

ARPES on $Tl_2Ba_2CuO_{6+\delta}$: Probing the Electronic Structure of Overdoped Cuprates

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QUANTUM MATERIALS AT UBC



■ Electronic Structure of Solids

*Theoretical modeling & fabrication
of nanostructured materials*

George Sawatzky

■ ARPES on Complex Systems

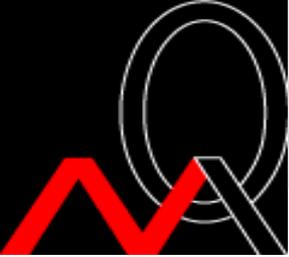
*Low-energy electronic structure
Photoelectron spectroscopies*

Andrea Damascelli

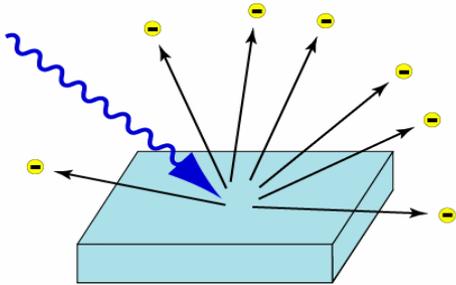
■ Scanning Tunneling Microscopy

*Self Assembly & atomic manipulation
of nanostructured materials*

Johannes Barth



ARPES ON COMPLEX SYSTEMS



Angle Resolved PhotoElectron Spectroscopy

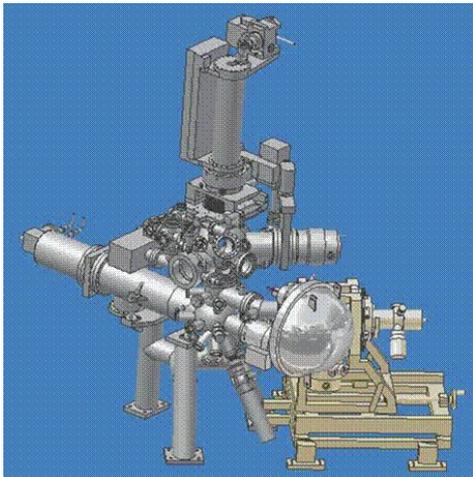
FIRST EVIDENCE FOR THE QUANTIZATION OF LIGHT!

Velocity and direction of the electrons in the solid

Low-energy Electronic Structure → Macroscopic Physical Properties

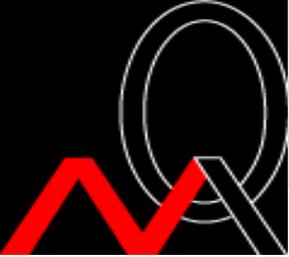
Superconductivity, Magnetism, Density Waves,

ARPES @ UBC



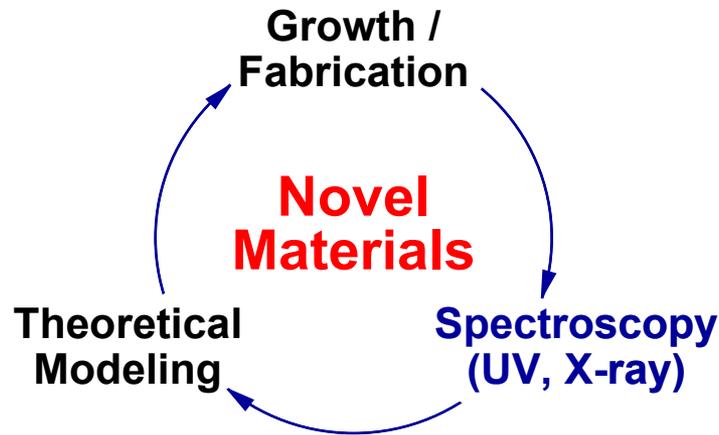
Synchrotron based spectroscopies





ARPES ON COMPLEX SYSTEMS

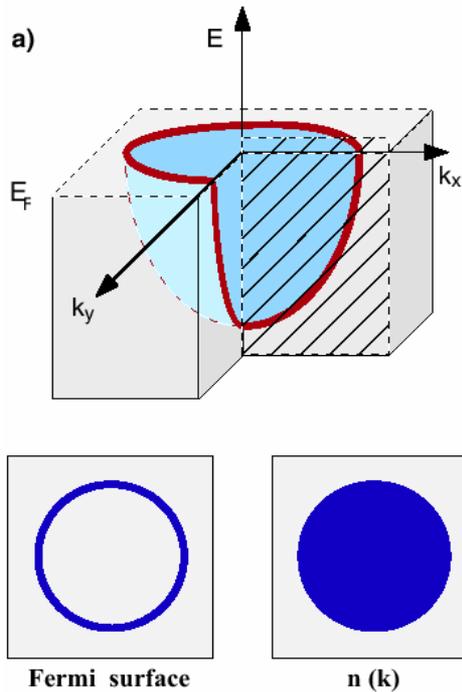
Comprehensive Material Science Program Across Canada



