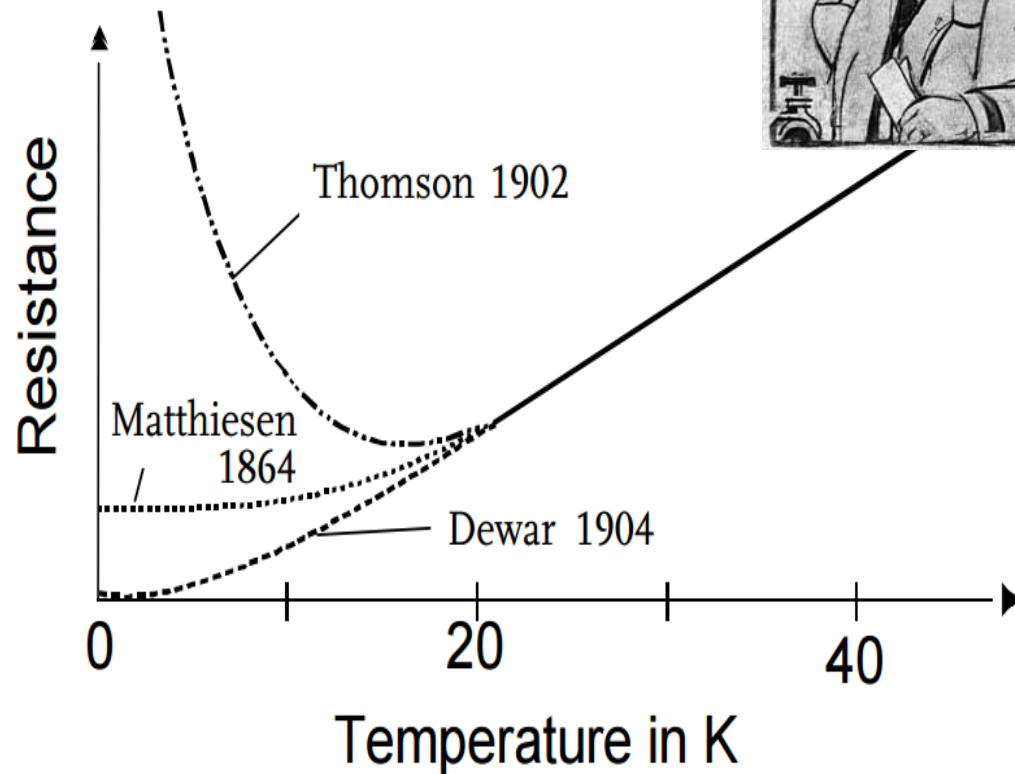
Heike Kamerlingh Onnes
1853-1926



$T_{\text{boiling}} = 4.2 \text{ K} = -269 \text{ }^{\circ}\text{C}$

The history of superconductivity: the beginning

1911

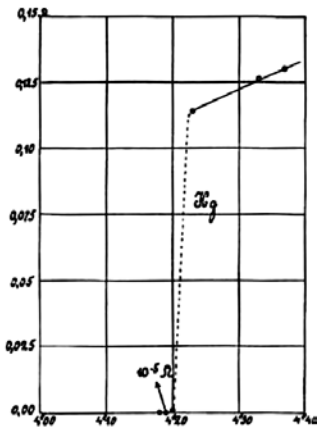


Hg, $T_c = 4.2\text{K}$

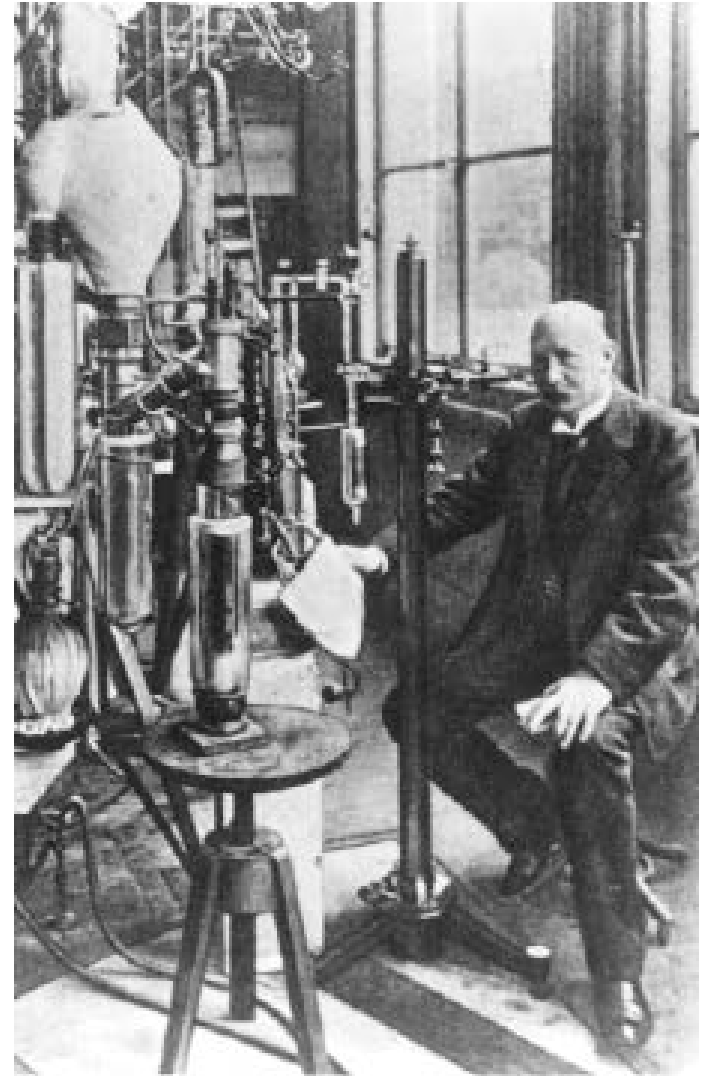
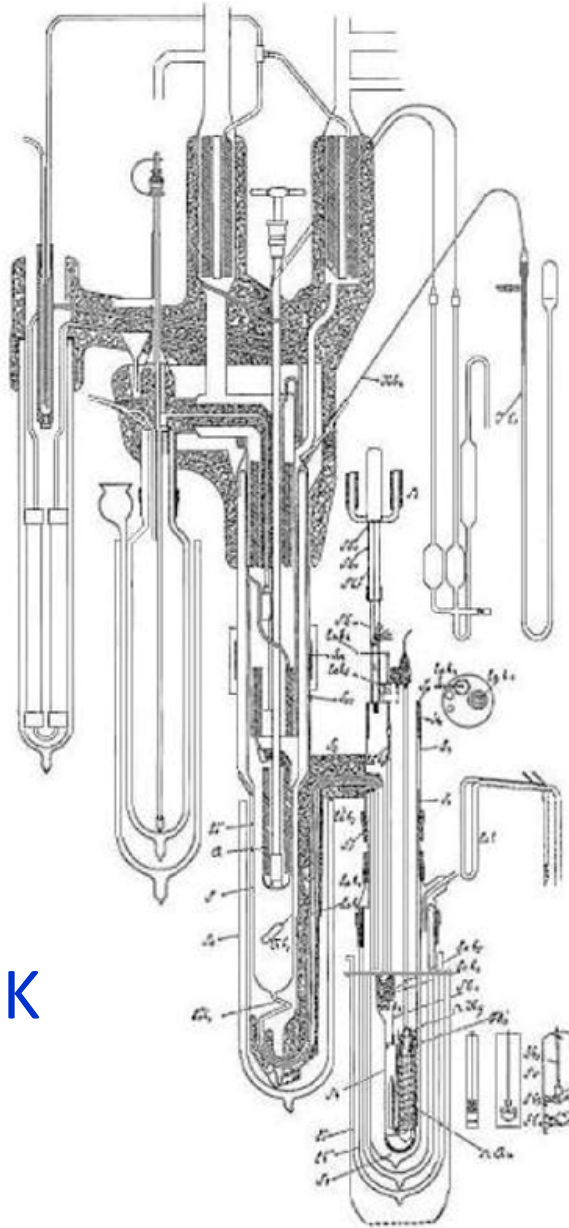
Why mercury?

The story of superconductivity started from LHe

1911



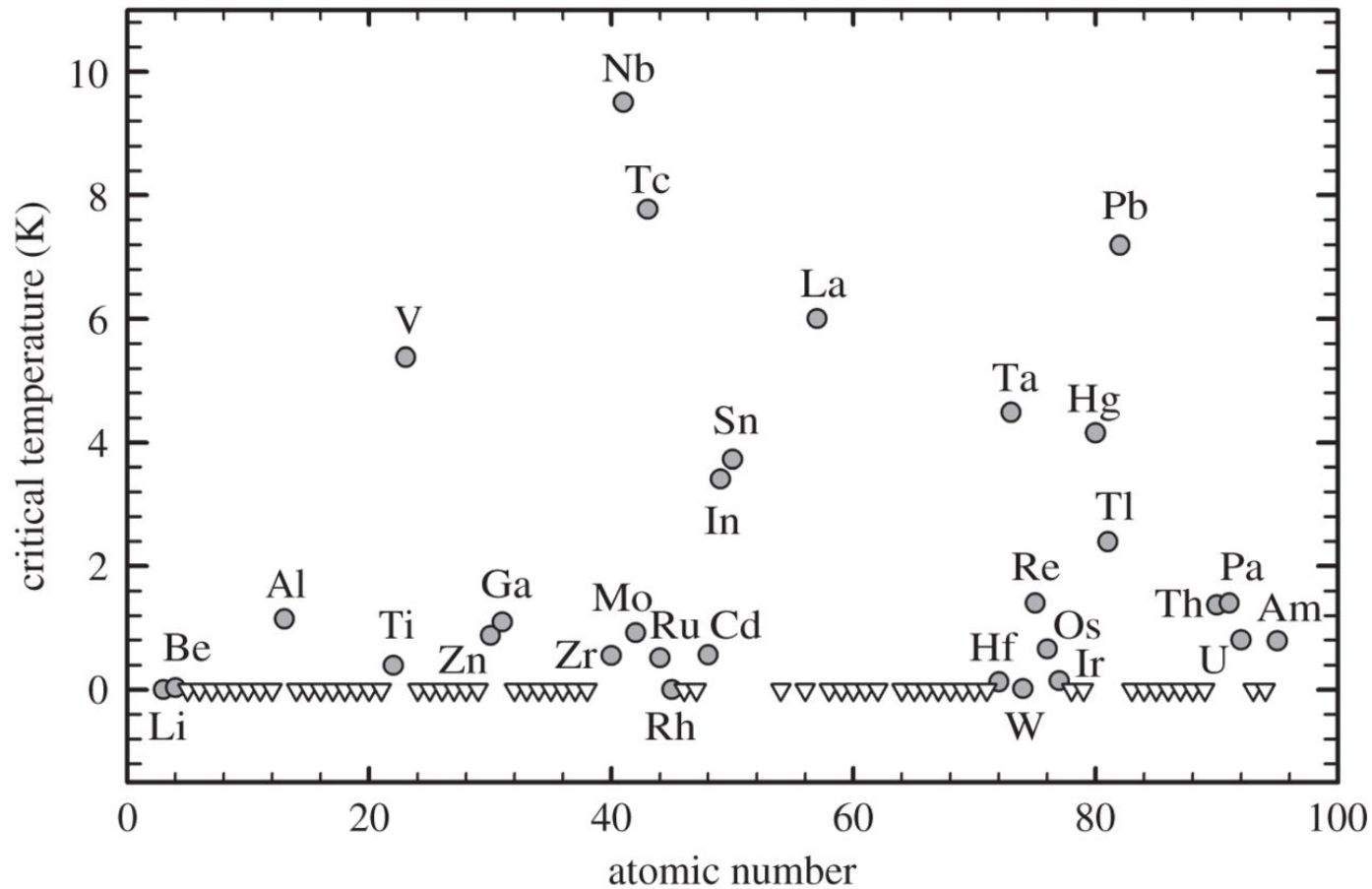
Hg, $T_c = 4.2\text{K}$



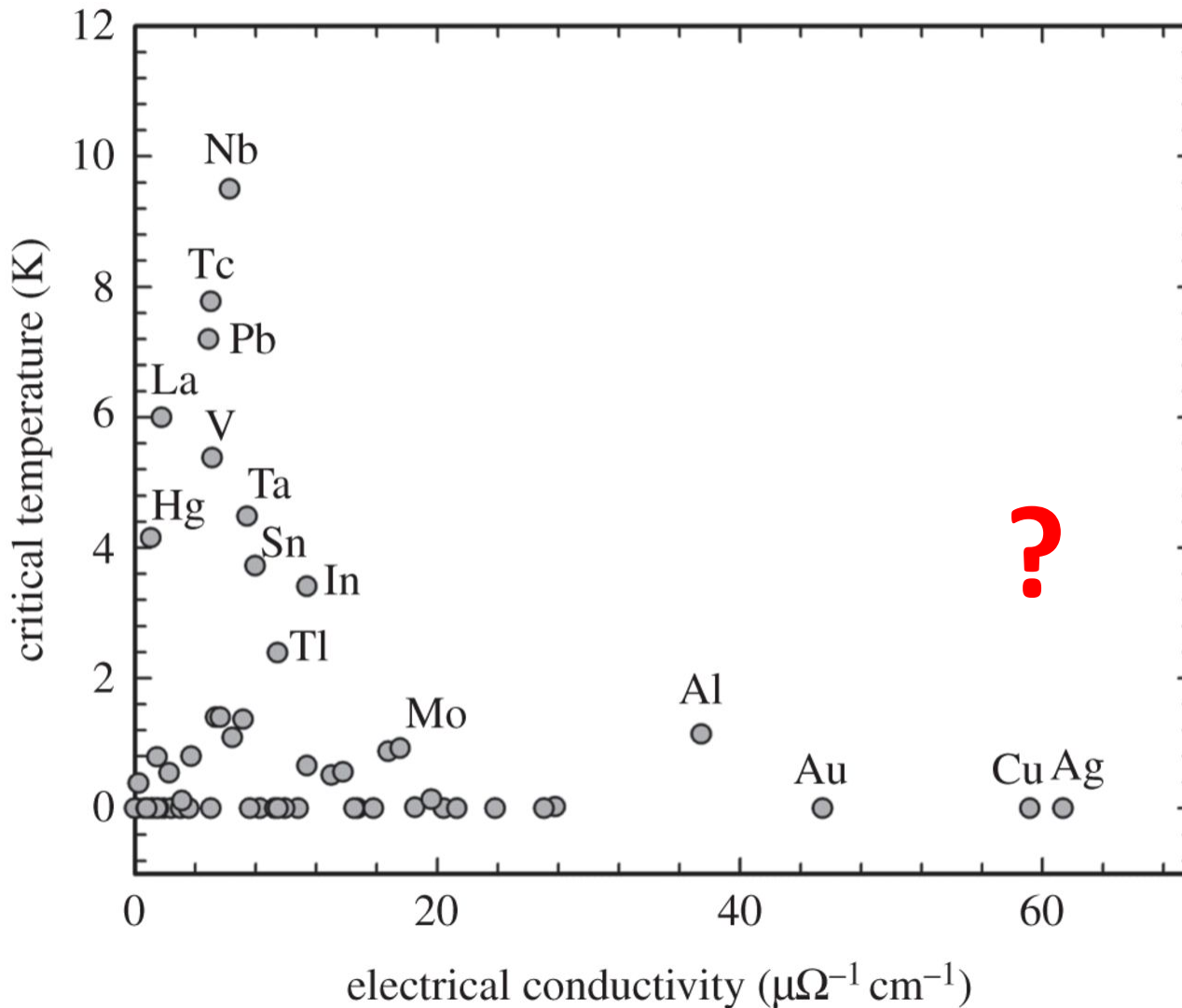
Superconducting Elements																		2
1 H																		He
3 Li	4 Be	<div> <div></div> In Bulk at Ambient Pressure <div></div> At High Pressure <div></div> In Modified Form </div>															10 Ne	
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar											
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	
87 Fr	88 Ra	89 Ac	104 Rf	105 Ha	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Uub							

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Superconducting Metals and Alloys



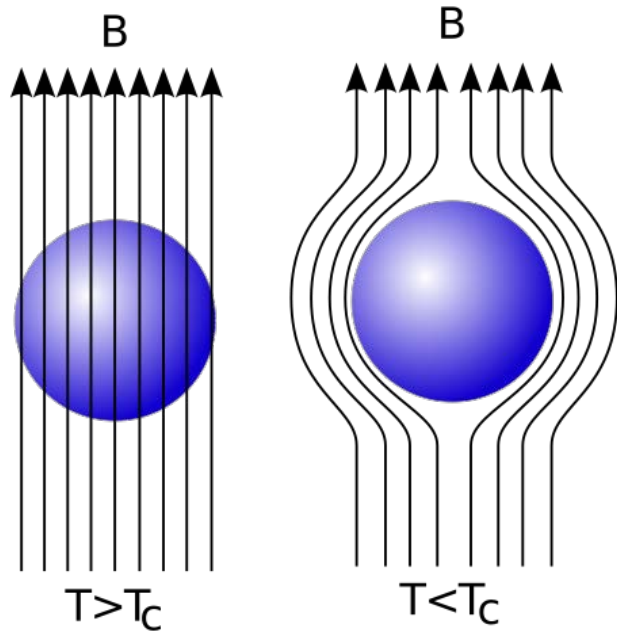
Superconducting Metals and Alloys



Element/ compound	T_c [K]
Al	1.19
Be	0.026
Ga	1.09
Hg	4.15
In	3.40
La	4.8
Nb	9.2
Pb	7.2
Sn	3.72
Ta	4.39
V ₃ Ge	6.0
V ₃ Si	17.1
Nb ₃ Ge	18.0
Nb ₃ Sn	23.2

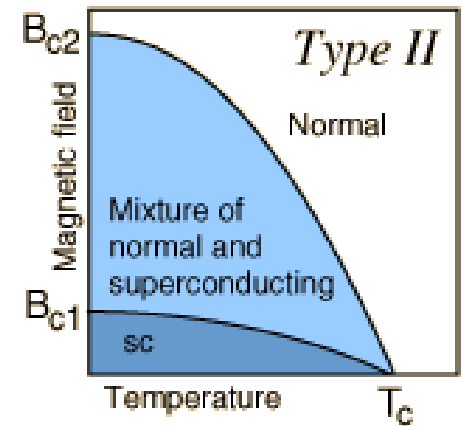
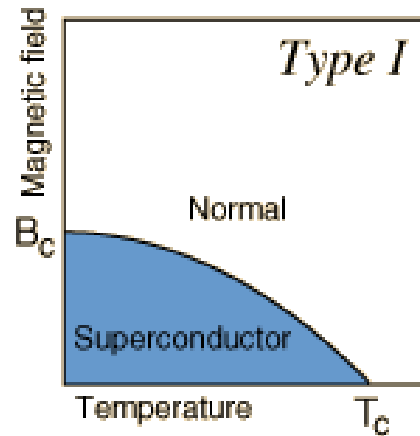
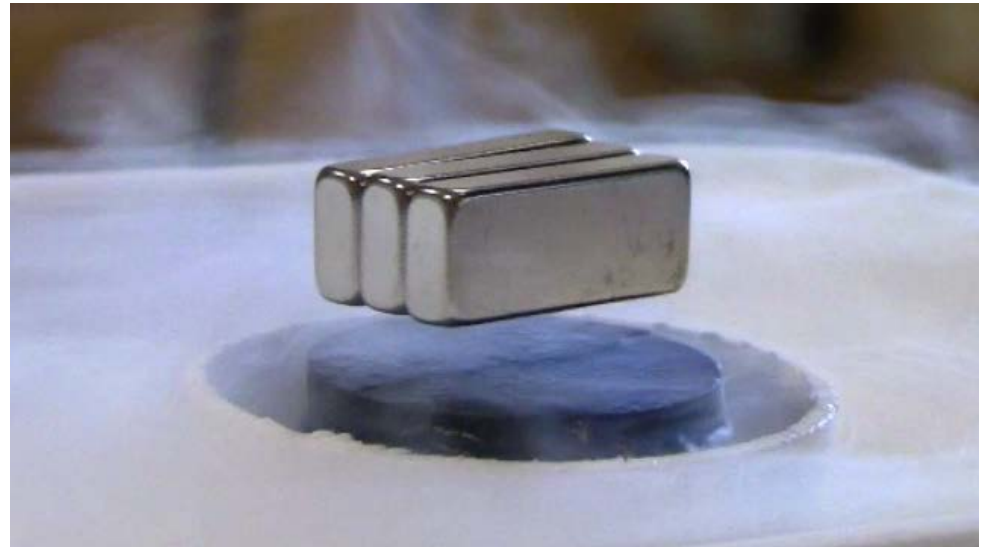
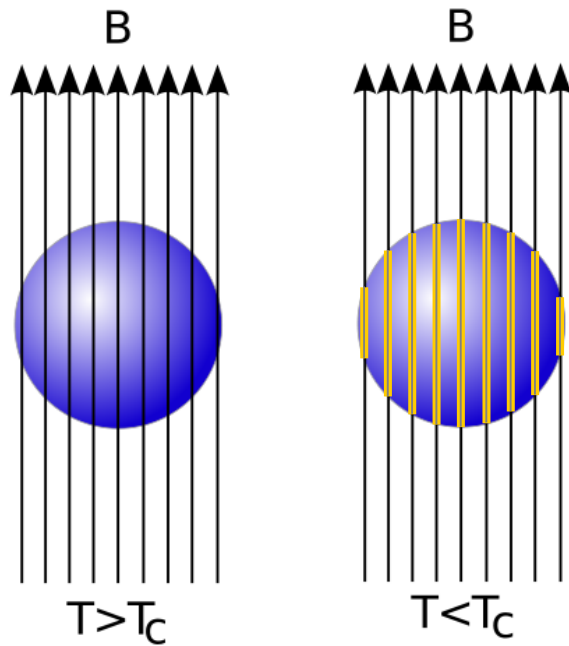
Meissner effect or vortex pinning ?

1933



Meissner effect or vortex pinning ?

1957



Two length scales in superconductors

1935: Londons equations

$$W_{\text{kin}} = n_s m v_s^2 / 2 = m j_s^2 / 2 n_s e^2 = \frac{\lambda^2}{8\pi} (\text{rot } \mathbf{H})^2$$

$$W_{\text{mag}} = H^2 / 8\pi$$

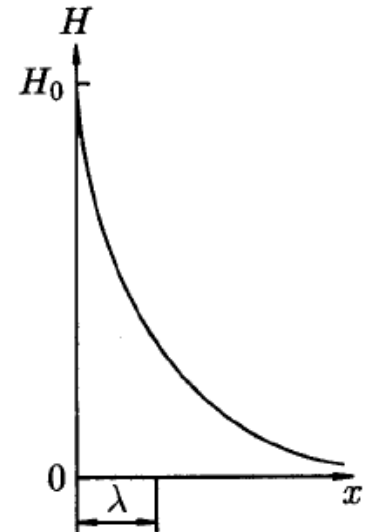
$$\lambda^2 = \frac{mc^2}{4\pi n_s e^2}$$

$$\mathcal{F}_{sH} = \mathcal{F}_{s0} + \frac{1}{8\pi} \int [\mathbf{H}^2 + \lambda^2 (\text{rot } \mathbf{H})^2] dV$$

2nd Londons equation:

$$\mathbf{H} + \lambda^2 \text{rot rot } \mathbf{H} = 0$$

$$d^2 H / dx^2 - \lambda^{-2} H = 0 \quad H = H_0 e^{-x/\lambda}$$



Two length scales in superconductors

1935: Londons equations

2nd Londons equation:

$$\mathbf{H} + \lambda^2 \text{rot rot } \mathbf{H} = 0$$

$$\mathbf{j}_s = -\frac{c}{4\pi\lambda^2} \mathbf{A}$$

Quantum generalization:

$$\Psi(\mathbf{r}) = (n_s/2)^{1/2} e^{i\theta(\mathbf{r})} \quad \hbar \nabla \theta = 2m\mathbf{v}_s + \frac{2e}{c} \mathbf{A}$$

$$\mathbf{j}_s = \frac{1}{c\Lambda} \left(\frac{\Phi_0}{2\pi} \nabla \theta - \mathbf{A} \right) \quad \Phi_0 = \frac{\pi \hbar c}{e} = \frac{hc}{2e}$$

Two length scales in superconductors

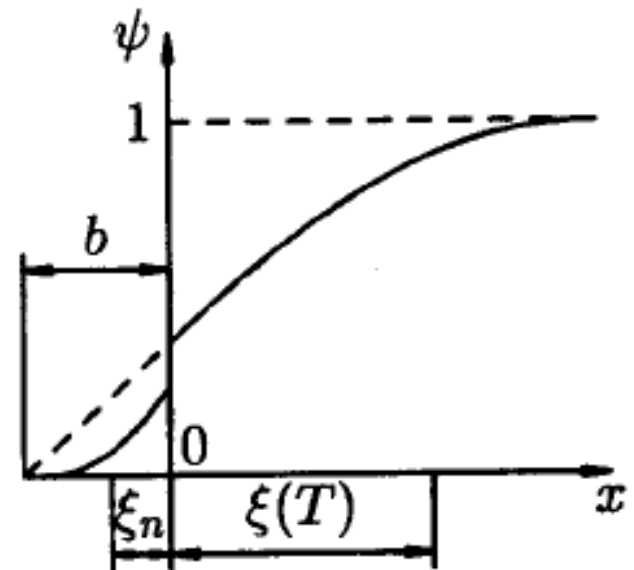
1950s: Ginzburg-Landau Theory

$$F = F_n + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \underbrace{\frac{1}{2m}|(-i\hbar\nabla - 2e\mathbf{A})\psi|^2}_{W_{\text{kin}}} + \frac{|\mathbf{H}|^2}{2\mu_0}$$

$$\xi^2 \left(i\nabla + \frac{2\pi}{\phi_0} \mathbf{A} \right)^2 \psi = \left(1 - \frac{|\psi|^2}{|\psi_0|^2} \right) \psi$$

$$\xi^2 = \frac{\hbar^2}{4m|\alpha|}$$

$$\phi_0 = \pi\hbar c/e$$





Two length scales in superconductors

1957: Abrikosov vortices

$$\kappa = \lambda / \xi$$

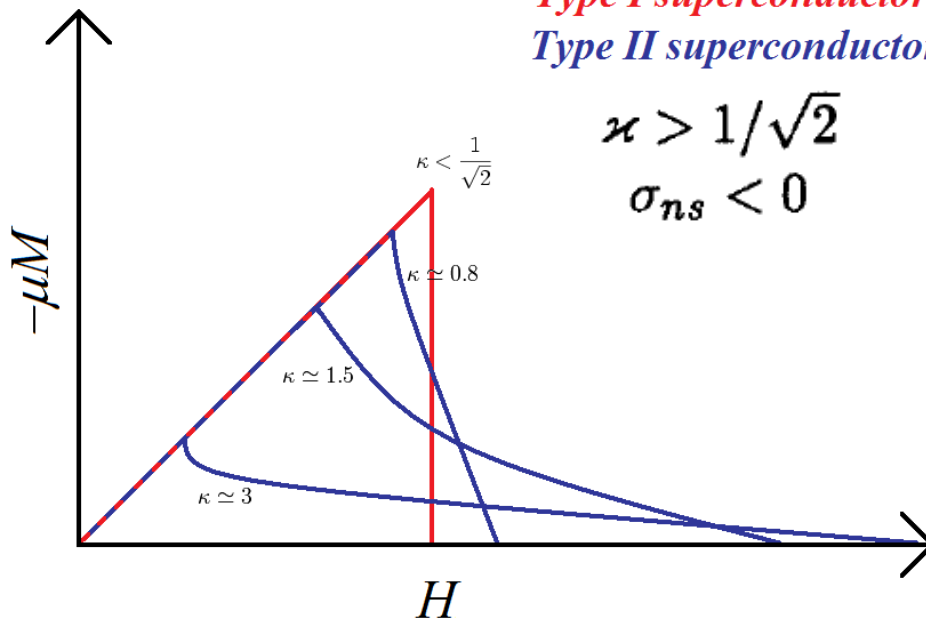
$$\kappa < 1/\sqrt{2}$$

$$\sigma_{ns} > 0$$

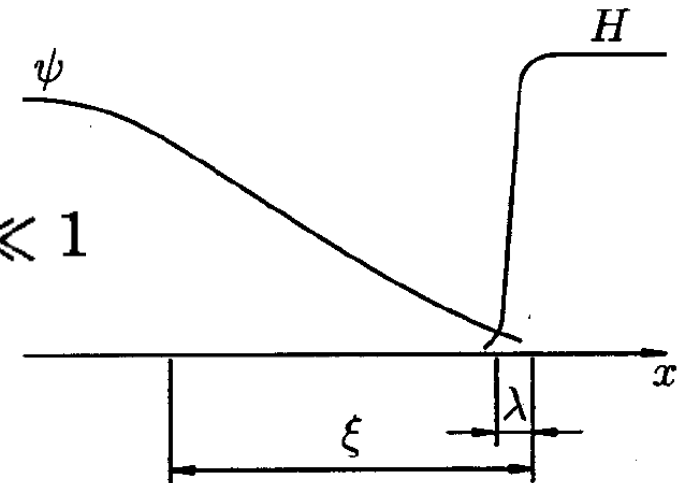
Type I superconductor
Type II superconductor

$$\kappa > 1/\sqrt{2}$$

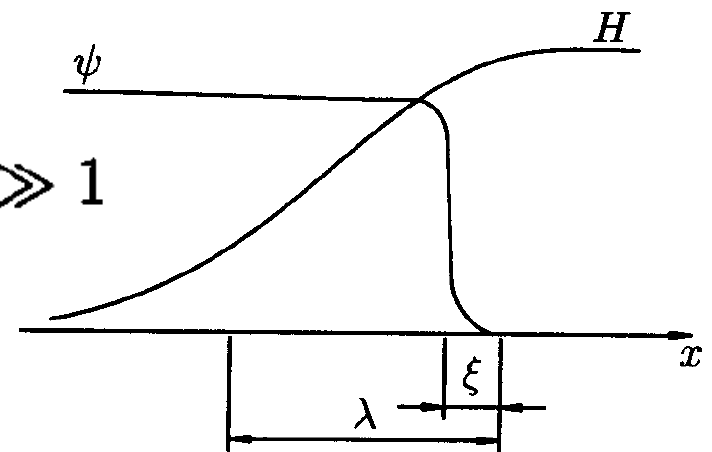
$$\sigma_{ns} < 0$$



$$\kappa \ll 1$$



$$\kappa \gg 1$$



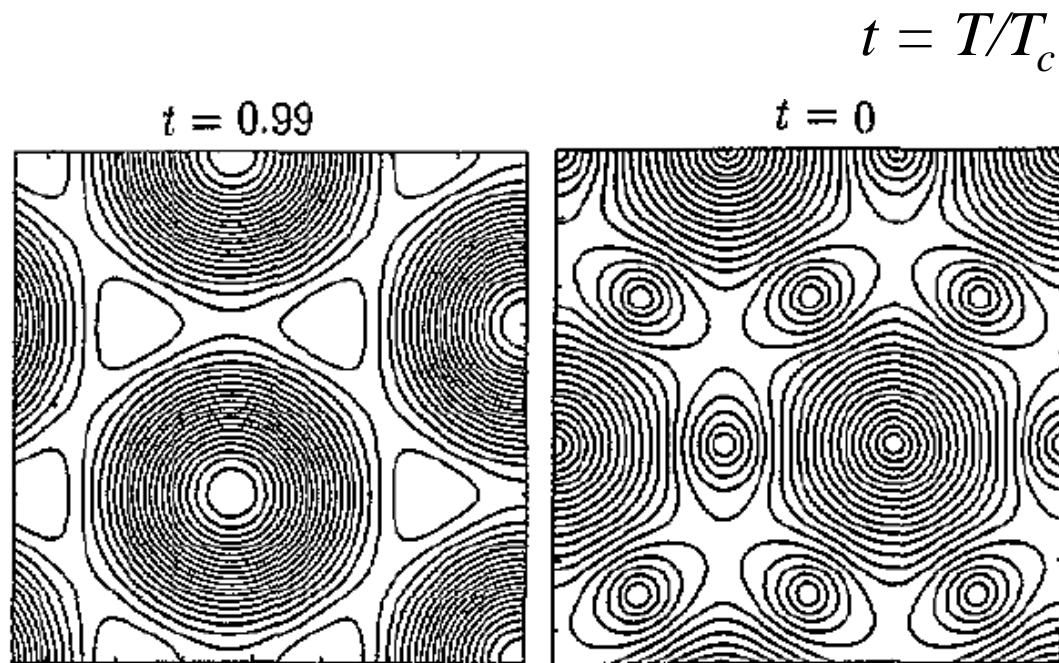
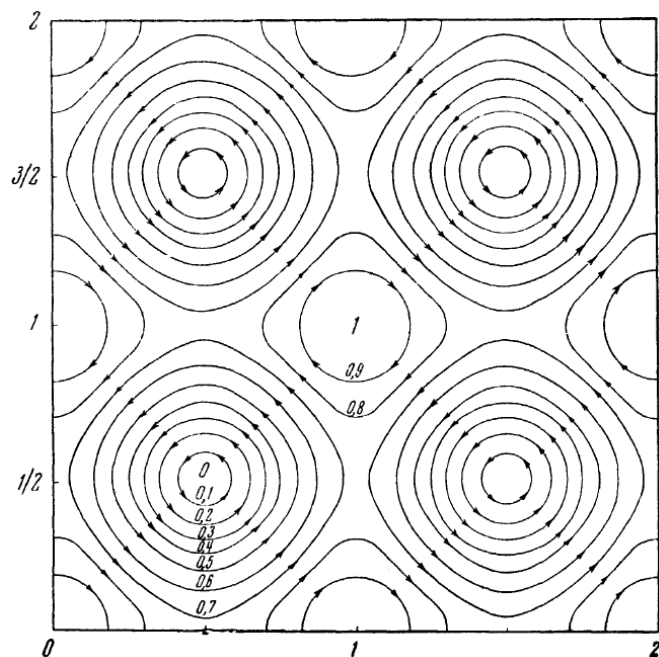
On the Magnetic Properties of Superconductors of the Second Group

A. A. ABRIKOSOV

Institute of Physical Problems, Academy of Sciences, U.S.S.R.

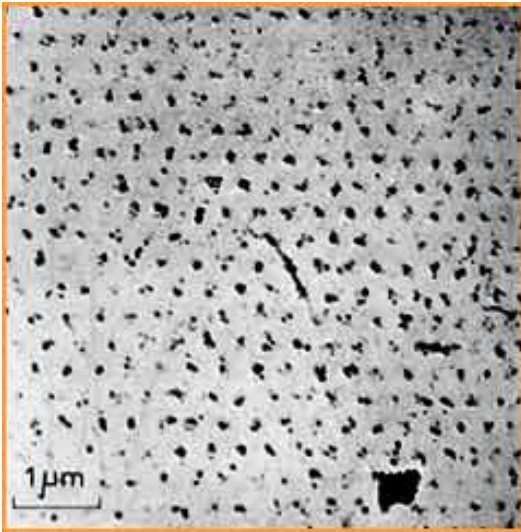
(Submitted to JETP editor November 15, 1956)

J. Exptl. Theoret. Phys. (U.S.S.R.) **32**, 1442-1452 (June, 1957)



E. H. Brandt, *Rep. Prog. Phys.* **58**, 1465 (1995)

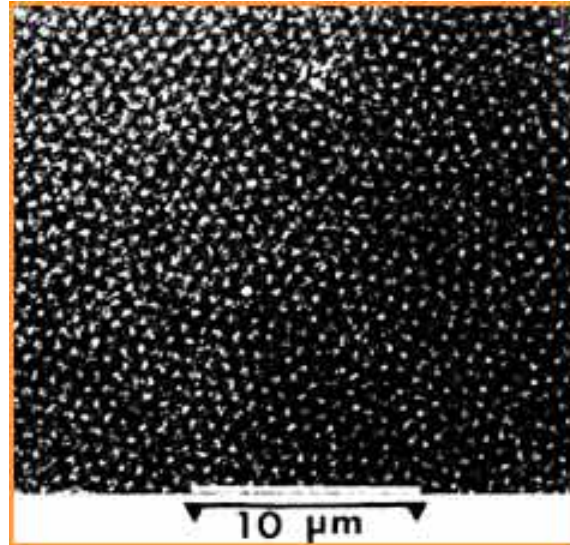
Abrikosov vortices



**First image of Vortex lattice,
1967**

Bitter Decoration
Pb-4at%In rod, 1.1K, 195G

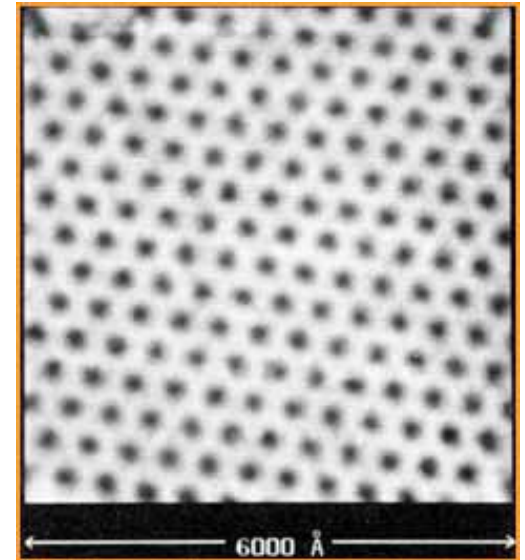
U. Essmann and H. Trauble
Max-Planck Institute, Stuttgart
[Physics Letters 24A, 526 \(1967\)](#)



**Vortex lattice in high-T_c
superconductor, 1987**

Bitter Decoration
YBa₂Cu₃O₇ crystal, 4.2K, 52G

P. L. Gammel et al.
Bell Labs
[Phys. Rev. Lett. 59, 2592 \(1987\)](#)

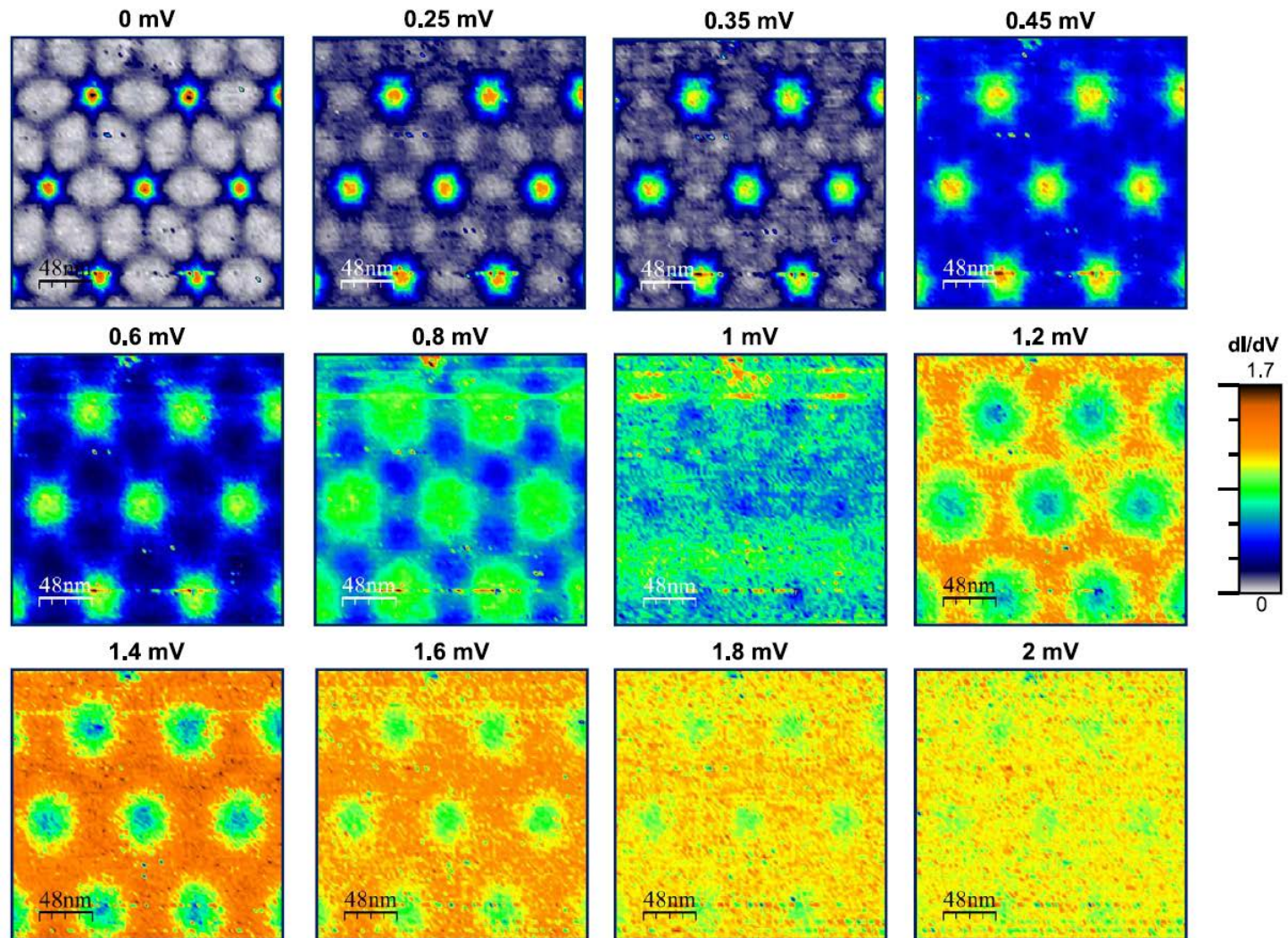


**STM image of Vortex lattice,
1989**

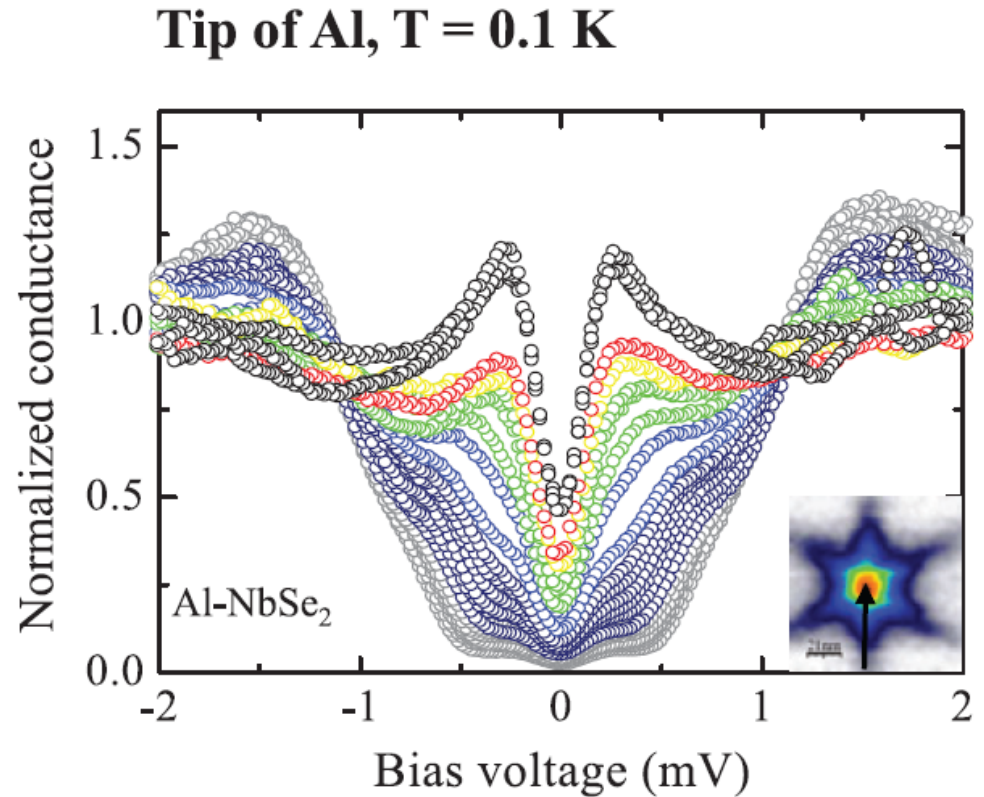
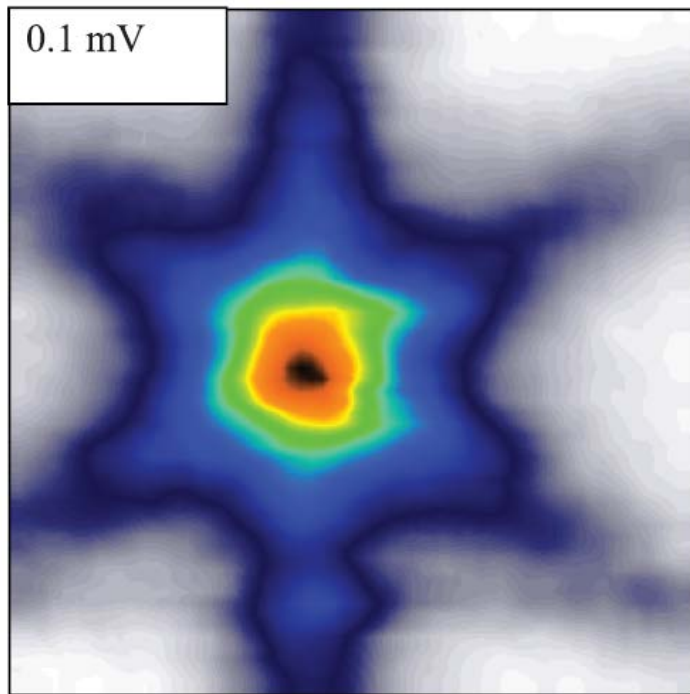
Scanning Tunnel Microscopy
NbSe₂, 1T, 1.8K

H. F. Hess et al.
Bell Labs
[Phys. Rev. Lett. 62, 214 \(1989\)](#)

Imaging superconducting vortex cores and lattices with a scanning tunneling microscope

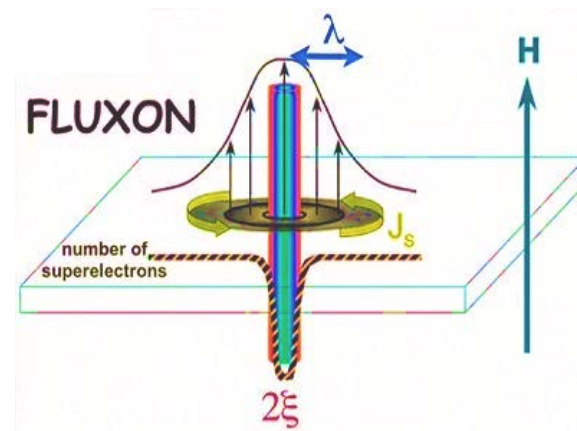
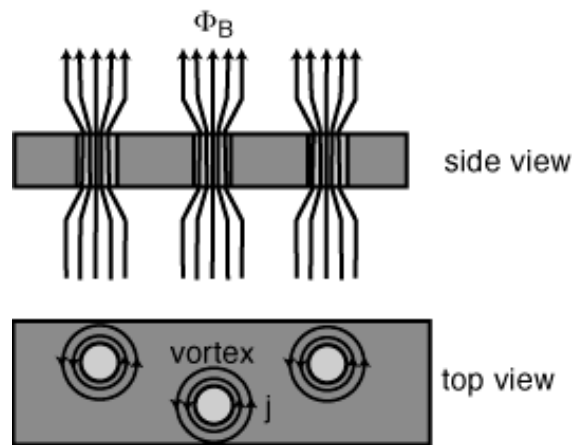
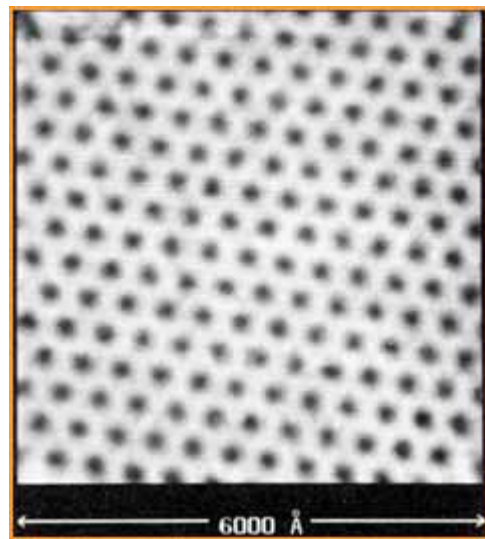
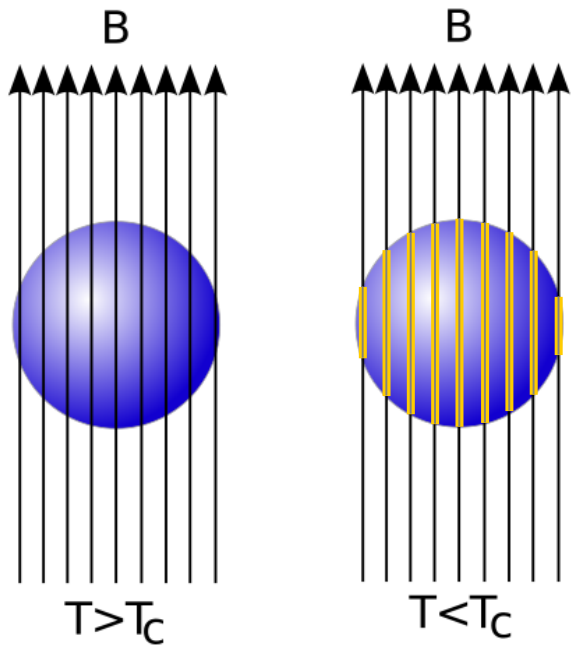


Imaging superconducting vortex cores and lattices with a scanning tunneling microscope

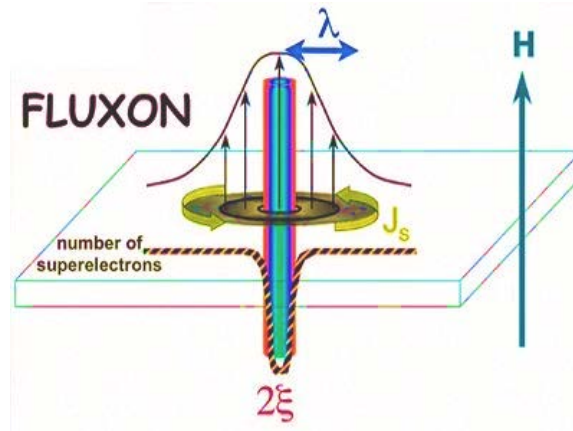
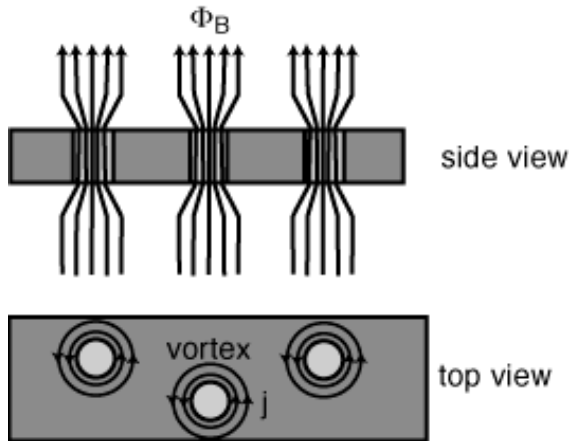


Suderow 2014, Guillamon 2008

Abrikosov vortices



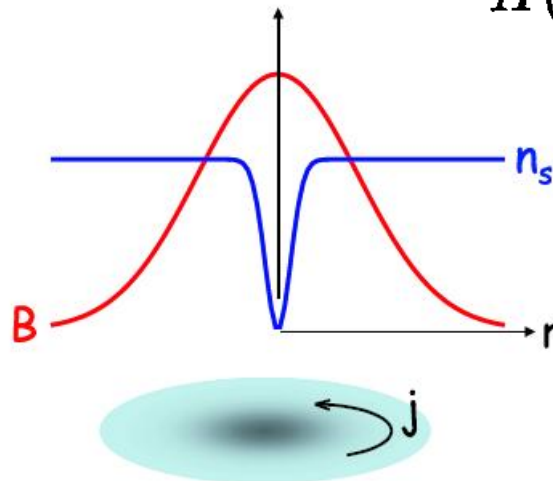
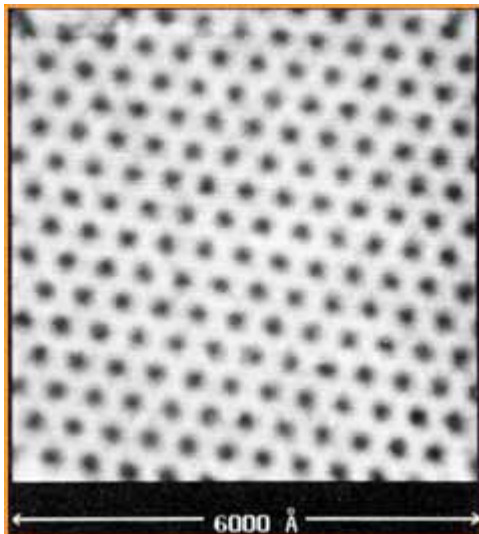
Abrikosov vortices



$$\Phi_0 = \frac{hc}{2e}$$

$$H(0) = \frac{\Phi_0}{2\pi\lambda^2} (\ln \kappa - 0.28)$$

$$\approx 2H_{c1}$$



Vortex mass?

$$M_e = \frac{3\pi}{2} m n \xi^2 \left(\frac{\Delta}{E_F} \right)^2,$$

$$M_J = M_e \frac{1}{3} \kappa^2 \left(\frac{v_F}{c} \right)^2$$

the basic idea that the electronic contribution to the vortex mass is due to the local change in dispersion within the vortex core. The number of electrons exposed to this change is given by $N(0)\pi\xi^2\Delta$, with $N(0)$ the density of states at the Fermi level and Δ denoting the energy gap. These electrons experience a relative change of their effective mass which is of the order of $m\Delta/E_F$.

Mass of a vortex in a superconducting film measured via magneto-optical imaging plus ultrafast heating and cooling

D. Golubchik et al. *Phys. Rev. B* **85**, 060504(R) (2012)

Vortex mass

Energy Absorption by a Single Abrikosov's Vortex in NbTi and YBaCuO Superconductors

S. Vasiliev · V.V. Chabanenko et. al

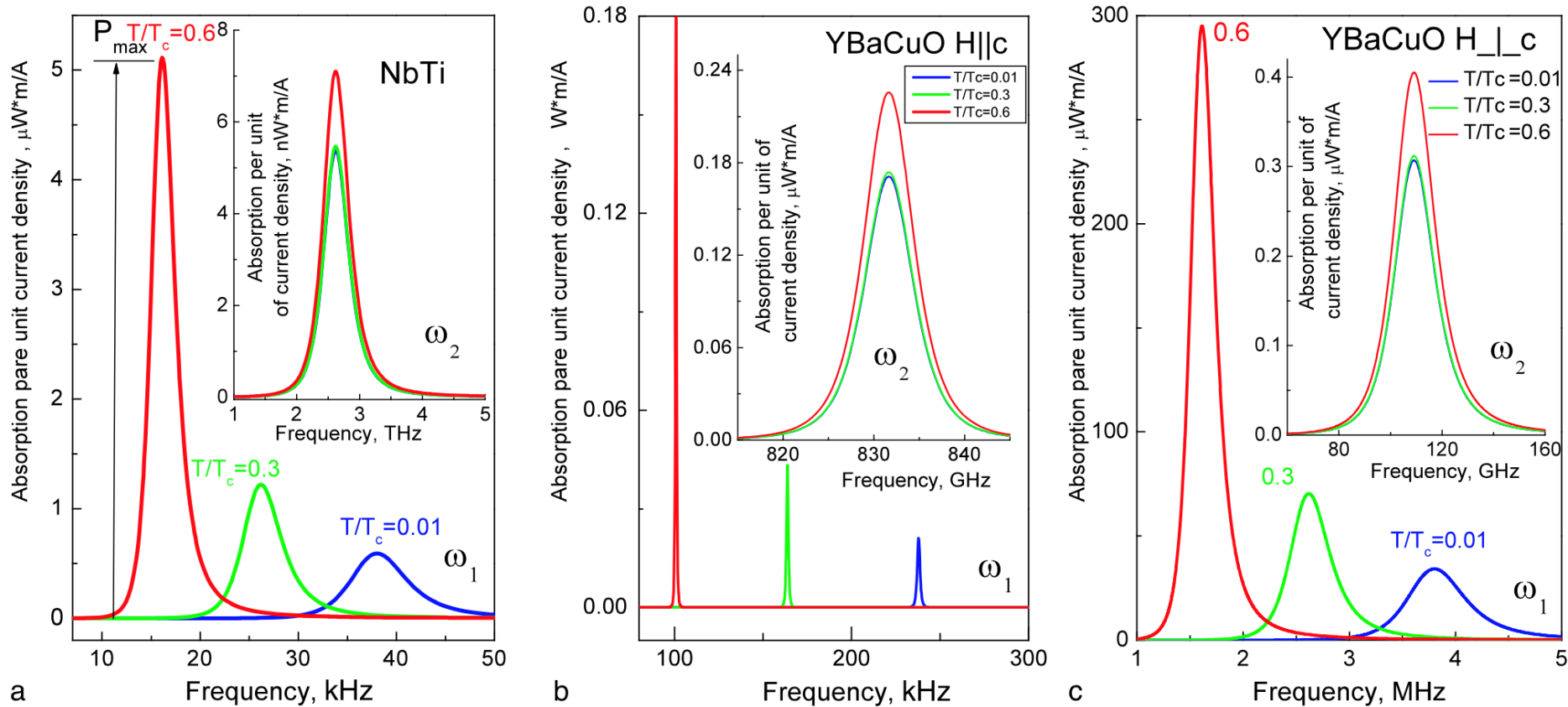


Fig. 1 Temperature dependence of absorption peaks $P_{\max}(\omega)$ of low-(ω_1) and high-frequency (ω_2) oscillation modes in (a) NbTi and in YBaCuO, for orientations (b) $H \parallel c$ and (c) $H \perp c$

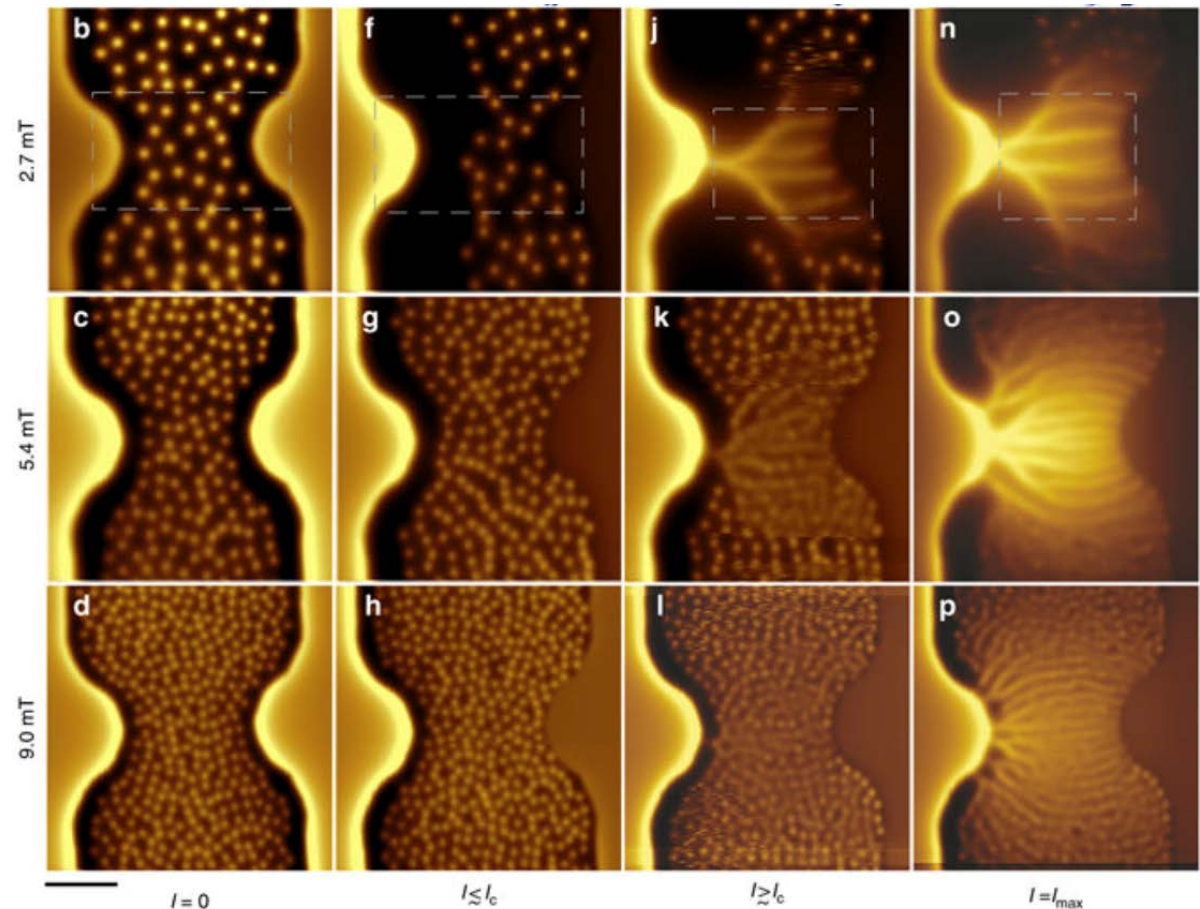
Vortex motion

Imaging of super-fast dynamics and flow instabilities of superconducting vortices

[L. Embon](#), et al.

Nature Commun. **8**, 85 (2017)

$$\eta_0 \simeq \phi_0^2 / 2\pi\xi^2 \rho_n$$



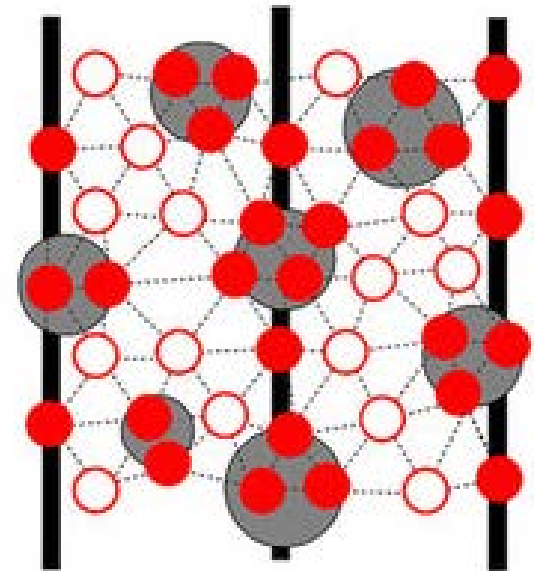
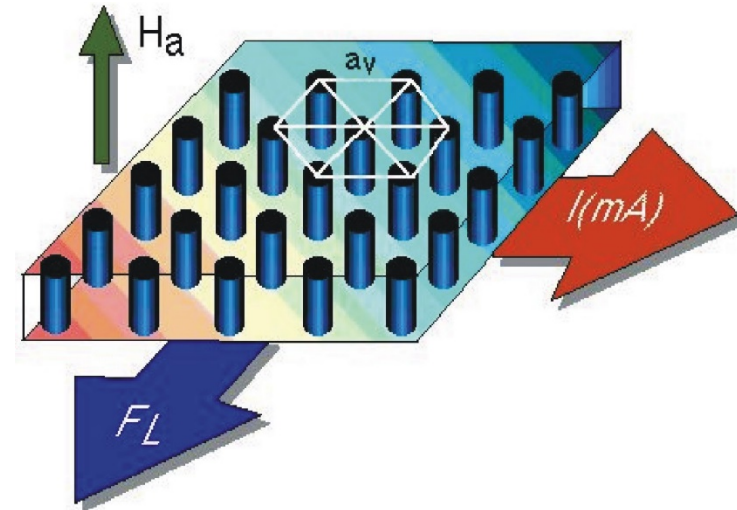
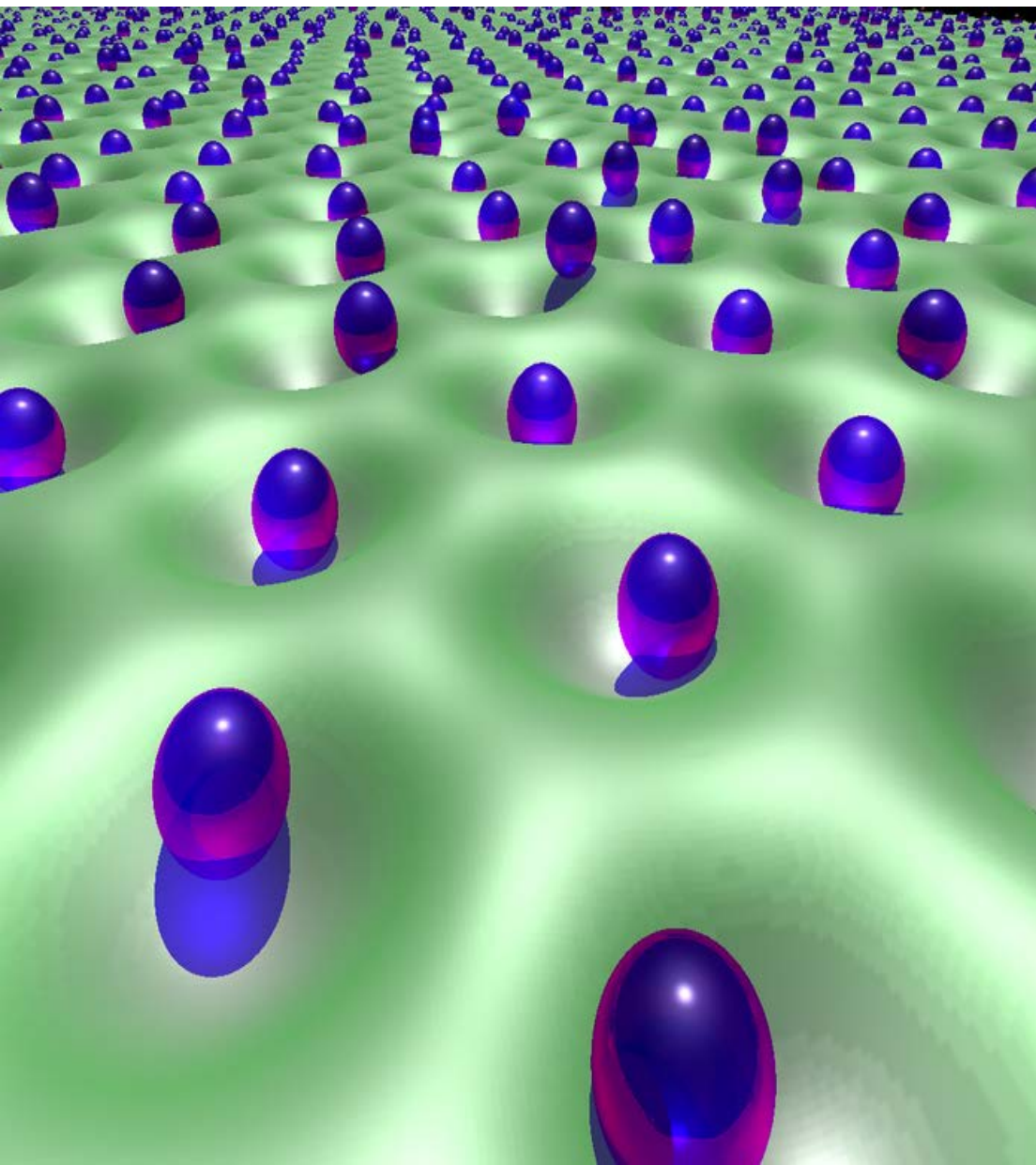
While the dynamic behavior of slow vortices has been thoroughly investigated, the physics of **ultrafast vortices** remains largely unexplored.

SQUID microscopy: velocities of up to **10s km/s**

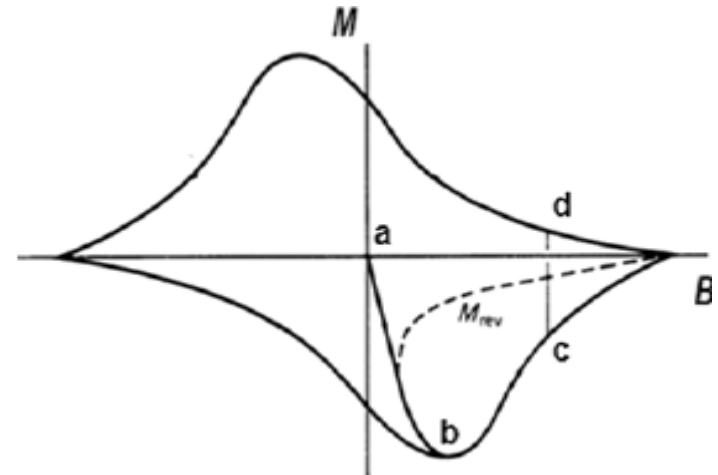
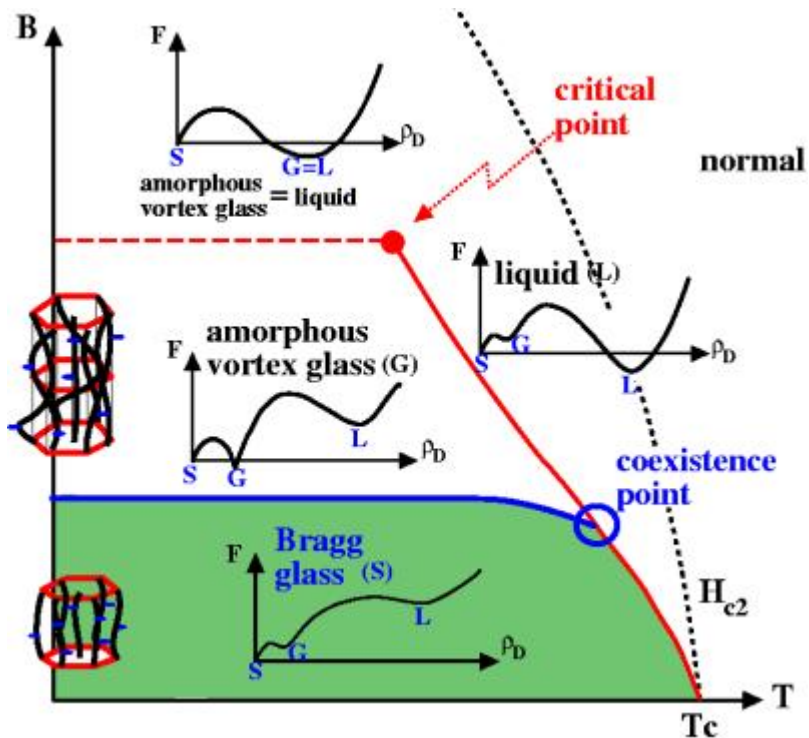
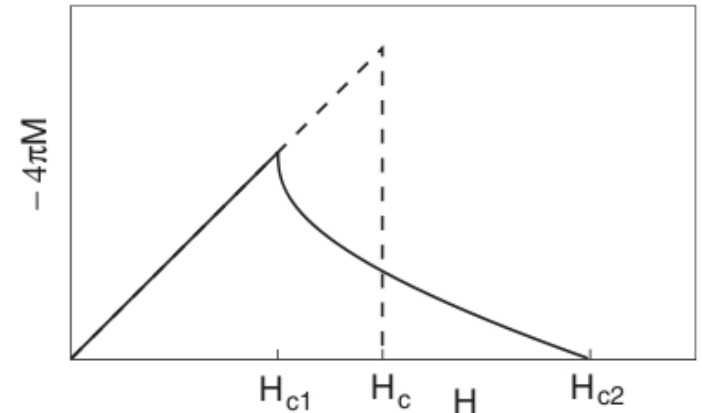
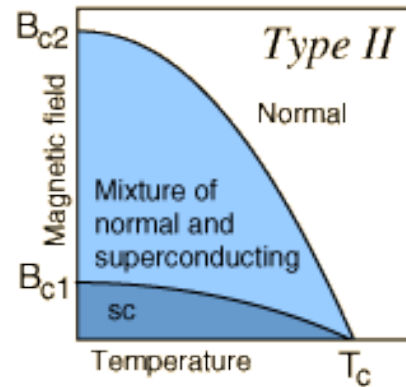
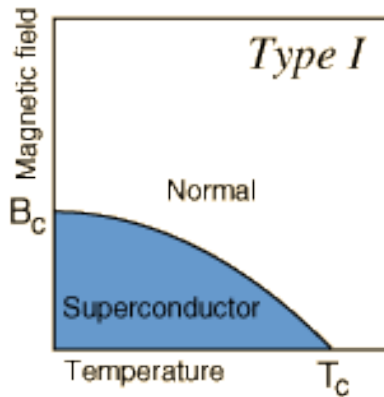
(much larger than the speed of sound and also exceed the pair-breaking speed limit of superconducting condensate)

$$v_{dp} = \Delta / mv_F = \hbar / \pi m \xi$$

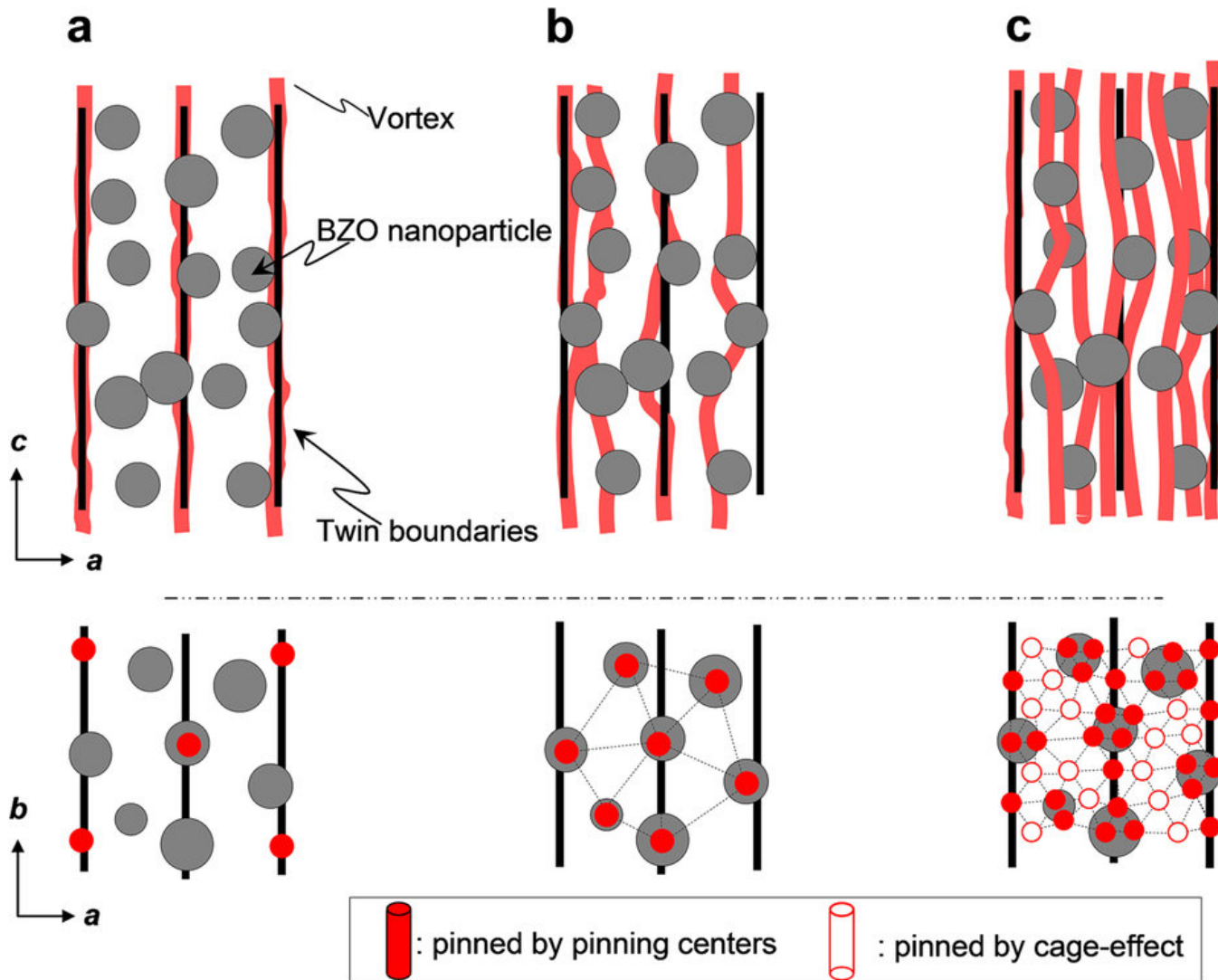
Vortex matter (H, T, J, F_p)



Vortex matter (H, T) – magnetic phase diagrams

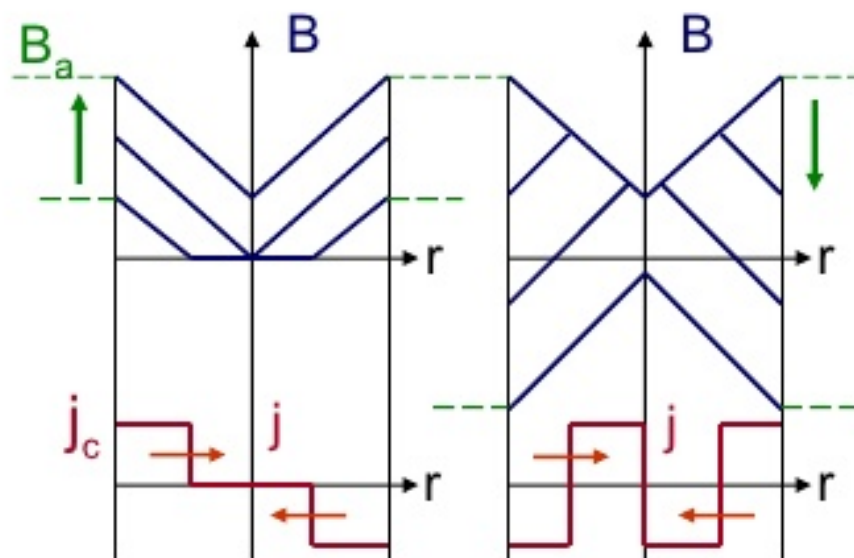
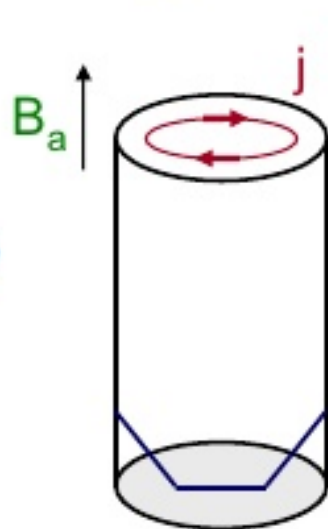


Abrikosov vortices: pinning

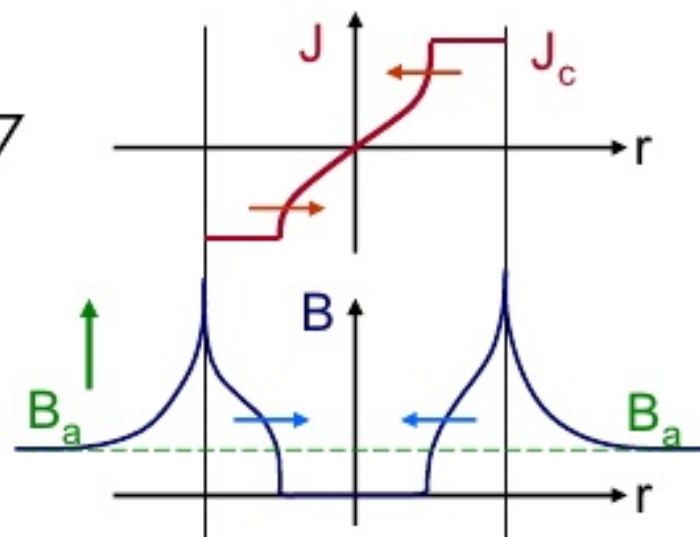
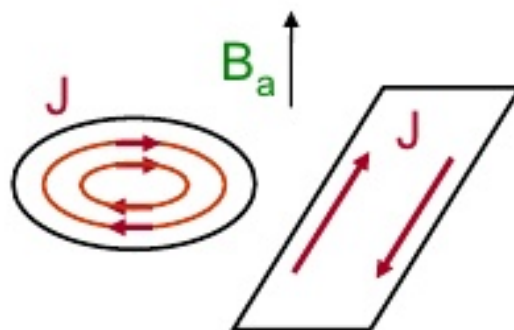


Importance of geometry

Bean model
parallel geometry
long cylinder or slab



Bean model
perpendicular geometry
thin disk or strip



analytical solution:

Mikheenko + Kuzovlev 1993: disk

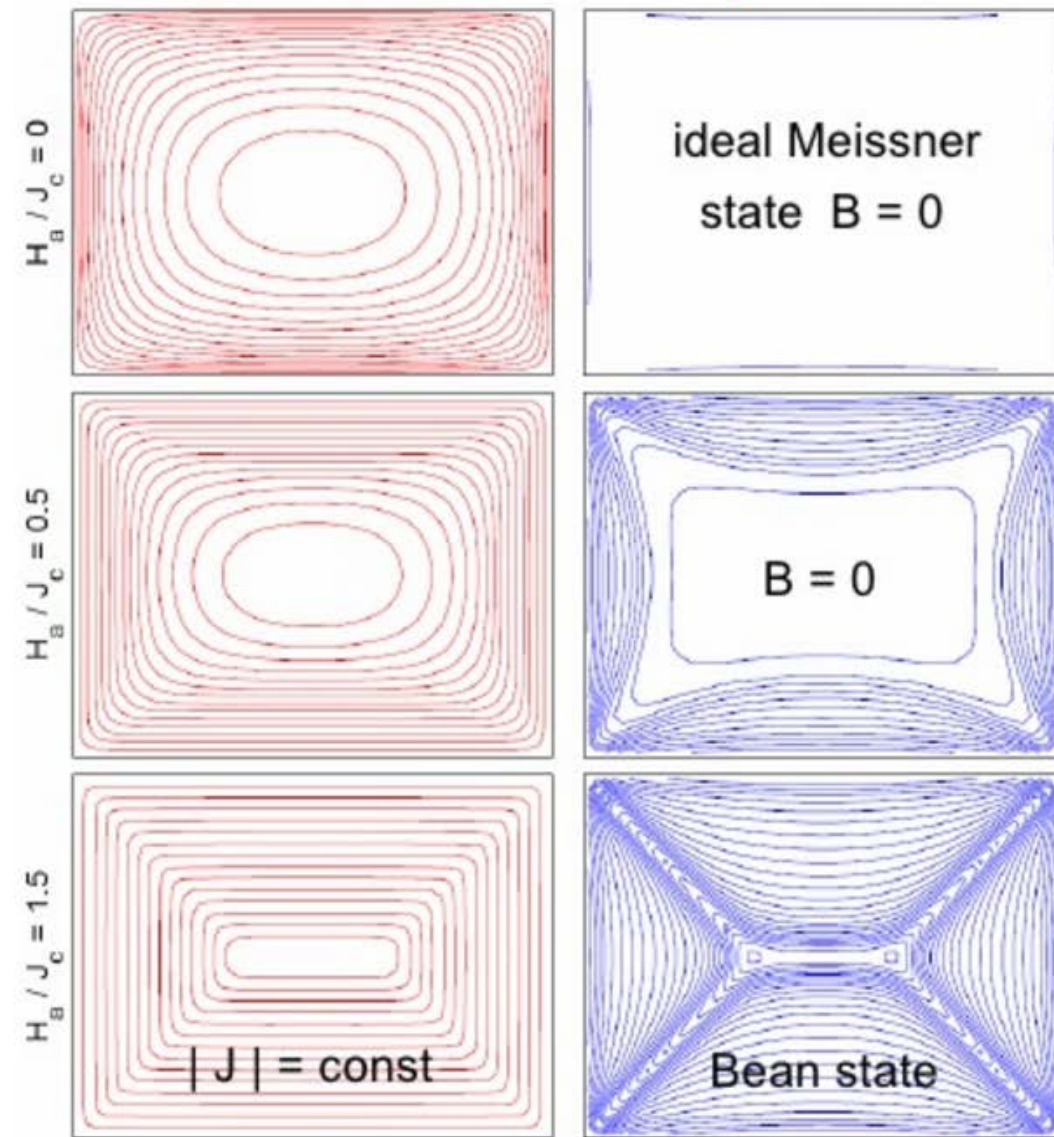
EHB+Indenbom+Forkl 1993: strip

Thin sc rectangle in perpendicular field

stream lines
of current

contours of
mag. induction

E.H. Brandt



Theory

EHB

PRB 1995

YBCO film

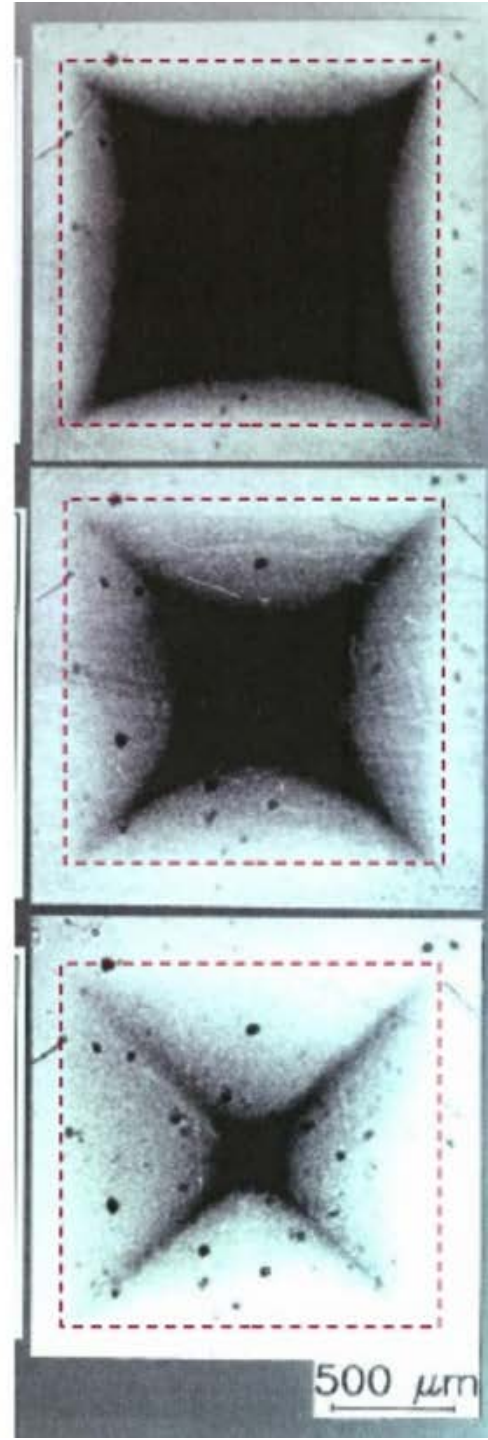
0.8 μm , 50 K

increasing field

Magneto-optics

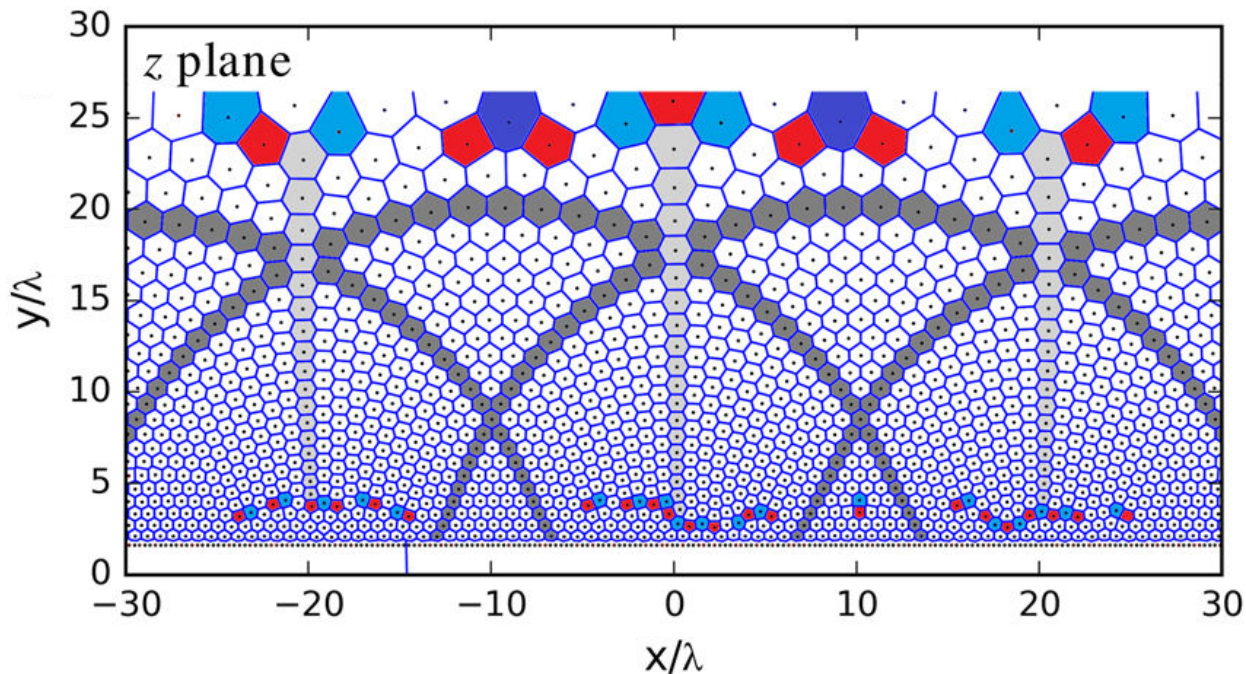
Indenbom +

Schuster 1995



Conformal Vortex Crystals

Raí M. Menezes & Clécio C. de Souza Silva
Scientific Reports **7**, 12766 (2017)

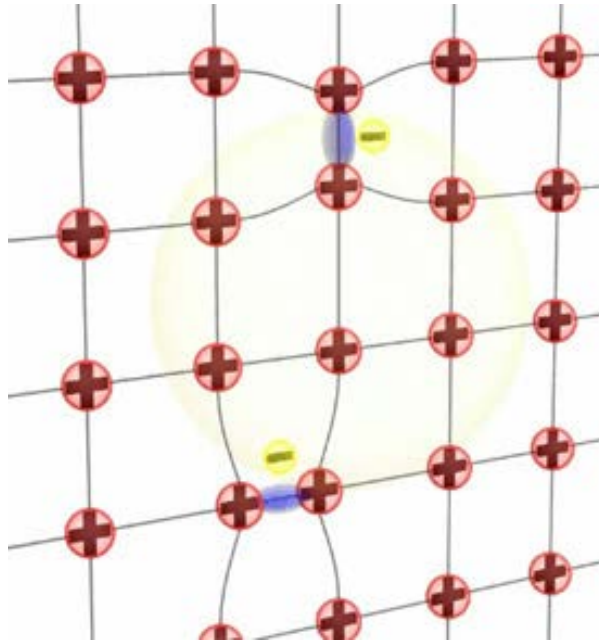


...we demonstrate that, for suitable choices of the force field, and below a certain transition temperature, the vortex system self-organizes into highly inhomogeneous conformal crystals in a way as to minimize the total energy. These nonuniform structures are topologically ordered and can be mathematically mapped into a triangular Abrikosov lattice via a conformal transformation.

History of superconductivity: BCS

1957

Phonons
 $T_c < 25\text{K}$



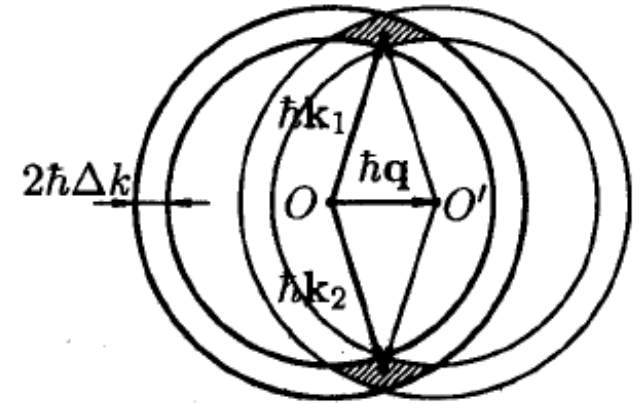
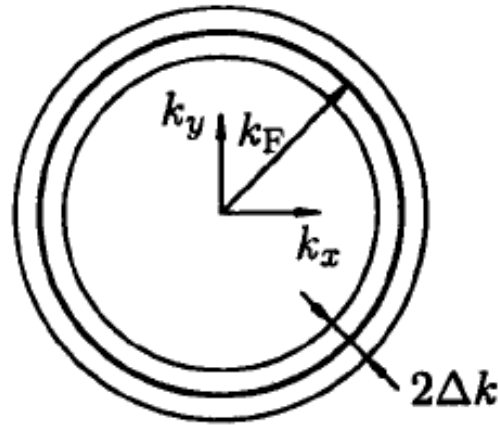
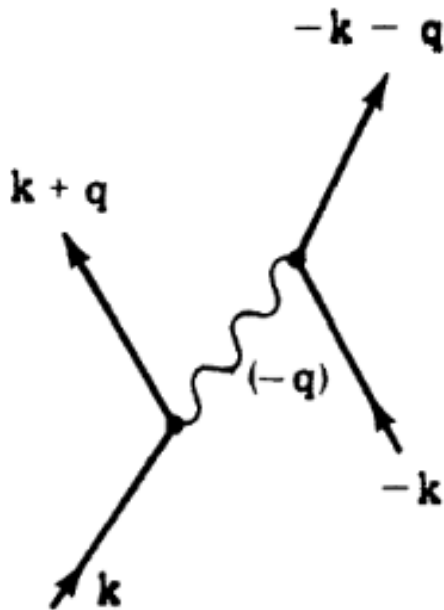
BCS

$$k_B T_c = 1.13 E_D e^{-1/N(0) V}$$

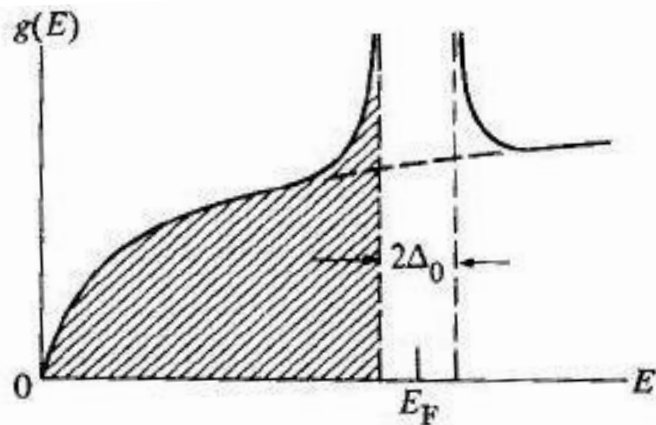
$$\Delta(T = 0) = 1.764 k_B T_c$$



History of superconductivity: BCS

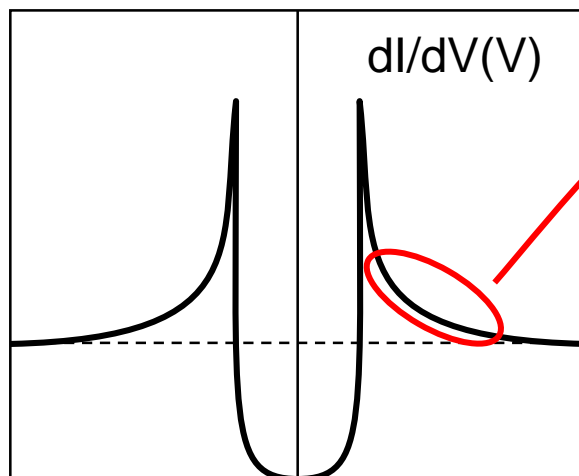
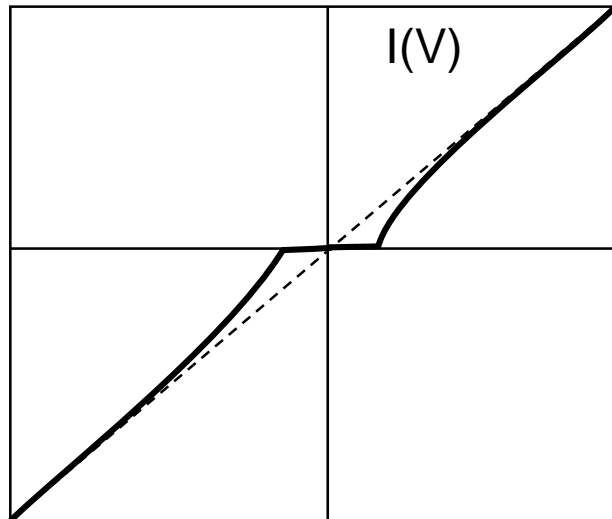


$$\Delta k/k_F \sim \hbar\omega_D/\epsilon_F, \quad \epsilon_F = \hbar^2 k_F^2/2m.$$

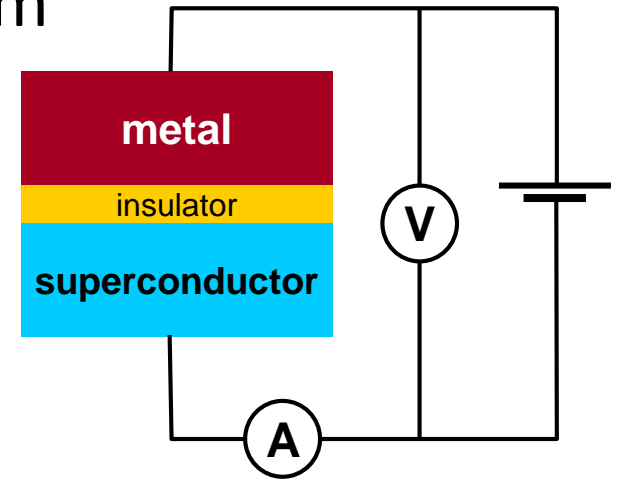
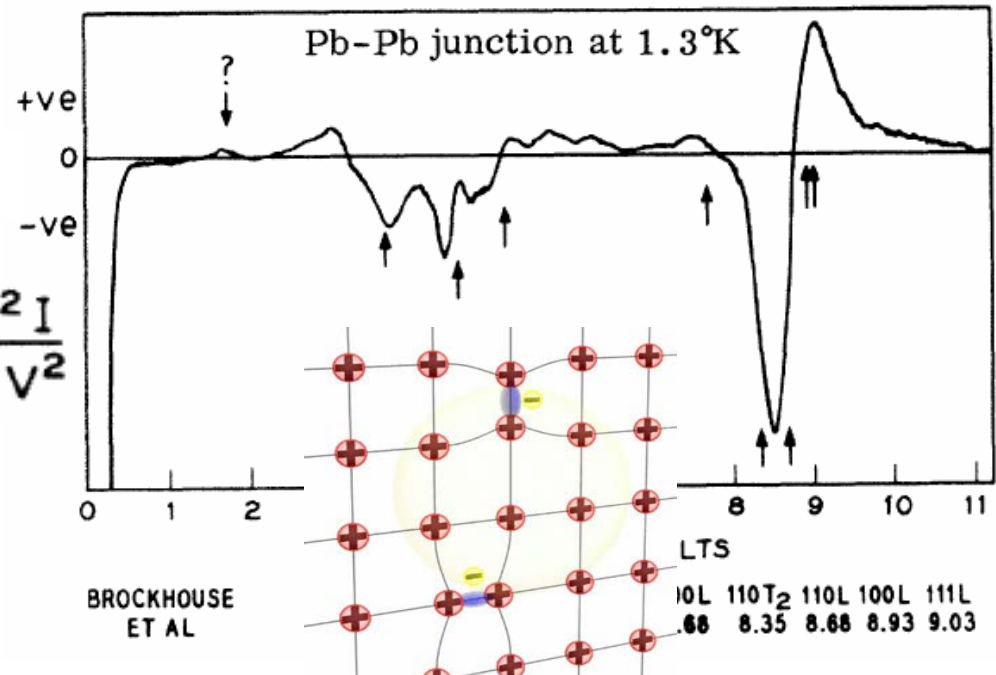


$$\Delta(T \rightarrow T_c) \approx 3.07 k_B T_c \sqrt{1 - (T/T_c)}$$

Experimental proof of the mechanism of superconductivity



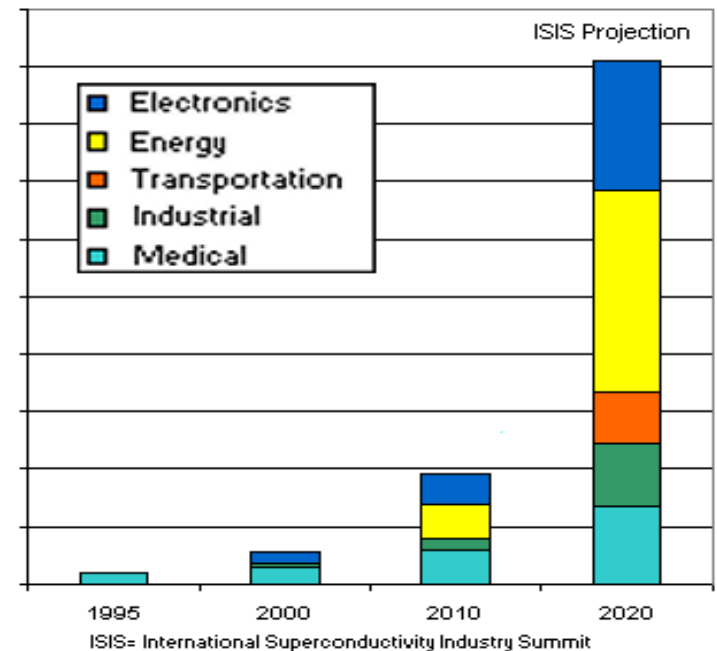
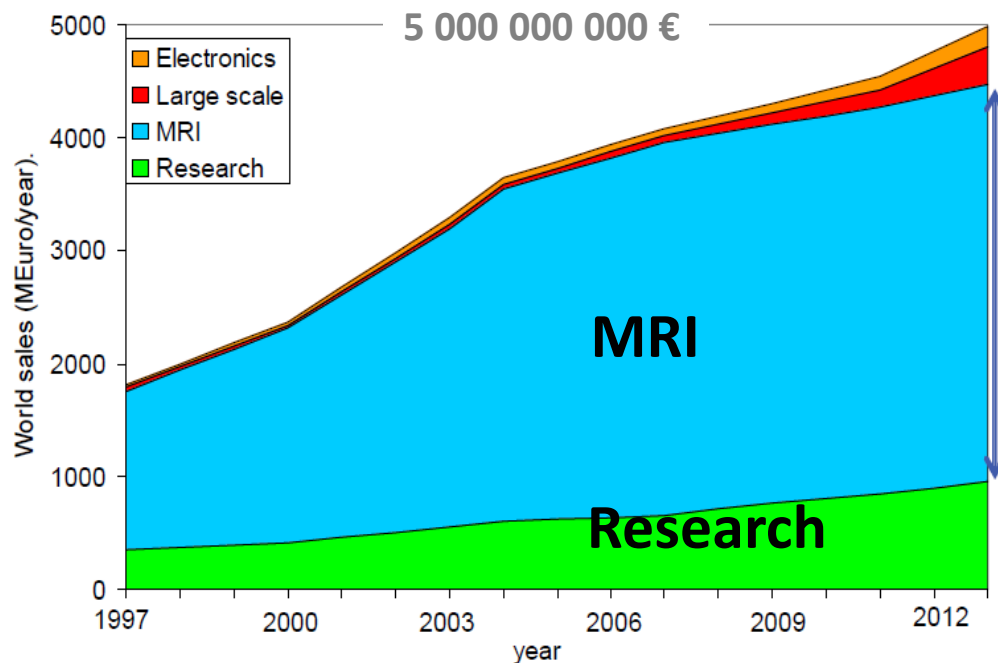
$$\frac{d^2I}{dV^2}$$

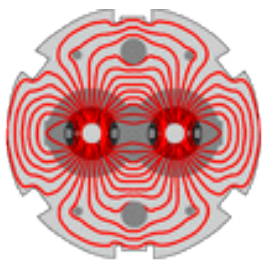


Application of superconductivity

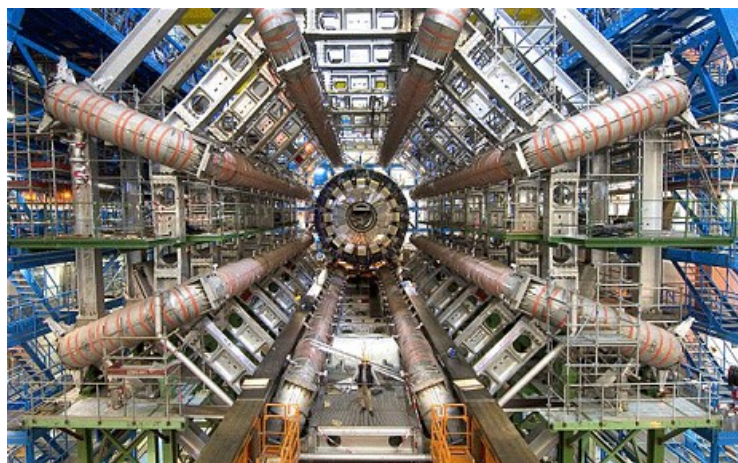


The main apps are magnets: MRI, NMR, accelerators and tokamaks. This is basically LTSC whose resource is already exhausted.





Large Hadron Collider



10 000 superconducting magnets
1200 tons of cable NbTi at 1.9 K
> 130 tons of LHe





The enormous toroidal superconducting magnet of ATLAS during its installation. Each of its eight coils, the last of which is being assembled in this photo, is 25 metres long.