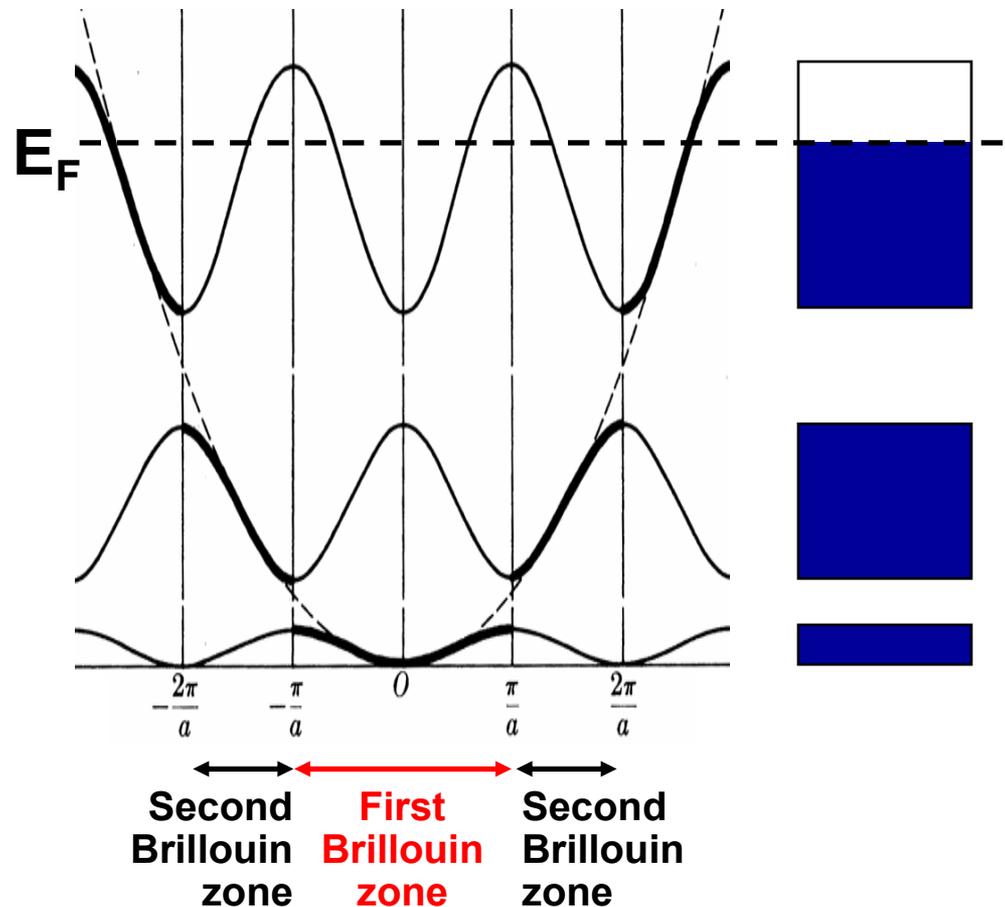
1. Orbital excitations in orbital-ordered ferromagnets
2. Magnetic fluctuations and p-wave superconductivity in $\text{Ca}_{2-x}\text{Sr}_x\text{RuO}_4$
3. Nanoscale phase separation and chemical disorder in the high- T_c superconductors
4. Challenging the Mystery of High- T_c Superconductivity: ARPES on $\text{Ti}_2\text{Ba}_2\text{CuO}_{6+d}$
5. TM-Oxide nanostructures: novel magnets, nanowires, and metal-insulator transition

Understanding the Solid State: Electrons in Reciprocal Space

Many **properties** of a solids are determined by **electrons near E_F** (**conductivity**, **magnetoresistance**, **superconductivity**, **magnetism**)