(Image: ATLAS/CERN)

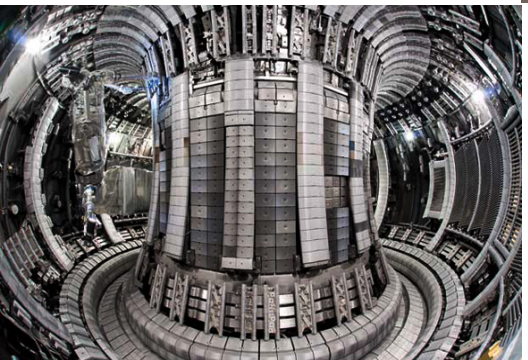
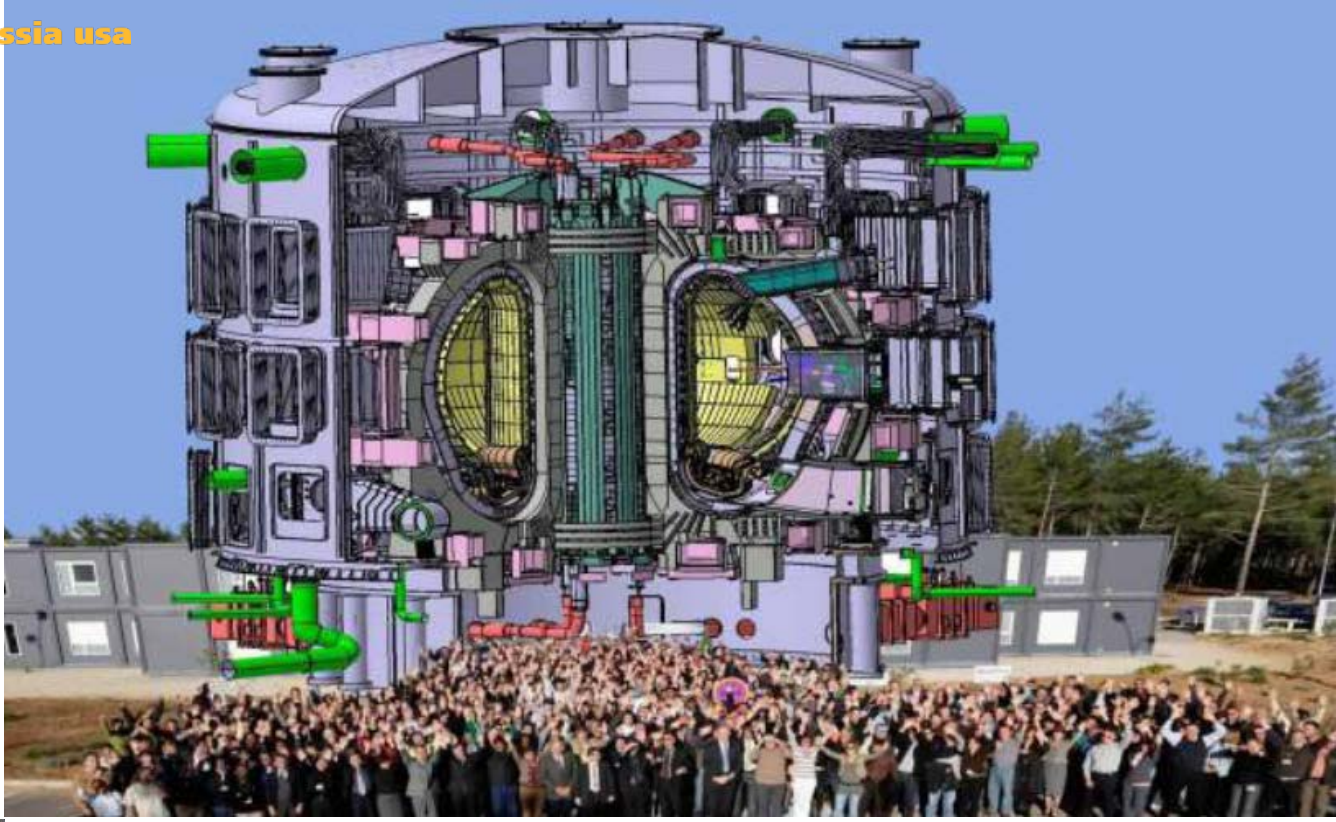


The new superconducting crab cavities being assembled at CERN. These cavities will be used in the future High-Luminosity LHC to tilt the particle bunches before they collide.
(Image: Jules Ordan/CERN)



International experimental thermonuclear reactor ITER

china eu india japan korea russia usa



T_C
 H_C
 J_C

ITER magnetic system:

600 tons of Nb₃Sn
600 tons of NbTi

Futurism



SUPERCOMPUTERS

To Moore's Law and Beyond

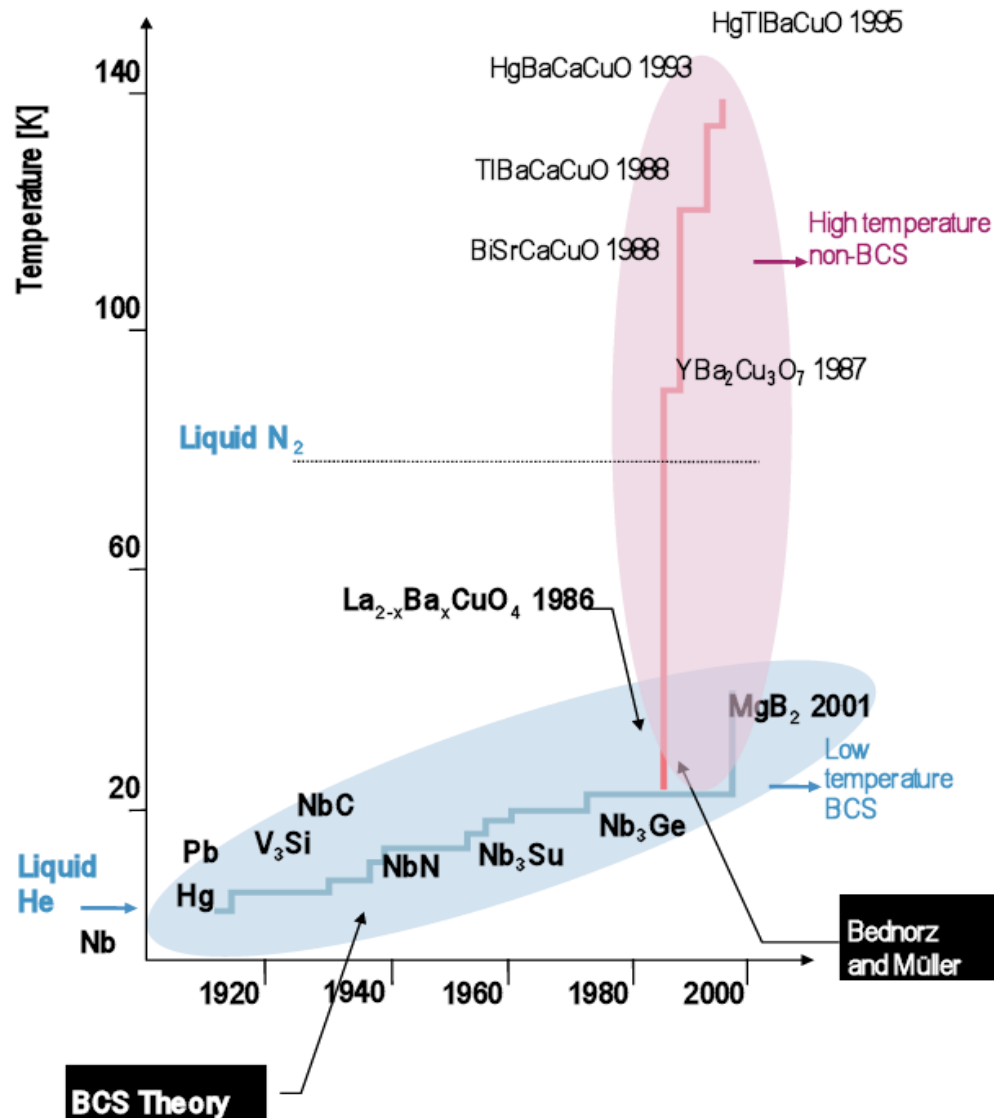
Історія надпровідності: ВТНП

1986



Muller & Bednorz

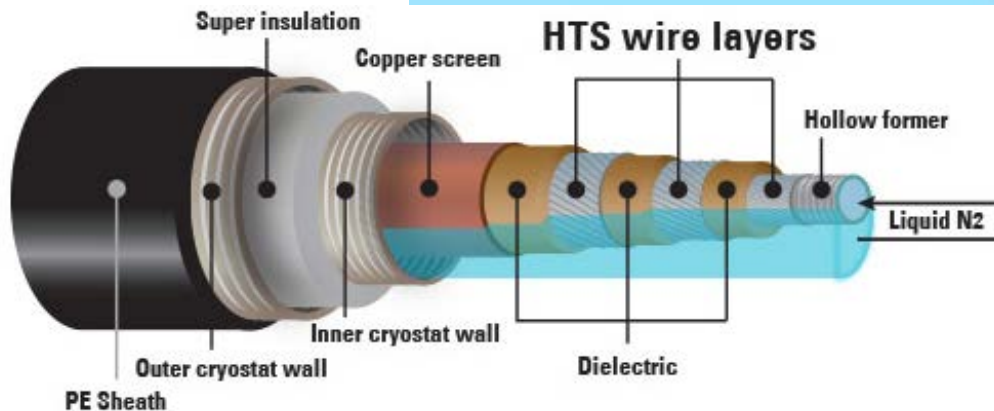
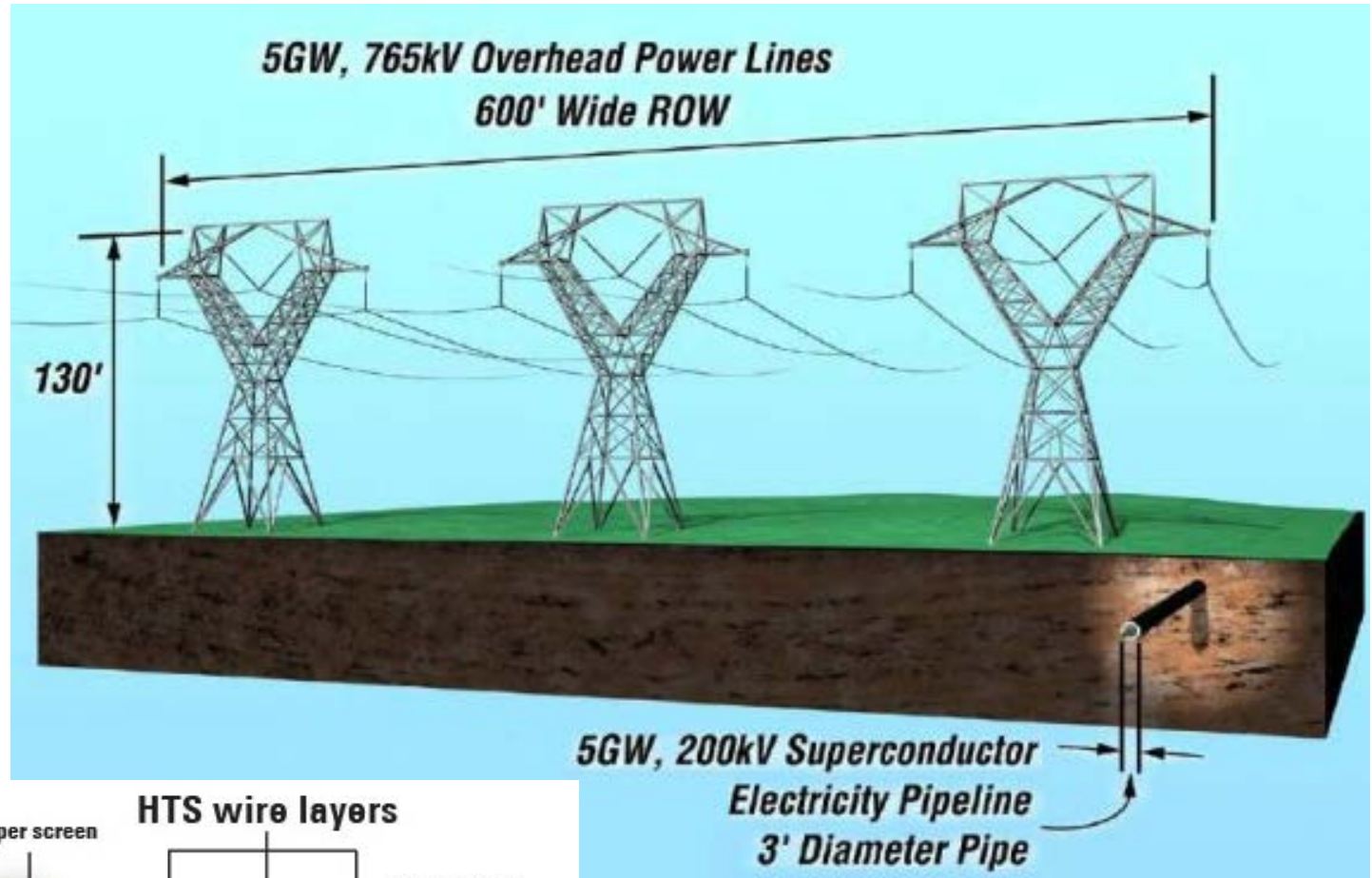
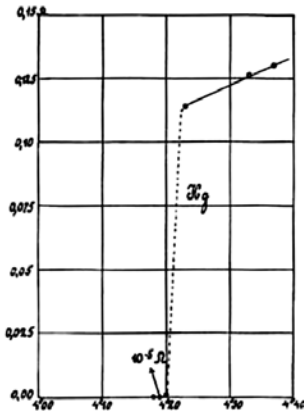
History of superconductivity: HTSC



Muller & Bednorz

compound	T_c (K)
Nd _{1.85} Ce _{0.15} CuO ₄	24
La _{1.85} Sr _{0.15} CuO ₄	40
YBa ₂ Cu ₃ O ₇	92
Bi ₂ Sr ₂ Ca ₂ Cu ₃ O ₁₀	110
Tl ₂ Ba ₂ Ca ₂ Cu ₃ O ₁₀	127
Hg ₂ Ba ₂ Ca ₂ Cu ₃ O ₈	134

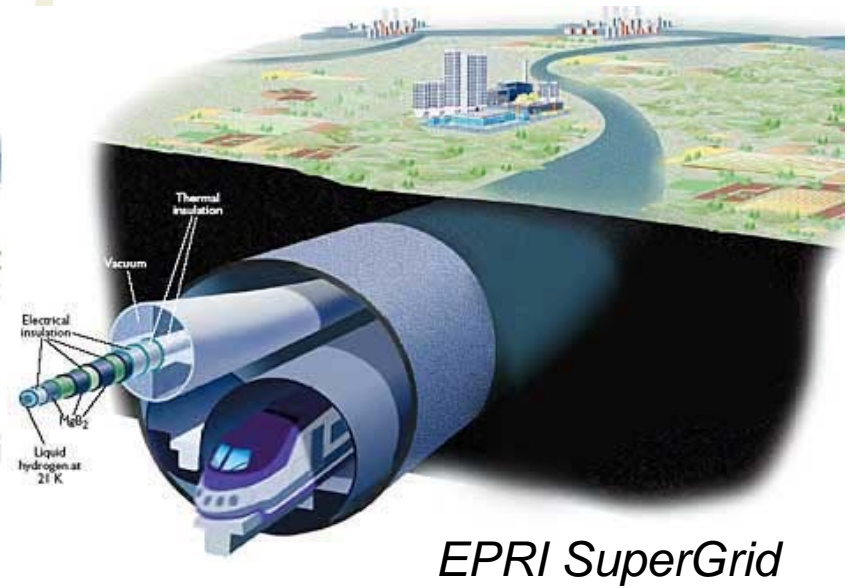
Application # 1 - Current



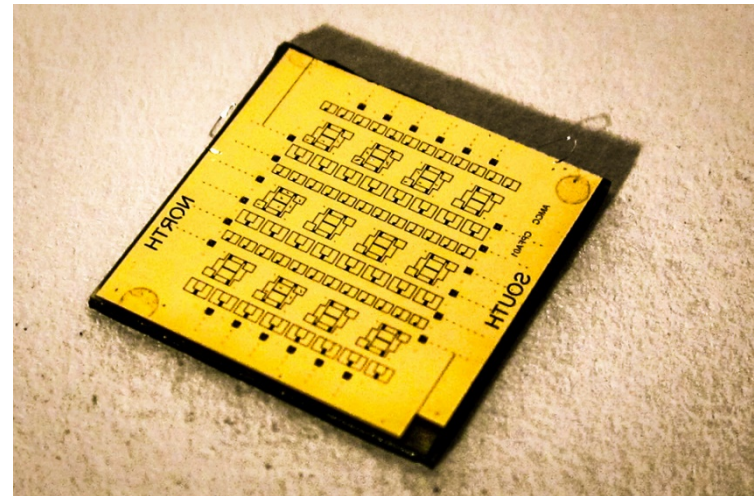
*American Superconductor
talk IREQ 2009*

Applications

Feature of Smart Grid



Superconducting
Supercomputer



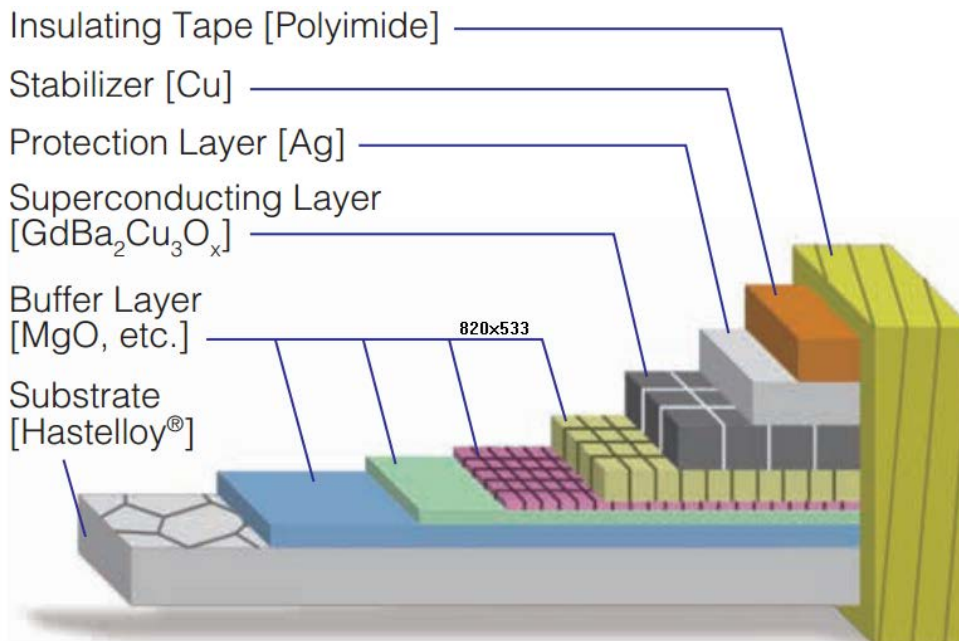
Superconducting cables



Wires of superconducting niobium-3 tin, a "low-temperature" superconductor, after partial removal of stainless steel jacket to reveal the internal components. Image by Carlos (Charlie) Sanabria / National MagLab

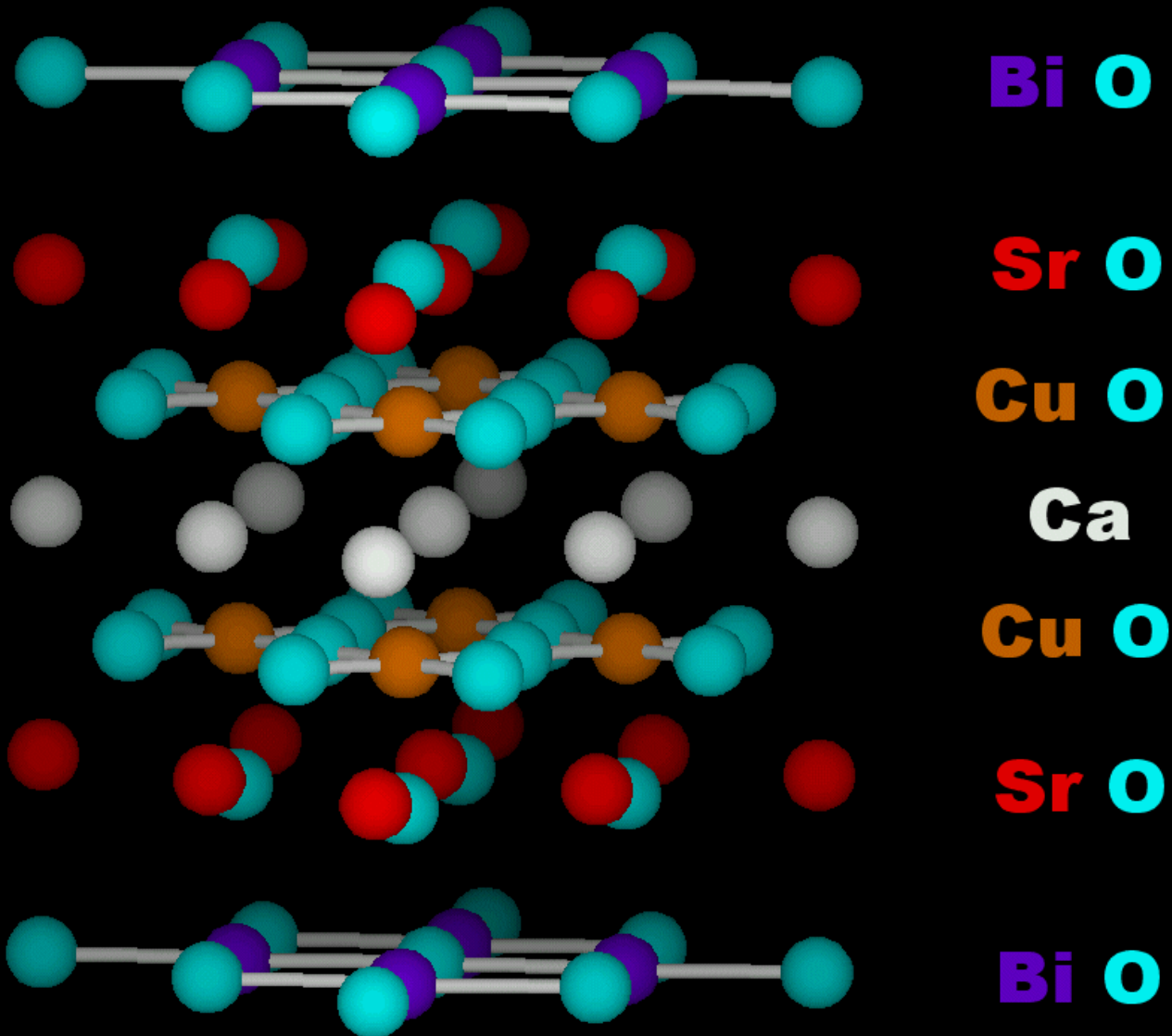
HTSC cables

Second-generation High Temperature Superconductor (2G HTS) wires utilising Yttrium and Gadolinium-based ceramics (YBCO)

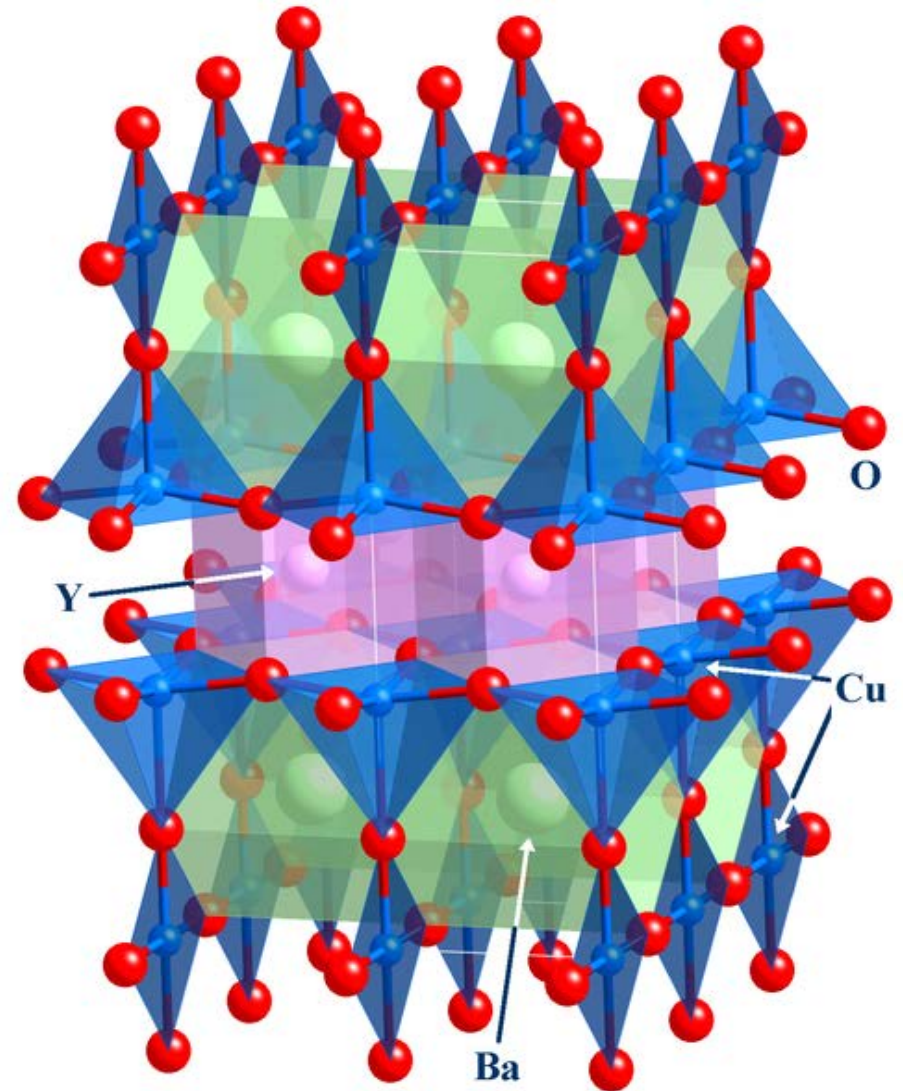
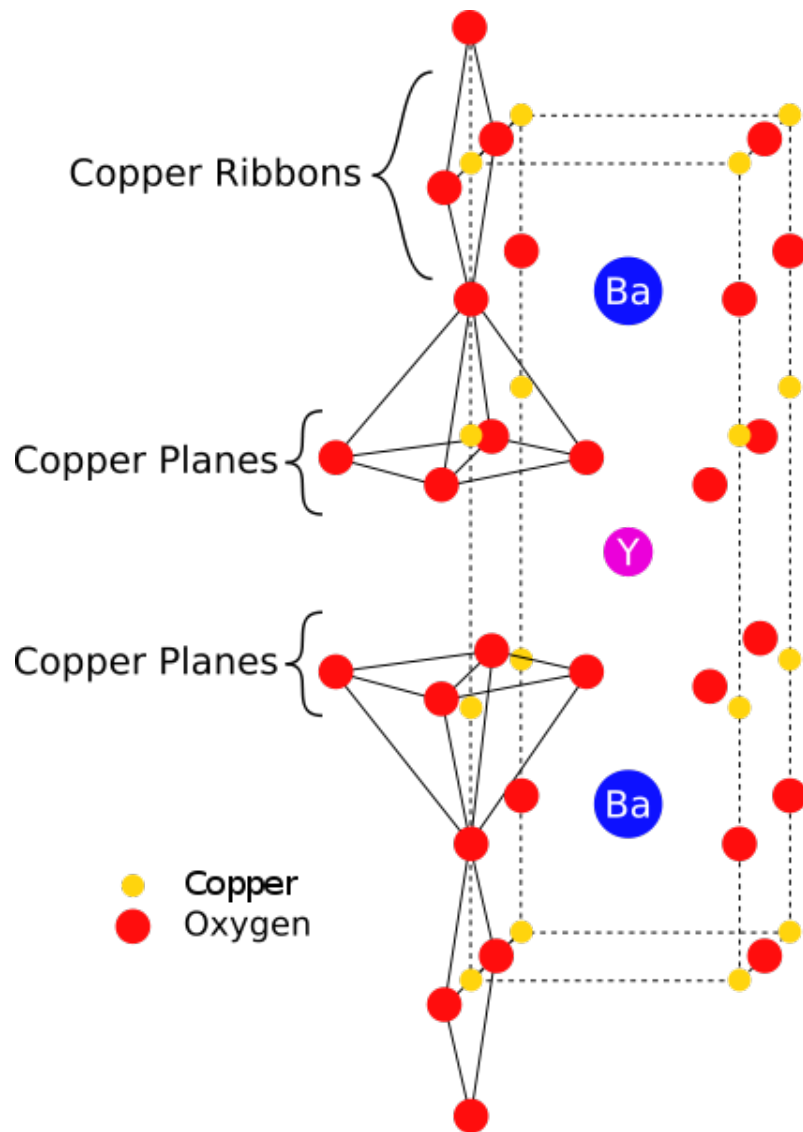




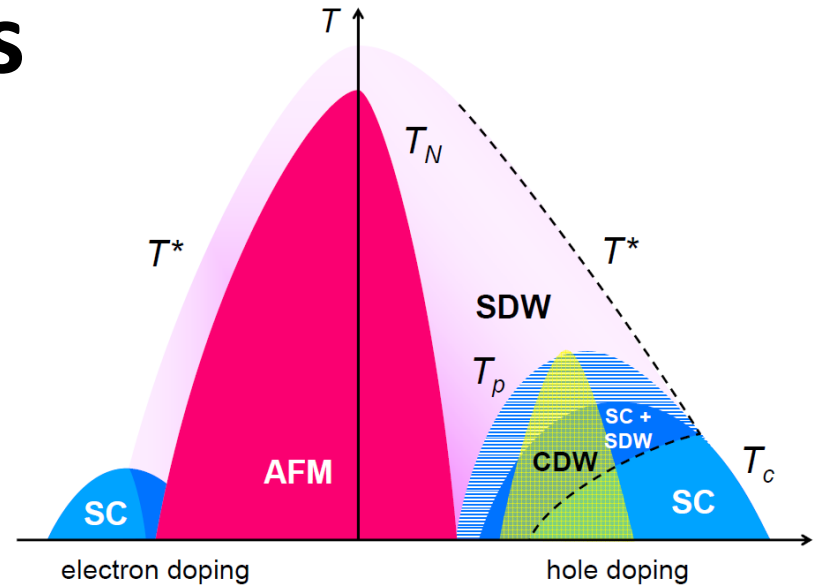
Prototype “Roebel” cable based on the high-temperature superconductor ReBCO (rare-earth barium-copper oxide) is being used to wind a demonstration accelerator dipole at CERN as part of the EuCARD-2 project. (Image: H Barnard/CERN)



HTSC: YBCO



Physics of cuprates



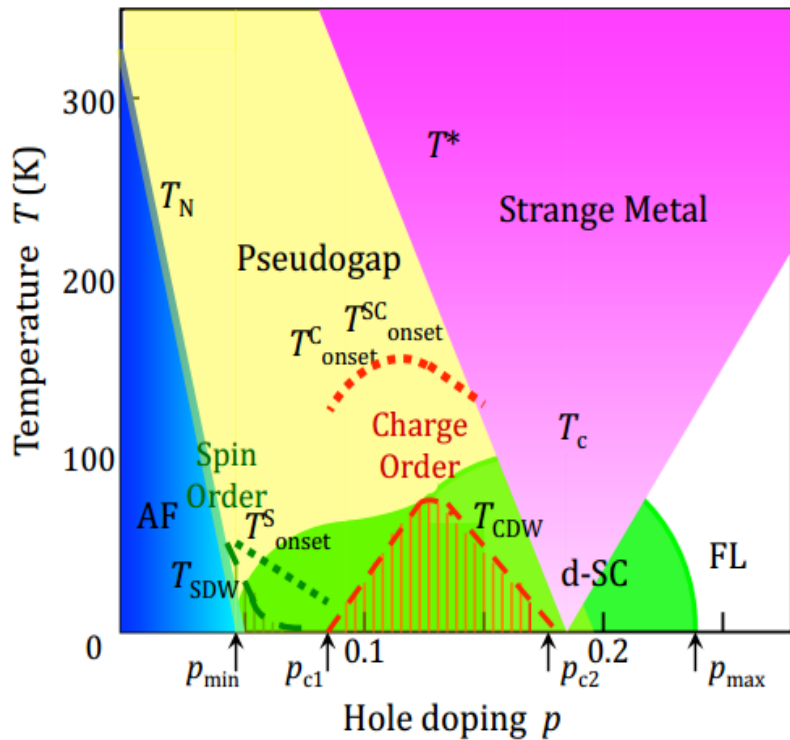
Physics is complex.

The structure is simple - the CuO₂ plane.

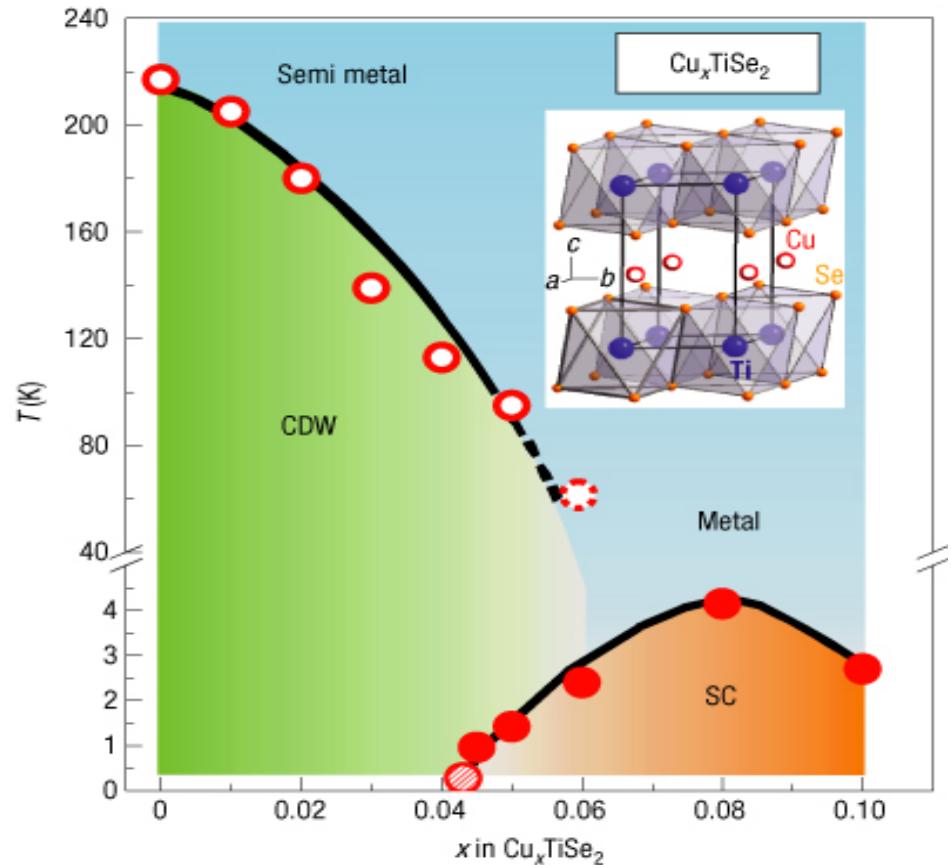
Simple electronic structure.

Smooth electronic interaction.

Competing orders relation to electronic structure?

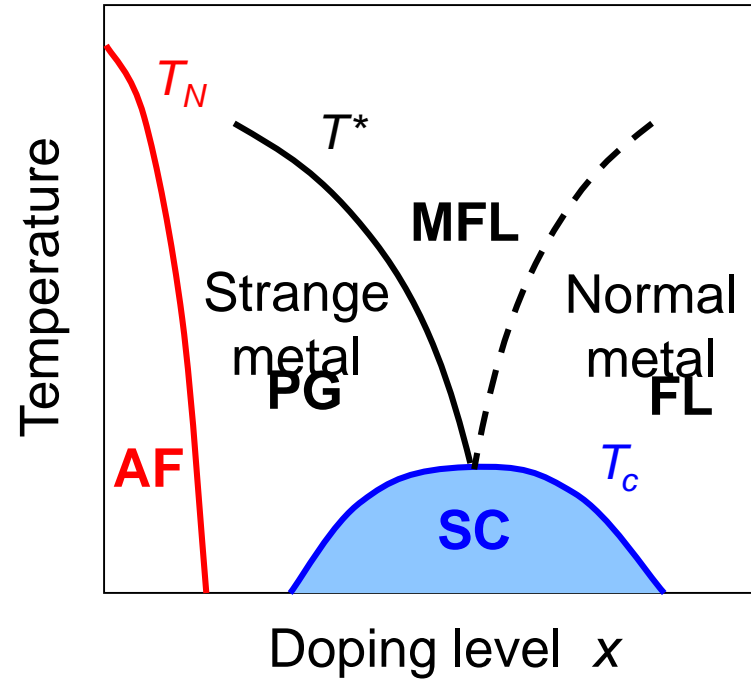
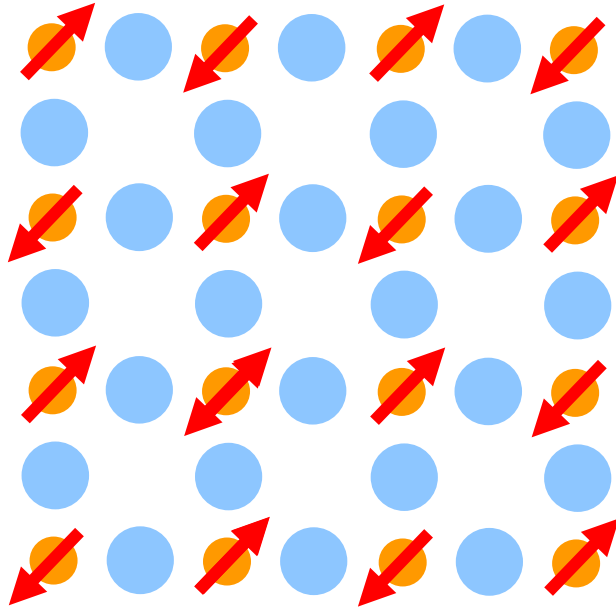


B Keimer, SA Kivelson,
MR Norman... 2014



Morosan *Nature Physics* 2006

Hole doping

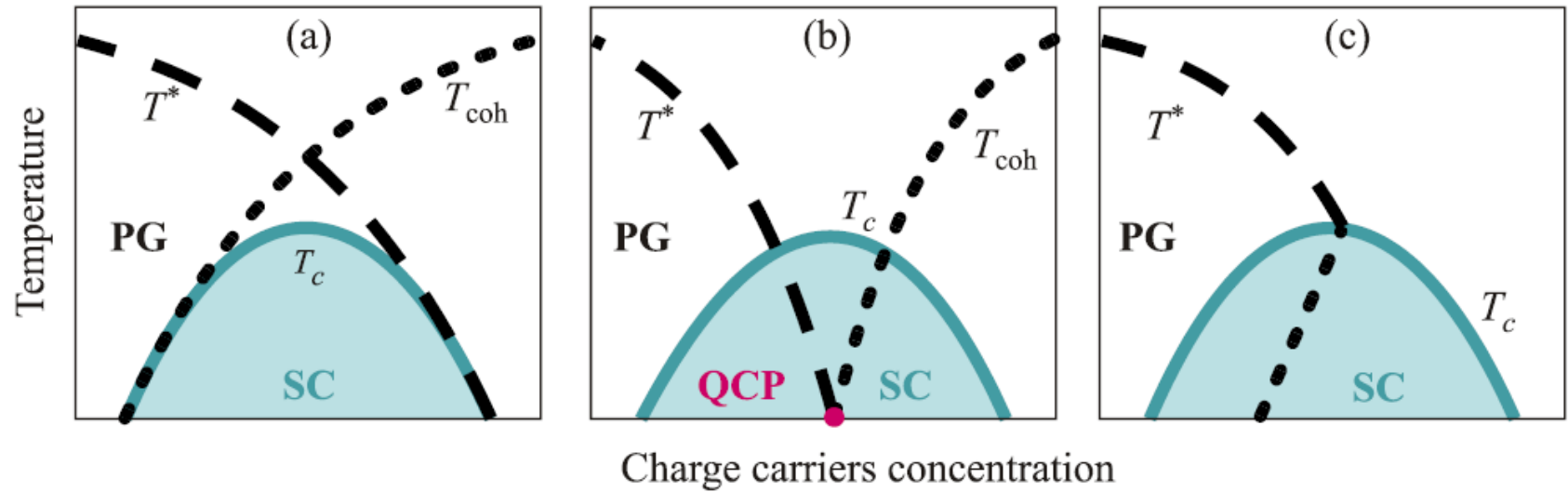


FL – Fermi Liquid

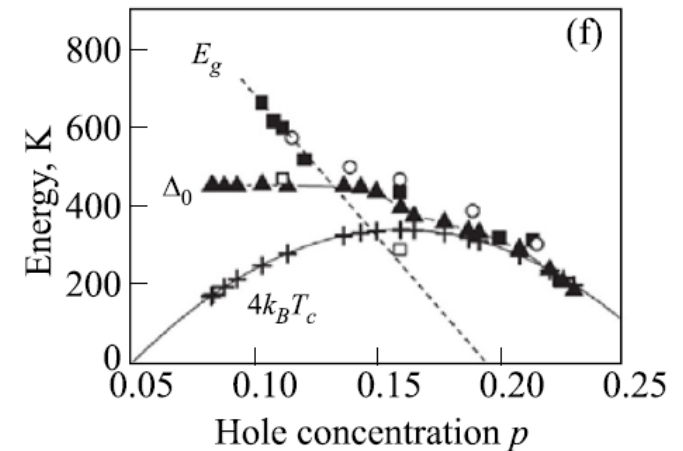
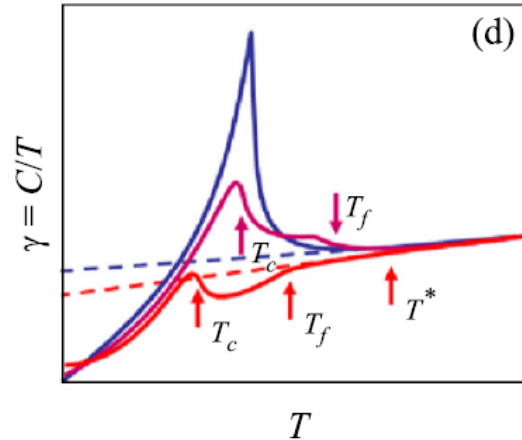
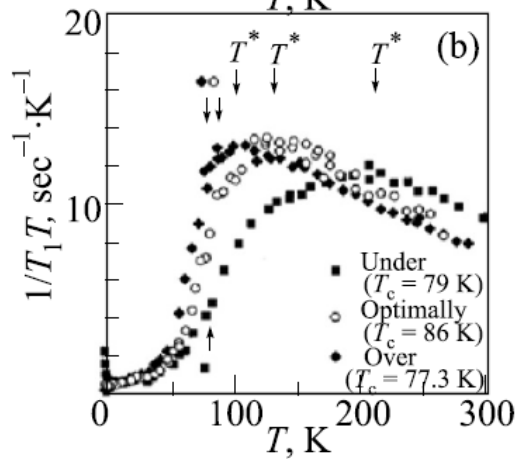
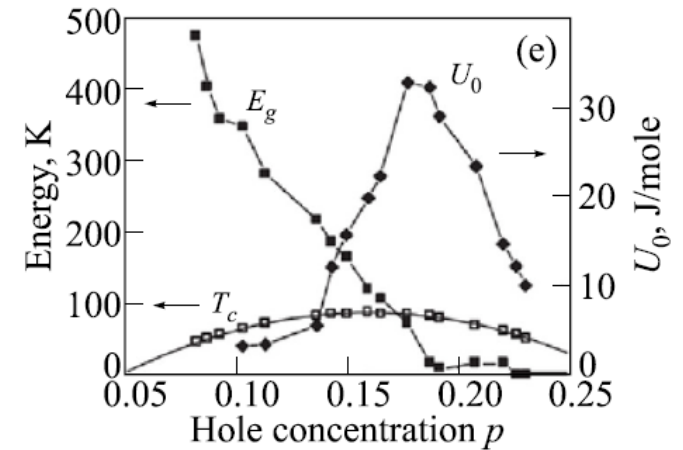
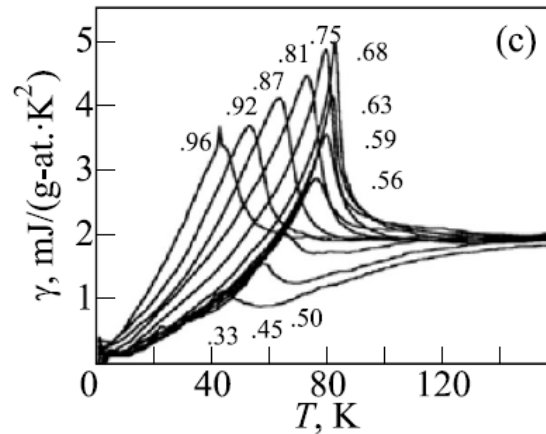
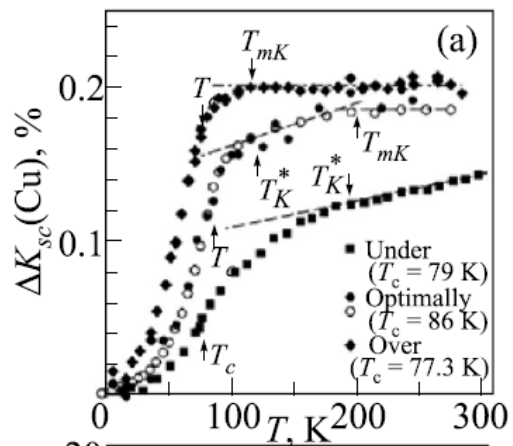
MFL – Marginal Fermi Liquid

PG – Pseudo Gap state

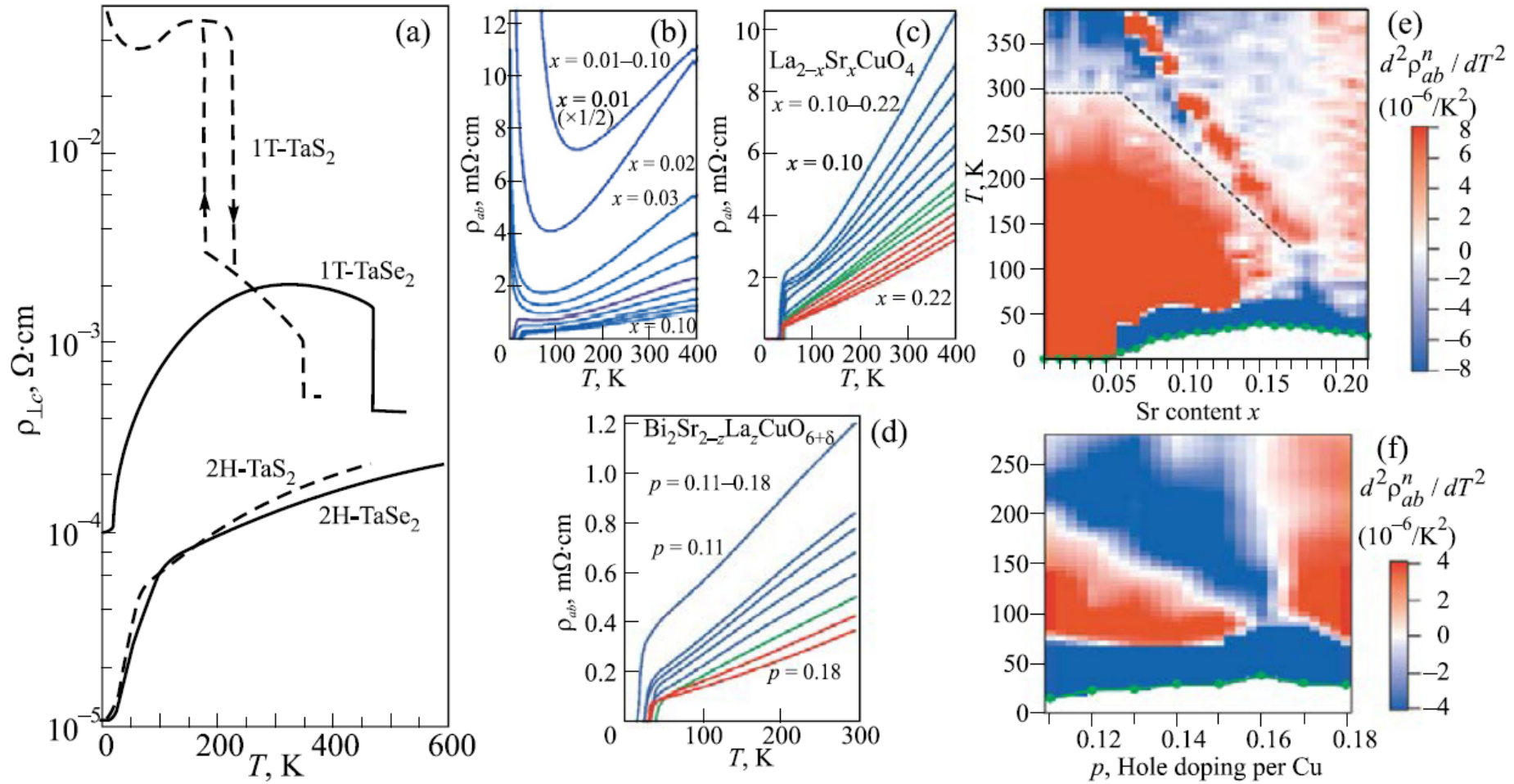
Theories of the pseudogap



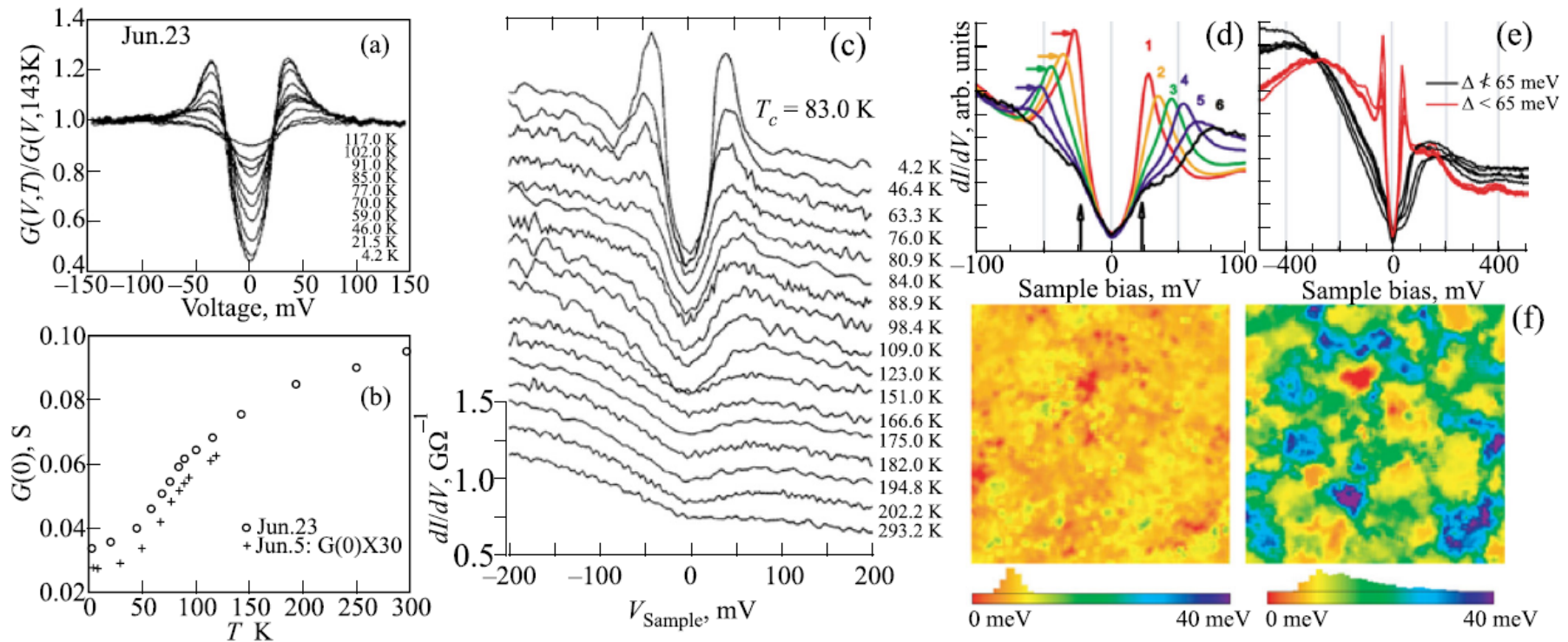
Pseudogap in NMR and heat capacity



Pseudogap in Resistivity



Pseudogap in Tunneling

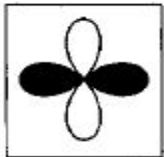


d-wave order: tri-crystal experiment

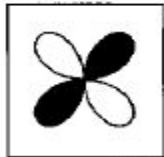
Pairing is d symmetry.

Phase sensitive measurements.

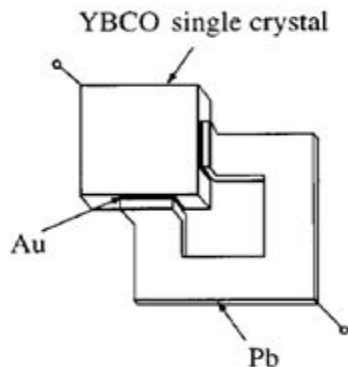
$$\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle \propto \Psi(\mathbf{k})$$



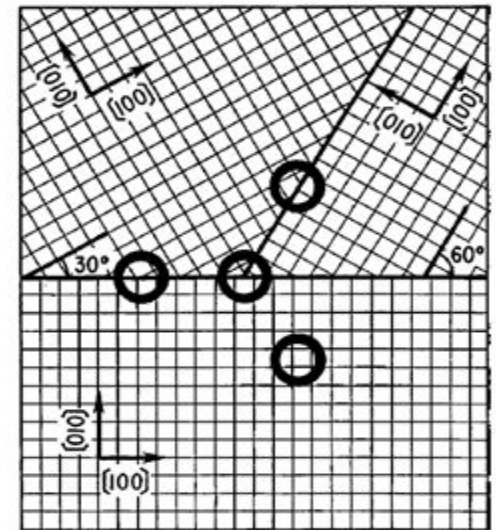
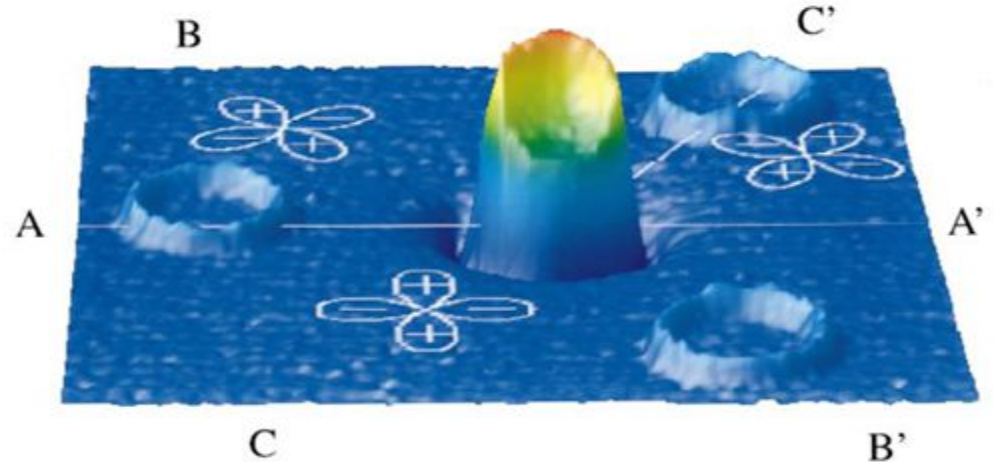
$$\Delta_{d_{x^2-y^2}}(\mathbf{k}) = \Delta_{d_{x^2-y^2}}^0 (\cos k_x - \cos k_y)$$



$$\Delta_{d_{xy}}(\mathbf{k}) = \Delta_{d_{xy}}^0 (\sin k_x \sin k_y)$$



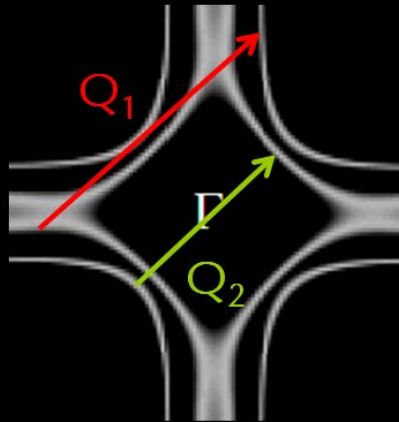
1. tri-crystal experiment, IBM 1993.
 $\frac{1}{2}$ flux vortex at the junction.
 Standard $hc/2e$ vortex everywhere else.
2. Corner SQUID.
 Wollman et al 1993.



Tsuei and Kirtley Rev Mod Phys 2000.

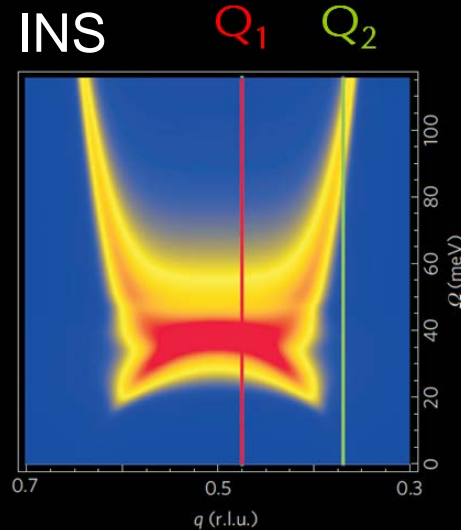
Spin-fluctuations and superconductivity

ARPES



$\text{Im } G_0(\mathbf{k}, \omega)$

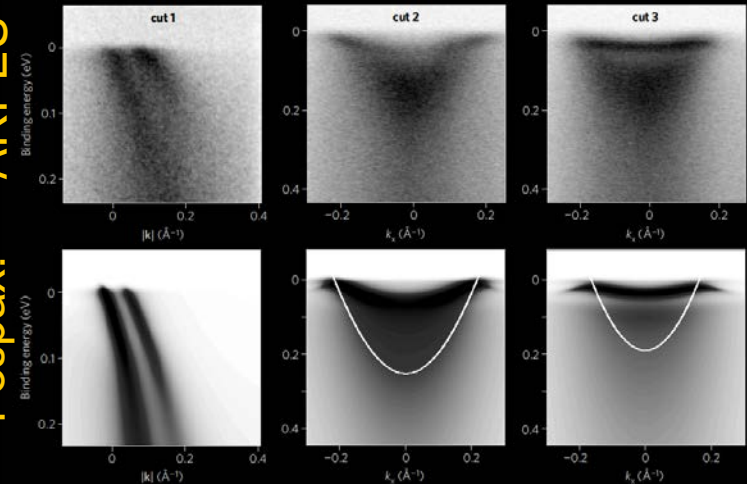
INS



$\text{Im } \chi(\mathbf{q}, \Omega)$

ARPES

Розрпax.



$\text{Im } G(\mathbf{k}, \omega)$

Formula of cuprates:

$$G_0^{-1} + \sum \alpha^2 G \star \chi = G^{-1}$$

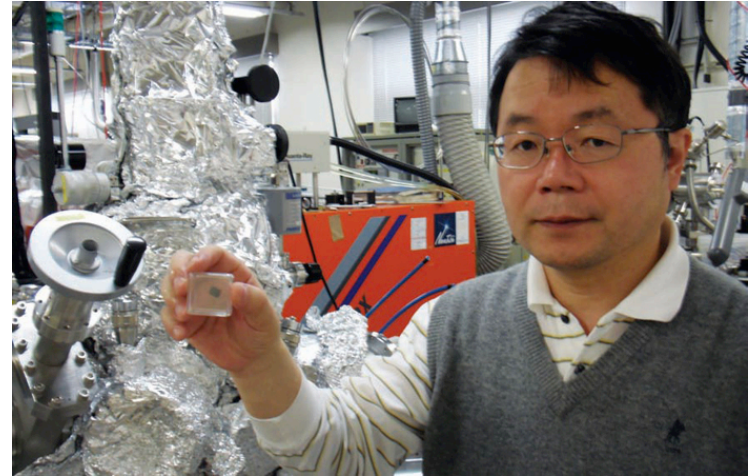
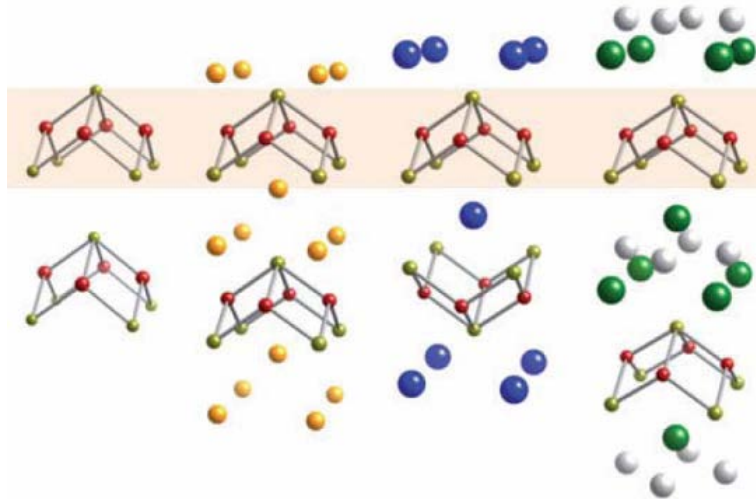
$$G_0^{-1} + \alpha^2 G \star G \star G = G^{-1}$$

1. ARPES and INS
→ spin-fluctuations
2. $T_c \sim 150$ K.

D. Inosov et al., [PRB 2007](#)
T. Dahm et al., [Nature Phys 2009](#)
A. Kordyuk et al., [EPJ ST 2010](#)

New history of superconductivity: Iron Age

2008

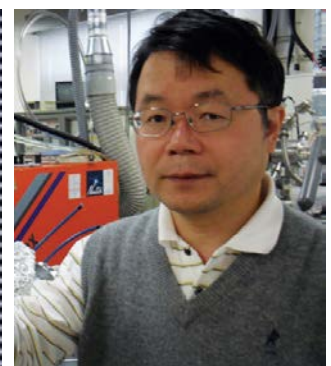
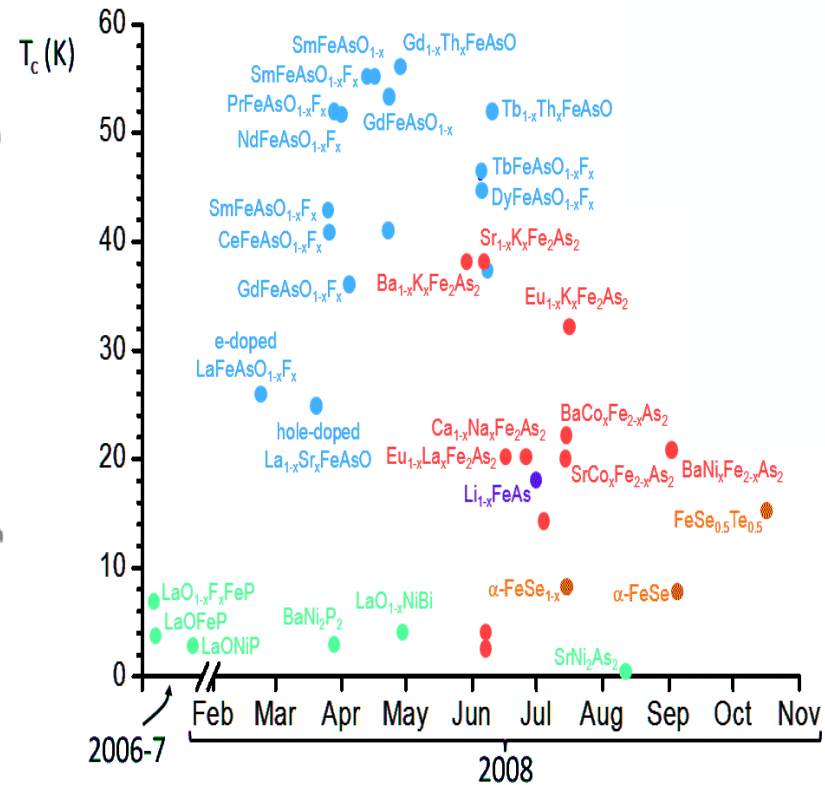
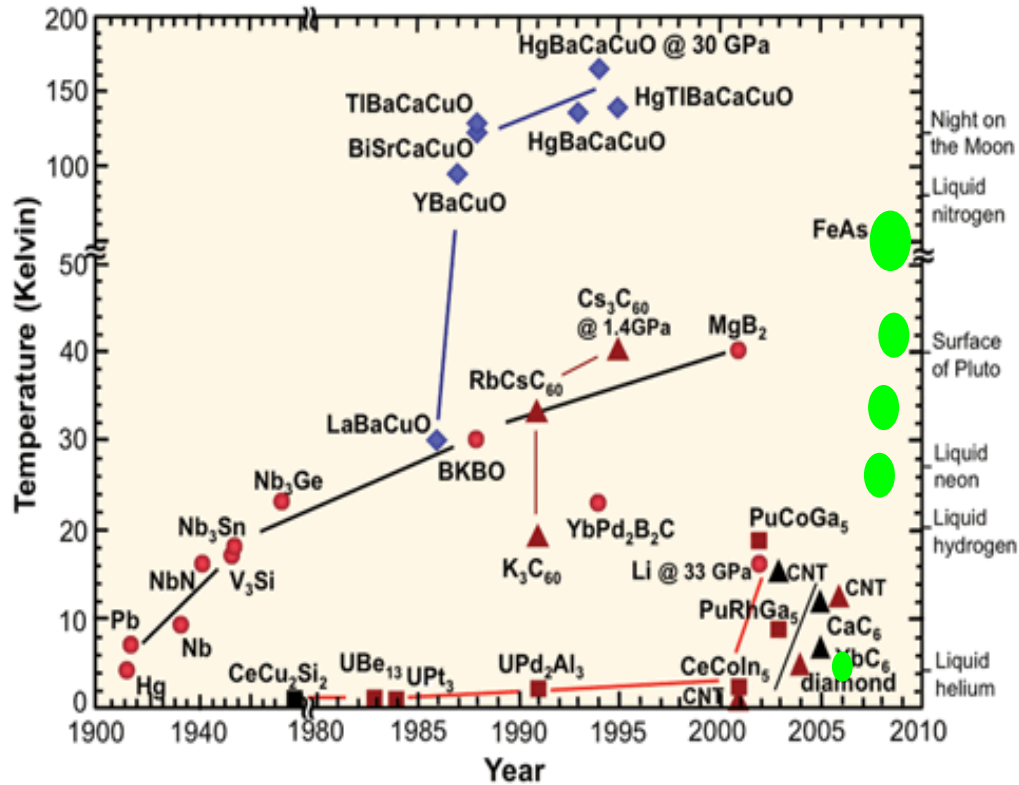


Hideo Hosono

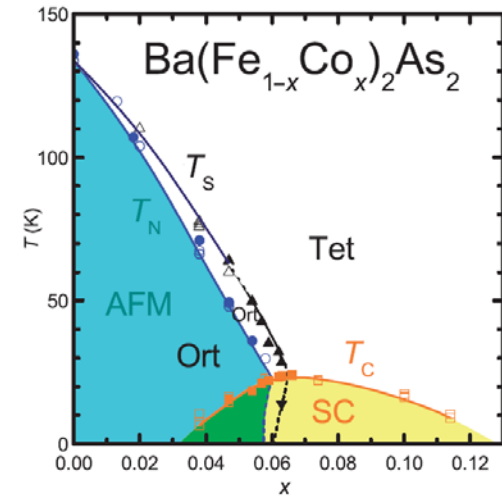
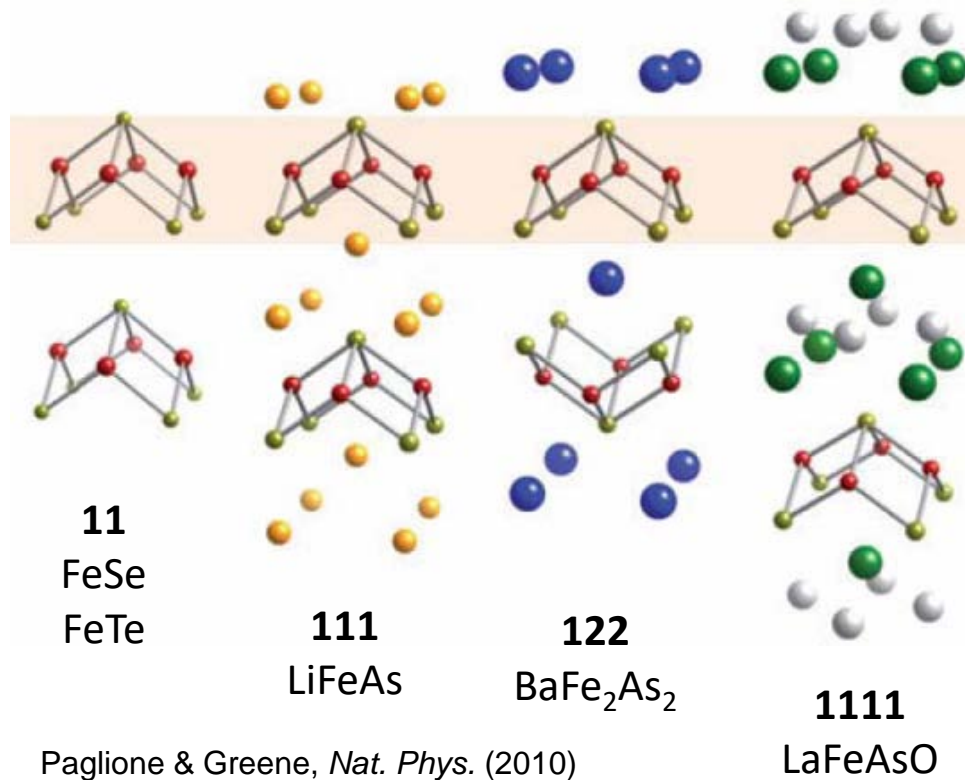
LaFeAs(OF) , $T_c = 26\text{K}$, up to 56K



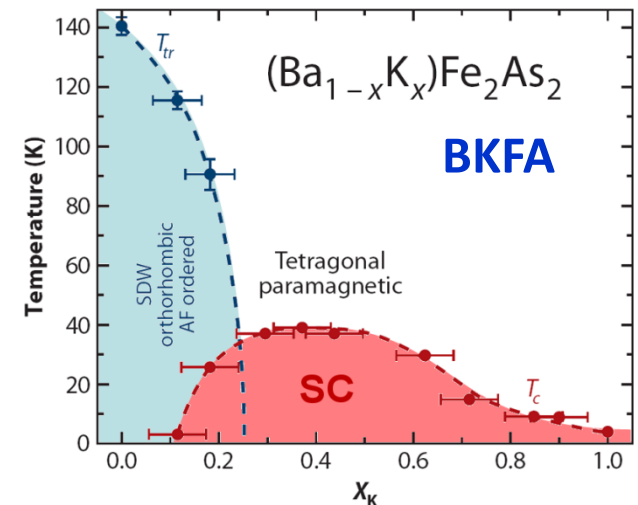
High-temperature superconductivity, HTSC



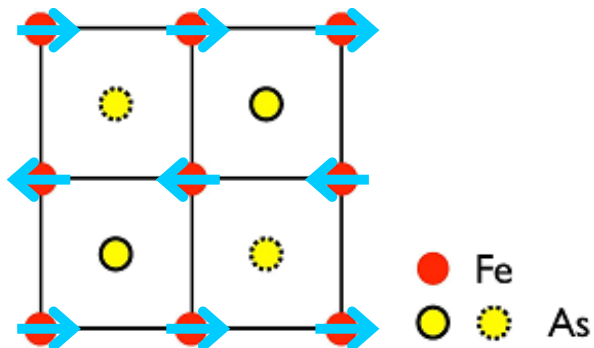
Iron-based superconductors (FeSC)



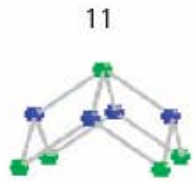
S.Nandi et al. [PRL 2010](#)



H.-H.Wen & S.Li [Annu. Rev. Cond. Mat. Phys. 2011](#)



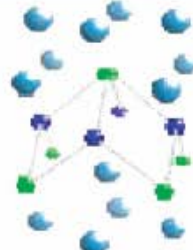
Iron-based superconductors



FeSe
FeTe

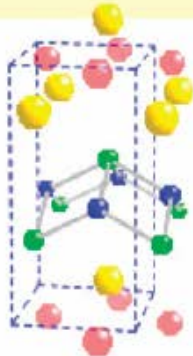
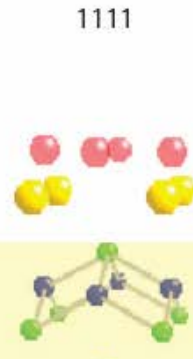
$T_c = 8 \text{ K}$

HP
 $T_c = 37 \text{ K}$



LiFeAs
NaFeAs

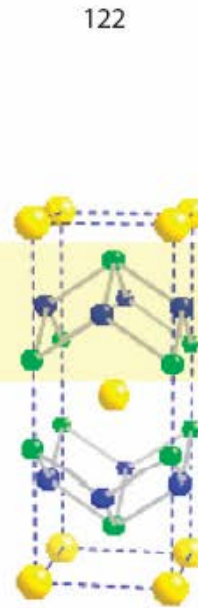
$T_c = 18 \text{ K}$



F-REFeAsO

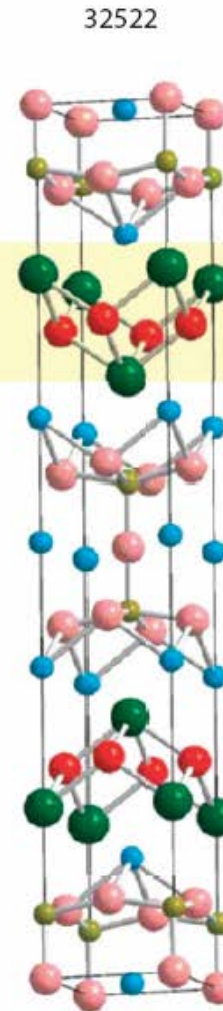
RE-CaFeAsF

$T_c = 57 \text{ K}$



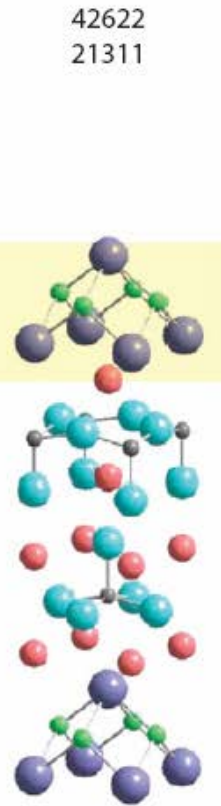
(Ba,K)Fe₂As₂
 $T_c = 38 \text{ K}$

Ba(Fe,Co)₂As₂
 $T_c = 26 \text{ K}$



(Sr₃Sc₂O₅)Fe₂As₂

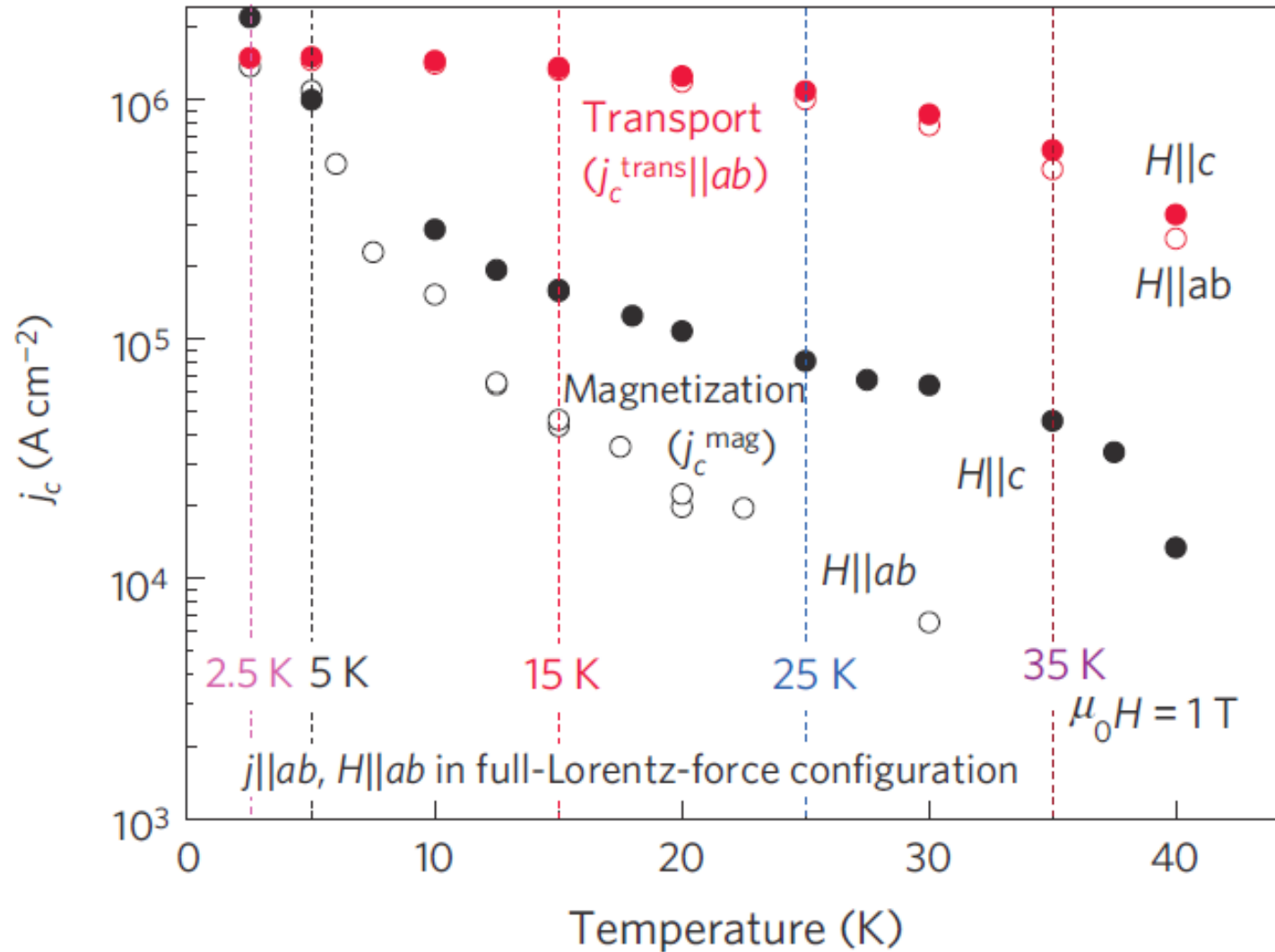
No SC



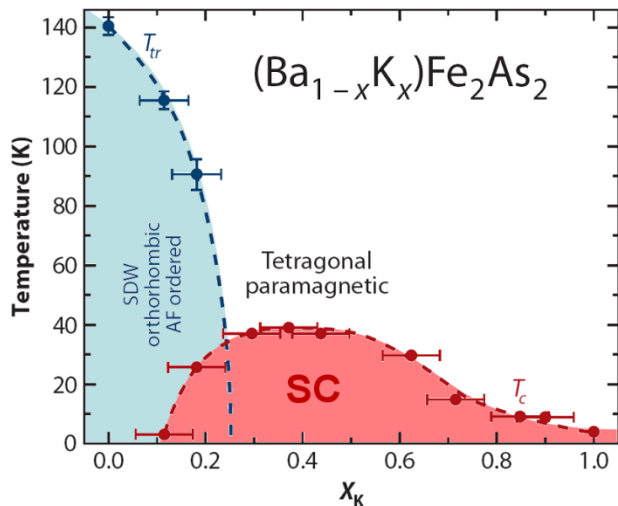
(Sr₄V₂O₆)Fe₂As₂

$T_c = 37 \text{ K}$
 $T_c = 46 \text{ K (HP)}$

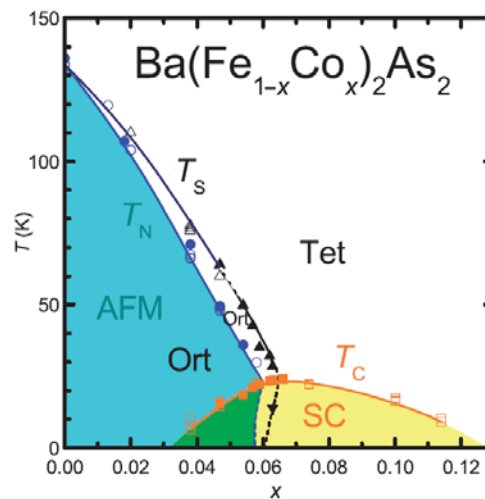
Critical current density FeSC



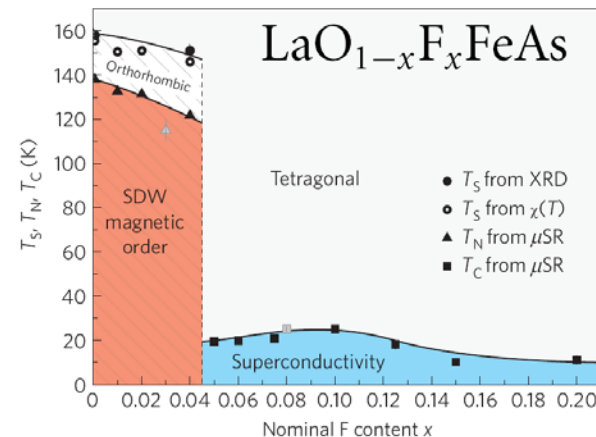
Phase diagrams



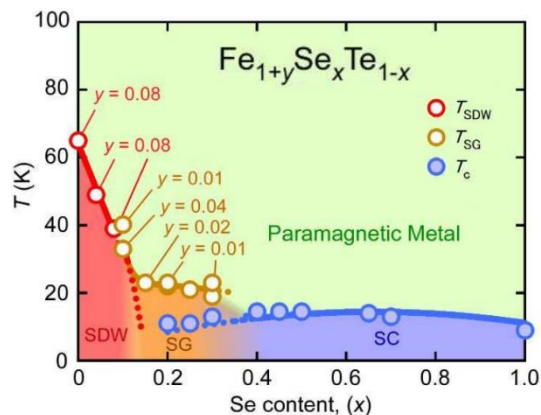
H.-H.Wen & S.Li [Annu. Rev. Cond. Mat. Phys. 2011](#)



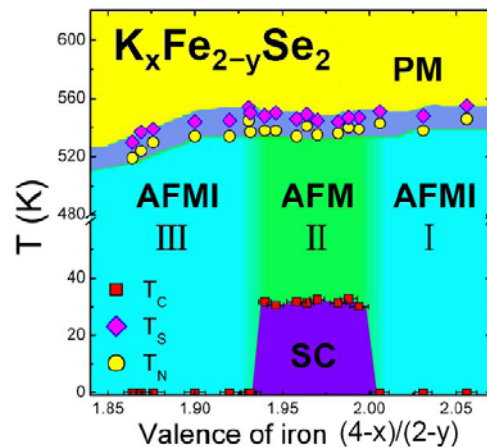
S.Nandi *et al.* [PRL 2010](#)



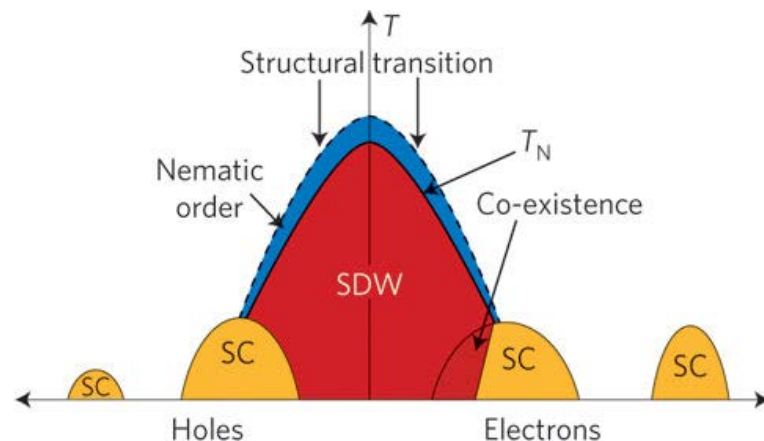
H.Luetkens *et al.* [Nature Mat. 2009](#)



N.Katayama *et al.* [arXiv:1003.4525](#)



Y.J.Yan *et al.* [arXiv:1104.4941](#)



Basov & Chubukov [Nature Phys. 2011](#)

Non-scientific conclusion

Among many theories of HTSC there is no one to predict new superconductors with higher T_c 's.

Empirical approaches should be used.

National Academy of Sciences of Ukraine
Institute for Metal Physics
Department of Superconductivity

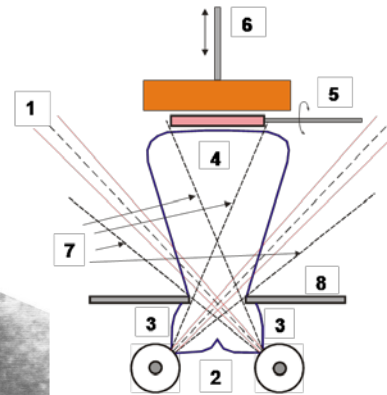
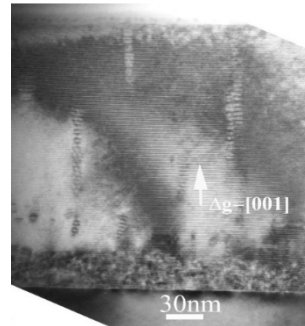
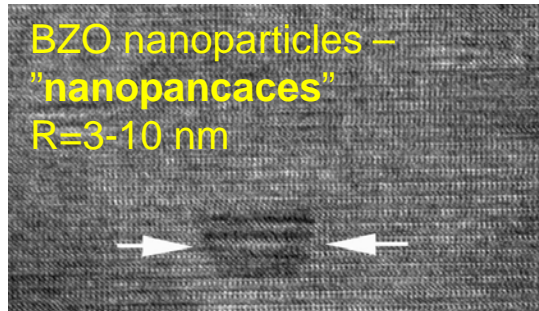
Directions of research:

- Optimization of magnetic flux pinning in thin films
- Novel Josephson Junctions
- Search for superconductors with higher T_c based on peculiarities of their electronic band structure

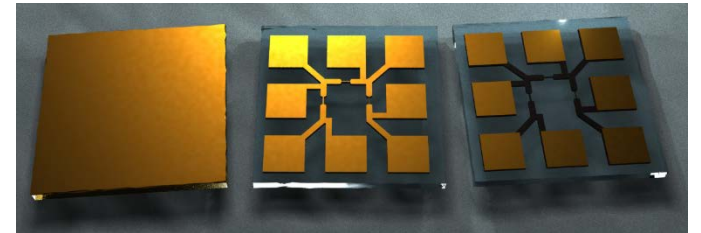
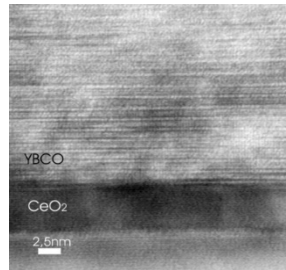
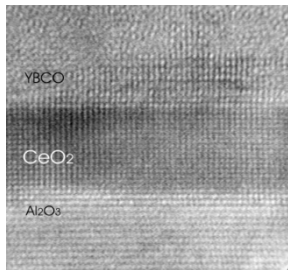
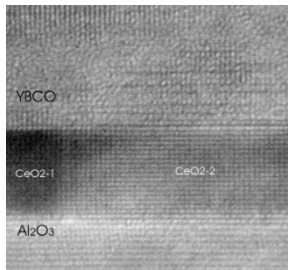
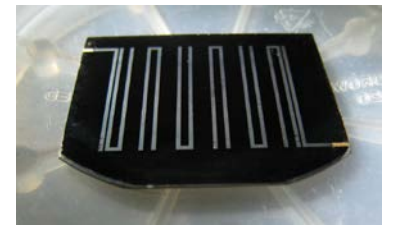
Optimization of magnetic flux pinning in thin films

Pulsed laser deposition (PLD) and
Magnetron scattering techniques

+ He Liquefier in operation!



Self-organized BZO
nanoparticles -
"nanorods"



Novel Josephson Junctions

PHYSICAL REVIEW LETTERS **120**, 067001 (2018)

Phase-Sensitive Evidence for the Sign-Reversal s_{\pm} Symmetry of the Order Parameter in an Iron-Pnictide Superconductor Using Nb/Ba_{1-x}Na_xFe₂As₂ Josephson Junctions

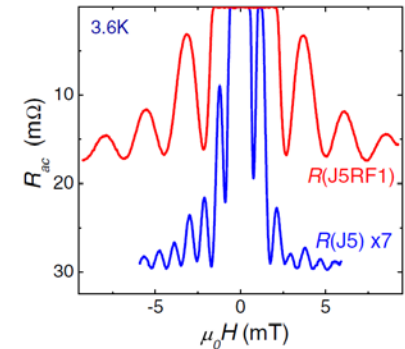
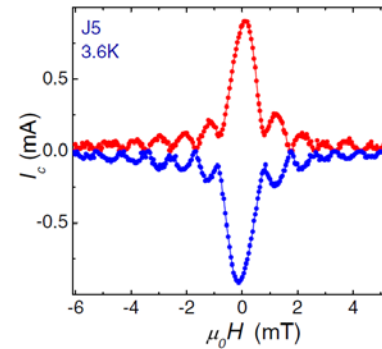
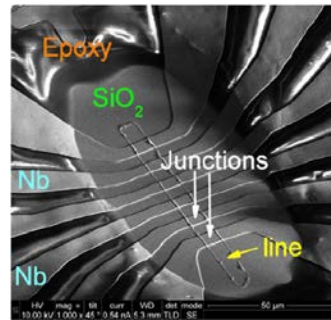
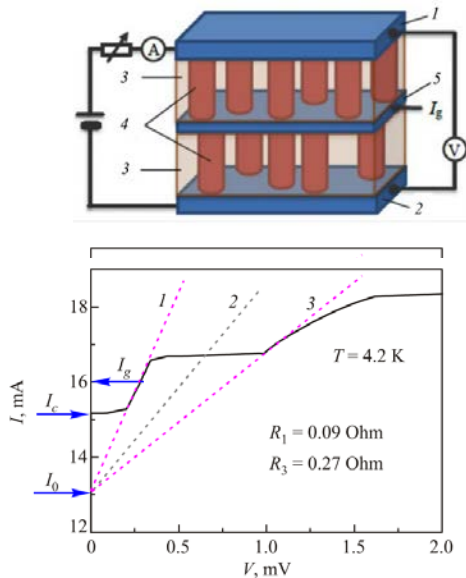
A. A. Kalenyuk,^{1,2} A. Pagliero,¹ E. A. Borodianskyi,¹ A. A. Kordyuk,^{2,3} and V. M. Krasnov^{1,*}

¹Department of Physics, Stockholm University, AlbaNova University Center, SE-10691 Stockholm, Sweden

²Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine

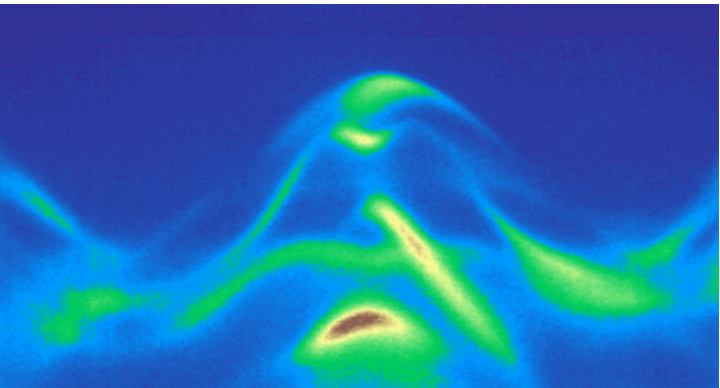
³Kyiv Academic University, 03142 Kyiv, Ukraine

MoRe/Si(W)/MoRe/Si(W)/MoRe device



Next:

Search for superconductors with higher T_c
based on peculiarities of their **electronic
band structure**



- Introduction to the electronic structure of superconductors

Outline

1. Introduction to

- ARPES (Large scale experimental facility)
- Electronic structure & electronic properties
(old results as starting point)

2. Band structure of Fe-SC and superconductivity

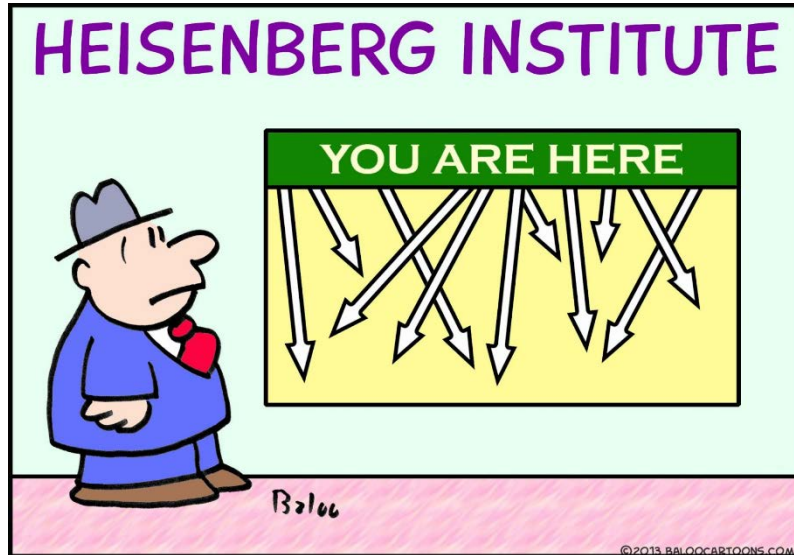
3. Are HTSC cuprates similar?

4. T-dependence of electronic structure

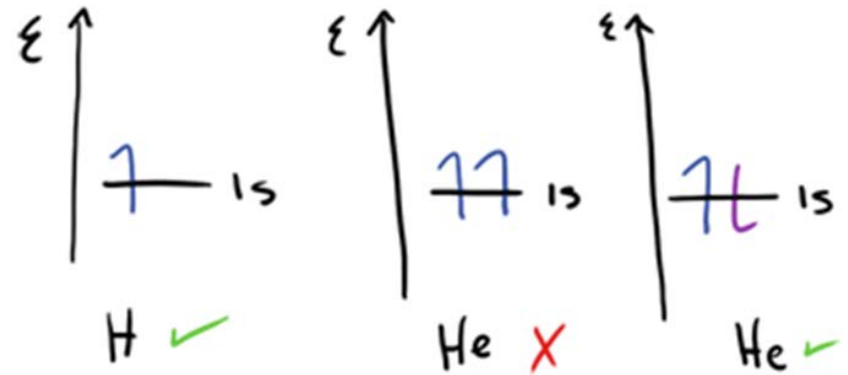
**ARPES
&
Electronic structure**

Electronic band structure

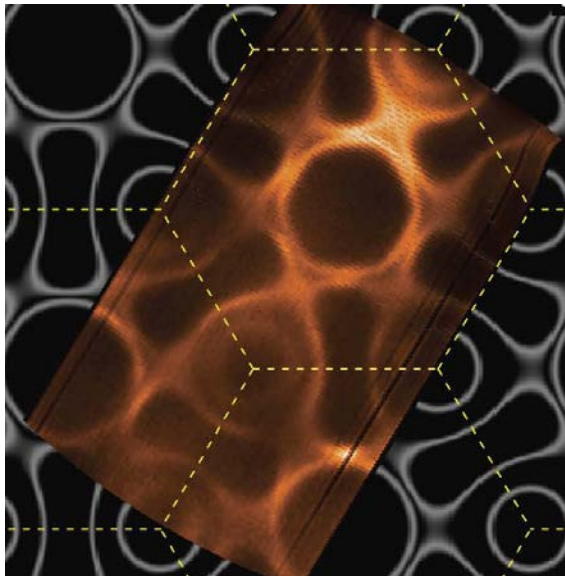
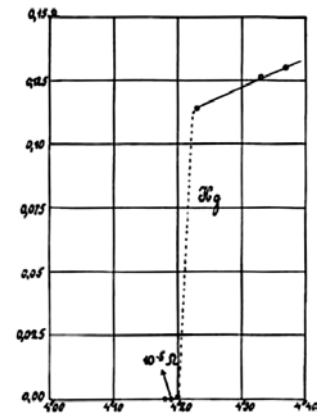
Quantum mechanics and everyday experience



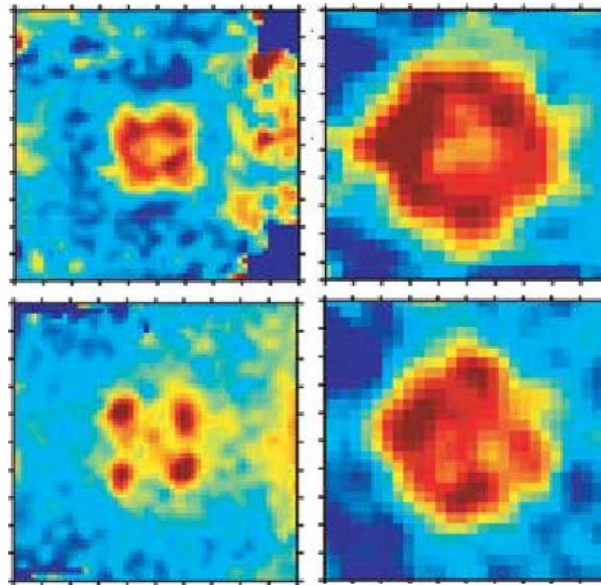
$$\Delta x \Delta p \geq \frac{\hbar}{2}$$



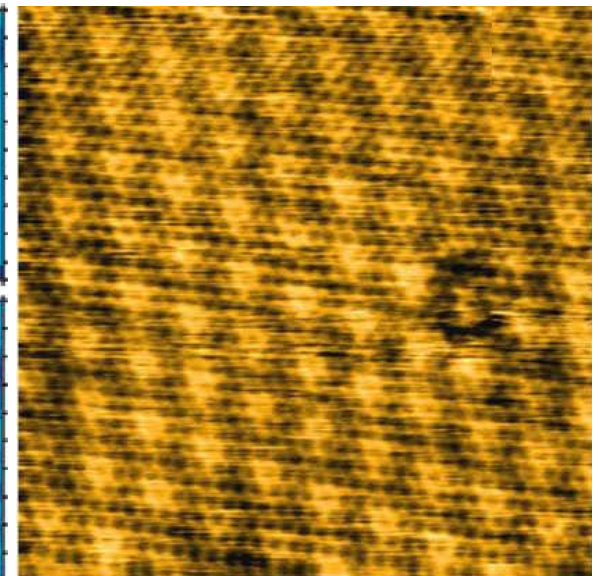
Modern research methods in condensed matter



Photoelectron
spectroscopy
(ARPES)

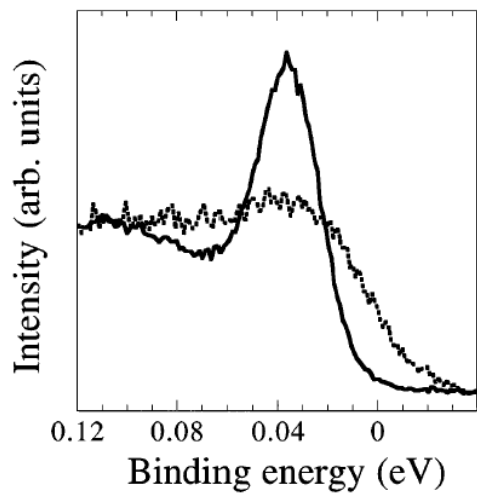
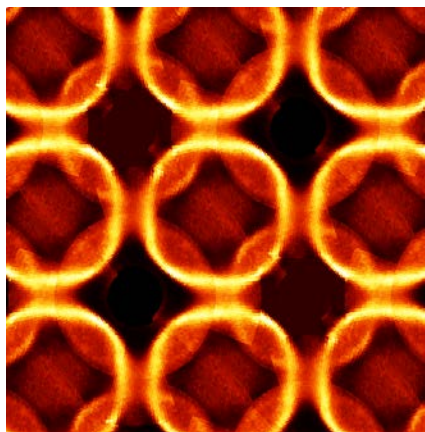


Inelastic neutron
scattering
(INS)

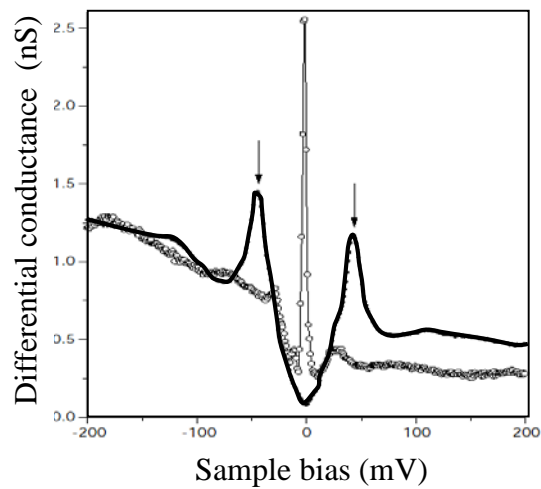
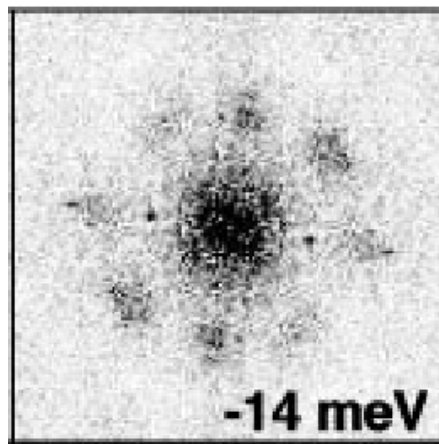


Scanning tunneling
spectroscopy
(STS)

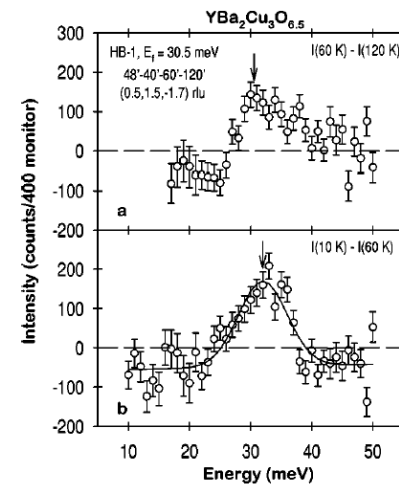
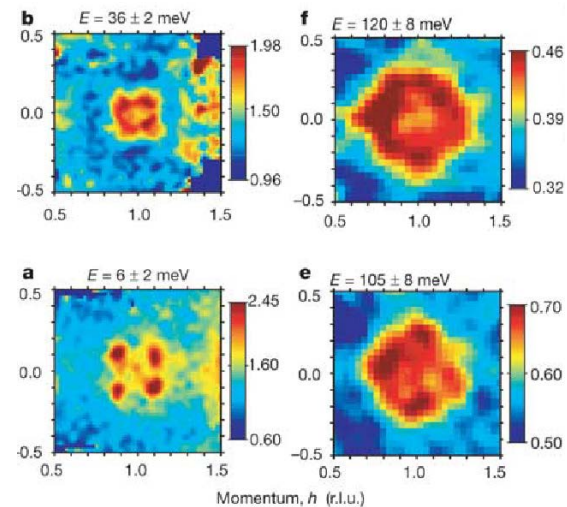
ARPES



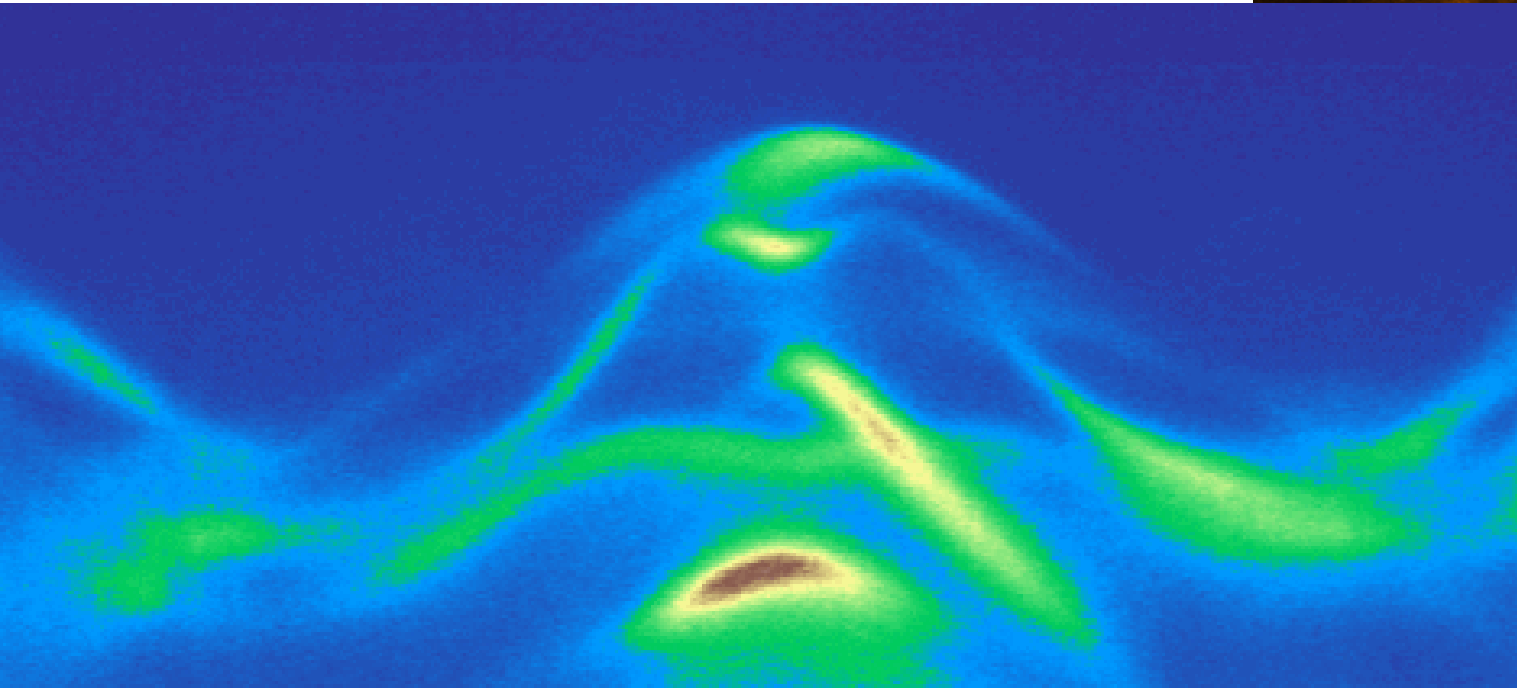
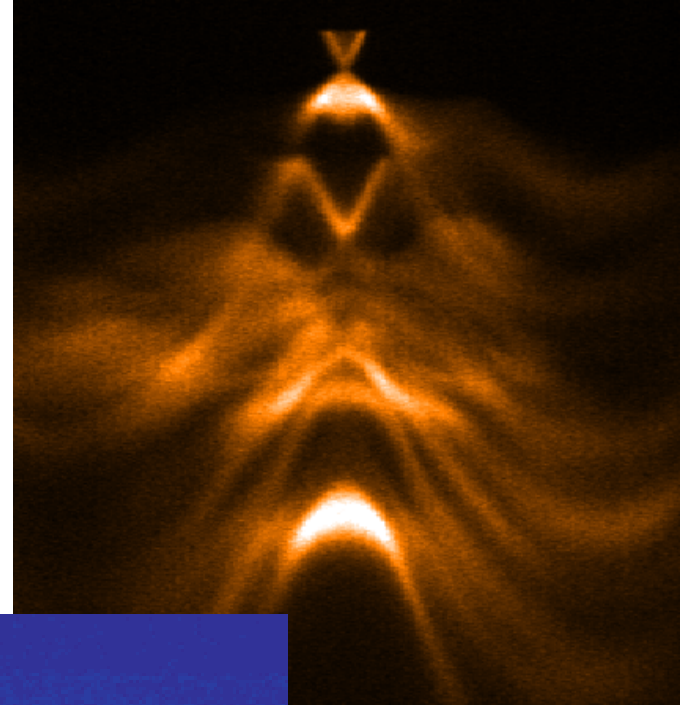
STS



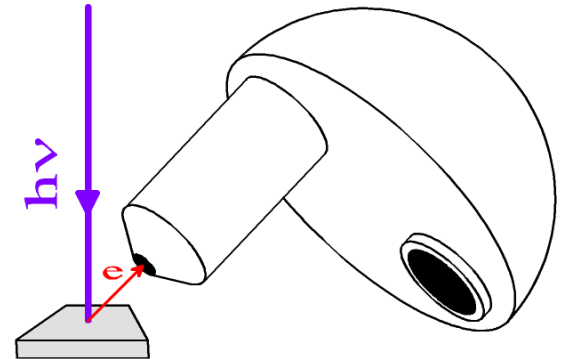
INS



Electrons in momentum-energy space

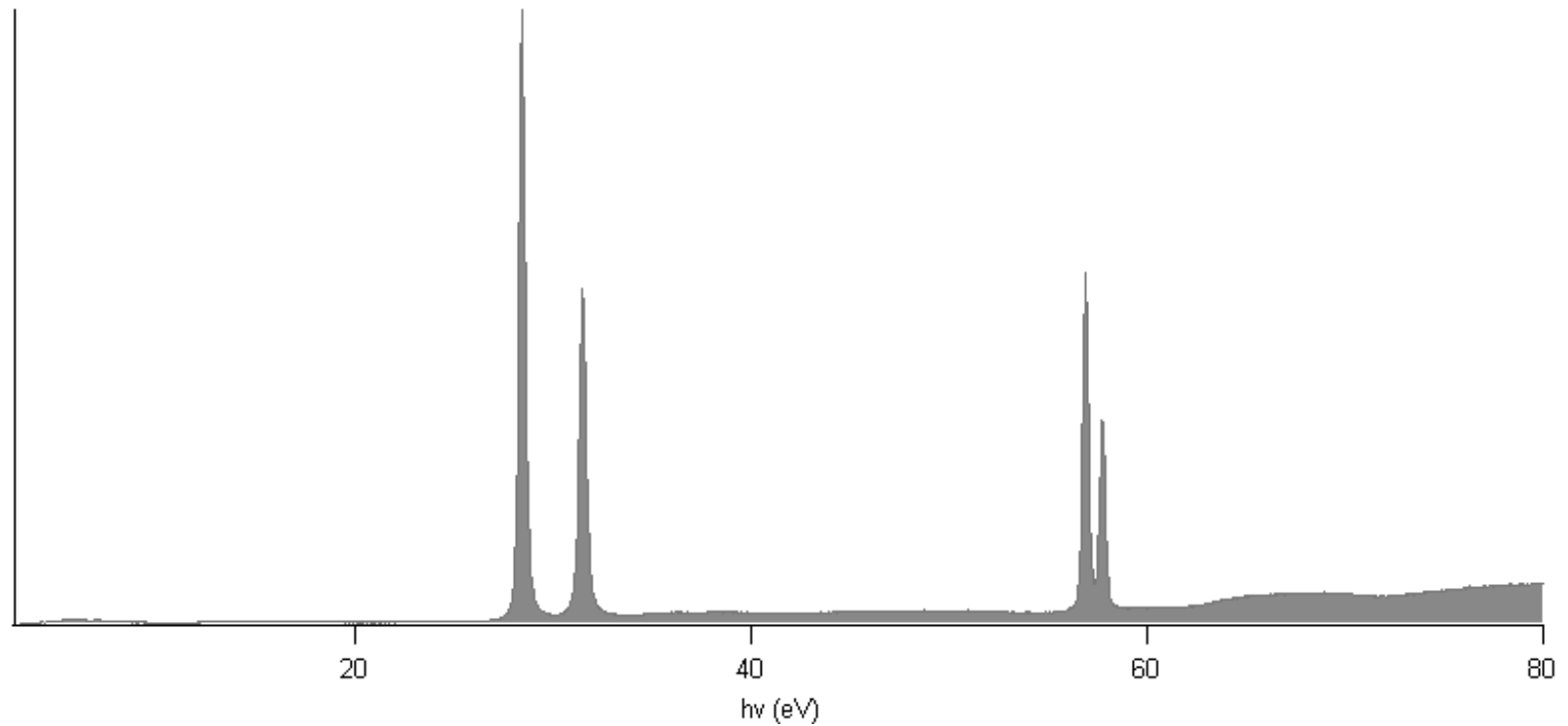


Photoelectron spectroscopy – Electronic band structure ?