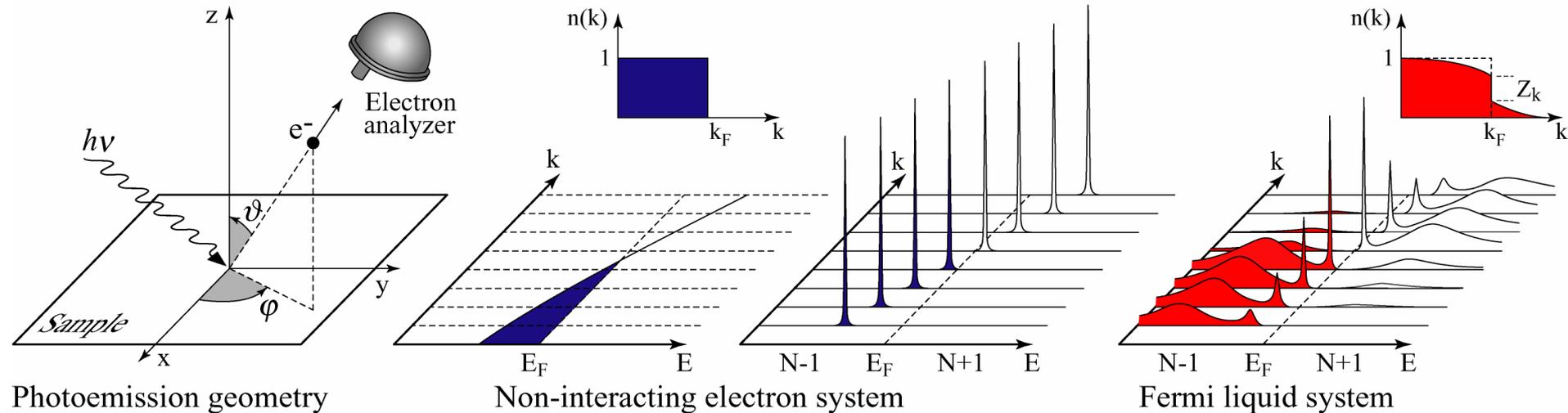
Allowed electronic states
Repeated-zone scheme



Only a **narrow energy slice** around E_F is relevant for these properties (**$kT=25$ meV** at room temperature)

ARPES: The One-Particle Spectral Function

A. Damascelli, Z. Hussain, Z.-X Shen, Rev. Mod. Phys. **75**, 473 (2003)



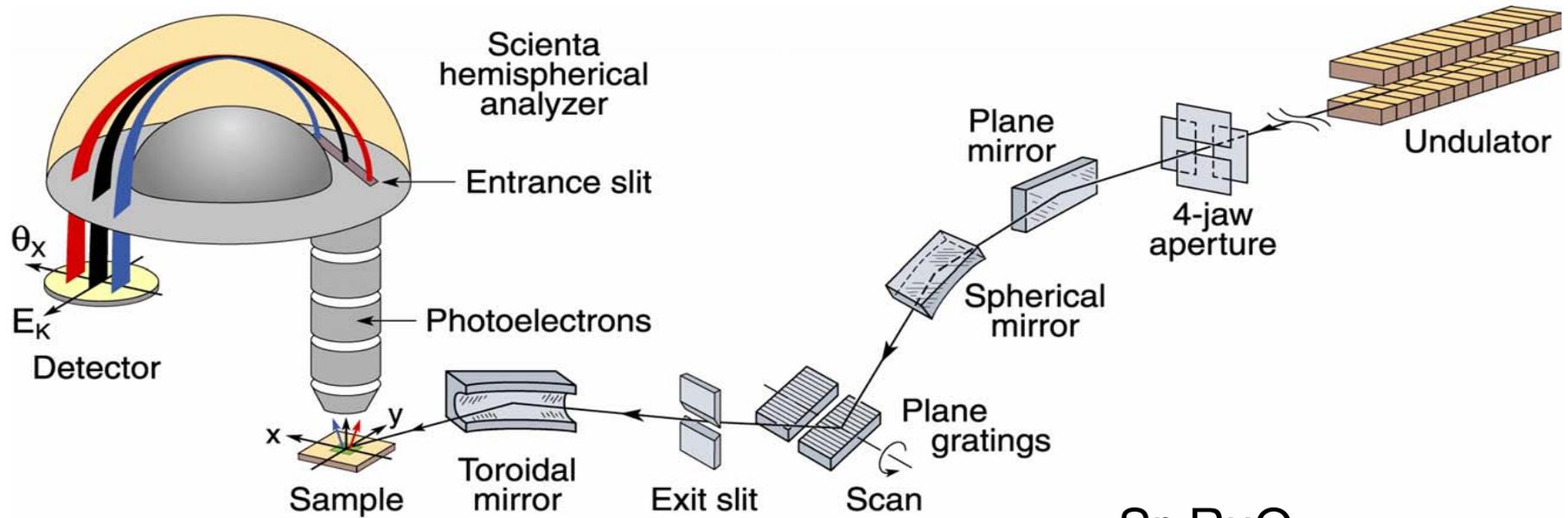
Photoemission intensity: $I(\mathbf{k}, \omega) = I_0 |M(\mathbf{k}, \omega)|^2 f(\omega) A(\mathbf{k}, \omega)$