Bi₂Se₃

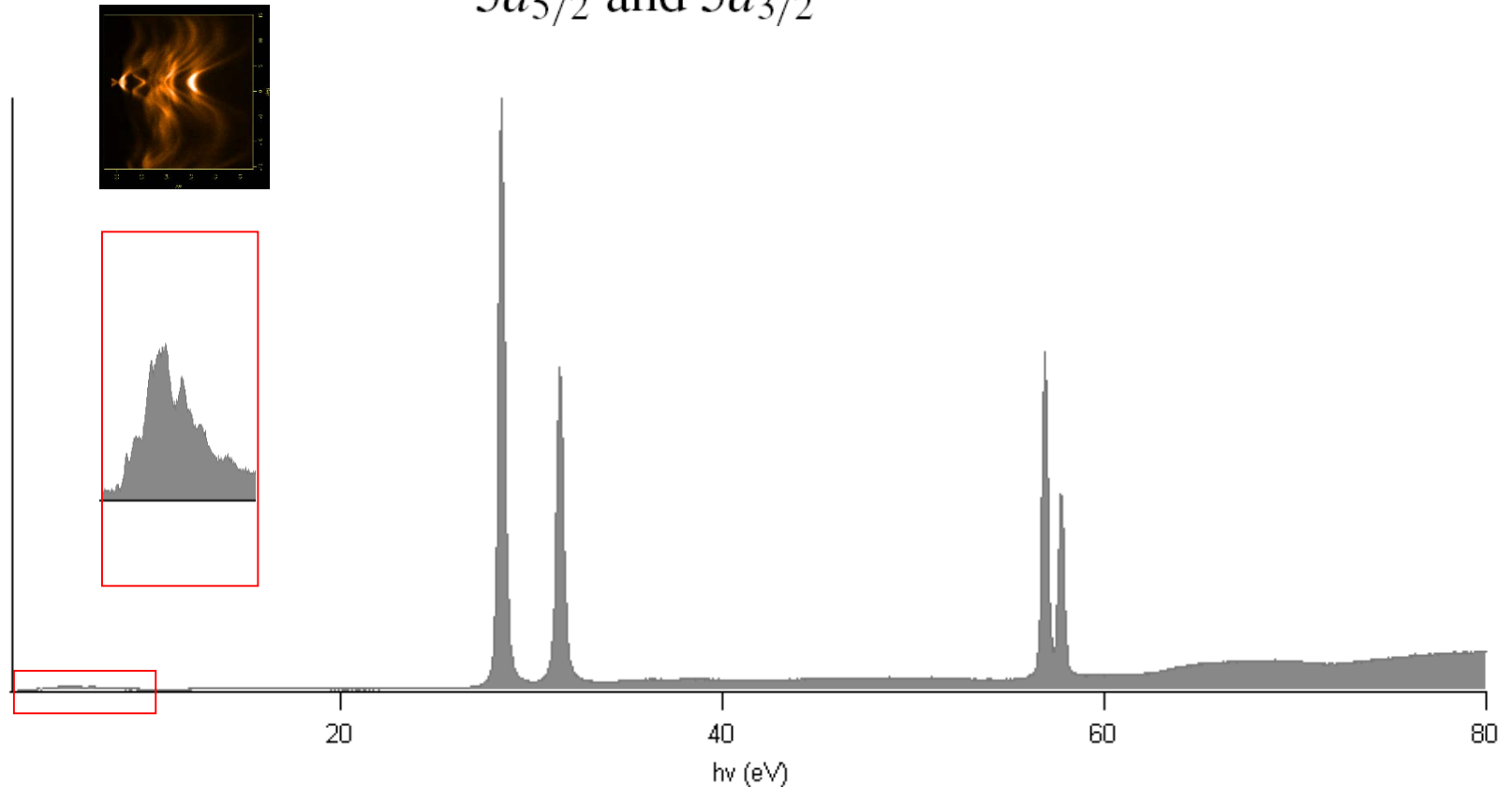
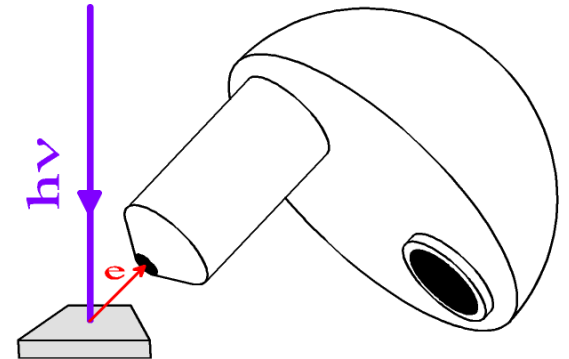
5d_{5/2} and 5d_{3/2}

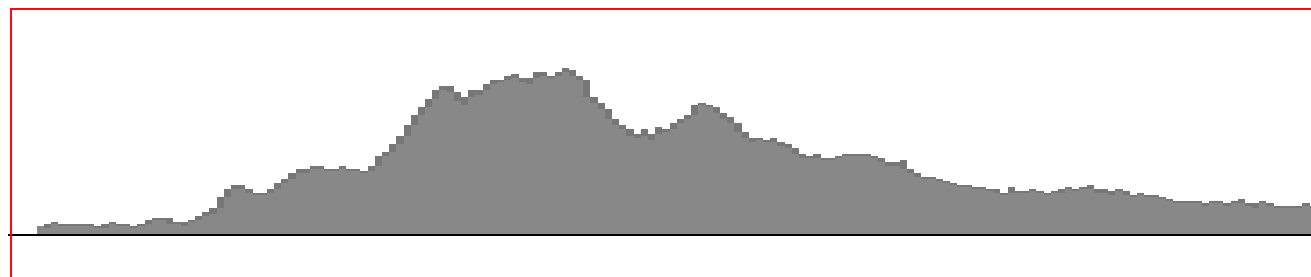
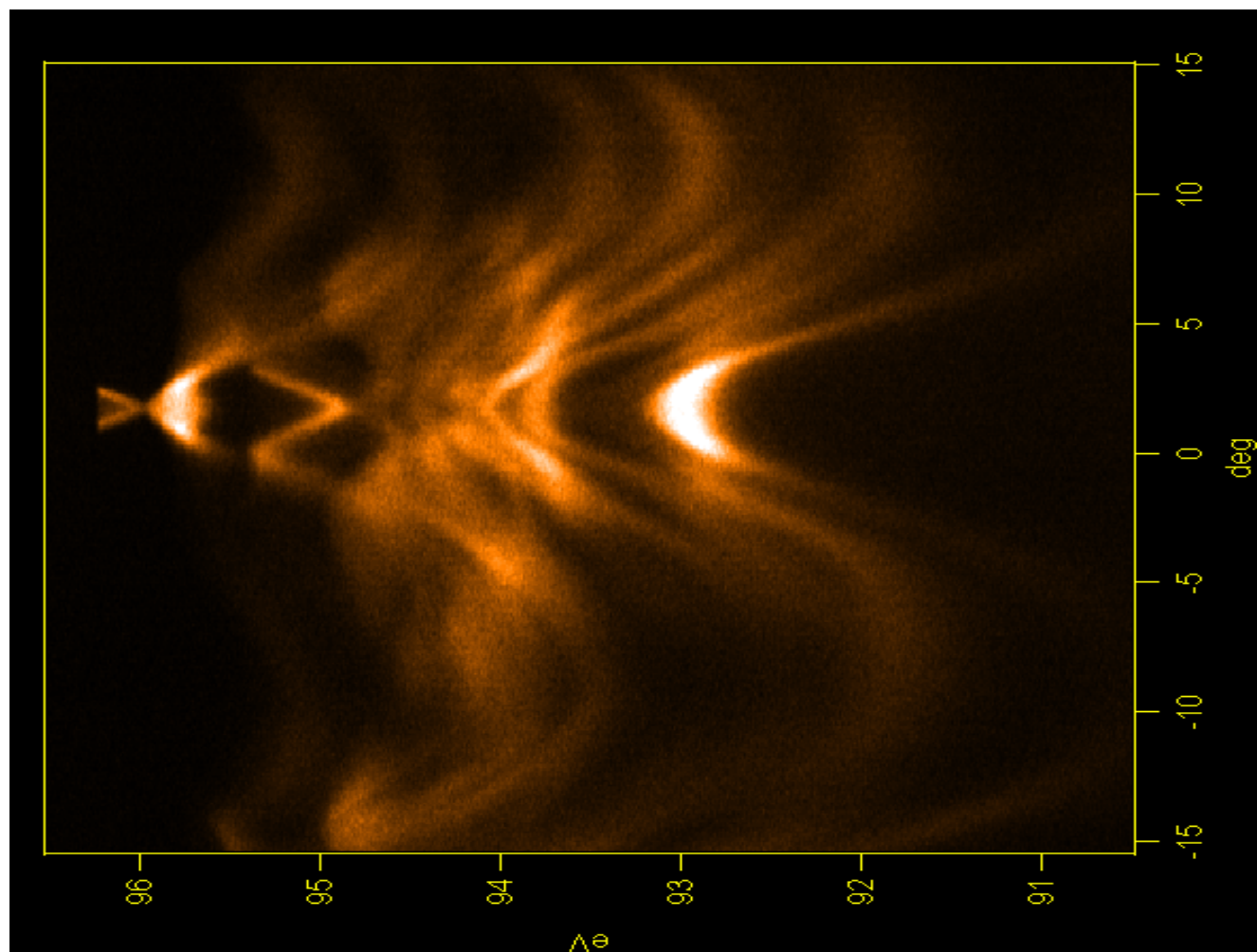


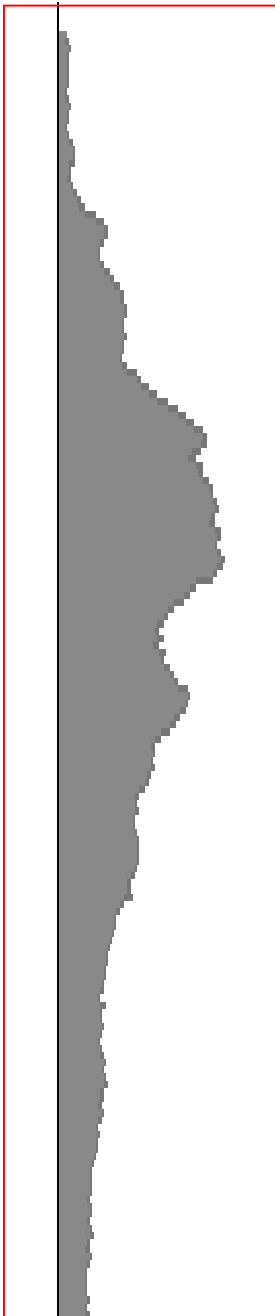
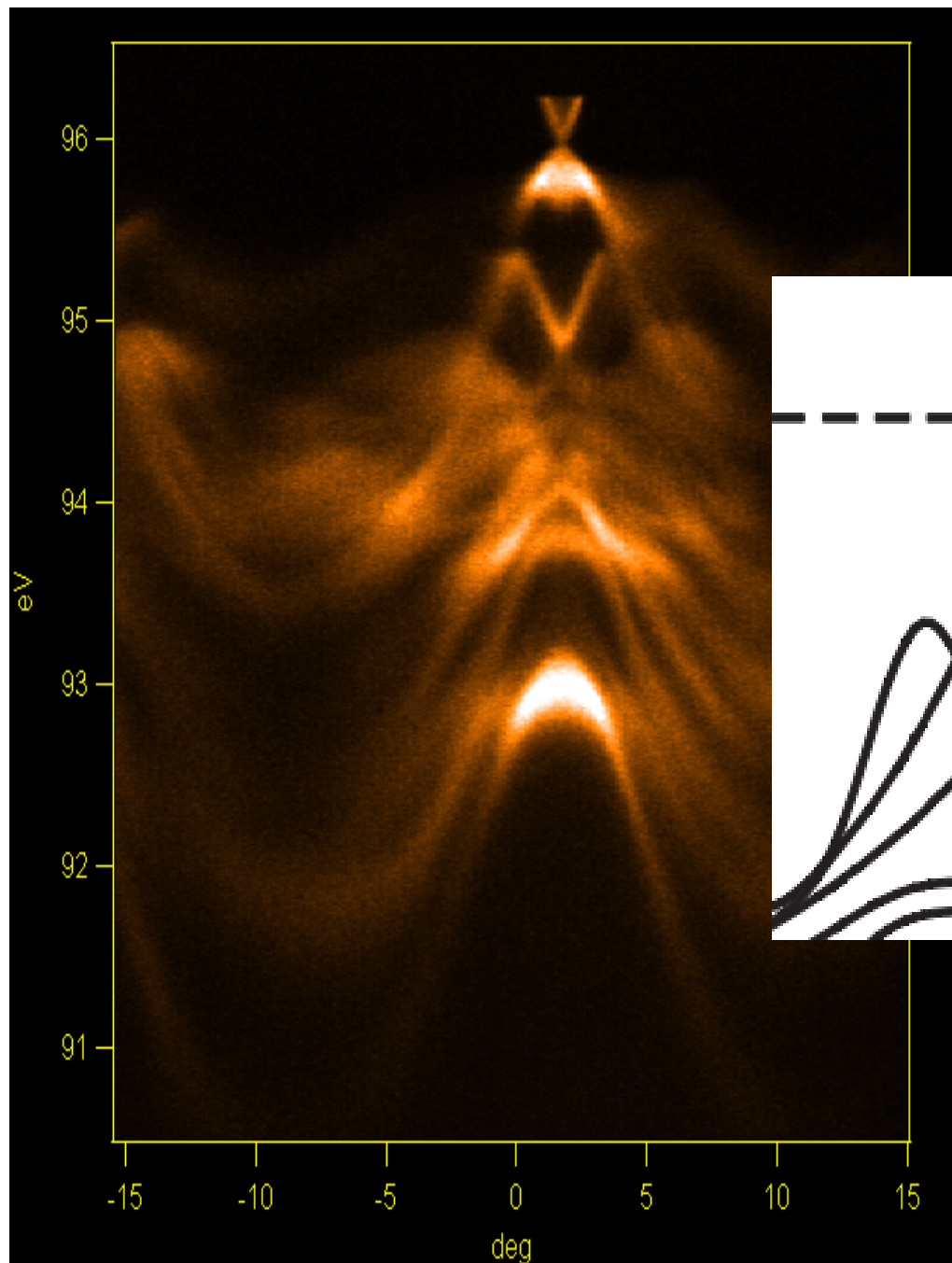
Photoelectron spectroscopy – Electronic band structure ?

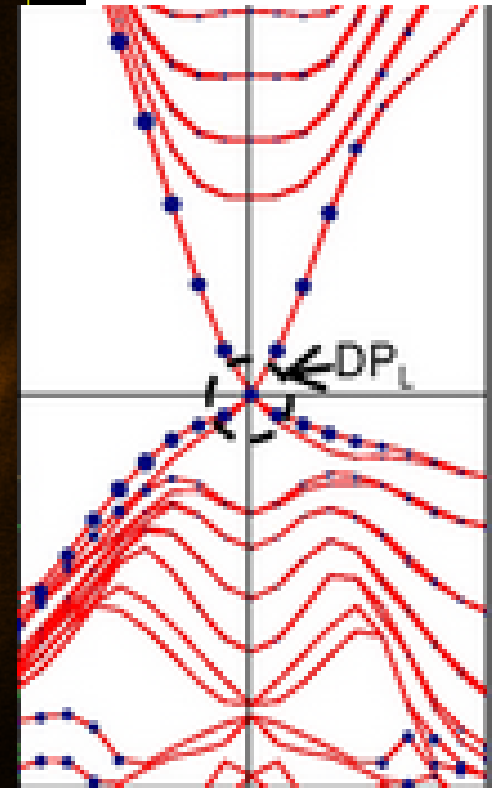
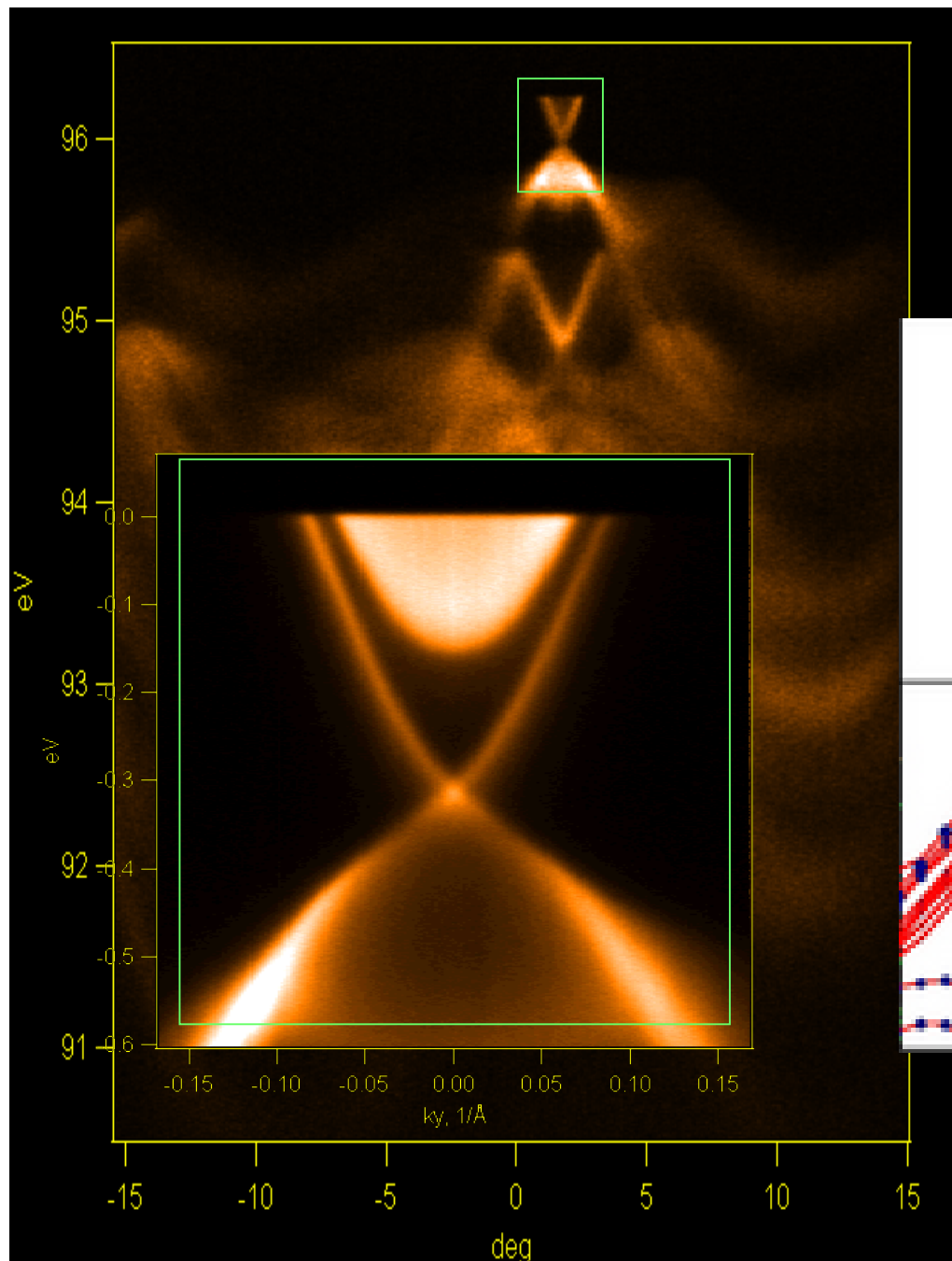
Bi₂Se₃

5d_{5/2} and 5d_{3/2}

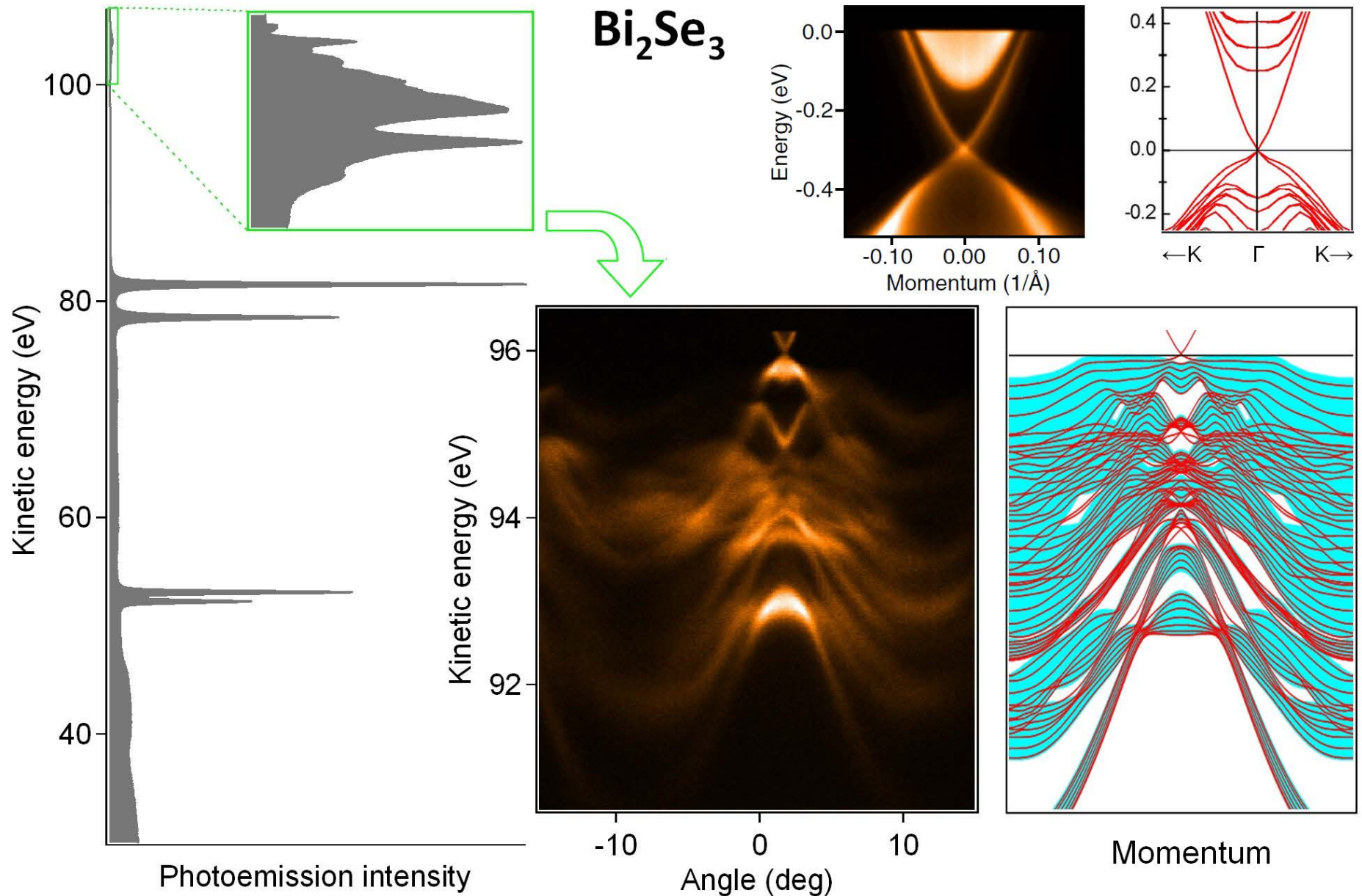




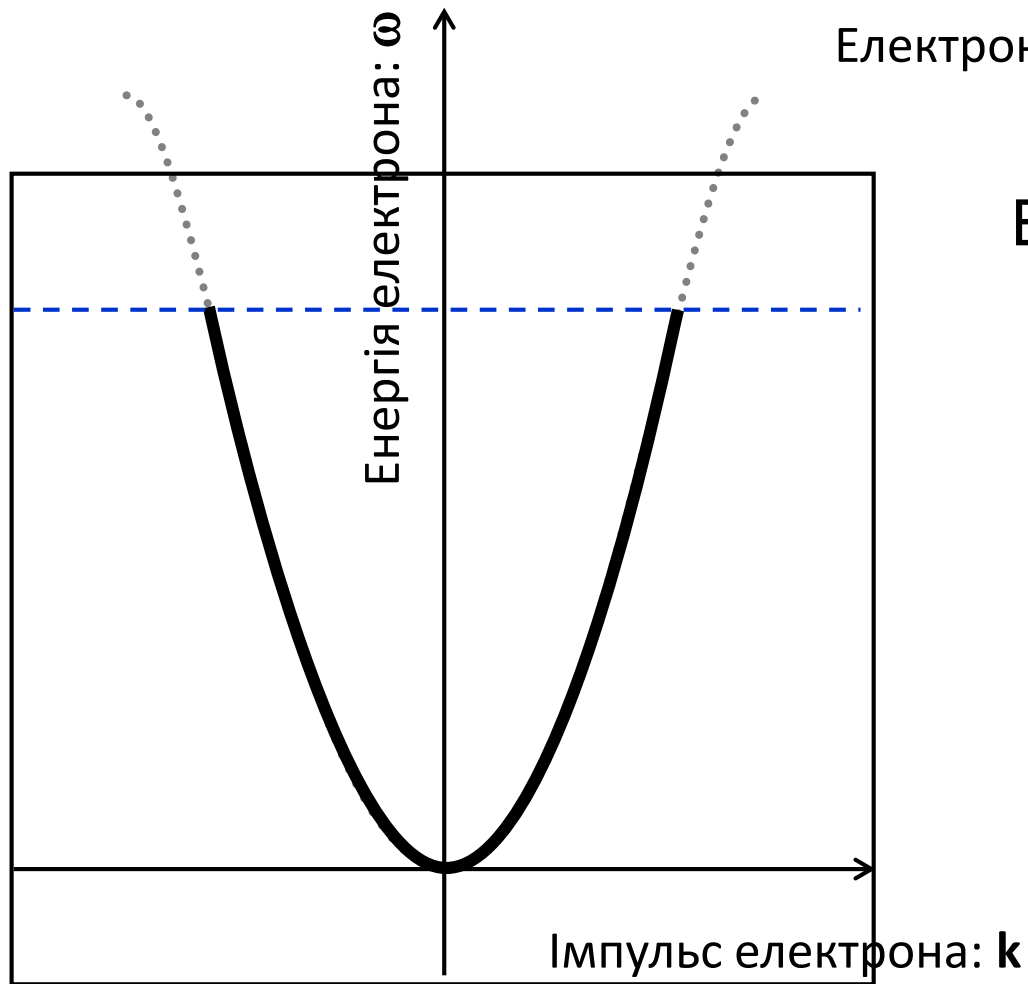




ARPES: Angle Resolved Photoemission Spectroscopy



Electronic structure

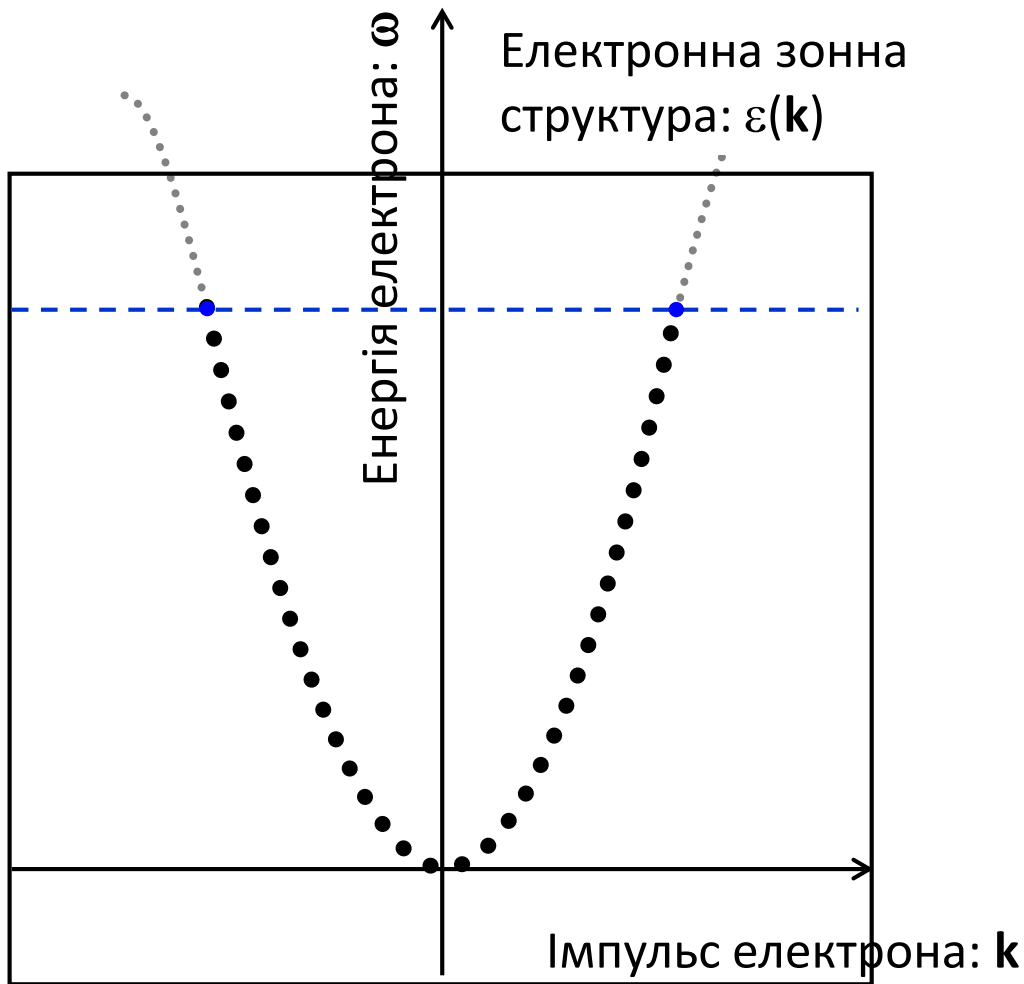
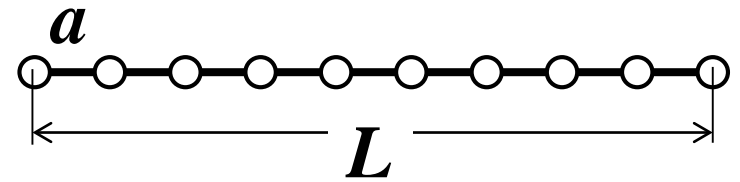


Електронна зонна структура: $\varepsilon(\mathbf{k})$

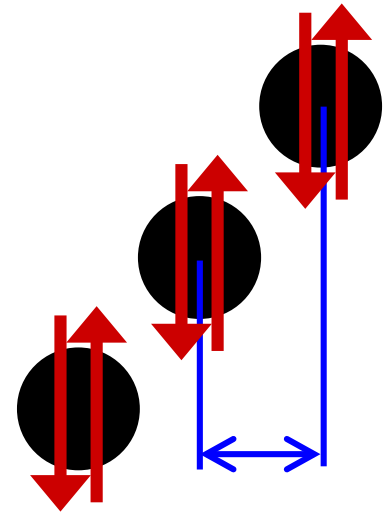
$$E = mv^2/2 = p^2/2m$$

$$p = \hbar k$$

Electronic structure

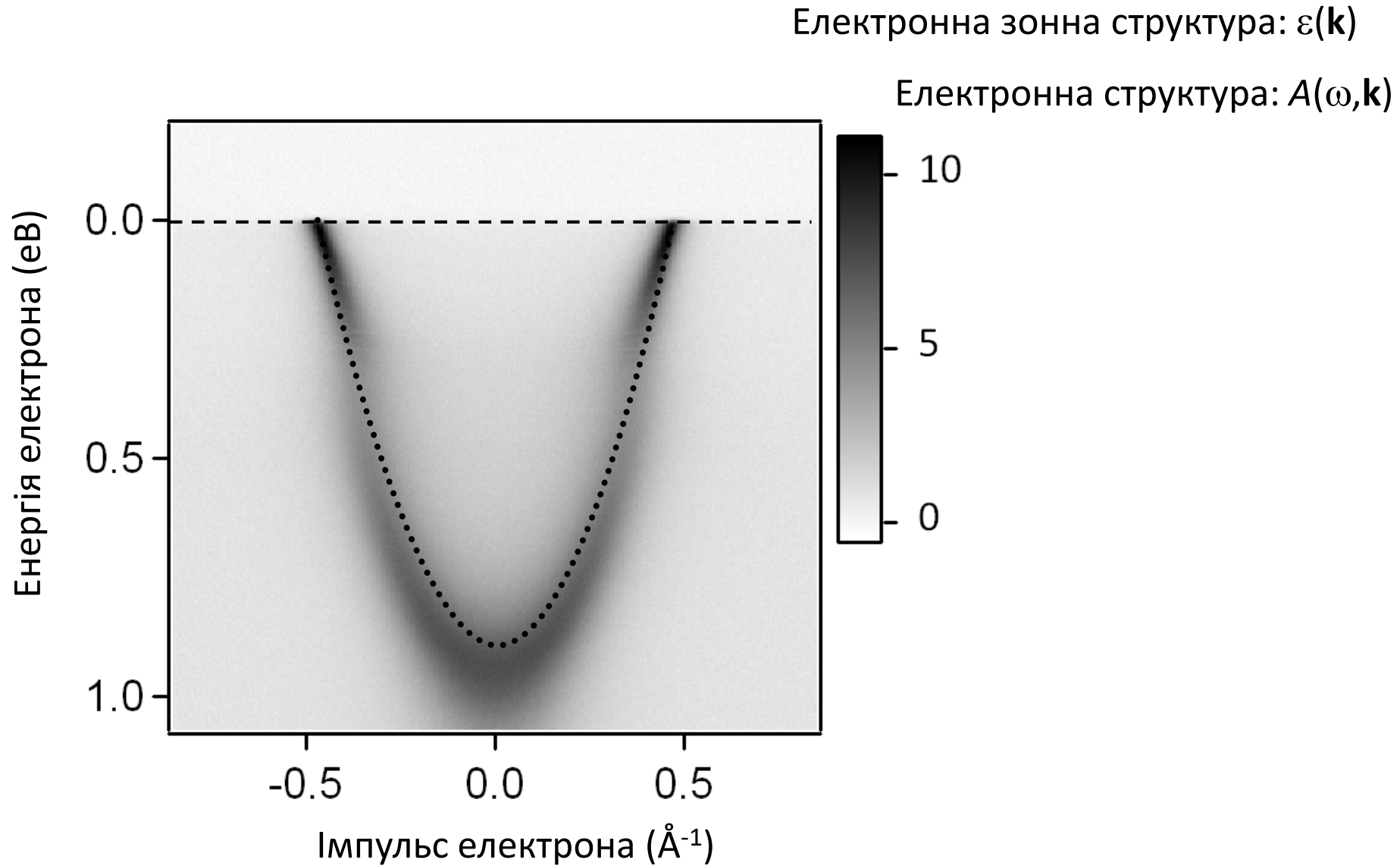


$$\Delta x \Delta p \geq \frac{\hbar}{2}$$



$$dk = 2\pi/L$$

Electronic structure



Electronic structure

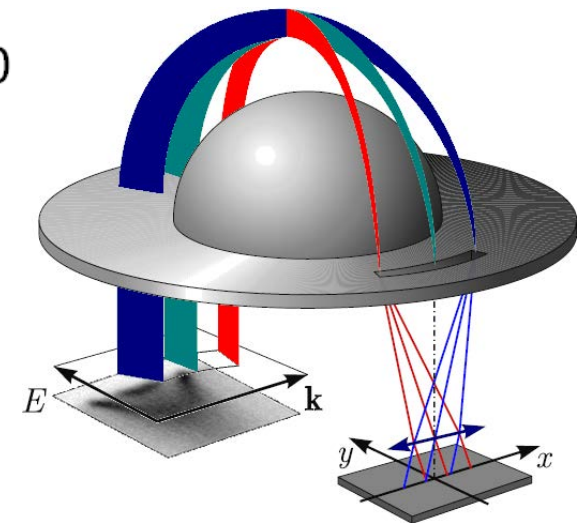
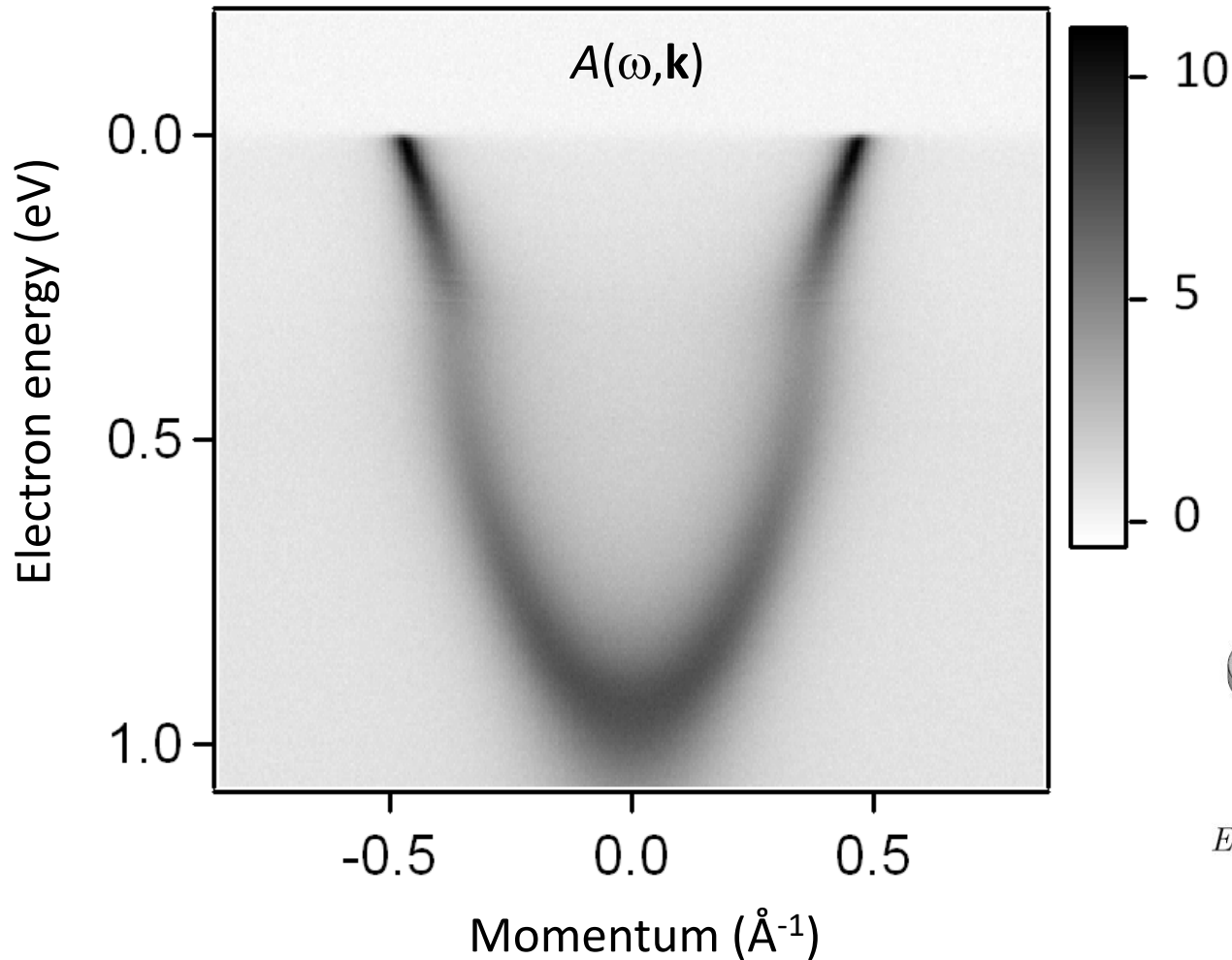
Electronic
structure

\equiv

Electronic excitation
spectrum

\equiv

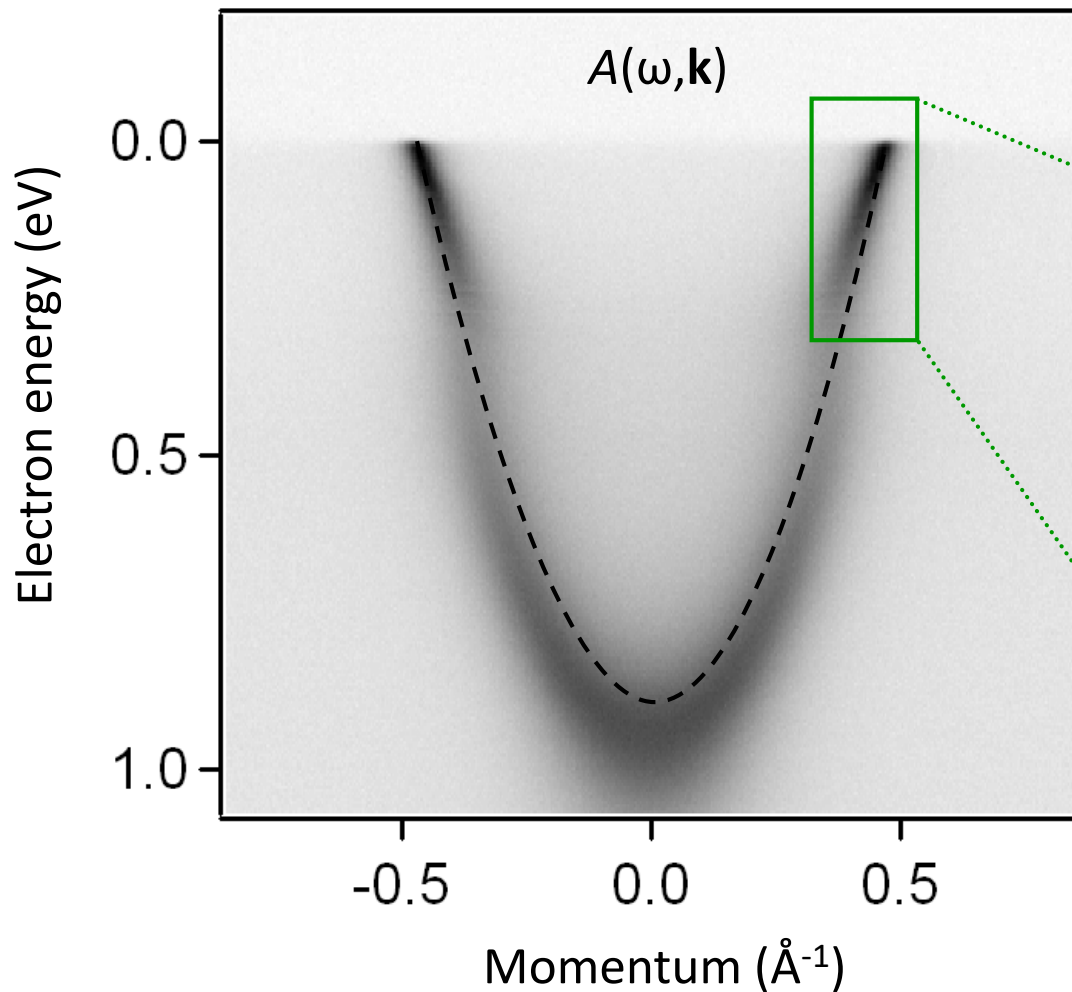
Probability to find electron
with momentum \mathbf{k}
and energy ω



Structure of electronic spectrum

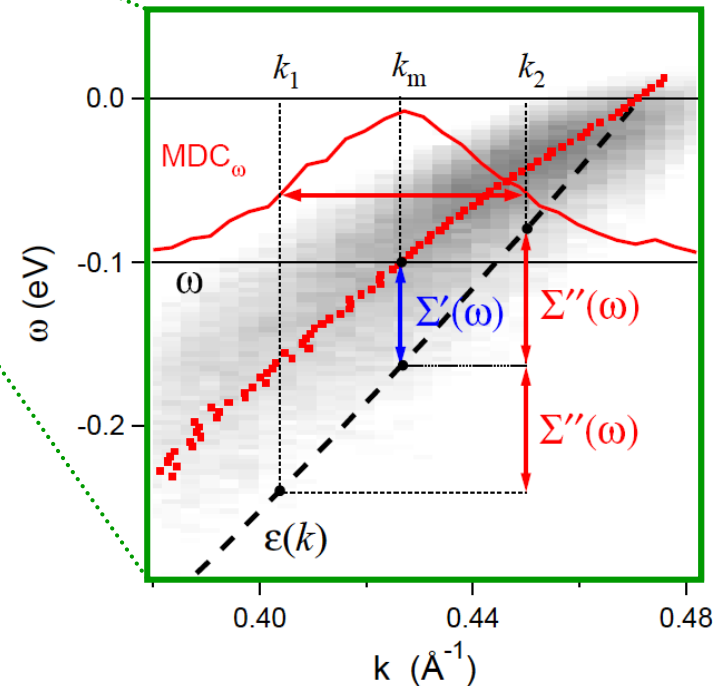
Spectral
function

$$A(\omega, \mathbf{k}) = -\frac{1}{\pi} \frac{\Sigma''(\omega)}{(\omega - \varepsilon(\mathbf{k}) - \Sigma'(\omega))^2 + \Sigma''(\omega)^2}$$

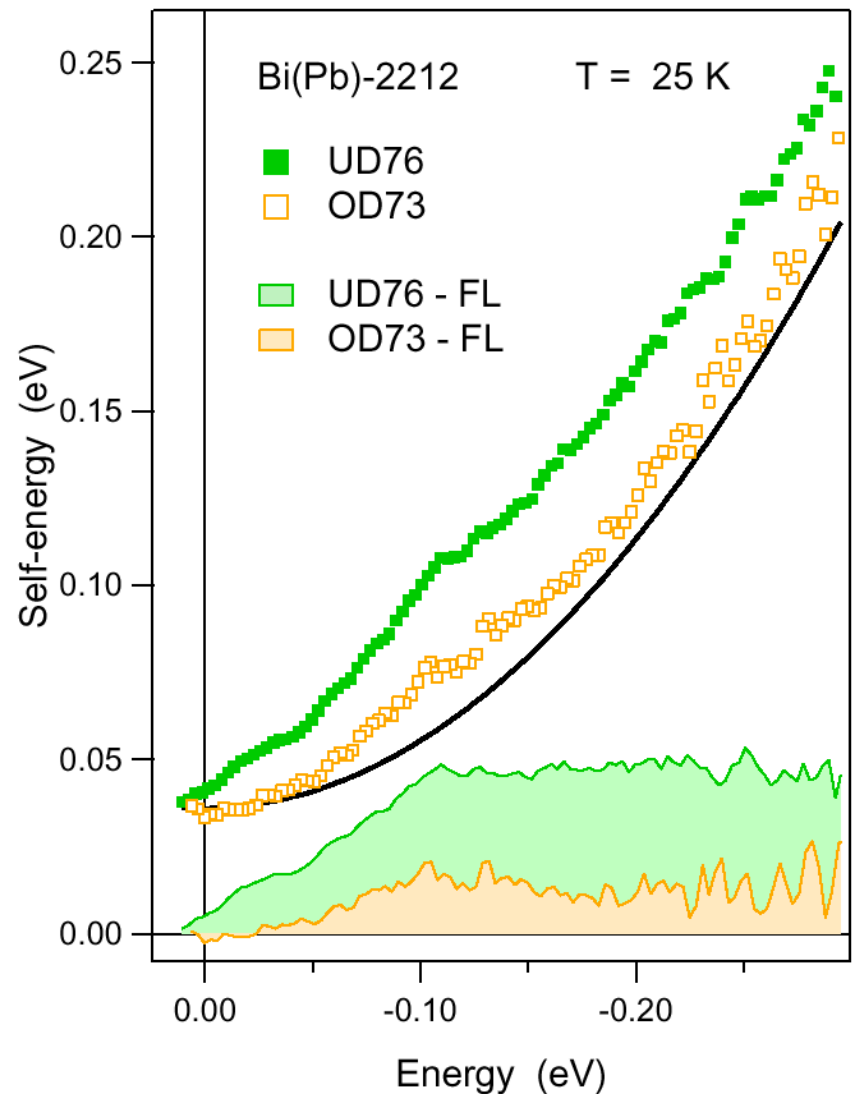
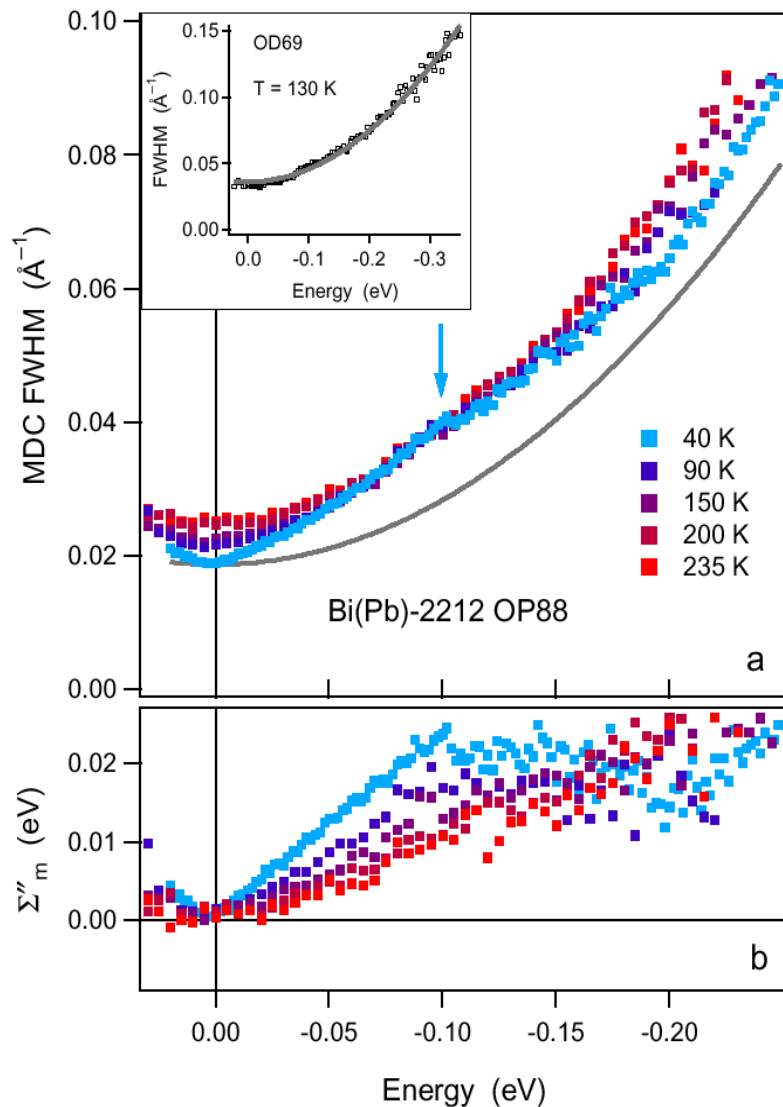


$\varepsilon(\mathbf{k})$ – “bare” electronic
band structure

$\Sigma(\omega, \mathbf{k})$ – self-energy

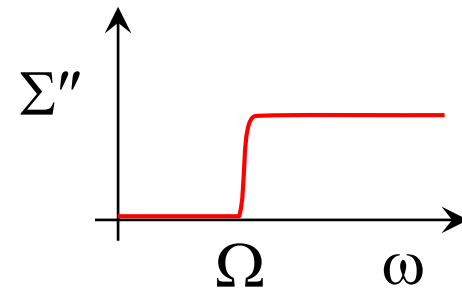
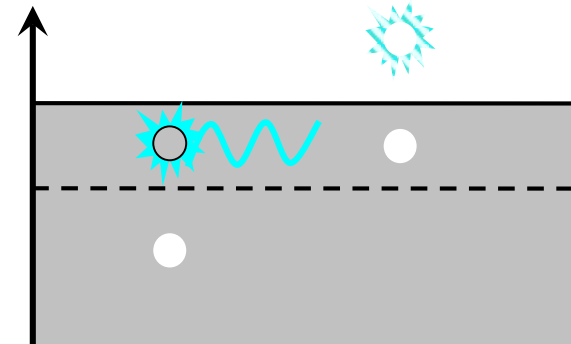
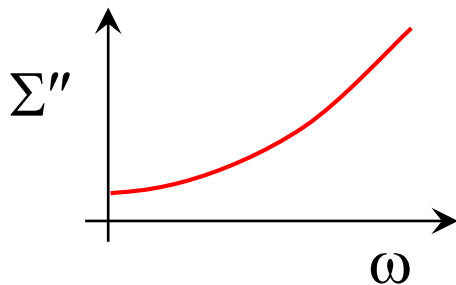
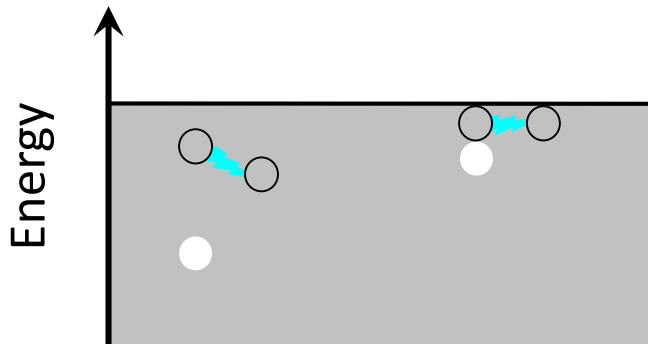
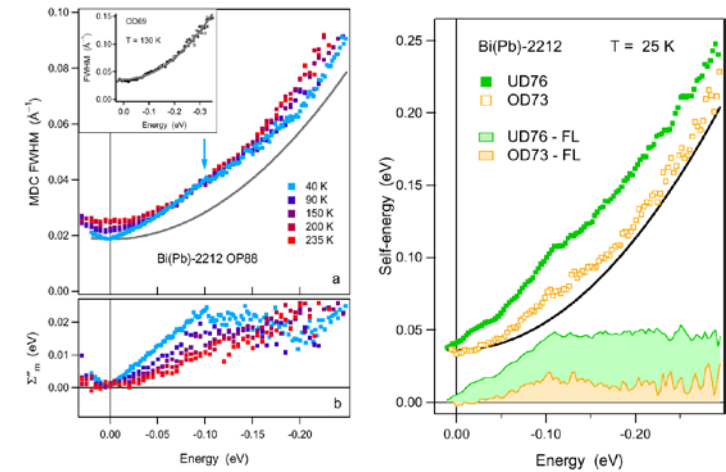


Scattering rate: T - and x -dependence

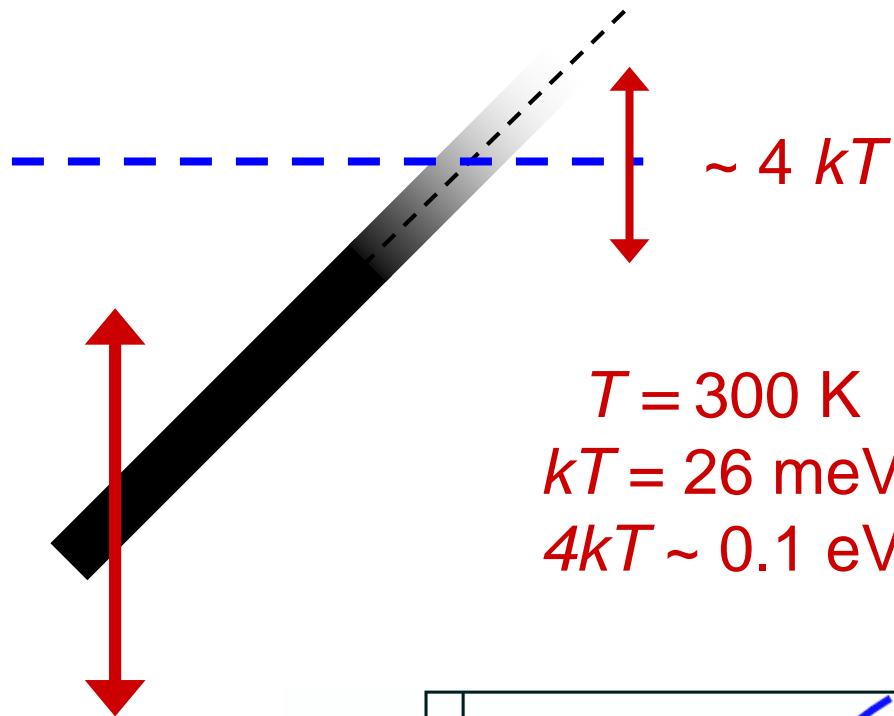
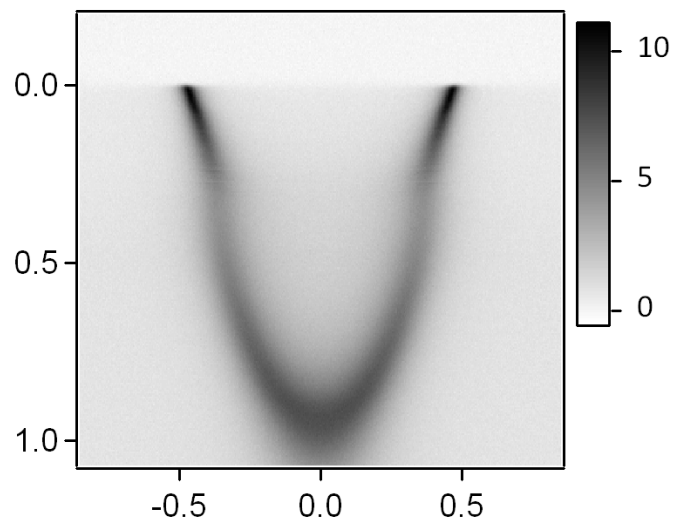
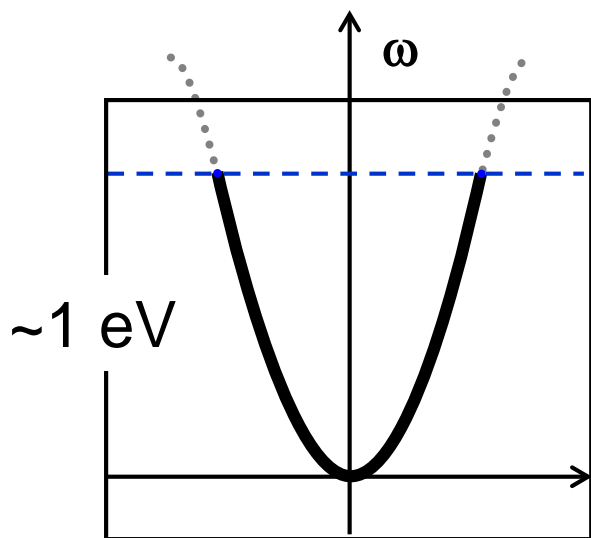


Scattering rate: Two channels

There are two channels:
1st electron-electron scattering and
2nd electron-boson scattering