Single-particle spectral function

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

$S(\mathbf{k}, \omega)$: the “self-energy” captures the effects of interactions

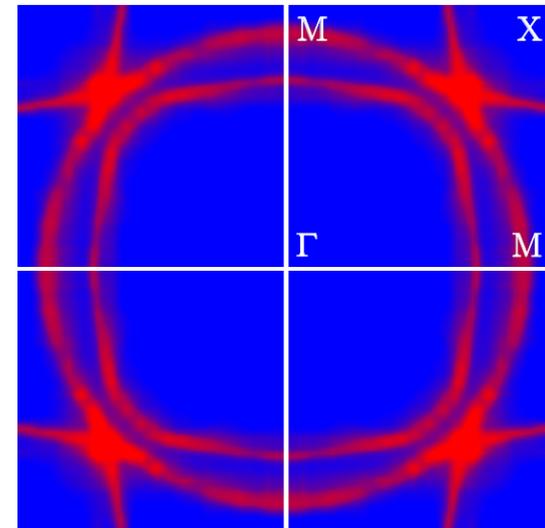
Angle-Resolved Photoemission Spectroscopy



Parallel multi-angle recording

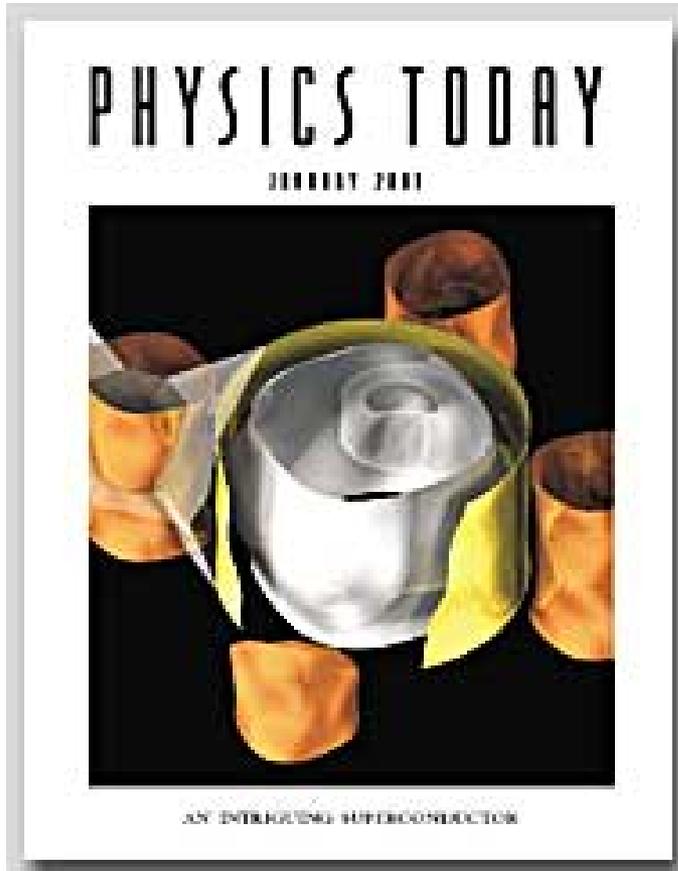
- Improved **energy resolution**
- Improved **momentum resolution**
- Improved **data-acquisition efficiency**

	ΔE (meV)	$\Delta\theta$
past	20-40	2°
now	2-10	0.2°



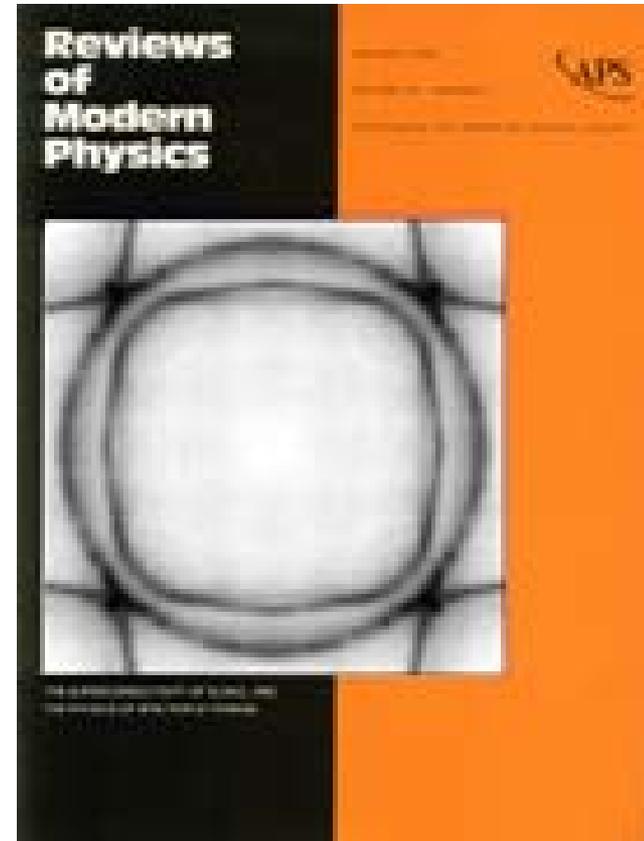
Normal State Fermi Surface of Sr_2RuO_4

de Haas-van Alphen

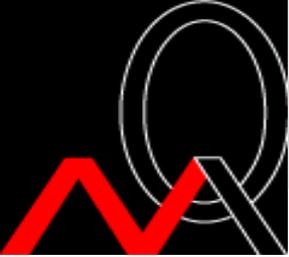


Maeno, Rice & Manfred, PT 1, 42 (2001)