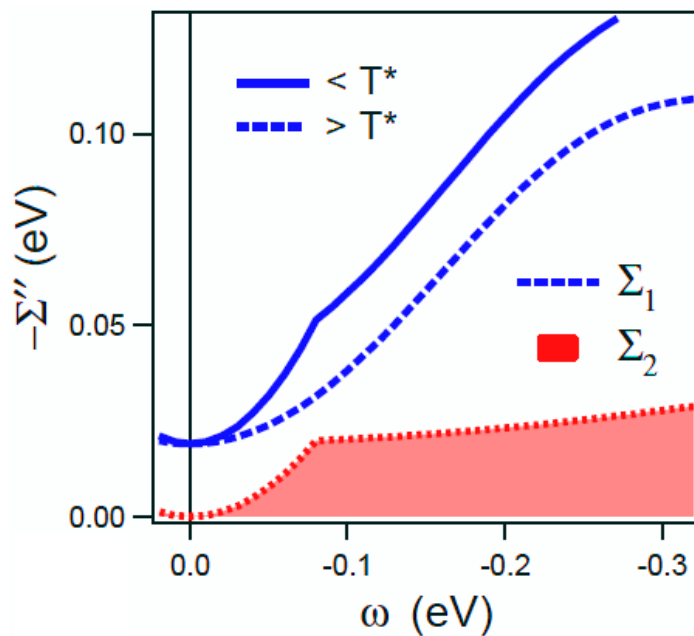


Energy scales

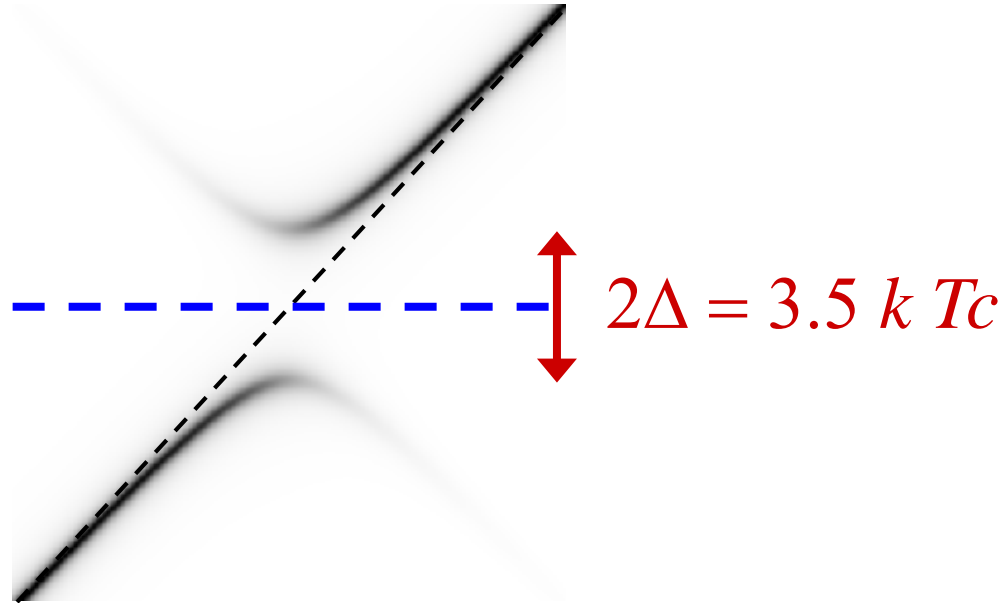


$T = 300 \text{ K}$
 $kT = 26 \text{ meV}$
 $4kT \sim 0.1 \text{ eV}$

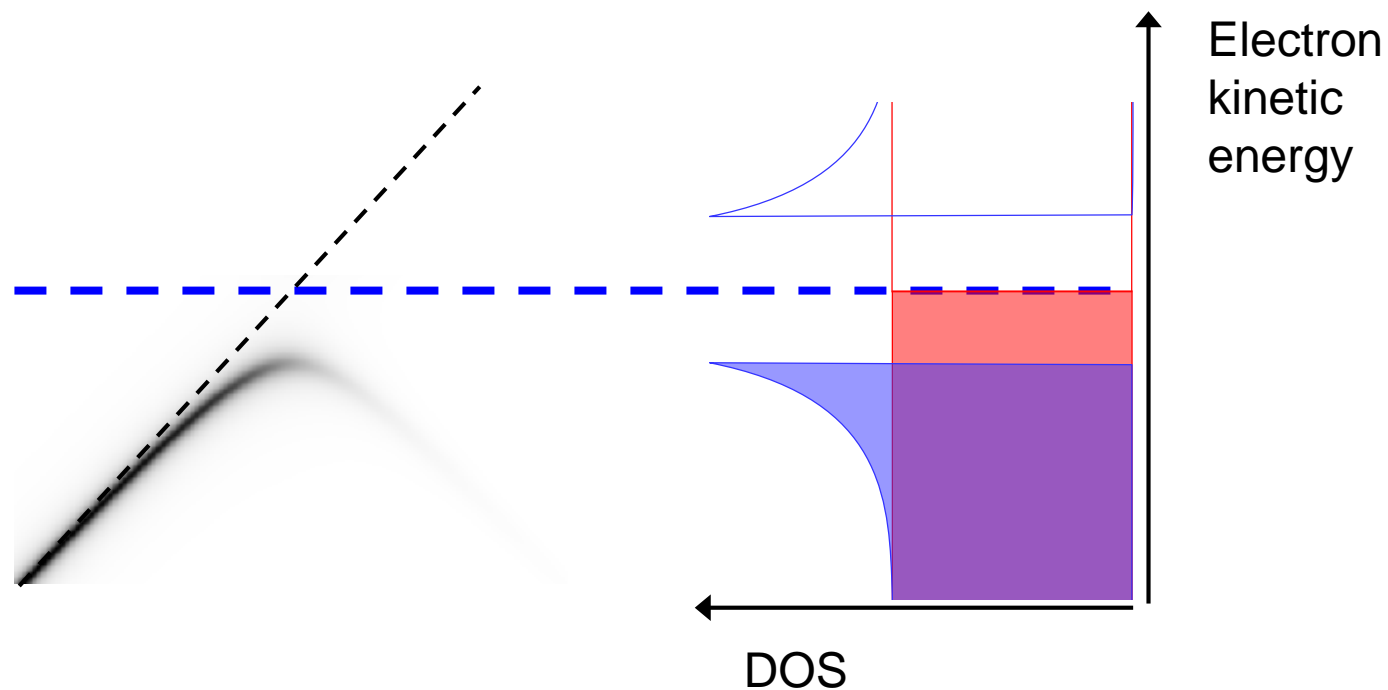
$$2\Sigma'' \sim \alpha \omega^2 + \beta T^2$$



Energy scales: superconducting gap

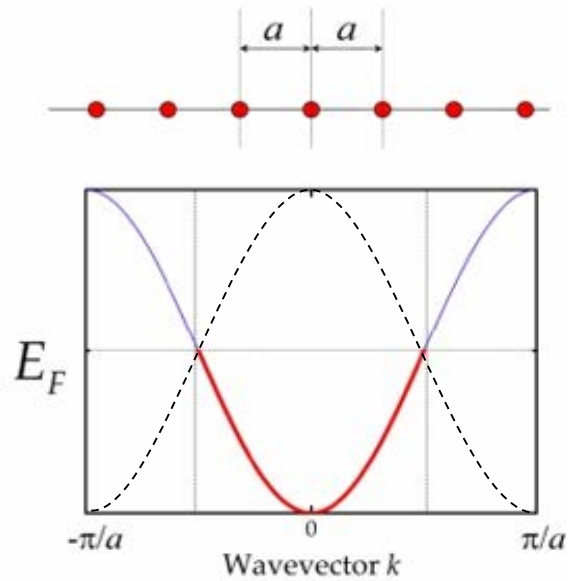


Energy scales: superconducting gap

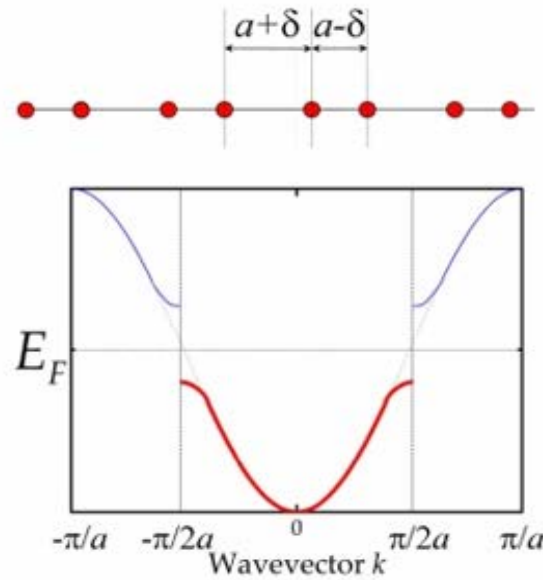


$$2\Delta = 3.5 k T_c$$

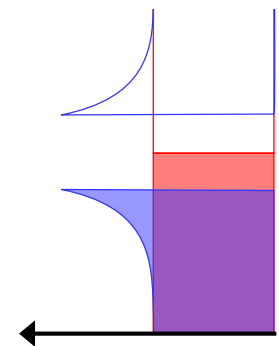
Peierls transition and Fermi surface nesting



(a)



(b)

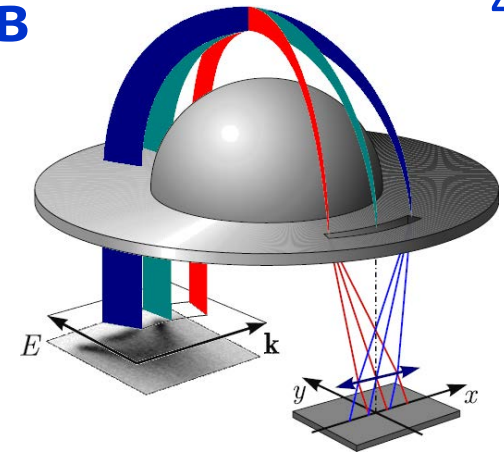
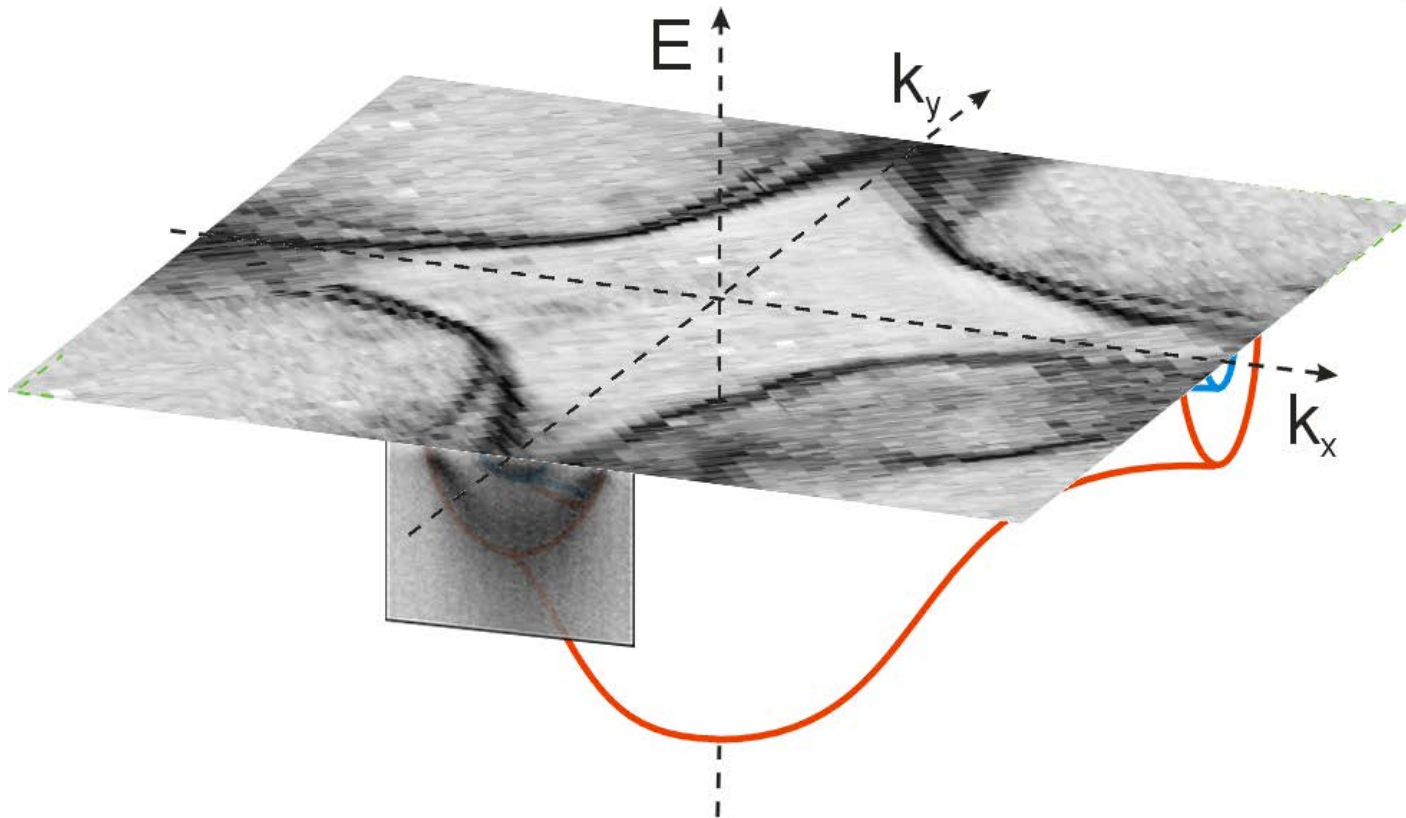


DOS

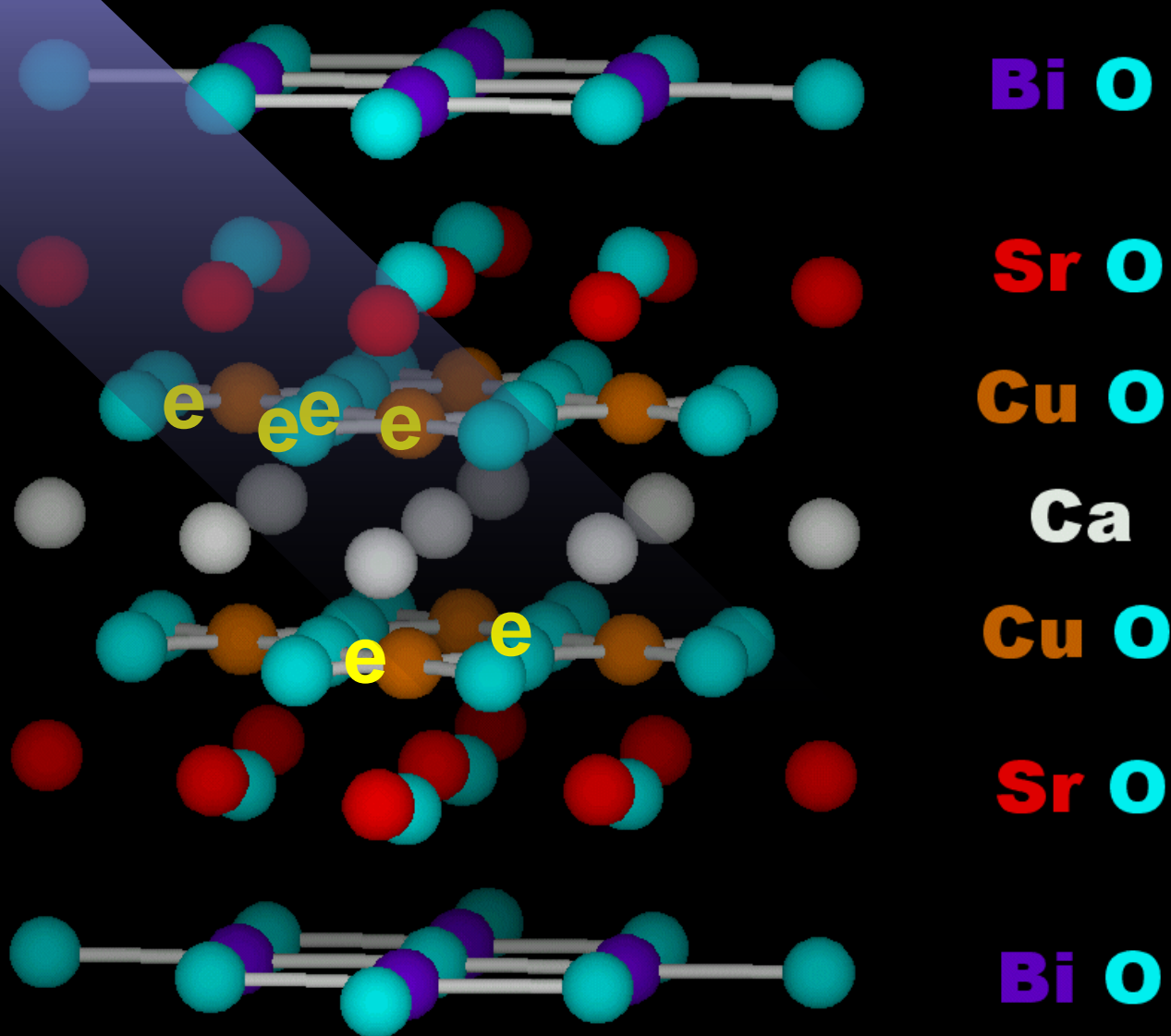
Електронна структура квазі-2D кристалів

4

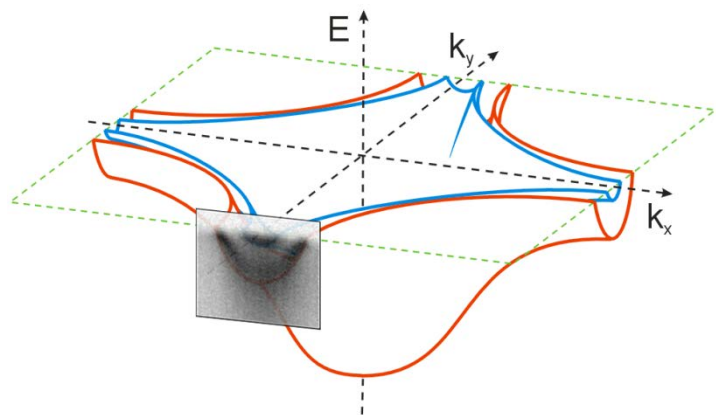
$$\varepsilon(k_x, k_y) \Rightarrow A(\omega, k_x, k_y)$$



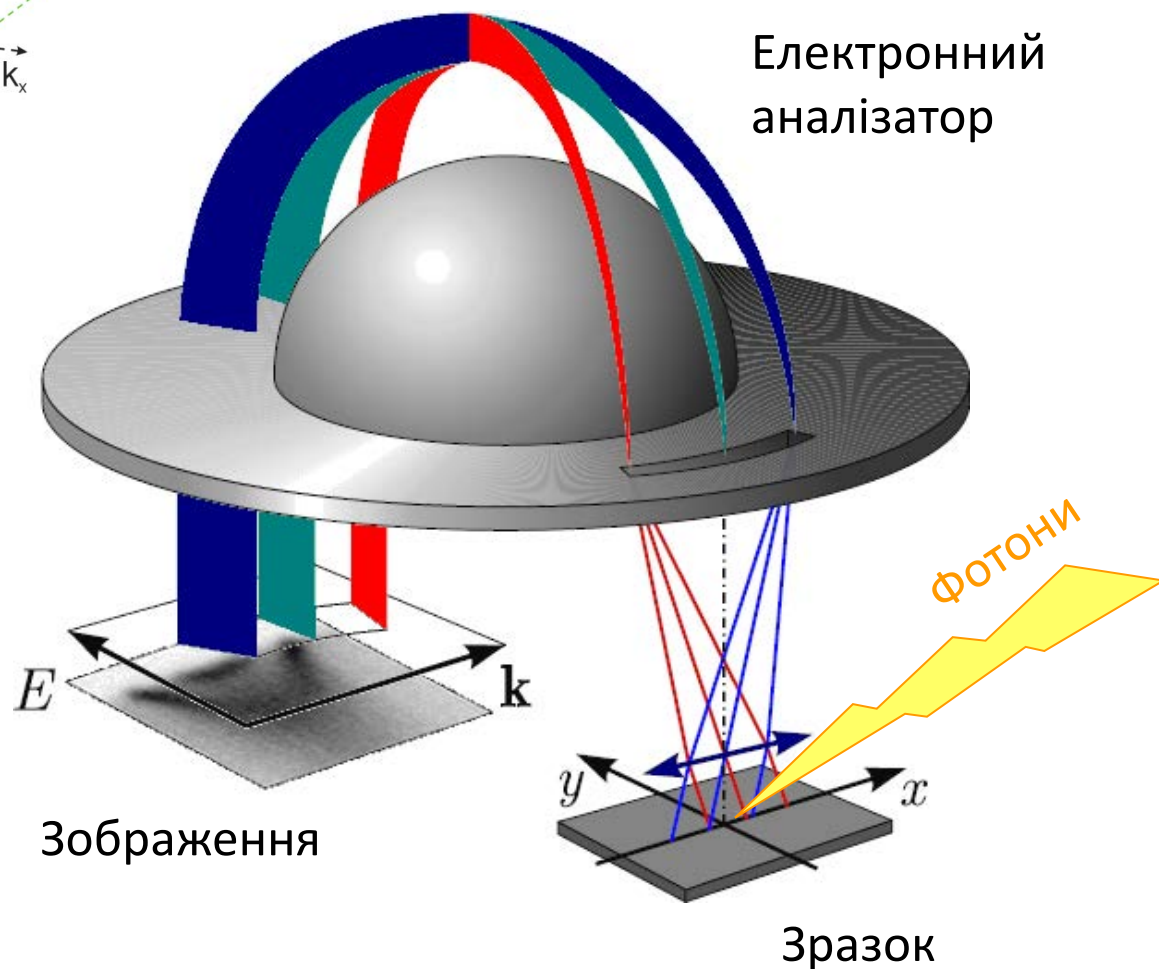
The most studied Bi-2212



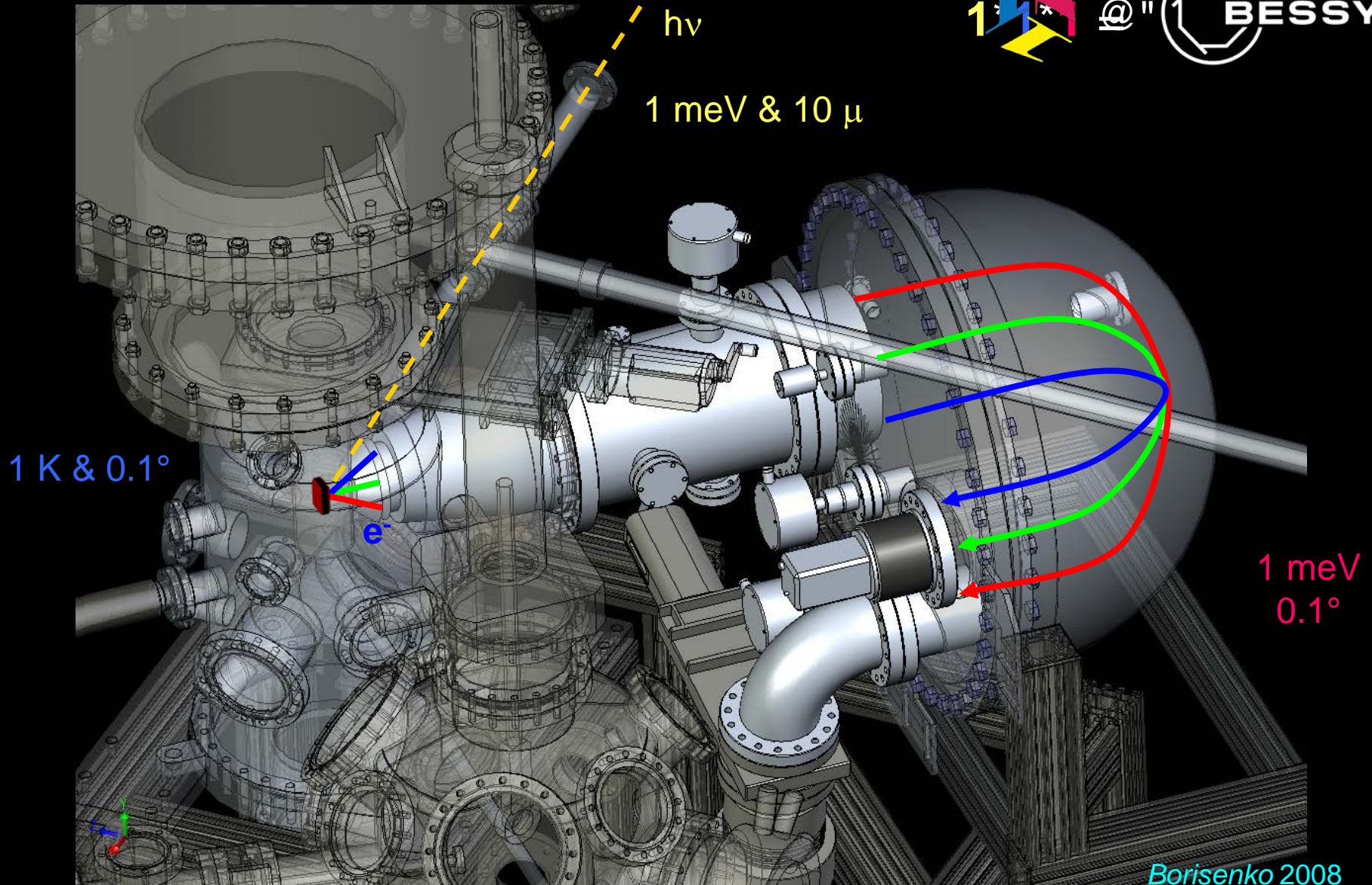
ARPES: Фотоелектронна спектроскопія з кутовим розділенням



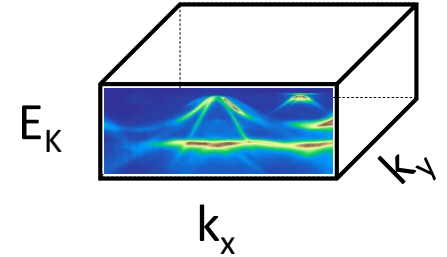
ARPES
=
фотоефект
+
аналізатор
+
маніпулятор



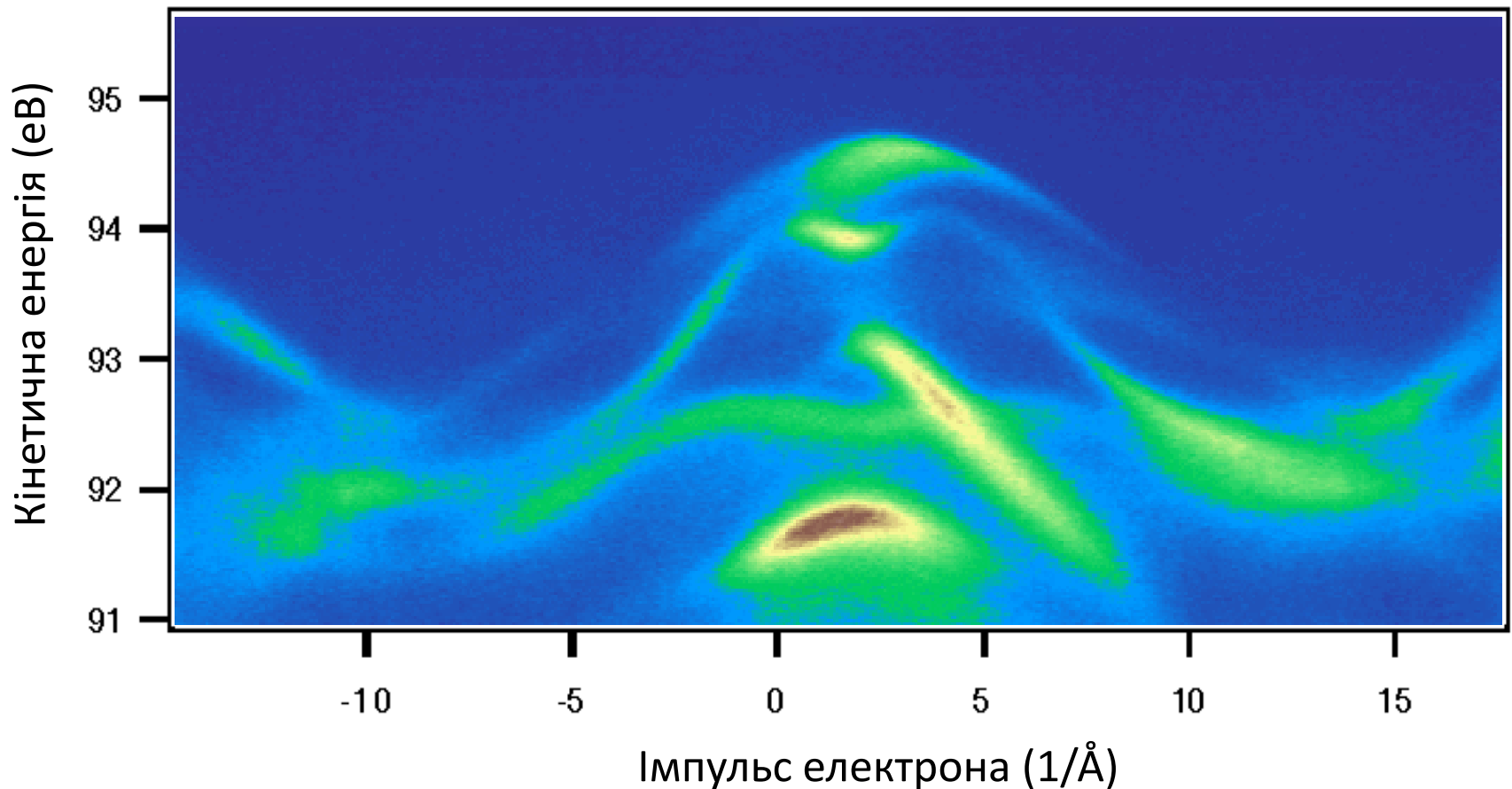
ARPES: анатомія експерименту



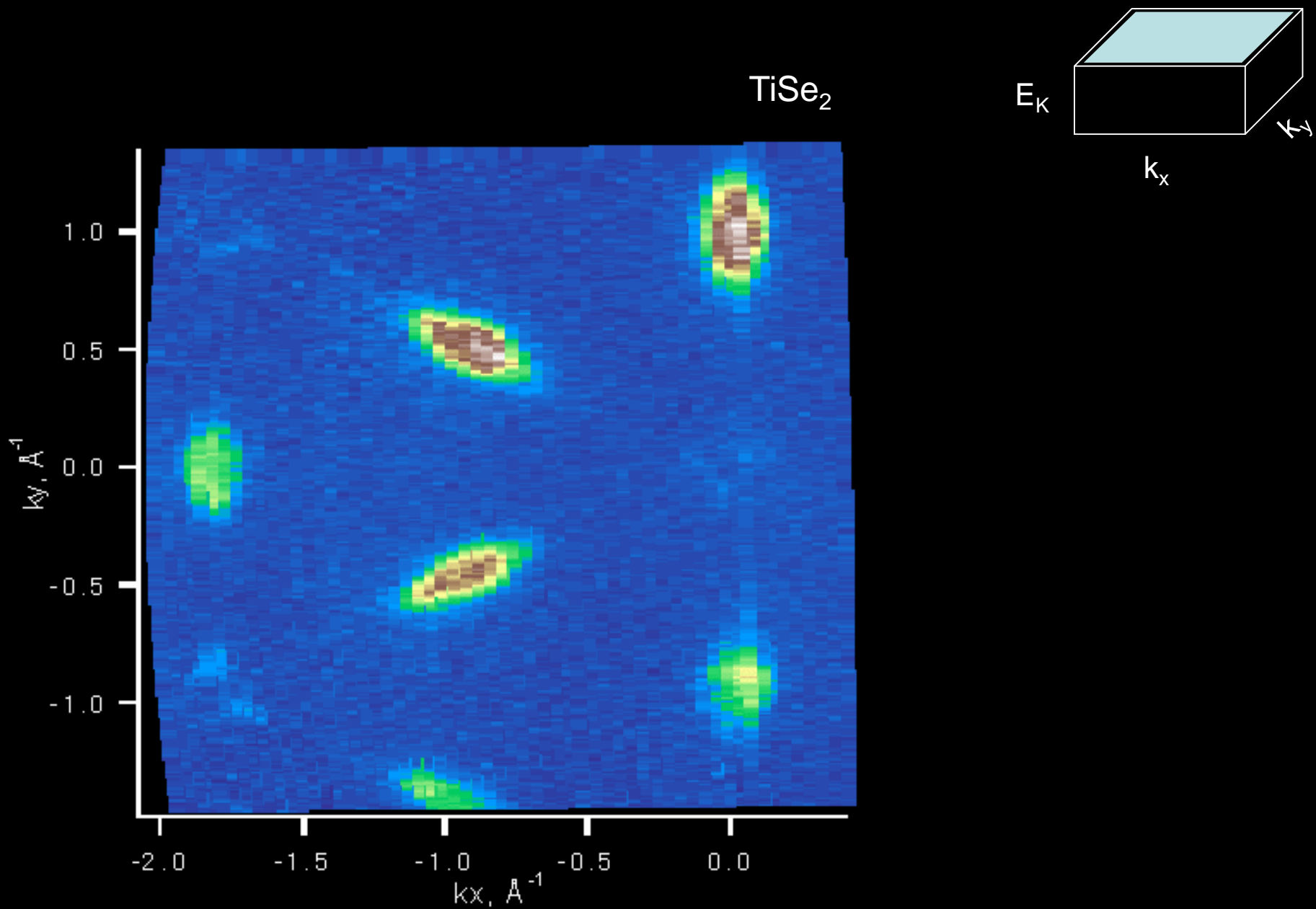
Електронний спектр у імпульсно-енергетичному 3D просторі



TiSe₂ - «ексітонний ізолятор»



Fermi surface (energy distribution) map



...travelling chamber



ARPES =

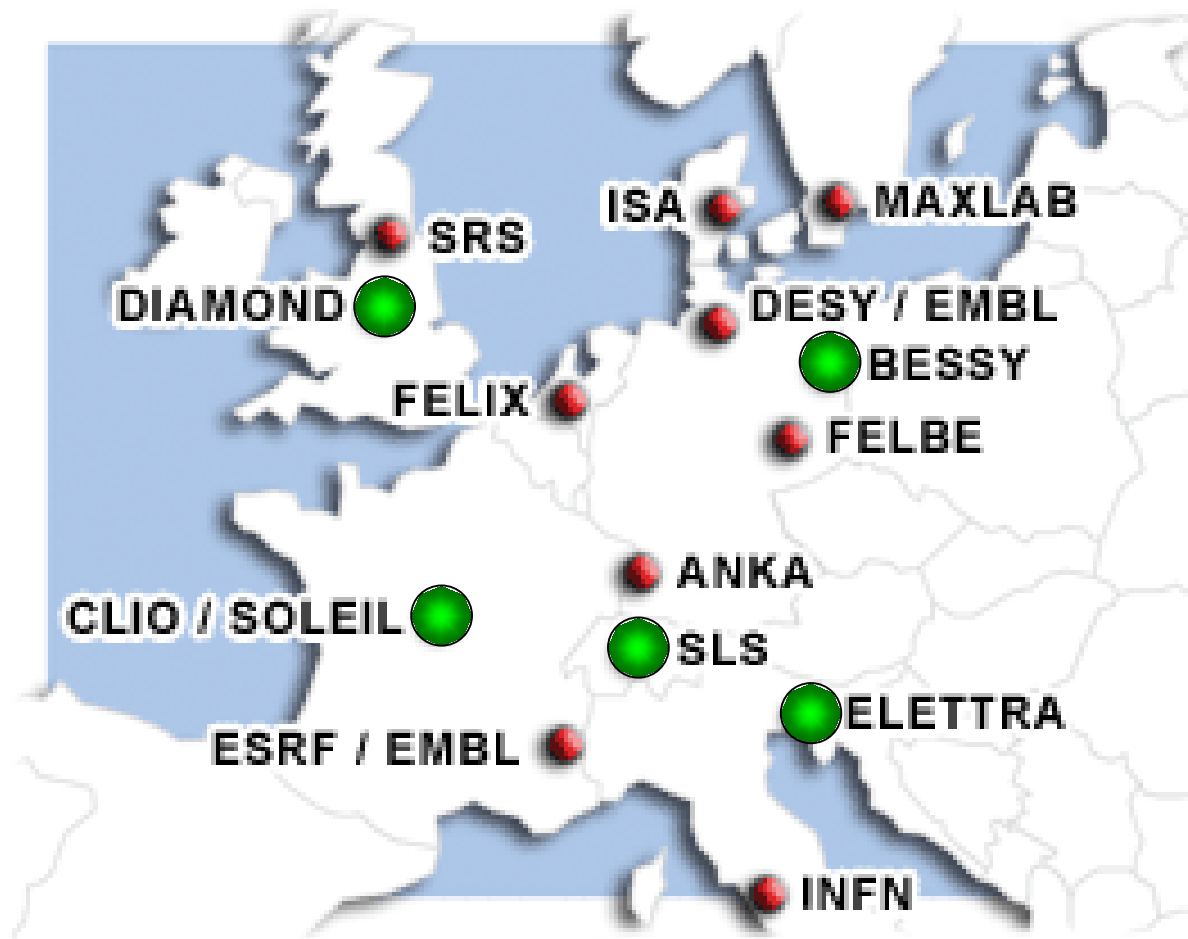
аналізатор + маніпулятор (10^6 €)
+ синхротрон



- Напрямок розвитку:
time resolved ARPES,
XFEL



Синхротронный эксперимент





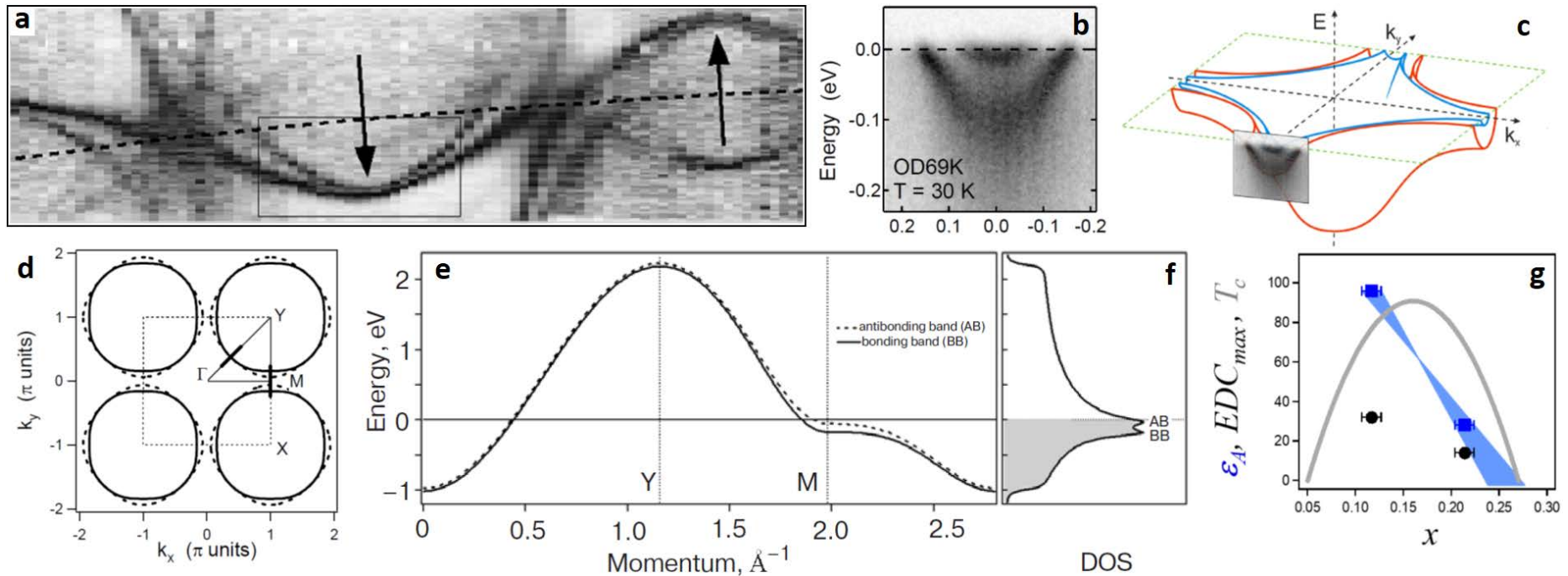
BESSY

SLS



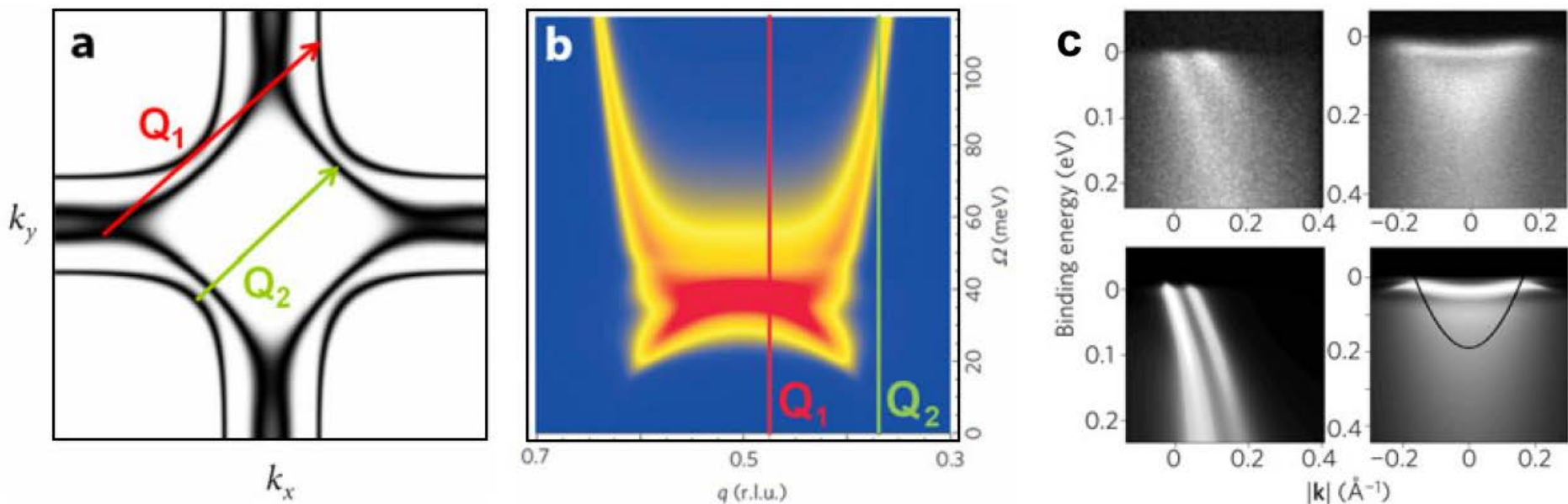
HTSC cuprates

Electronic structure of Cu-SC ...



PRB 66, 014502 (2002); PRL 89, 077003 (2002); PRB 67, 064504 (2003);
 PRL 90, 207001 (2003); PRL 91, 167002 (2003); PRB 70, 214525 (2004);
 PRB 69, 224509 (2004); PRL 92, 207001 (2004); Nature 431, (2004);
 PRL 99, 237002 (2007)...

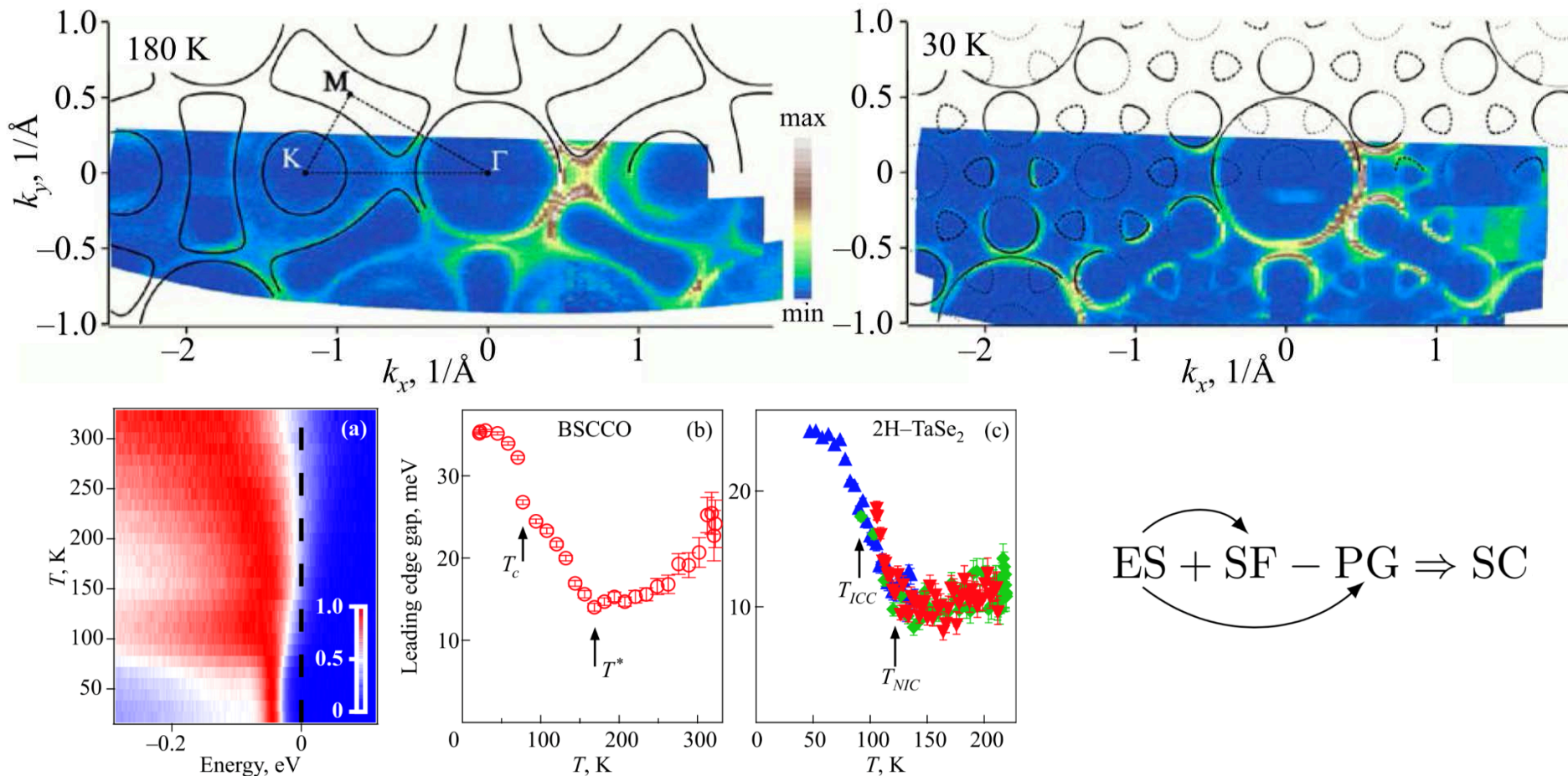
Electronic structure of Cu-SC defines their spin-fluctuation spectrum



$$G^{-1} = G_0^{-1} - \bar{U}^2 G \star \underbrace{G \star G}_{\chi}$$

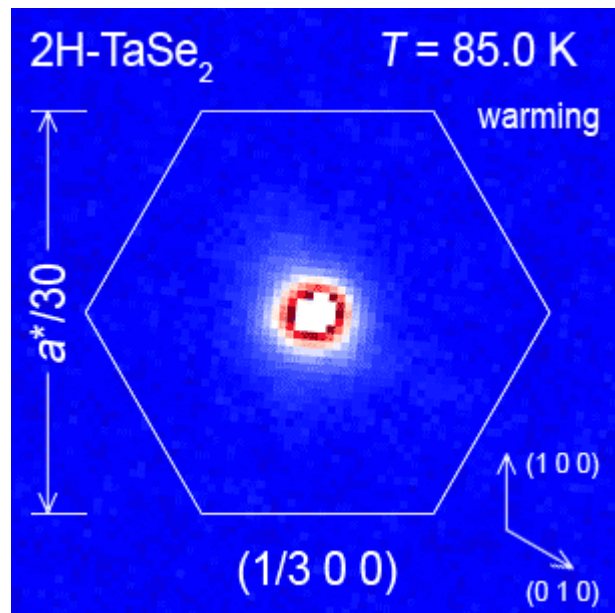
PRL 92, 257006 (2004); PRB 71, 214513 (2005); PRL 96, 067001 (2006);
 PRL 96, 117004 (2006); PRL 96, 037003 (2006); PRL 97, 017002 (2006);
 PRB 75, 172505 (2007); Nature Phys. 5, 217 (2009)...

... and the electronic ordering, which forms the
pseudogap state



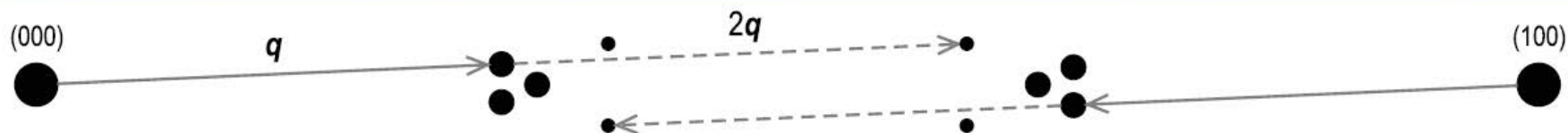
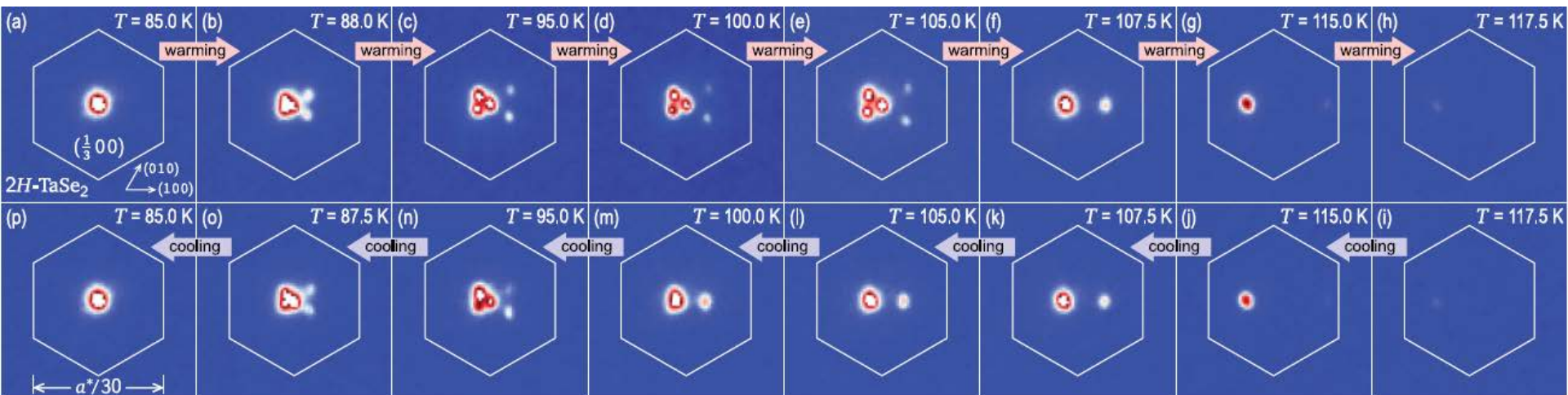
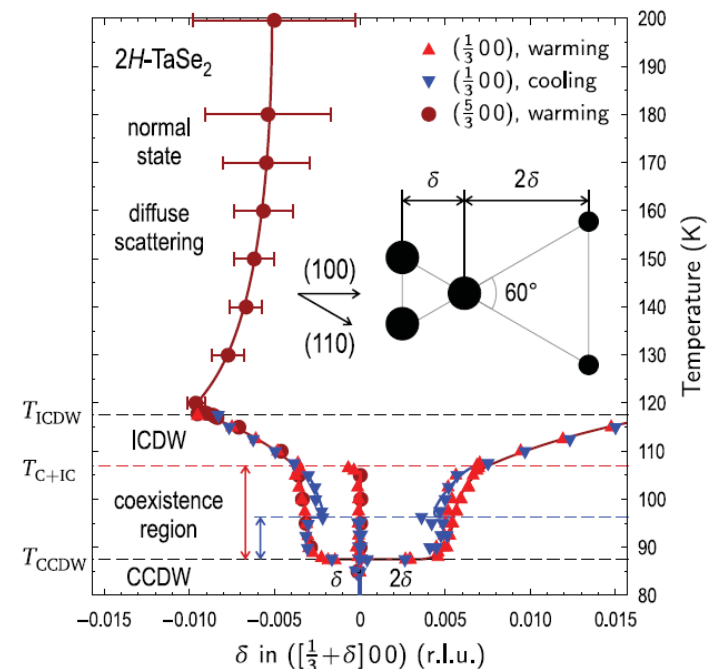
$$\text{ES} + \text{SF} - \text{PG} \Rightarrow \text{SC}$$

PRL 100, 196402 (2008); PRL 100, 236402 (2008); PRB 79, 020504 (2009);
PRL 102, 166402 (2009); PRB 85, 064507 (2012)...