ARPES

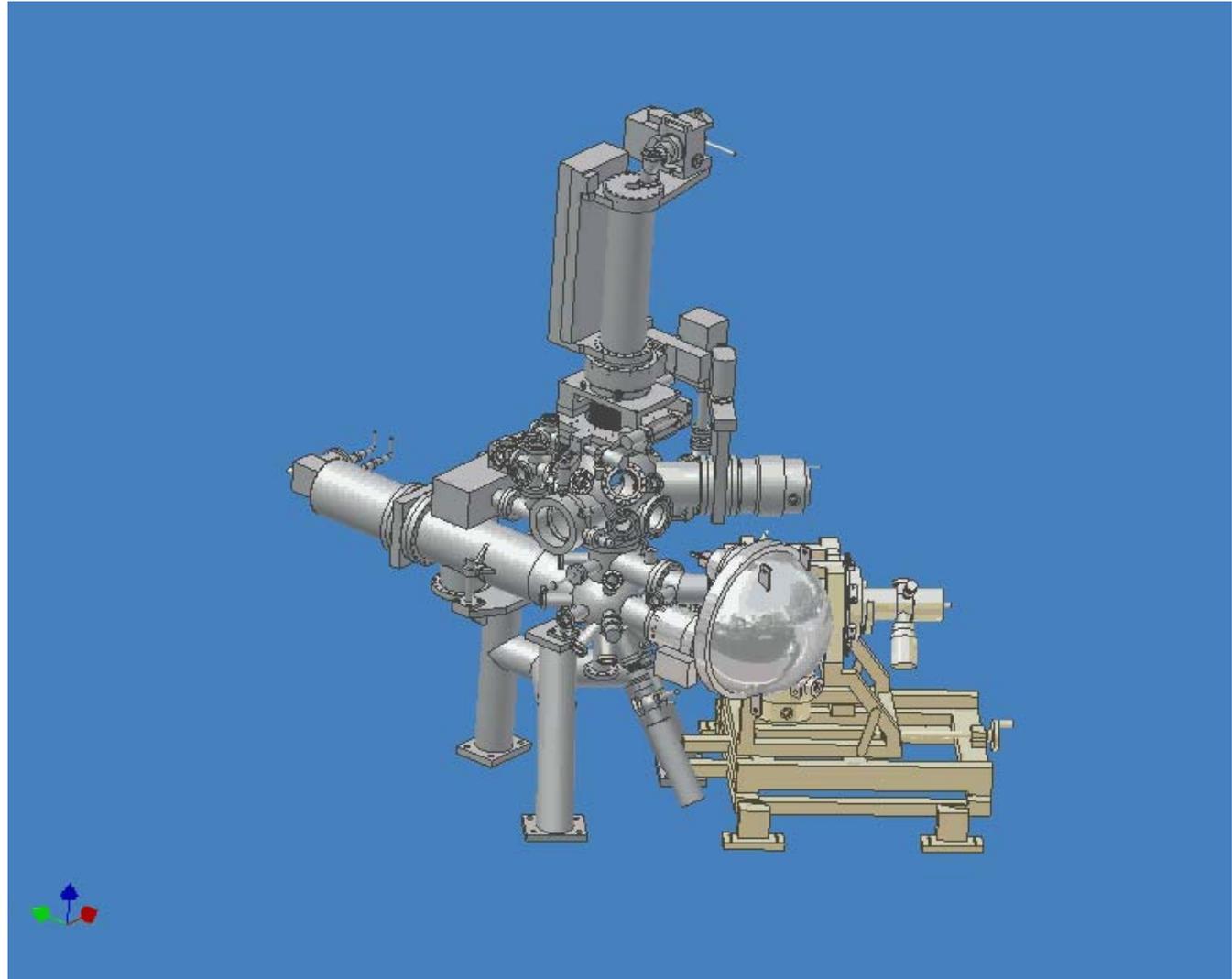


Mackenzie & Maeno, RMP 75, 657 (2003)