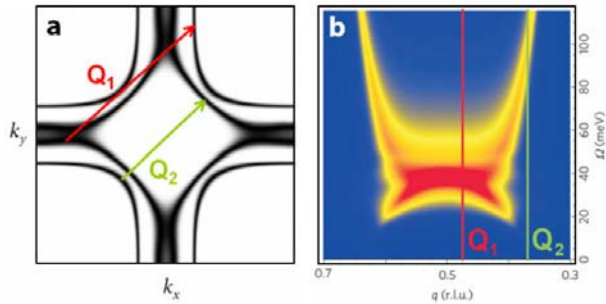
Competing CDW and temperature-dependent nesting in 2H-TaSe₂

Leininger... Inosov, PRB 2011

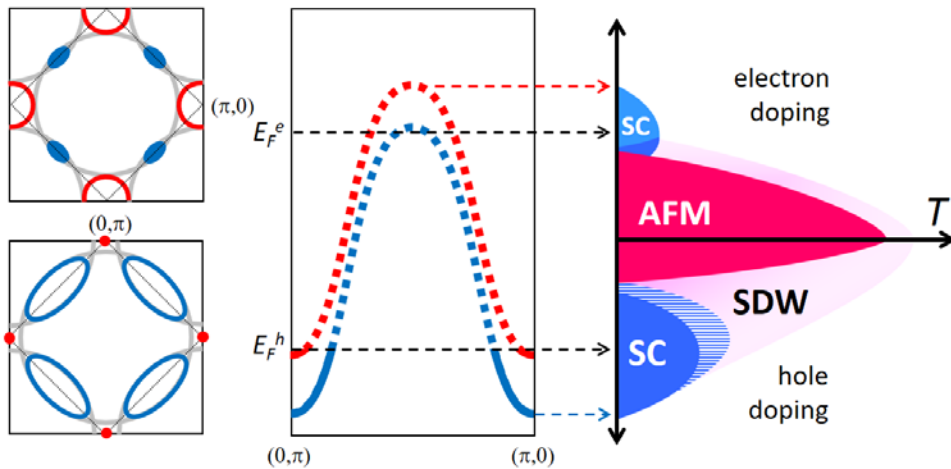


To Fe-SC and back again

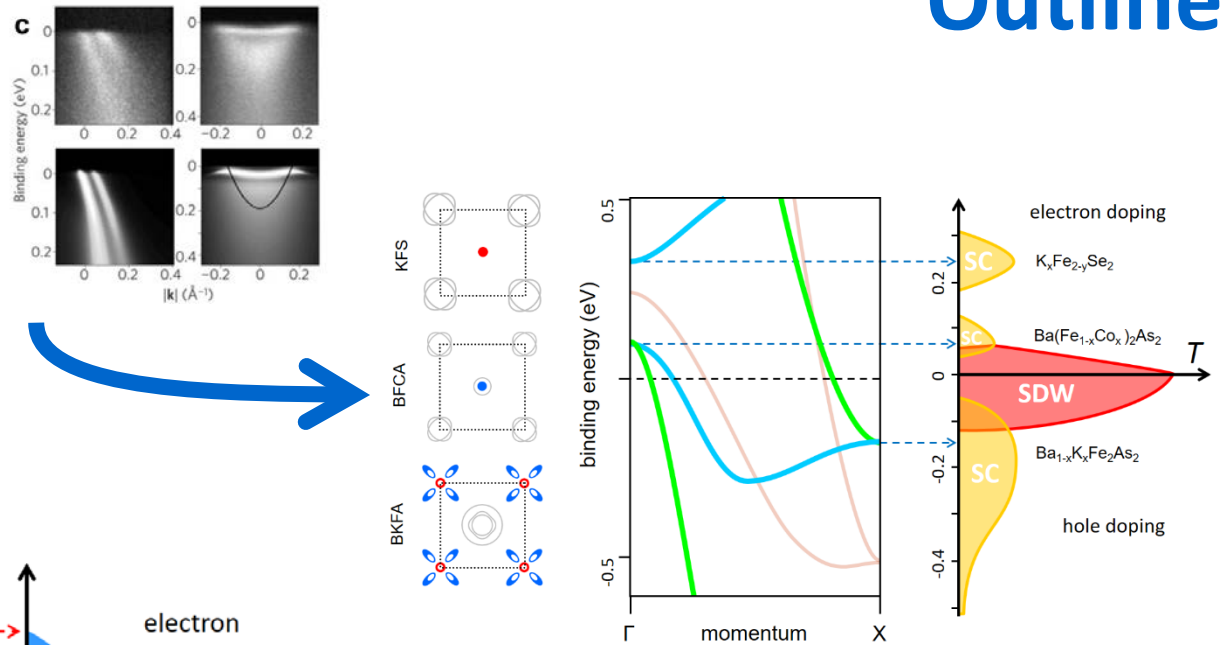
Outline



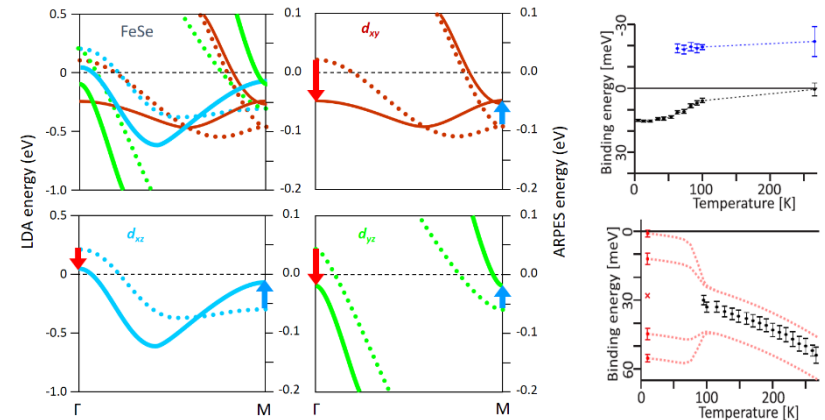
Band structure is important for Cu-SC



...and in Cu-SC, if...

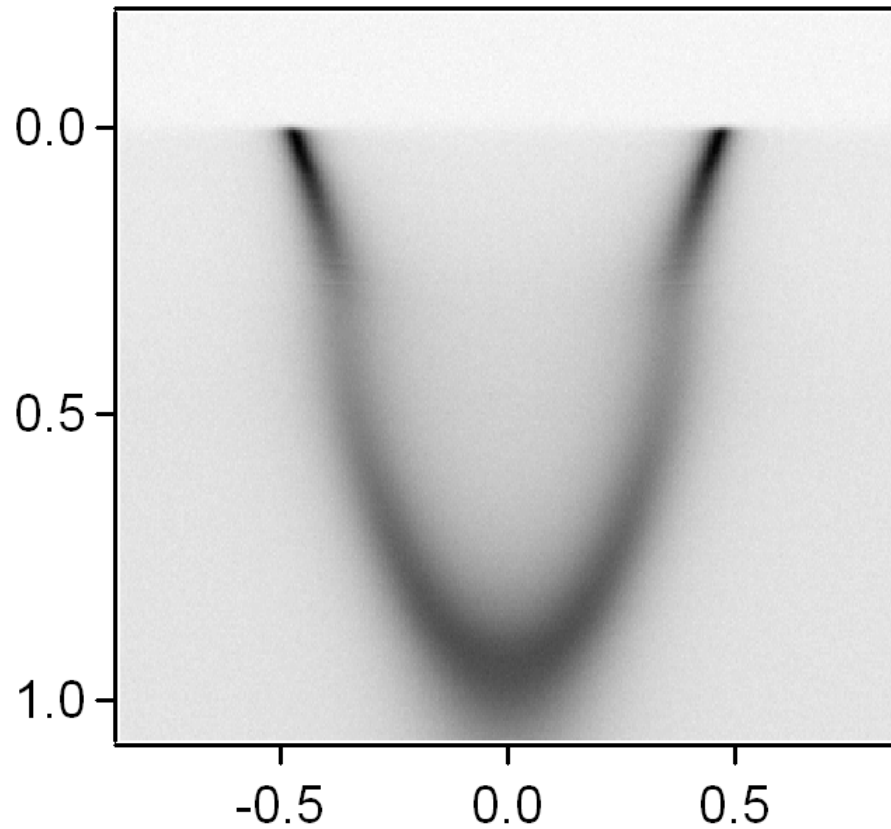


It correlates with T_c in Fe-SC

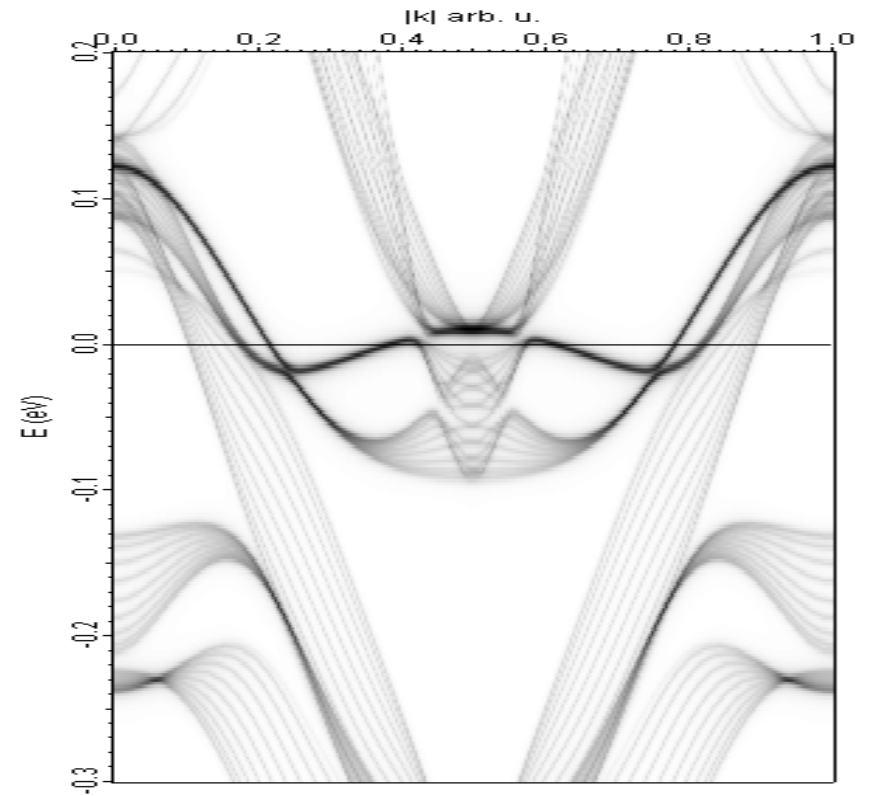


Fe-SC: Complex electronic structure

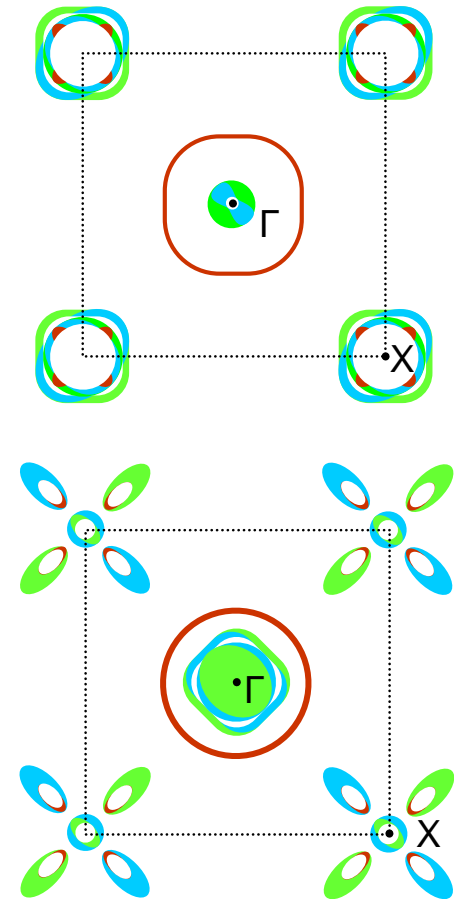
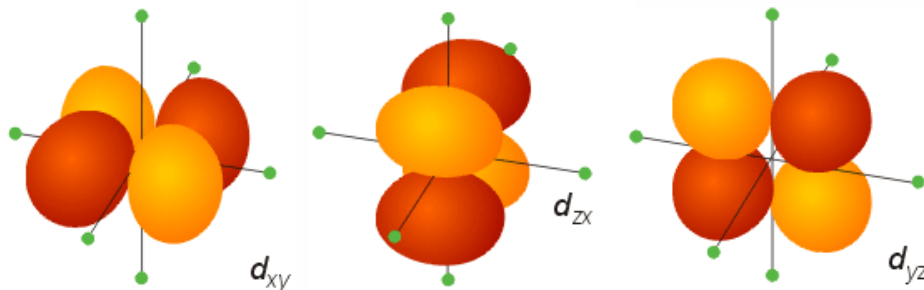
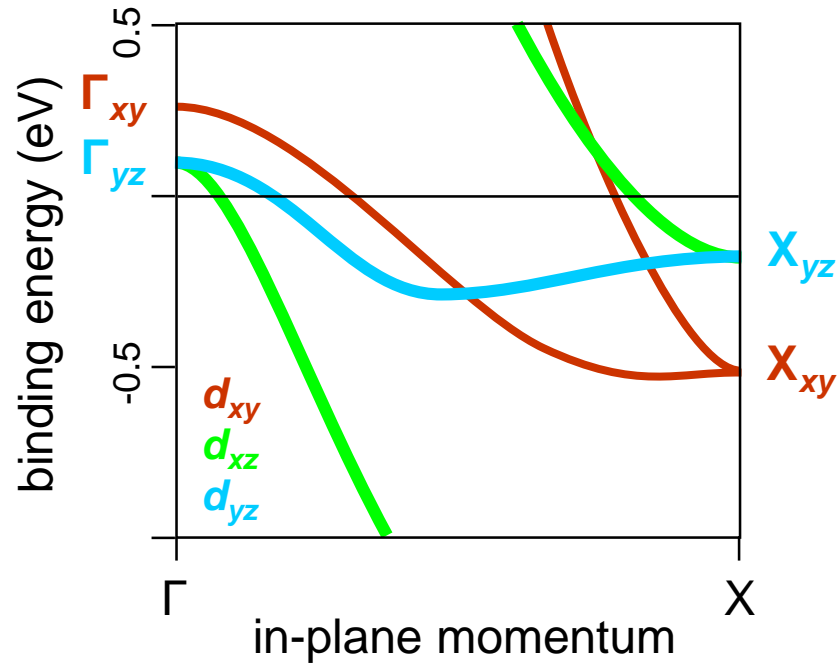
HTSC cuprates



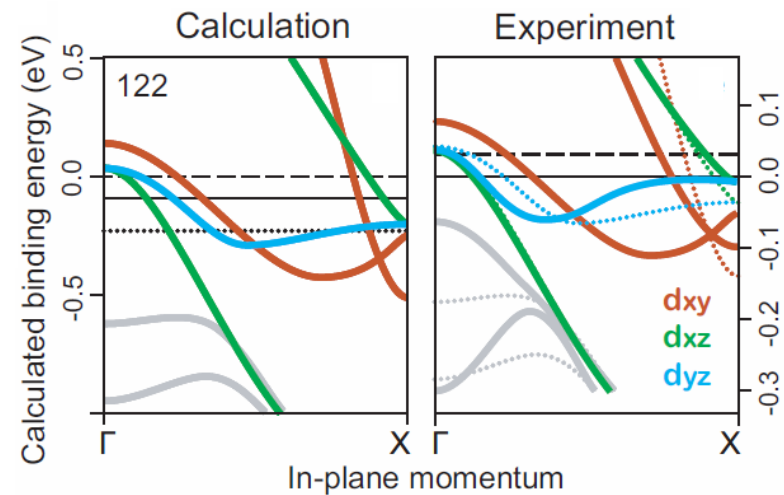
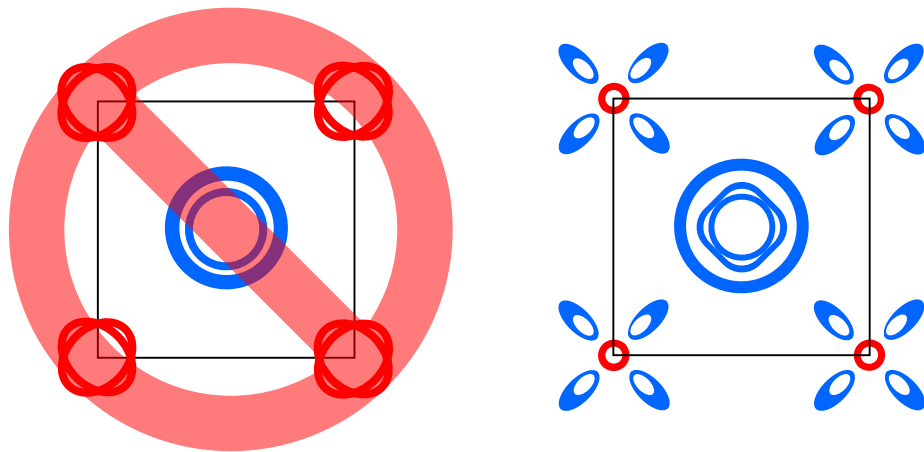
Fe-SC



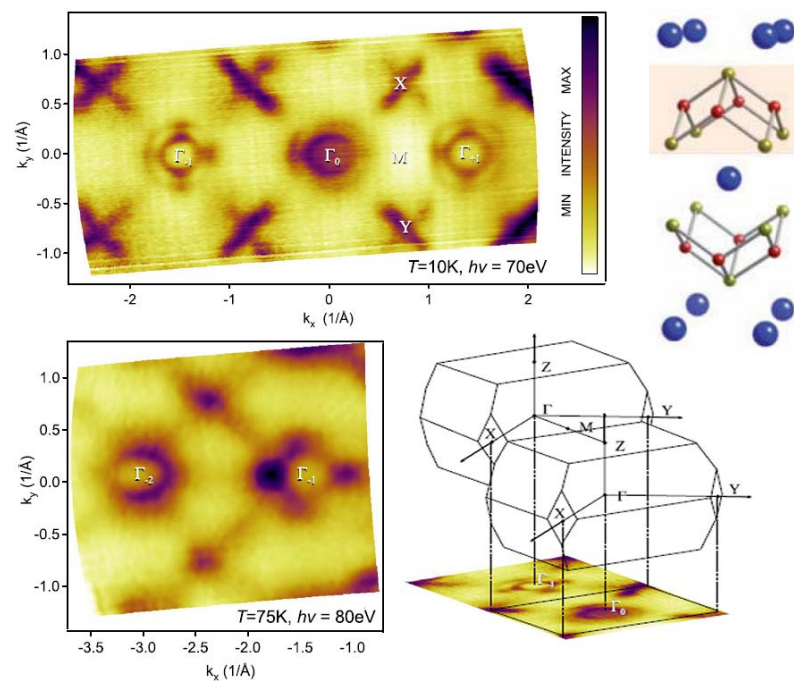
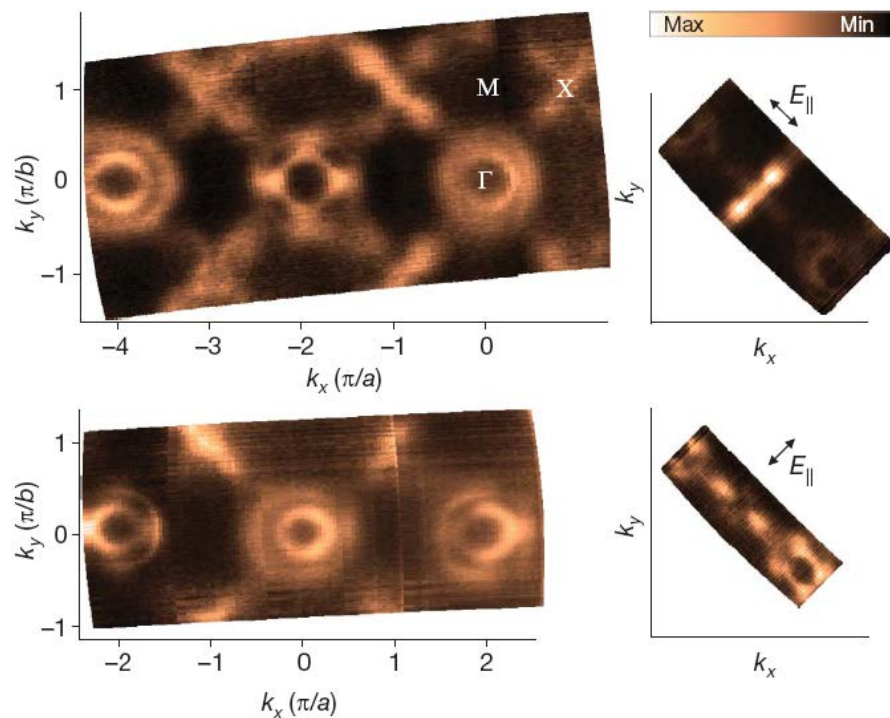
Iron-based superconductors: electronic structure



Fermi surface of BKFA

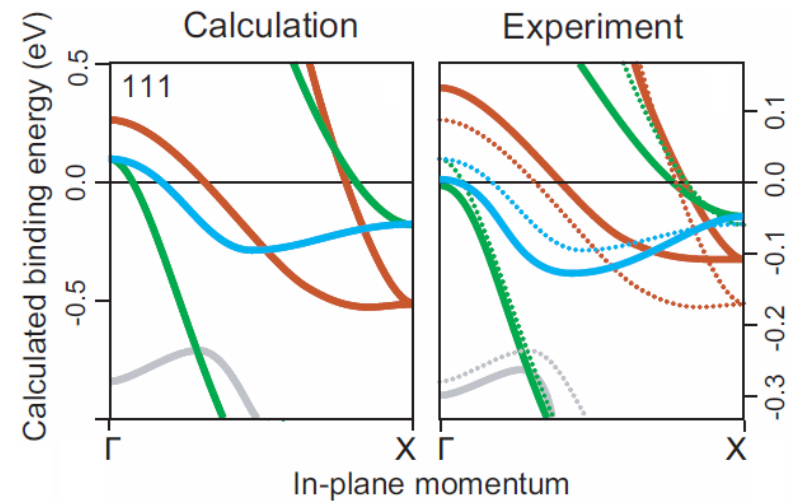
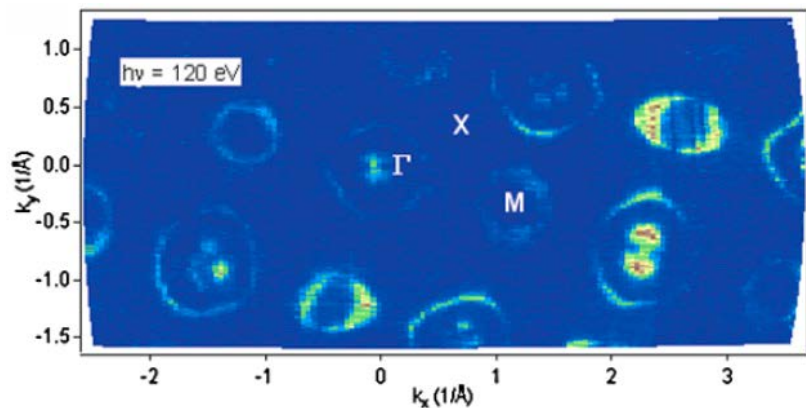
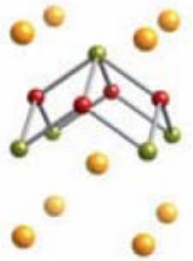
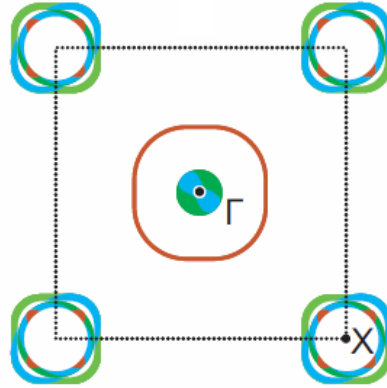
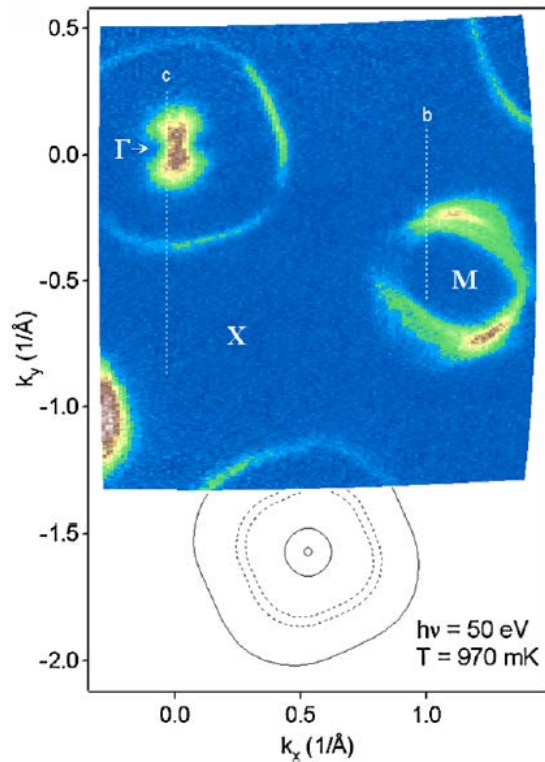


A. A. Kordyuk, *J. Supercond. Nov. Magn.* 2013

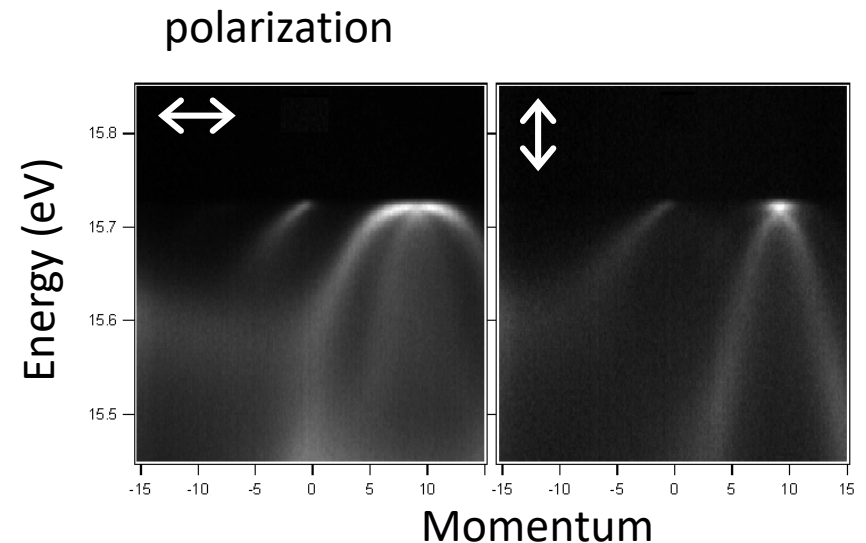


V. Zabolotnyy *Nature* 2009

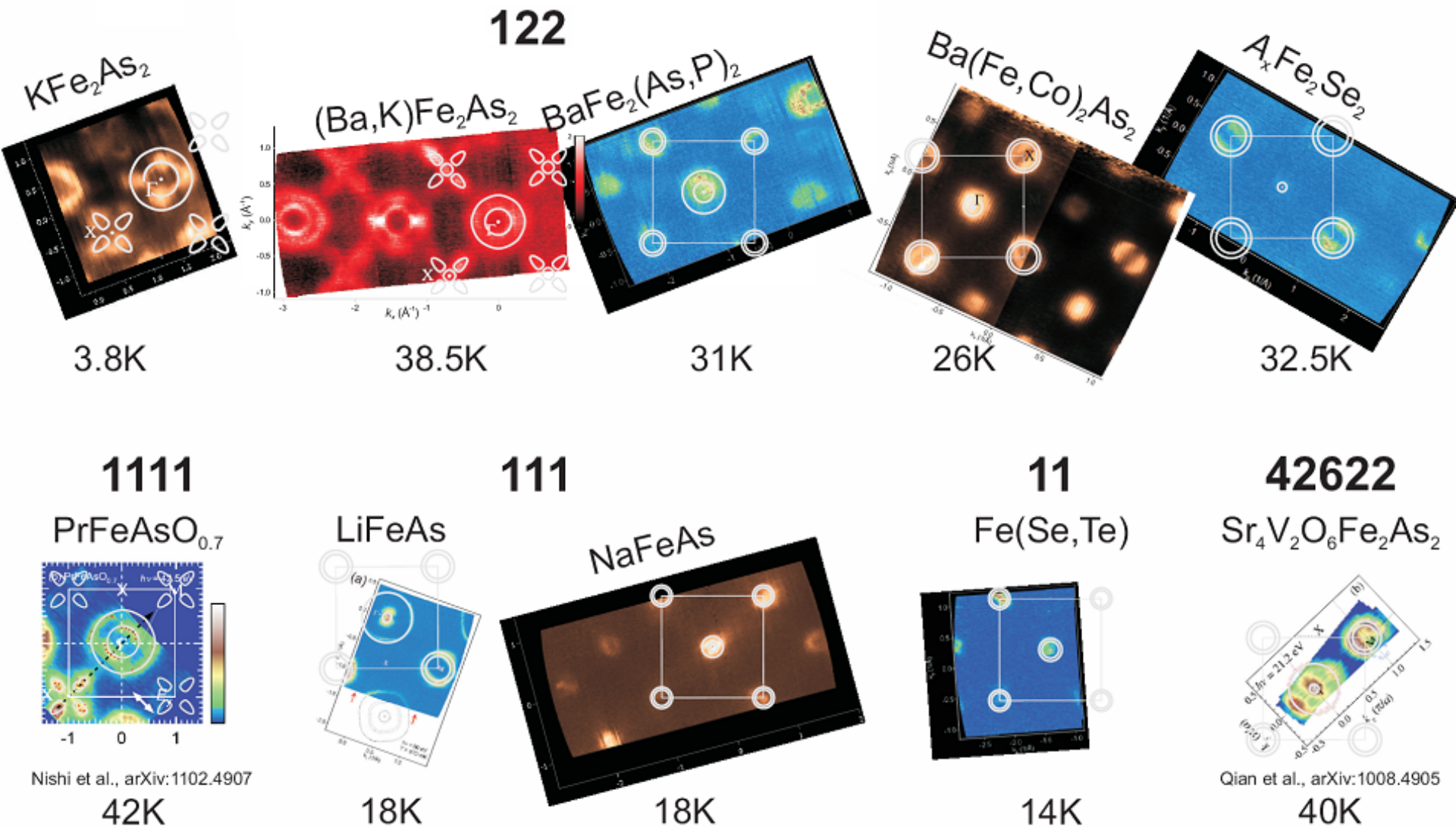
Fermi surface of LiFeAs



Kordyuk, *J. Supercond. Nov. Magn.* 2013

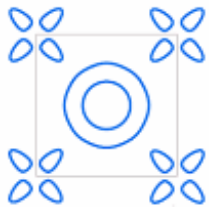
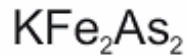


FS's of iron-based superconductors

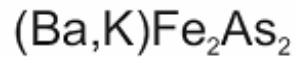


FS's of iron-based superconductors

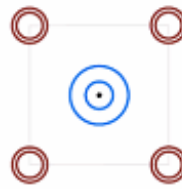
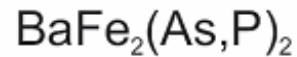
122



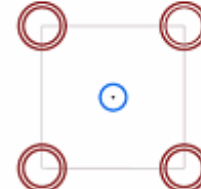
3.8K



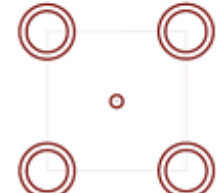
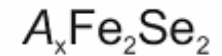
38K



31K

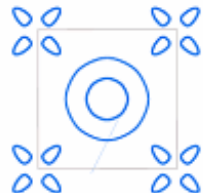


26K



31K

1111

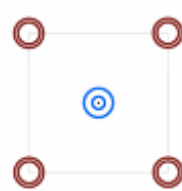


42K

111

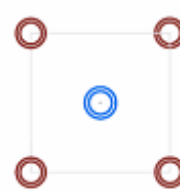


18K



18K

11



14K

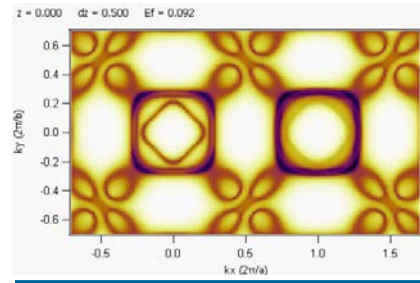
42622



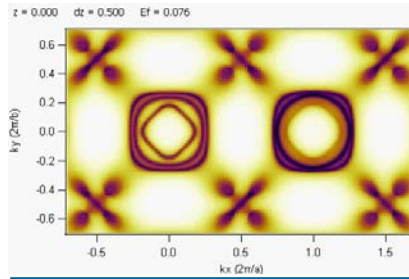
40K

BFA: density of states

Hole doped KFA

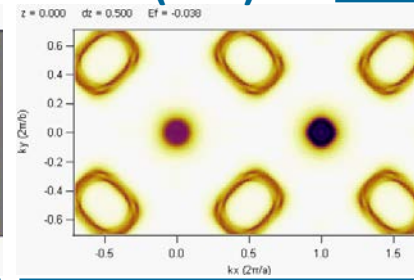


BKFA (38K)

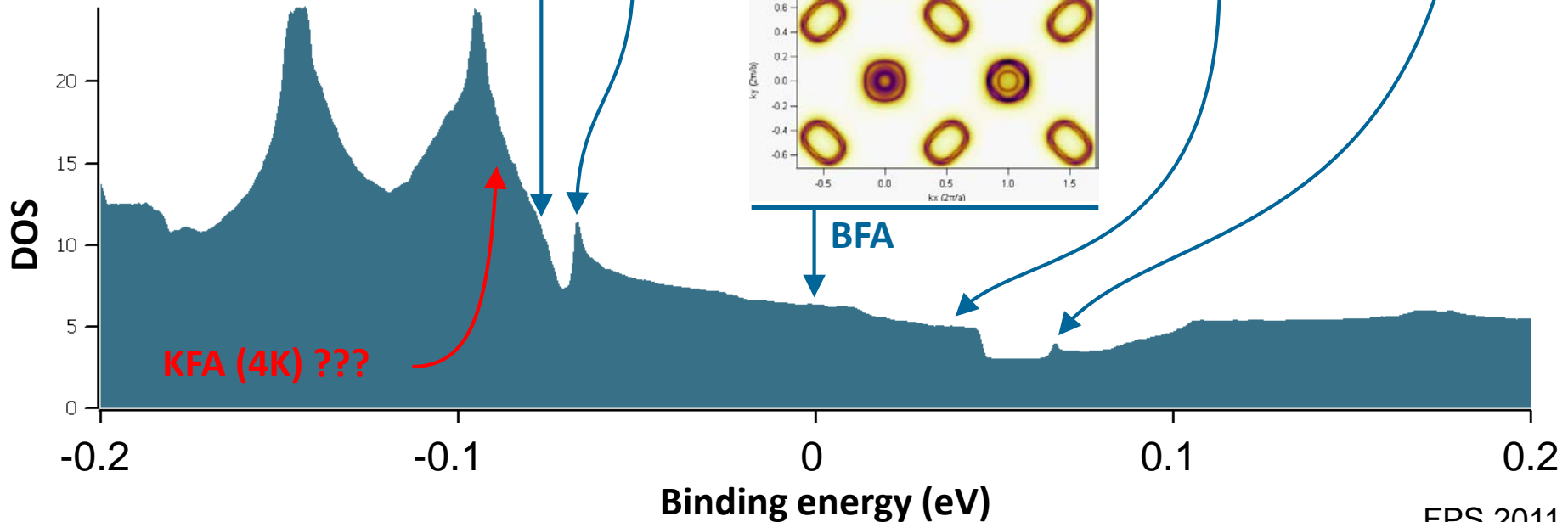
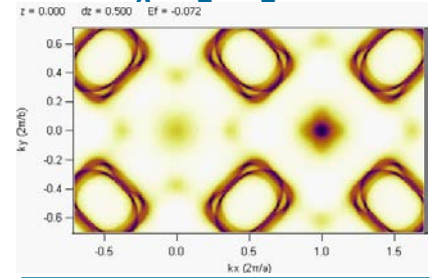


BFCA (26K)

LiFeAs (18K)



$A_x\text{Fe}_2\text{Se}_2$ (31K)



"Topological" superconductivity

=

Small Fermi surfaces

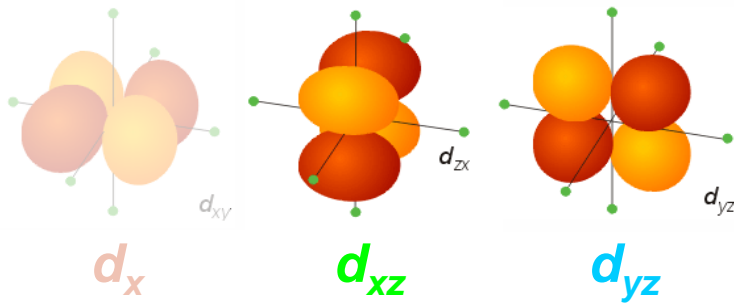
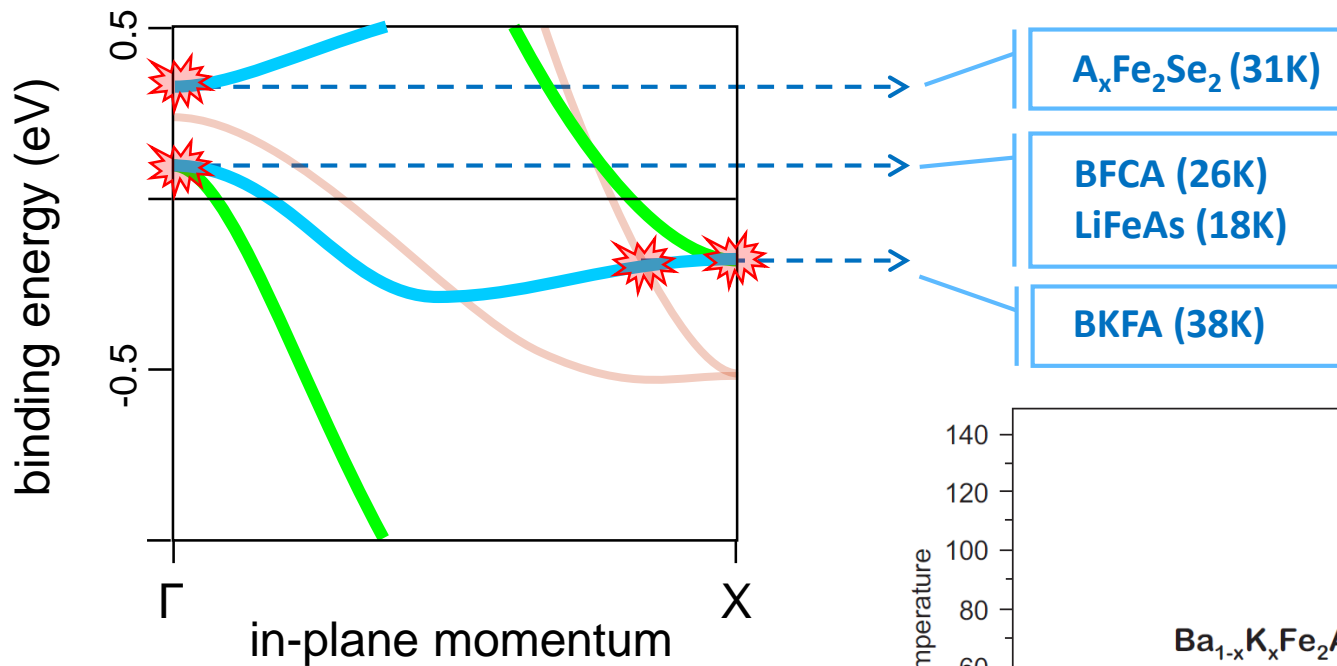
=

vicinity to Lifshitz transition

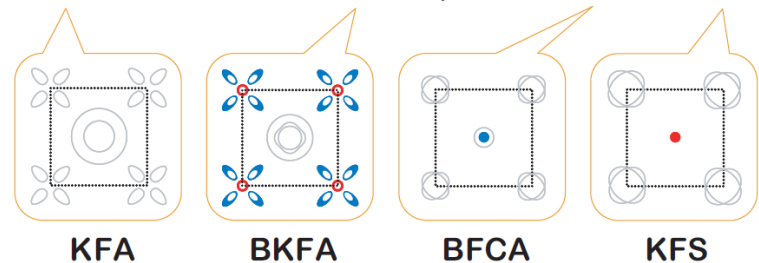
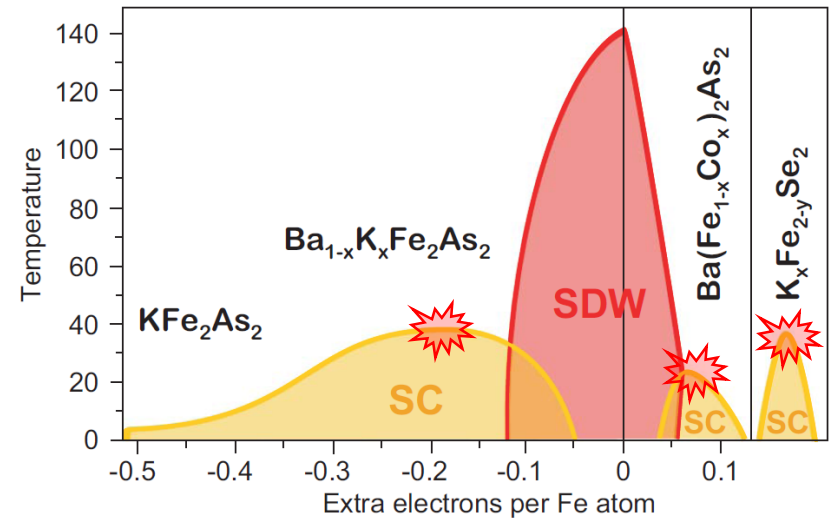
=

vicinity to 2D-3D crossover

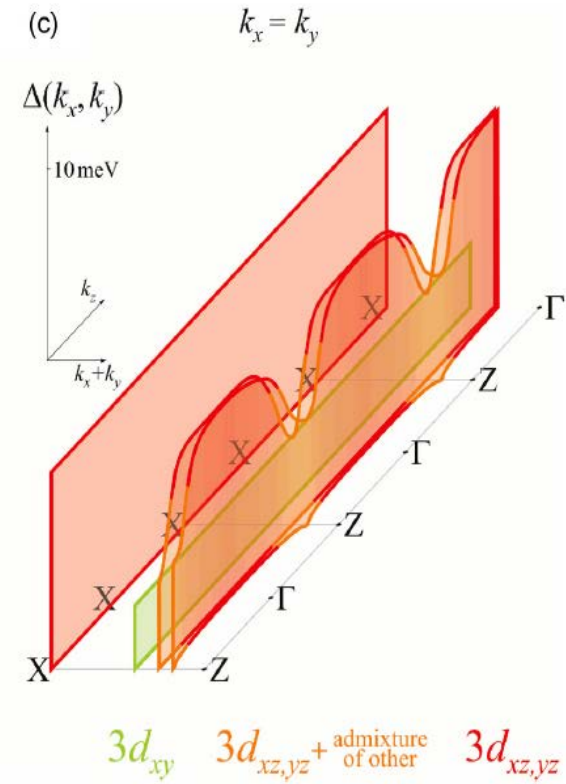
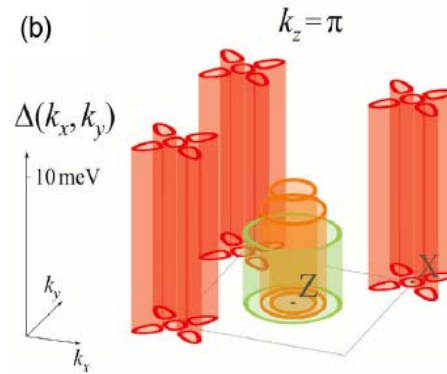
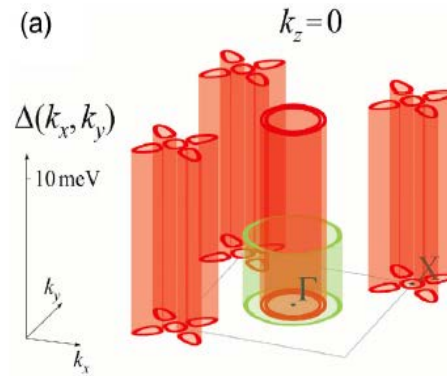
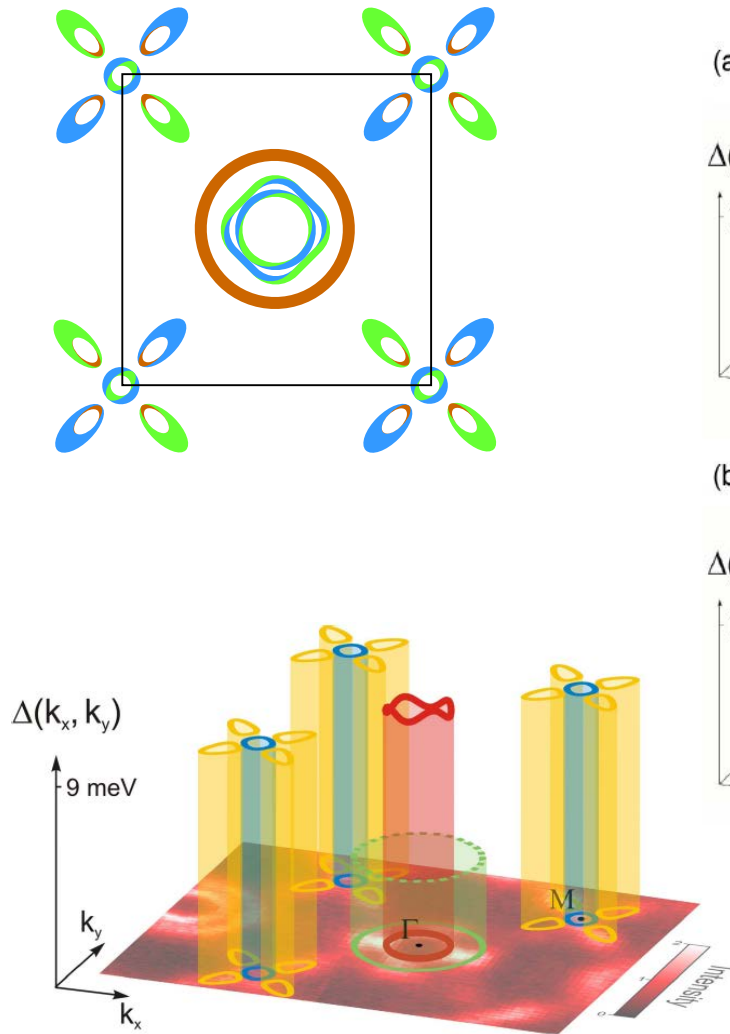
FeSC: electronic structure and superconductivity



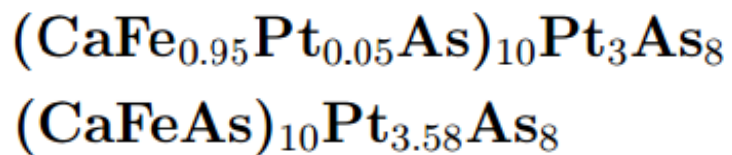
correlates with SC gap!!! - Daniil



BKFA: Fermi surface and gaps

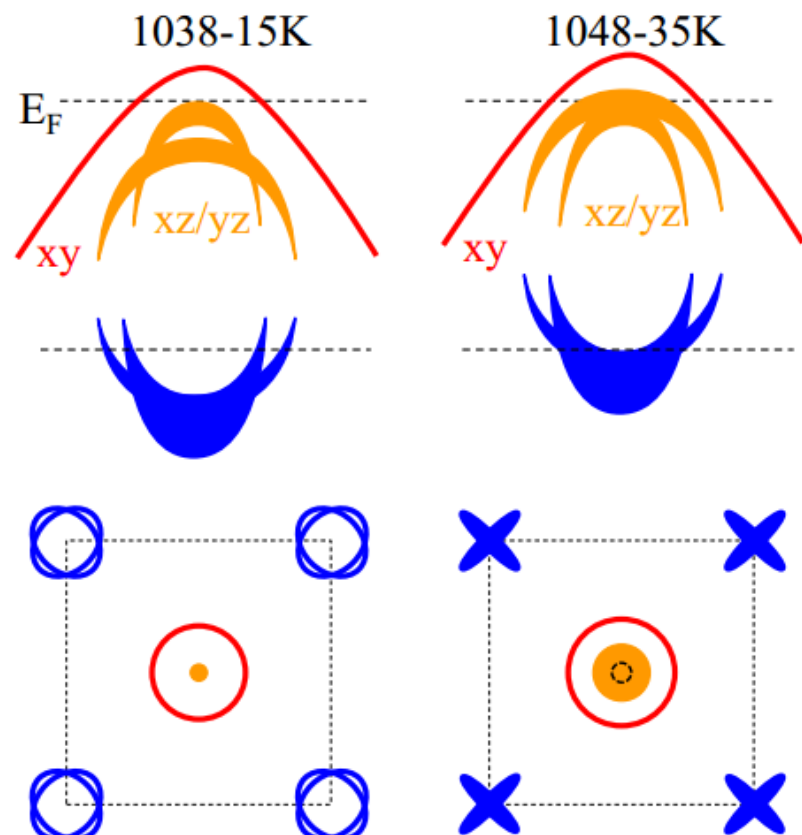
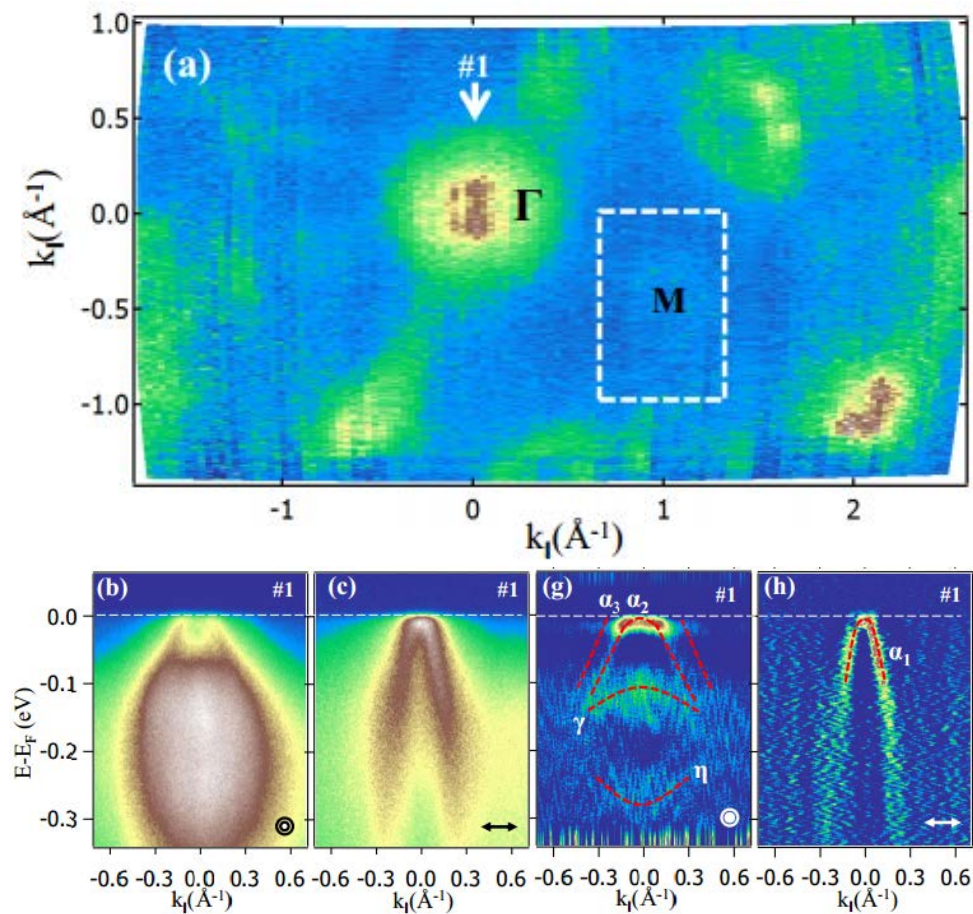


Δ correlates with the orbital composition:
 $\Delta = 3\text{--}4 \text{ meV}$ for $3d_{xy}$ and $3d_{z^2}$
 $\Delta = 10.5 \text{ meV}$ for $3d_{xz/yz}$.



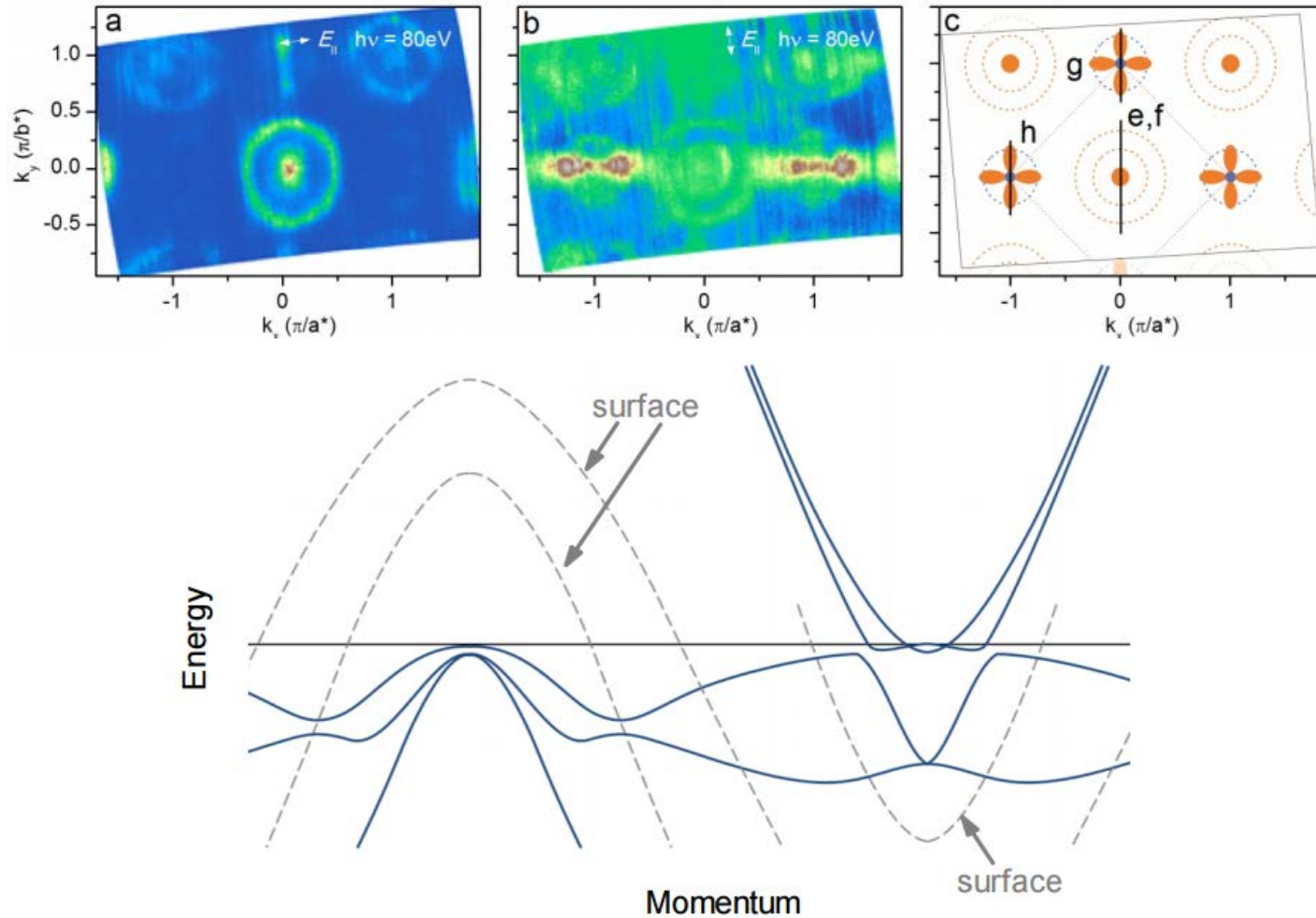
“10 3 8” – 15K

“10 4 8” – 35K



1111

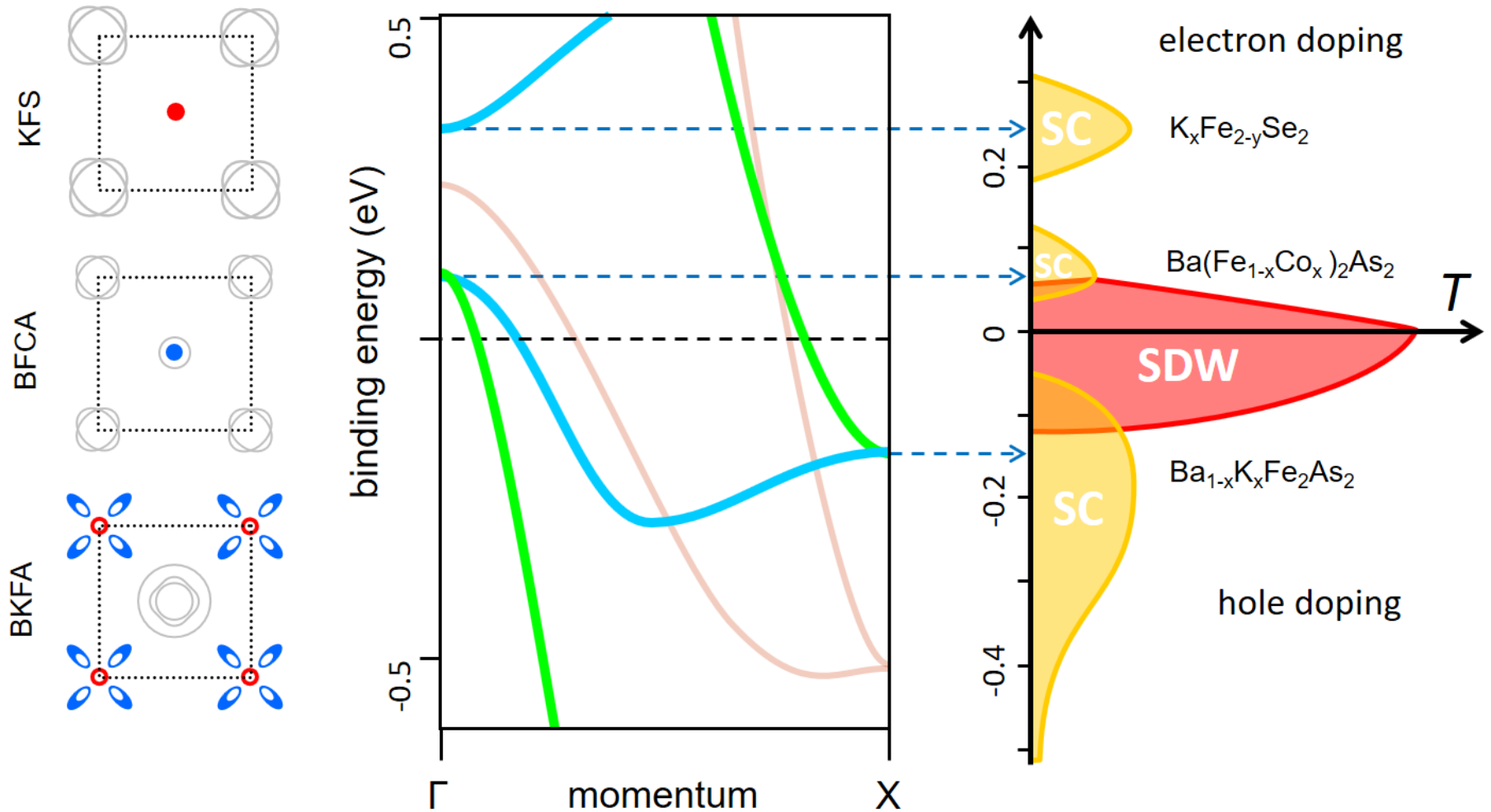
LaFeAsO-type materials $\text{SmFe}_{0.92}\text{Co}_{0.08}\text{AsO}$



Charnukha et al. *Sci. Rep.* **5**, 10392 (2015)

- The band structure of Fe-SC is well captured by LDA but do not take it too literally. The calculated Fermi surface is usually bad starting point for theory.
- T_c 's for different compounds *almost 100%* correlate with the position of the Van Hove singularities (Lifshitz transitions) for the xz- and yz-bands.