ARPES ON COMPLEX SYSTEMS

- High energy resolution
 $\Delta E < 1 \text{ meV}$
- High angular precision
 $\pm 0.1^\circ$
- Low base temperature
 $\sim 2 \text{ K}$
- Photon energies
 $\text{H}_2, \text{He}, \text{Ne}$
- Polarization control
linear
- Ultra-high vacuum
 $\sim 10^{-11} \text{ torr}$
- Surface / Thin films
- LEED - RHEED



Tl₂Ba₂CuO_{6+δ}: Collaborators

- **ARPES at UBC:**

M. Platé, J. Mottershead, S. Hossain, S. Wang, P. Bloudoff,
T. Pedersen, R. Norman, F. Cao, N. Ingle, **A. Damascelli**

- **Band Structure Calculations:**

Ilya Elfimov

- **Samples:**

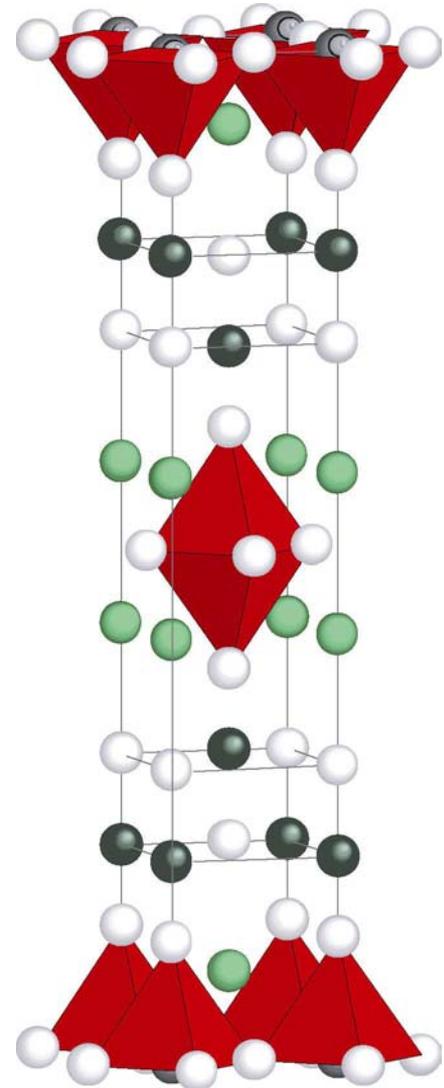
Tl₂Ba₂CuO_{6+δ}

D. Peets, Ruixing Liang, D.A. Bonn, W.N. Hardy

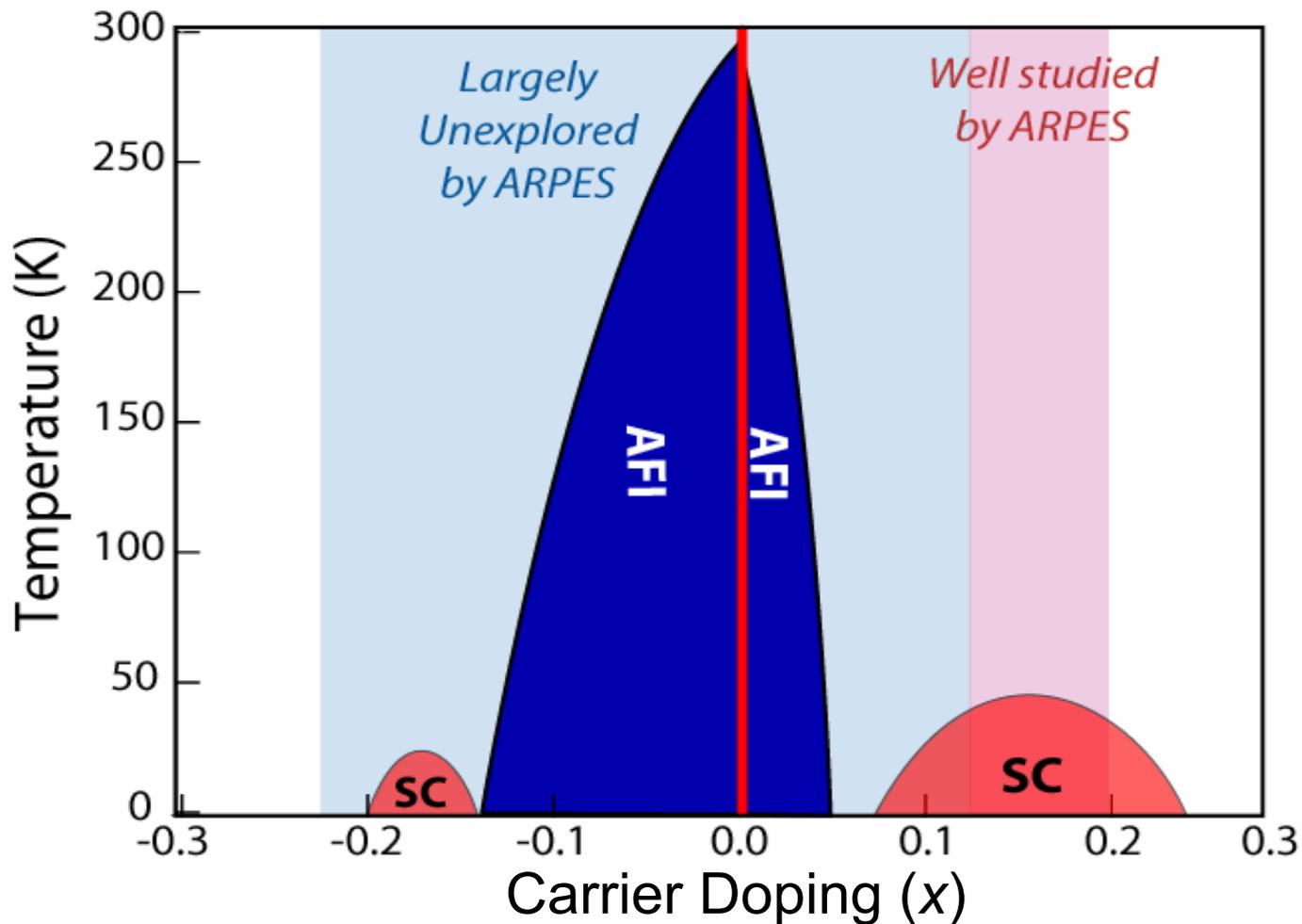
- **ARPES Experiments:**

Swiss Light Source – SIS Beamline

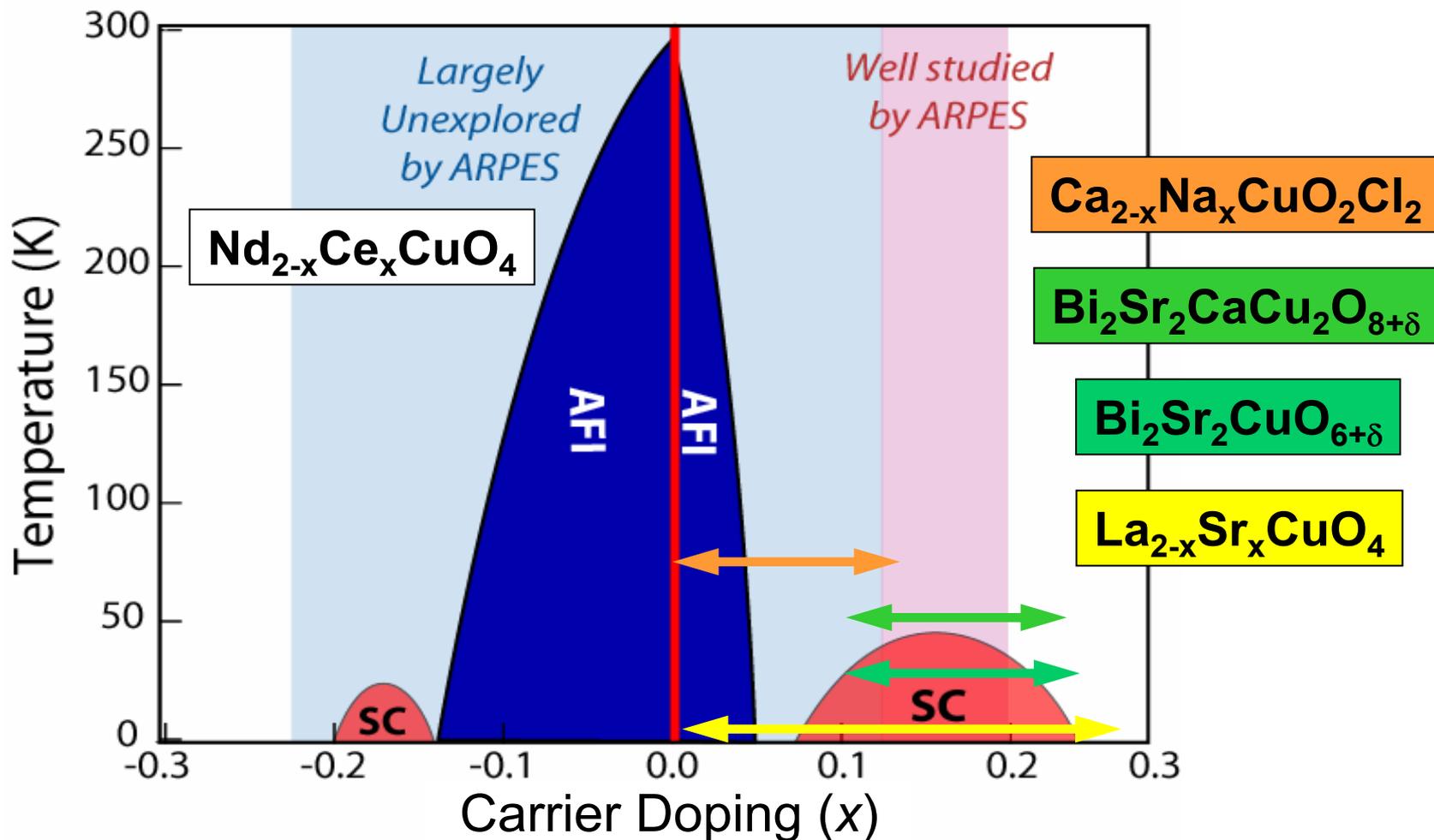
S. Chiuzaian, M. Falub, M. Shi, L. Patthey