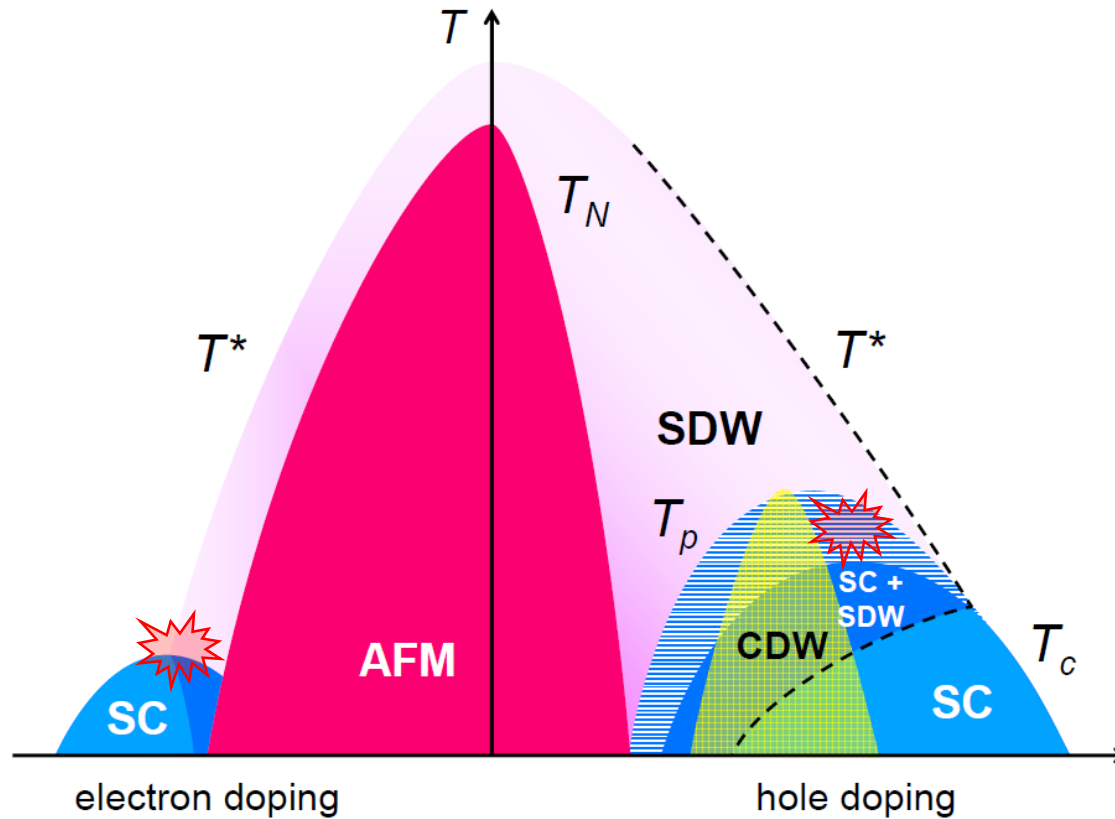
"Topological" superconductivity in Fe-SC



LTP 38, 888 (2012); JSNM 26, 2837-2841 (2013); PRB 88, 134501 (2013);
PRB 89, 064514 (2014), **LTP (2018)**...

**back to
HTSC cuprates**

"Topological" superconductivity in Cu-SC



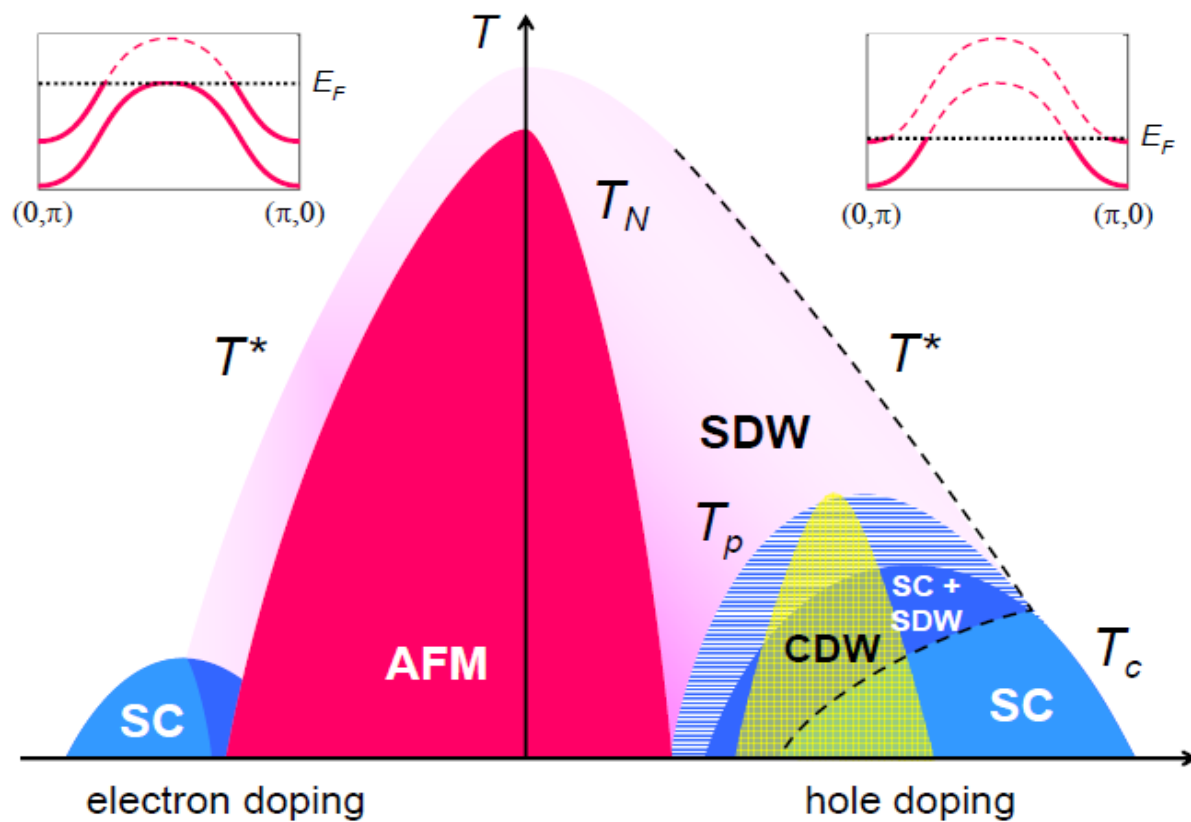
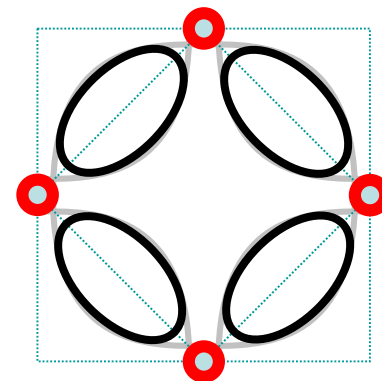
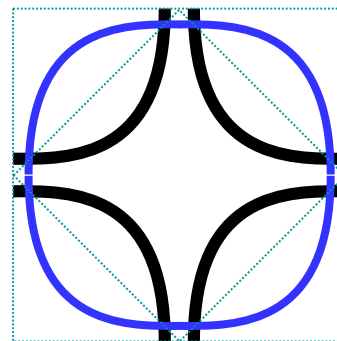
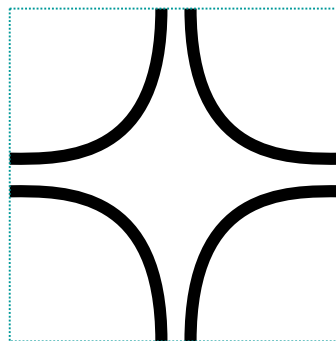
Pseudogap in cuprates

There are at least **three** mechanisms that form the pseudogap in the hole doped cuprates:

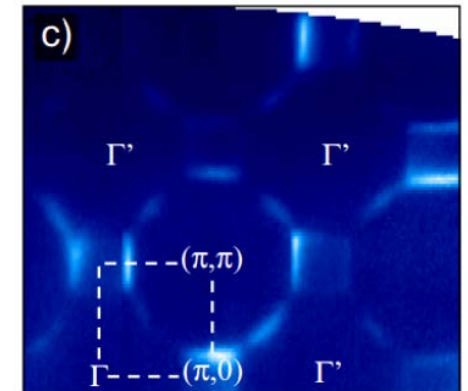
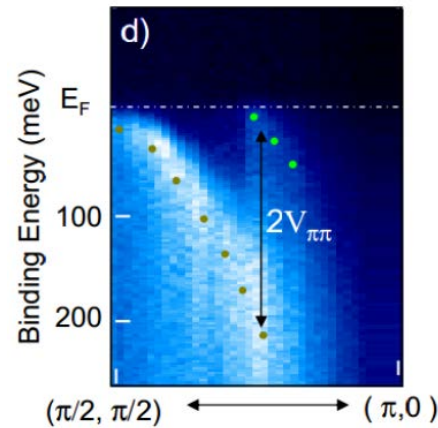
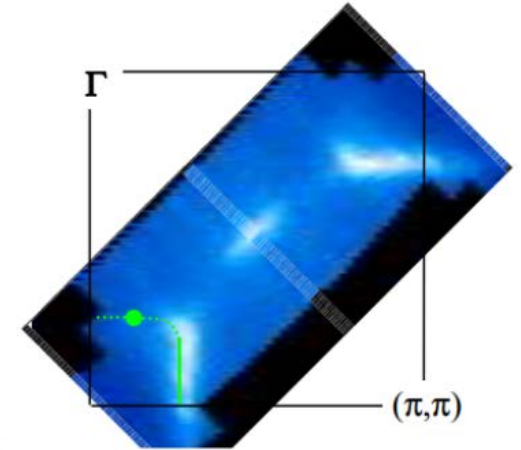
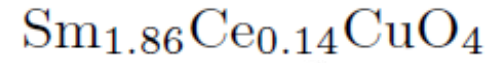
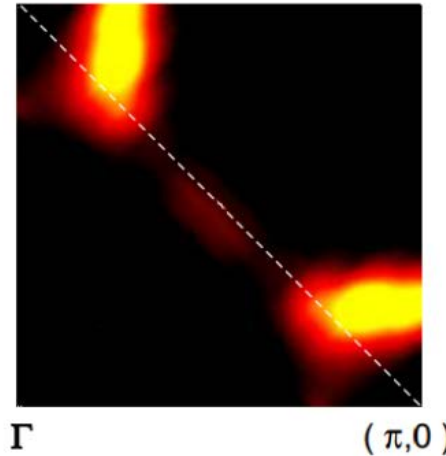
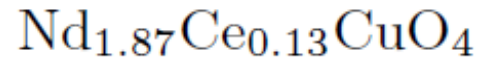
- 1 the preformed pairing;
- 2 the incommensurate CDW due to nesting of the straight parallel Fermi surface sections around $(\pi, 0)$ and $(0, \pi)$;
- 3 **SDW** which is **dominant** constituent of the pseudogap associated with T^* and is either causing or caused by the Mott localization.

These phases occupy different parts of the phase diagram and gap different parts of the Fermi surface competing for it.

VHS nesting

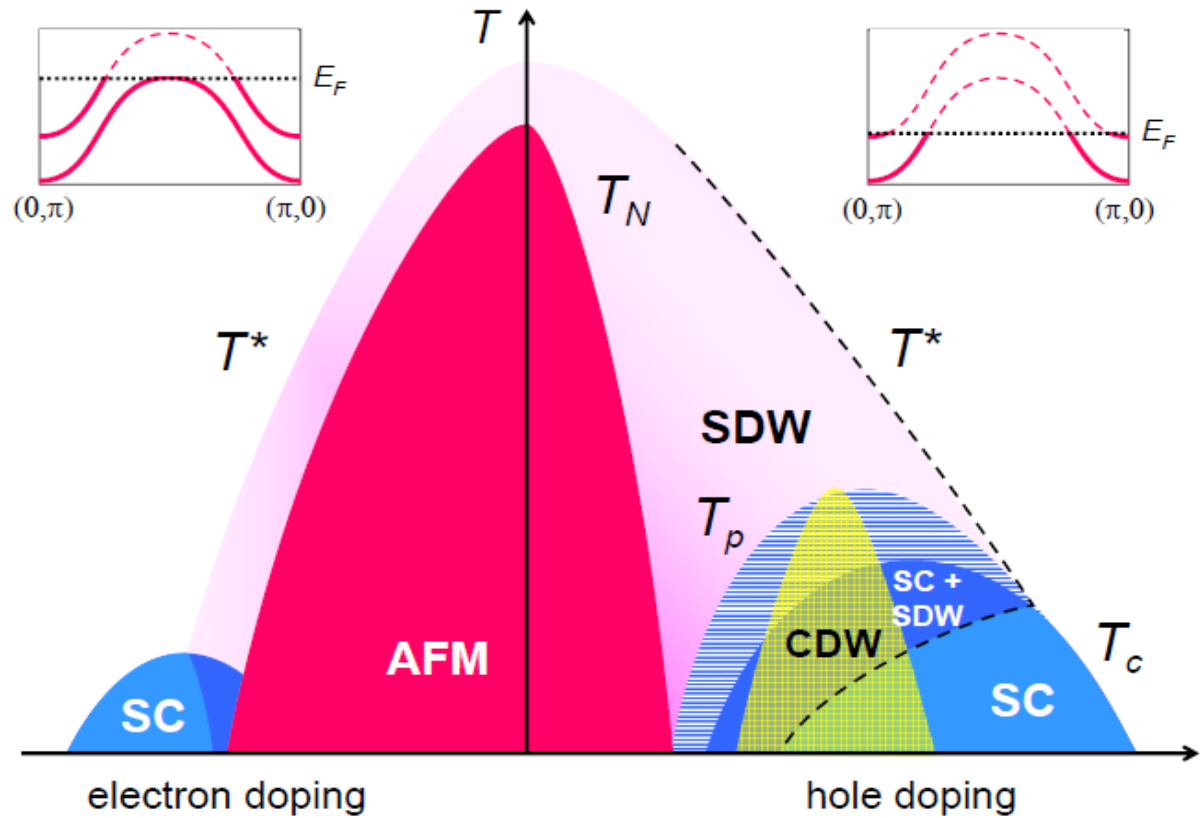
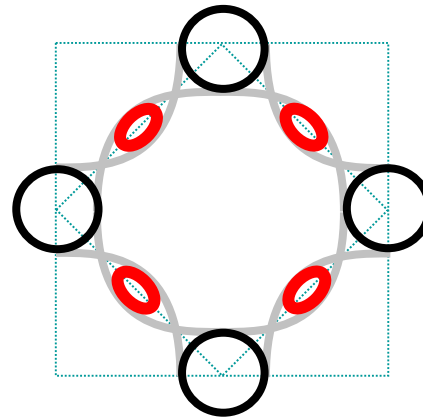
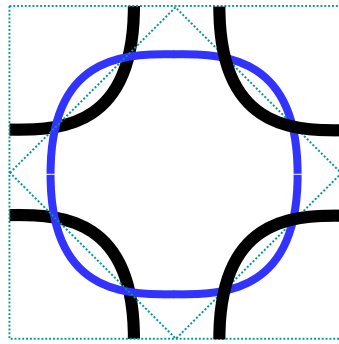
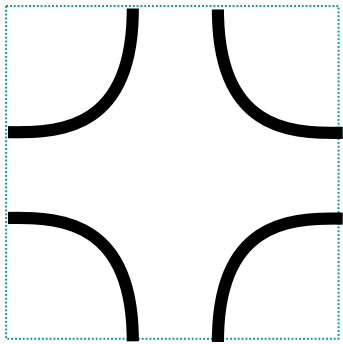


SDW in electron-doped cuprates



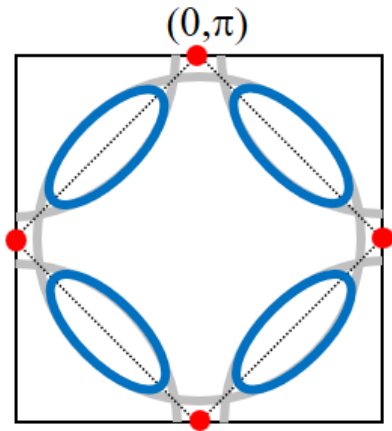
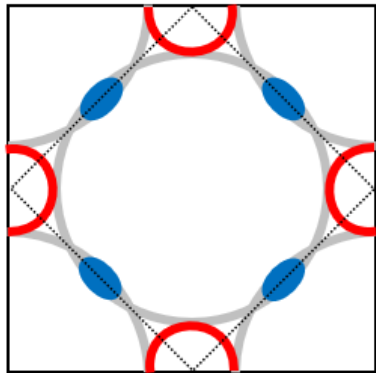
H. Matsui et al., *PRL* **94**, 047005 (2005)
 S. R. Park et al., *PRB* **75**, 060501 (2007)

Nodal nesting

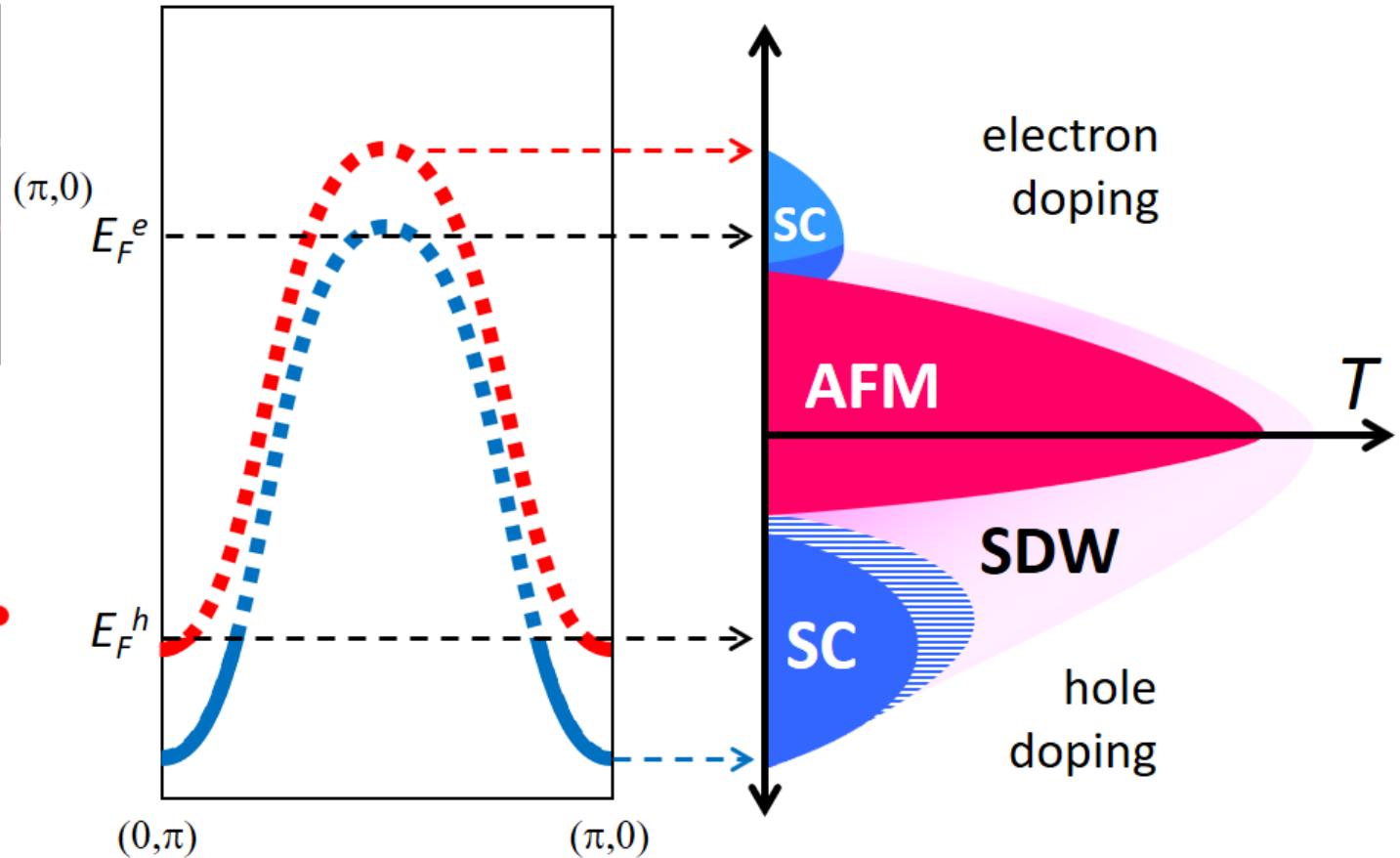


SDW and superconductivity

Nodal nesting

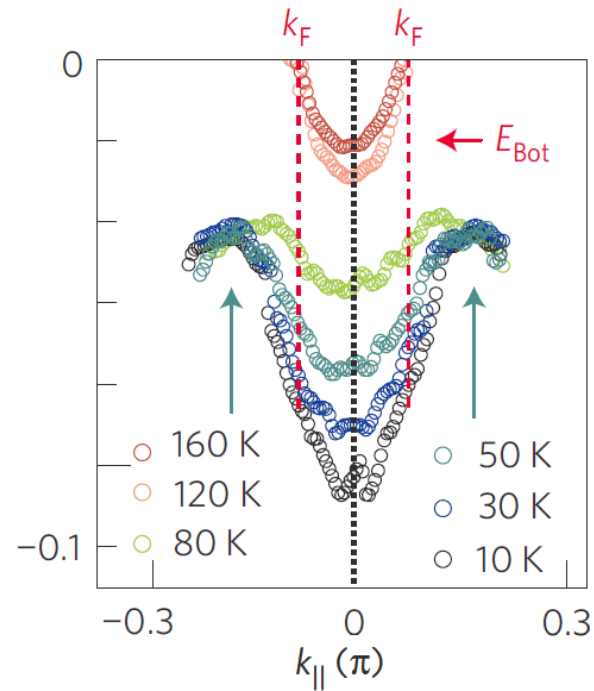
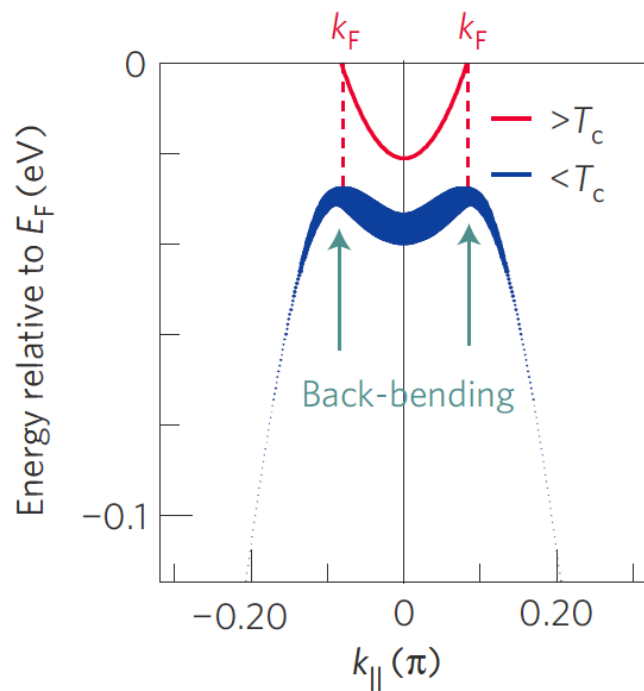
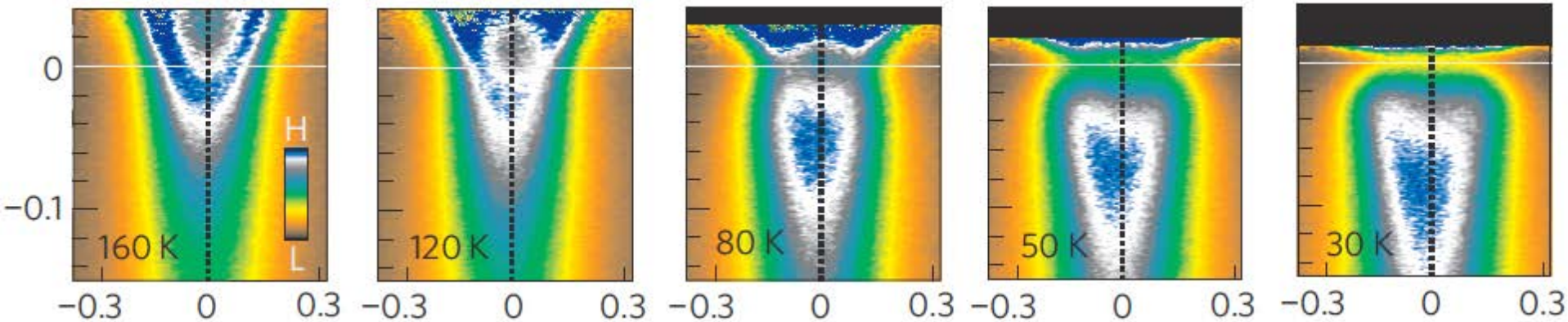


VHs nesting

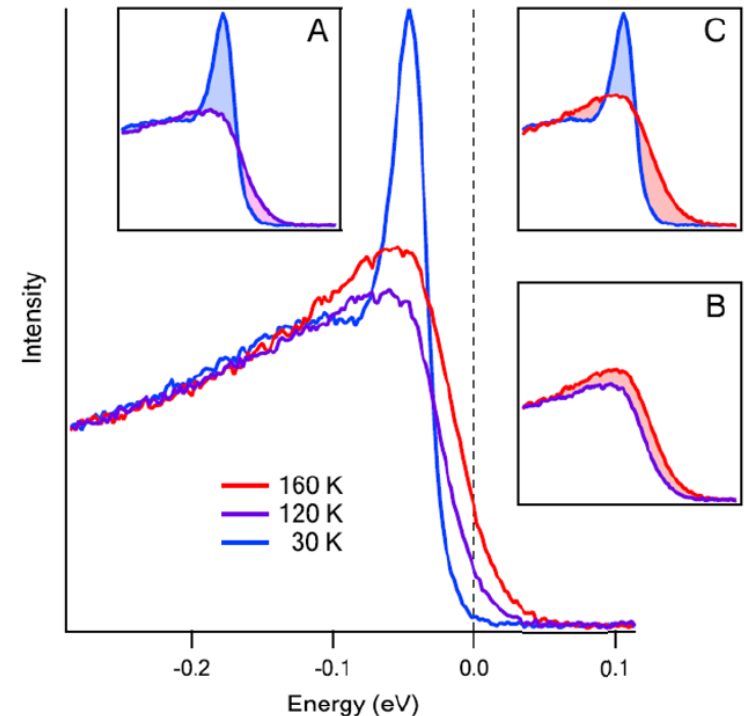
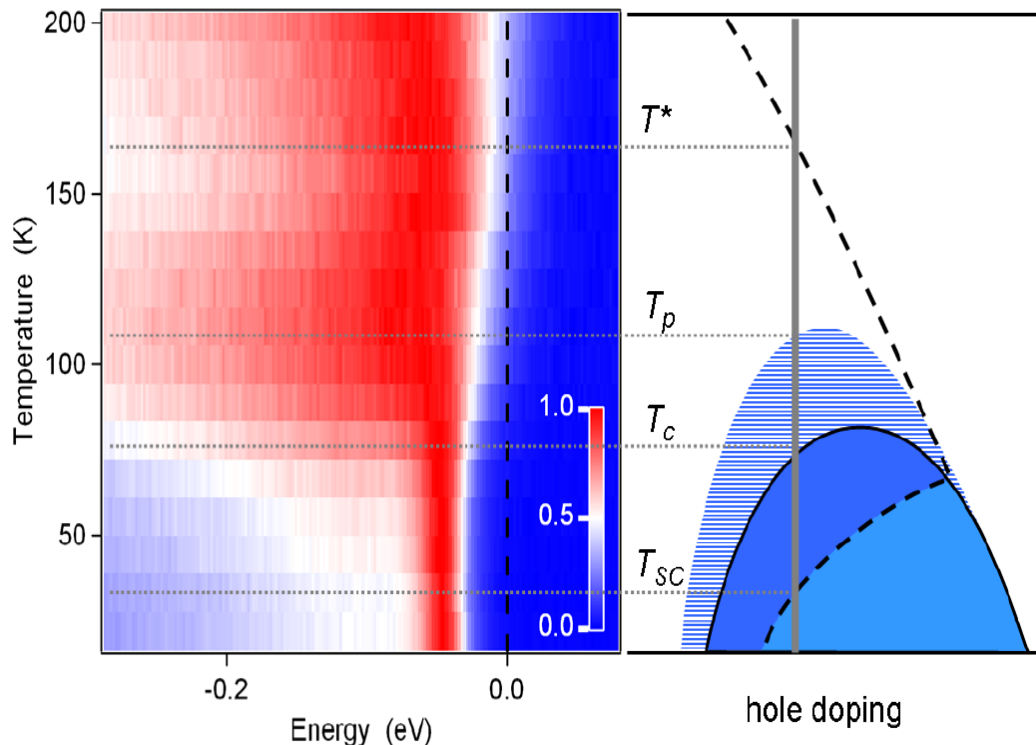


$(0,\pi)$ SDW

Pb-Bi2201 $T_c = 34$ K, $T^* = 125$ K



Pseudogap in cuprates



Temperature evolution of the hot spot EDC for underdoped BSCCO ($T_c = 77$ K).

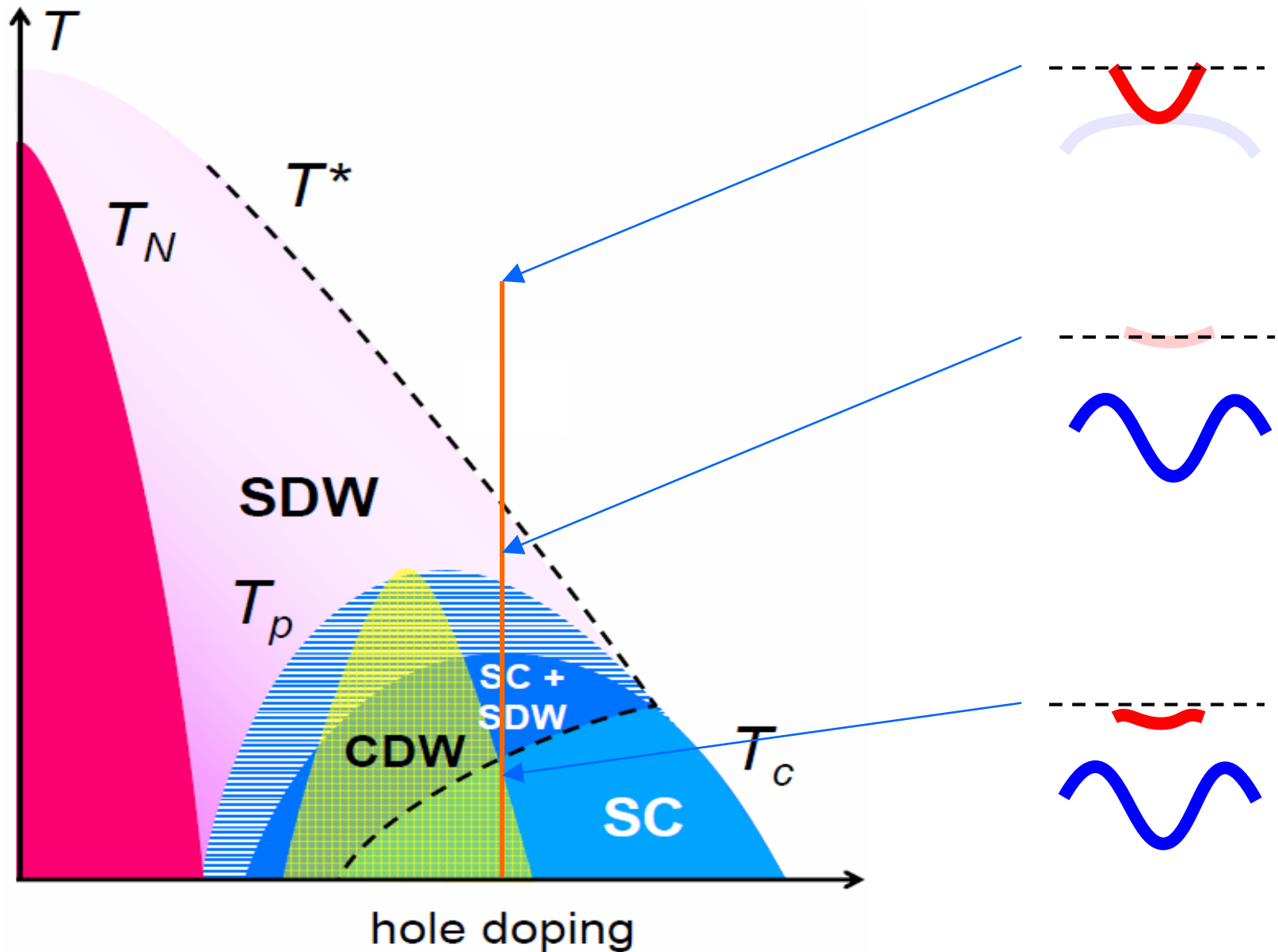
T^* - the pseudogap starts to increase rapidly, the spectral weight starts to decrease;

T_p - the spectral weight starts to increase;

T_c - the superconducting gap opens, the spectral weight continues to increase up to **T_{sc}** .

The examples of non-normalized EDC's at 160 K, 120 K, and 30 K (right) illustrate the spectral weight evolution.

Pseudogap in hole-doped cuprates

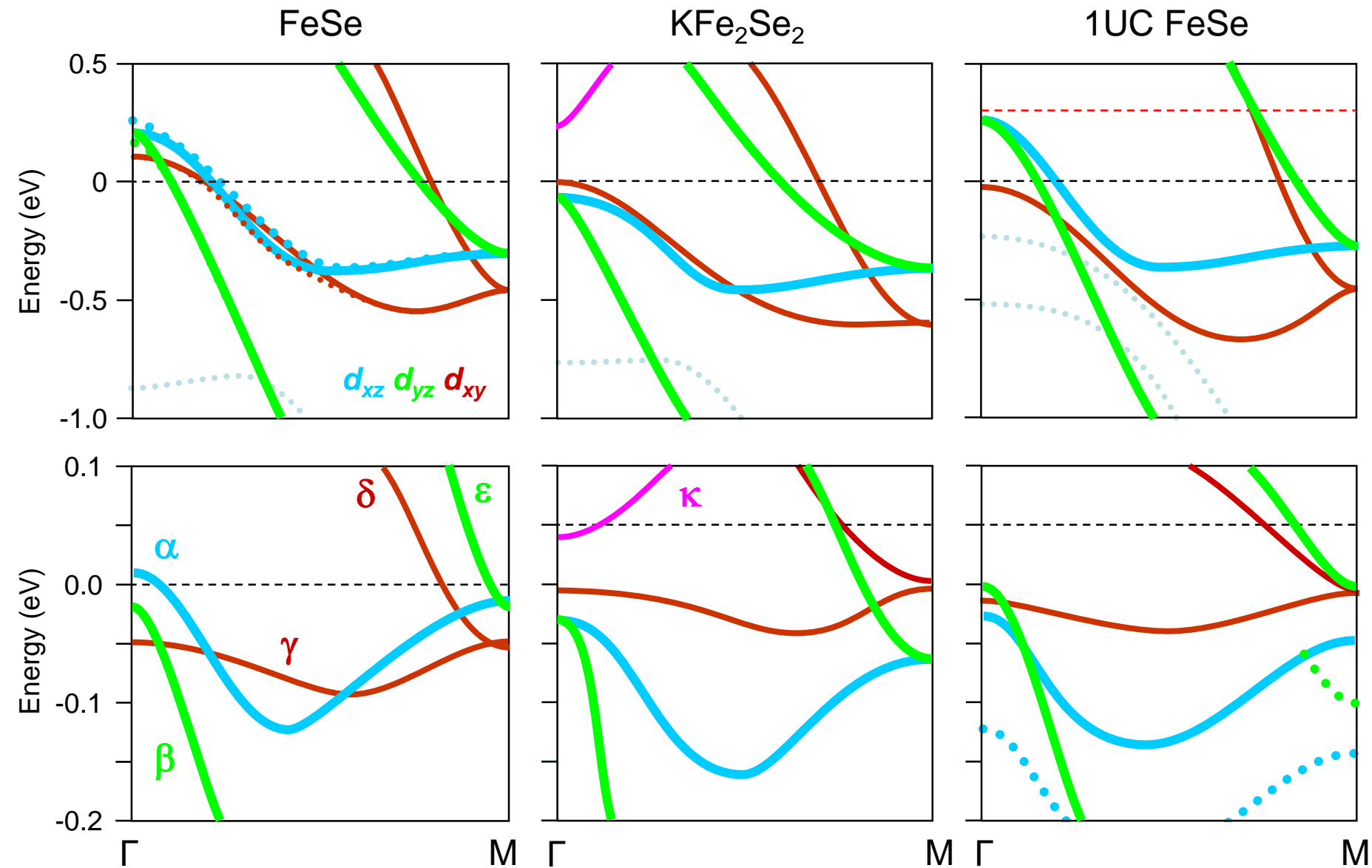


Conclusions

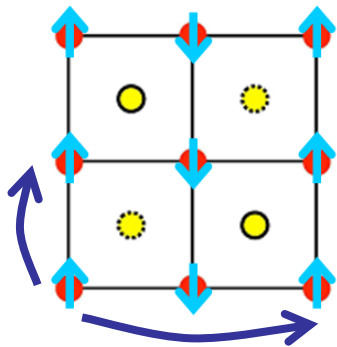
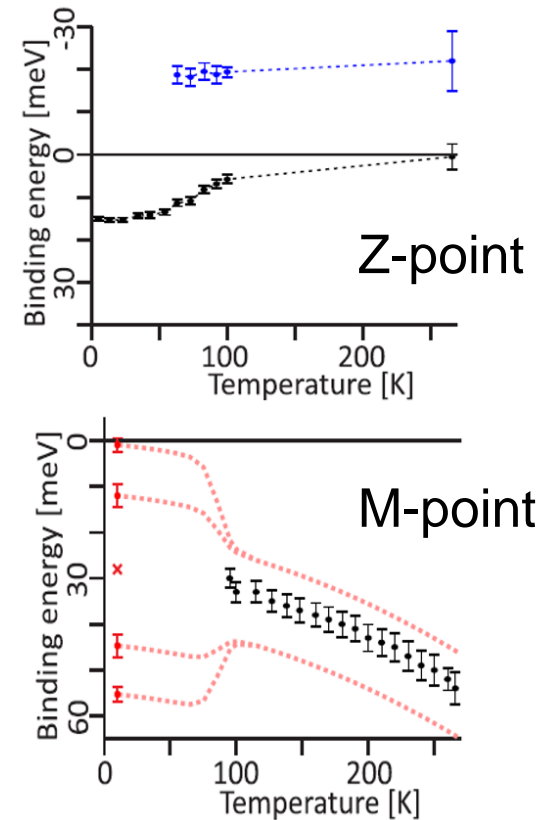
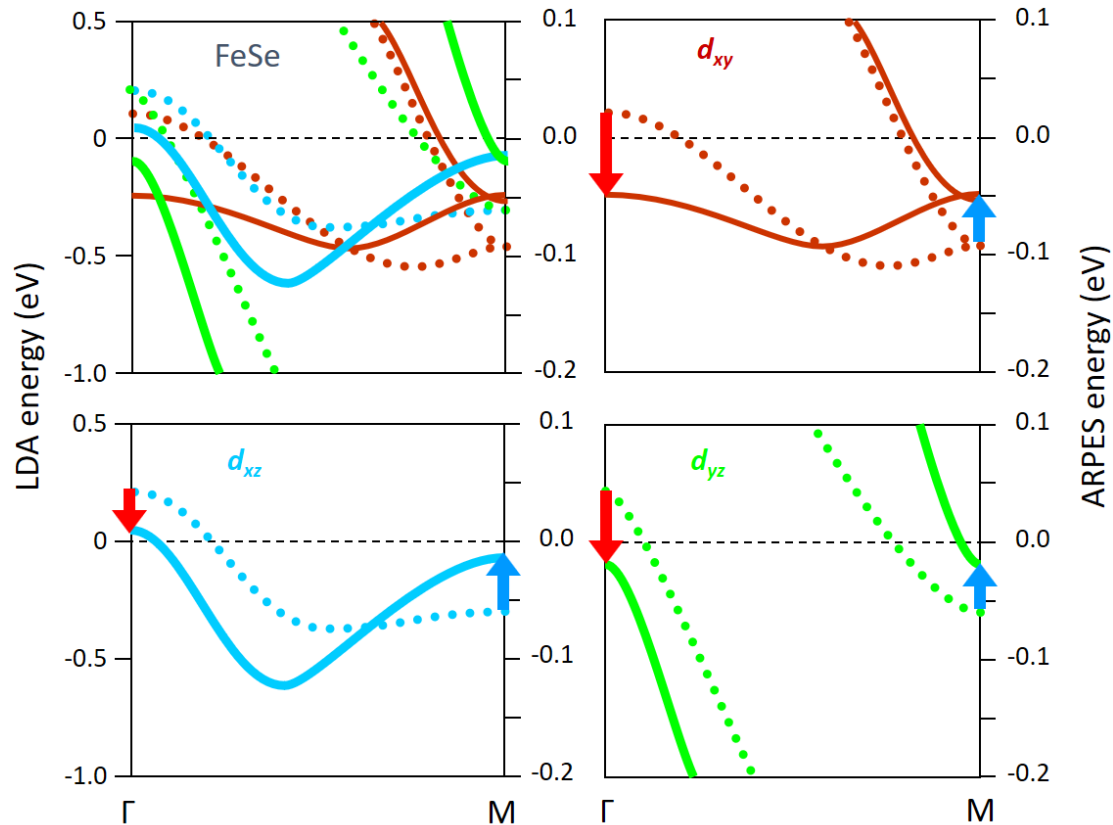
- The SDW and superconductivity in HTSC cuprates competes for the phase space but, on the other hand, the **SDW-reconstructed Cu-SC** share with Fe-SC the empirical correlation between the T_c maximum and the proximity of the Fermi surface to the topological **Lifshitz transition**. This suggests that **"topological superconductivity"** could be a general mechanism for high temperature 2D superconductors.
- SDW (AF) in cuprates could be initiated by nodal nesting and VFs nesting for the electron and hole doped Cu-SC, respectively.

back to Fe-SC

FeSe: electronic band structure (LDA & ARPES)

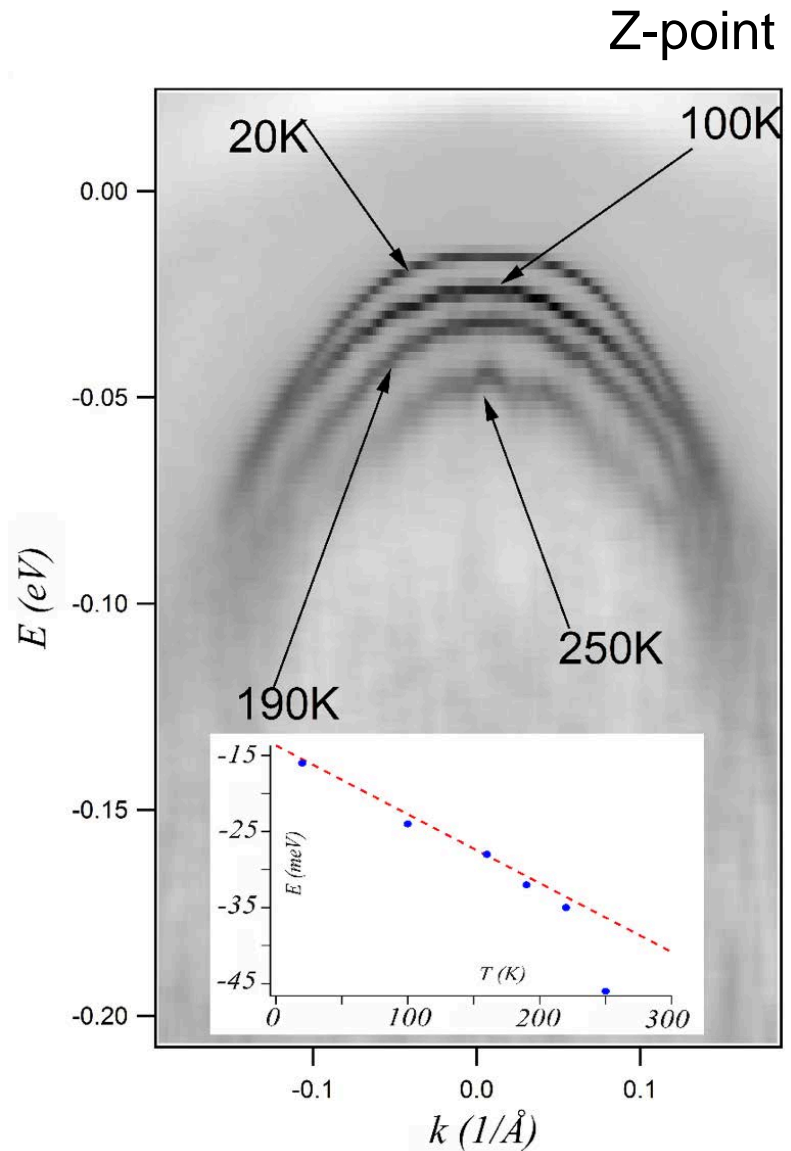
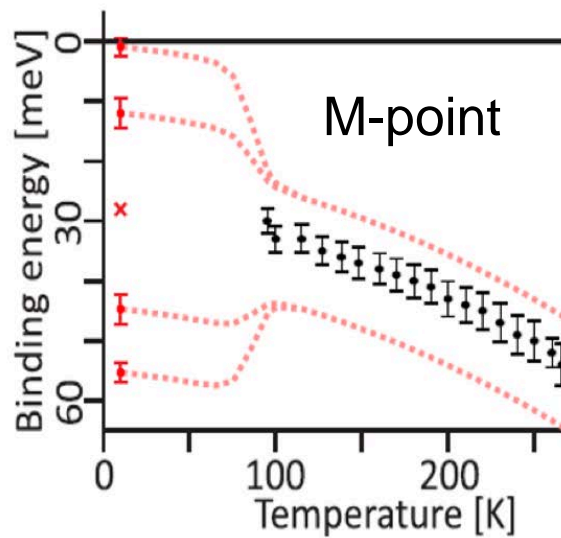
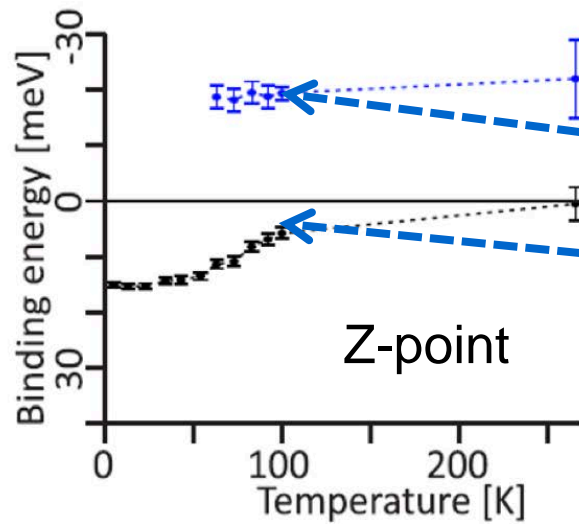


“Red-blue shift” in Fe-SC



$$\varepsilon(k) = \varepsilon_0 + t_1 \cos(ka) + t_2 \cos(2ka)$$

“Red-blue shift” in Fe-SC



Conclusions

- There is an empirical correlation between electronic structure and T_c : maximal T_c (optimally doped SC) is observed when proximity of the ES to topological Lifshitz transition takes place.
- This is observed for all Fe-SCs and for Cu-SC (both for hole- and electron-doped ones) in the antiferromagnetic Brillouin zone, i.e., assuming that the PG is caused by the AF-like electronic ordering.
- This correlation can be used to **search for new high-temperature superconductors with much higher transition temperatures.**

Collaboration



IMP

Yuriy Pustovit
Vladimir Bezguba
Alexander Plyushchay
Yurii Toporov

ARPES, IFW Dresden

Sergey Borisenko
Volodymyr Zabolotny
Daniil Evtushinsky
Yevhen Kushnirenko
Timur Kim
Jörg Fink

ARPES Worldwide

Mark Golden
Toni Valla
Veronique Brouet

Neutron Scattering

Vladimir Hinkov
Bernhard Keimer
Dmytro Inosov

STM & Transport

Bernd Buehner
Cristian Hess
Alexey Pan

Theory

Alexander Yaresko
Eugene Krasovskii
Thomas Dahm
Doug Scalapino
Andrey Chubukov
Ilya Eremin

Synchrotron Light

BESSY

Rolf Follath
Andrei Varykhalov

SLS

Ming Shi
Vladimir Strocov
Luc Patthey

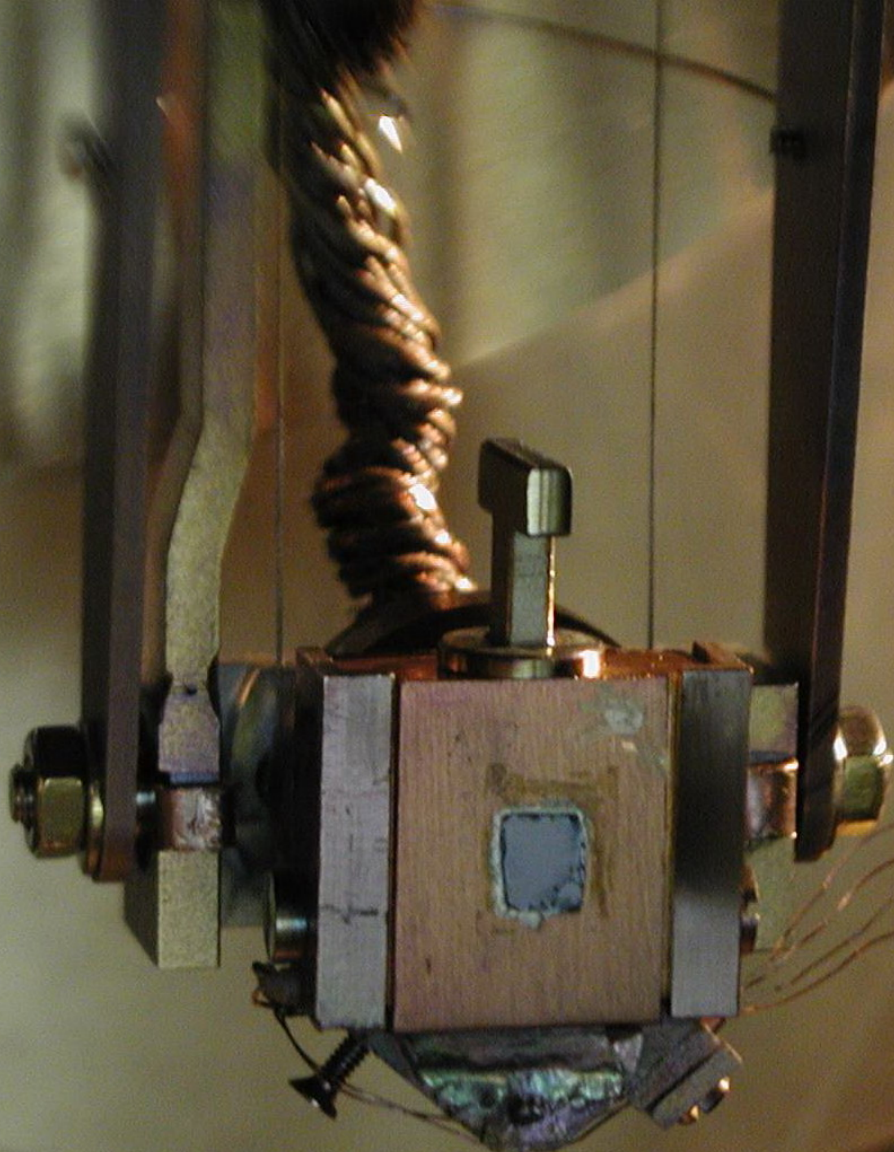
ELETTRA

Luca Petaccia

SOLEIL

Veronique Brouet





Single Crystals

Cuprates

Helmut Berger (EPFL Lausanne)

Chengtian Lin (MPI Stuttgart)

S. Ono, Yoichi Ando (CRIEPI Tokyo)

Iron based superconductors

Igor Morozov (MSU)

Alexey Chareev (Chernogolovka)

Chengtian Lin (MPI Stuttgart)

S. Aswartham (IFW)

S. Wurmhel (IFW)

Hai-Hu Wen (IoP Beijing)

Topological insulators

Helmut Berger

S. Wurmhel

Thank you!