High-Temperature Superconductors

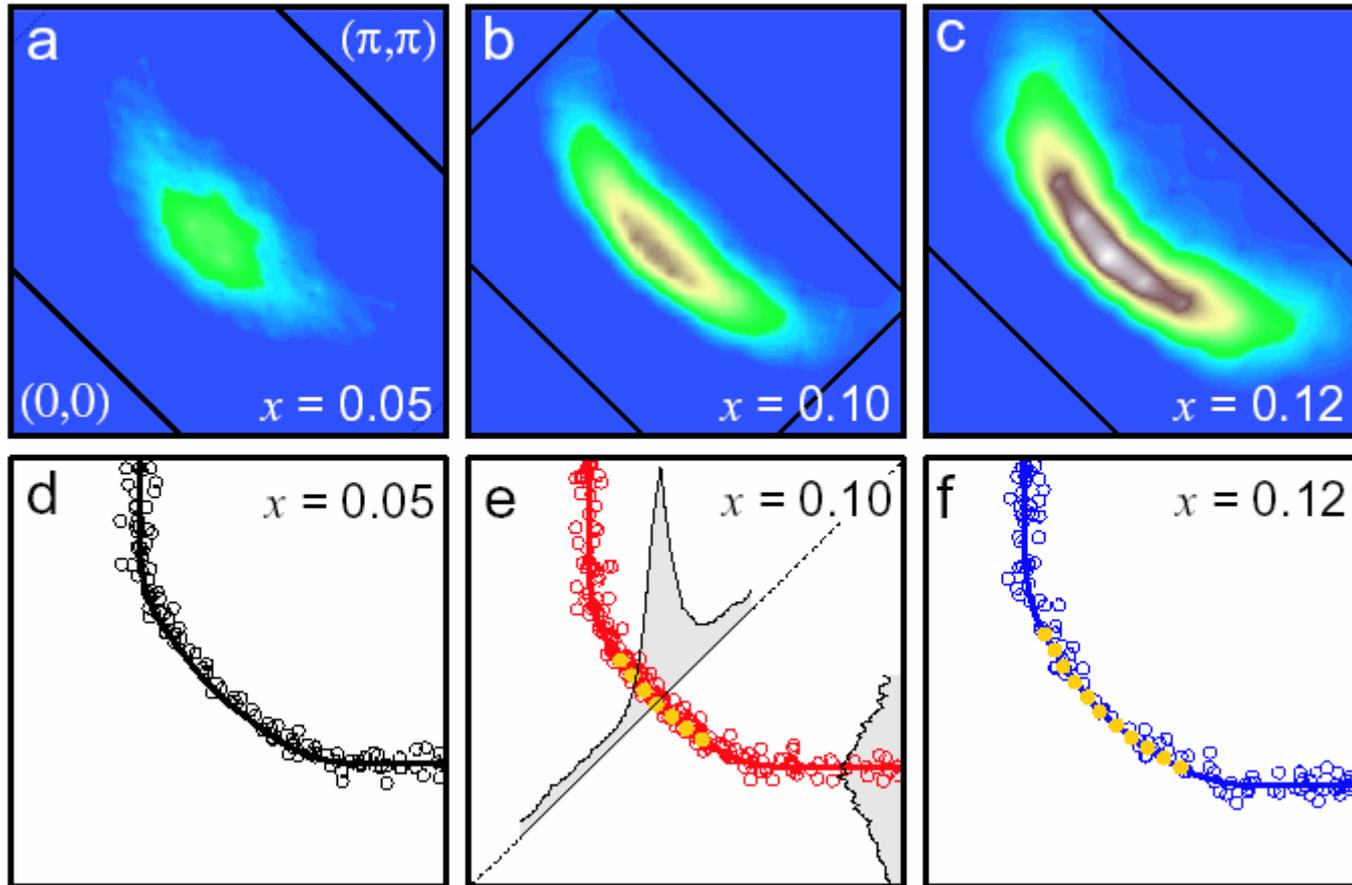


High-Temperature Superconductors



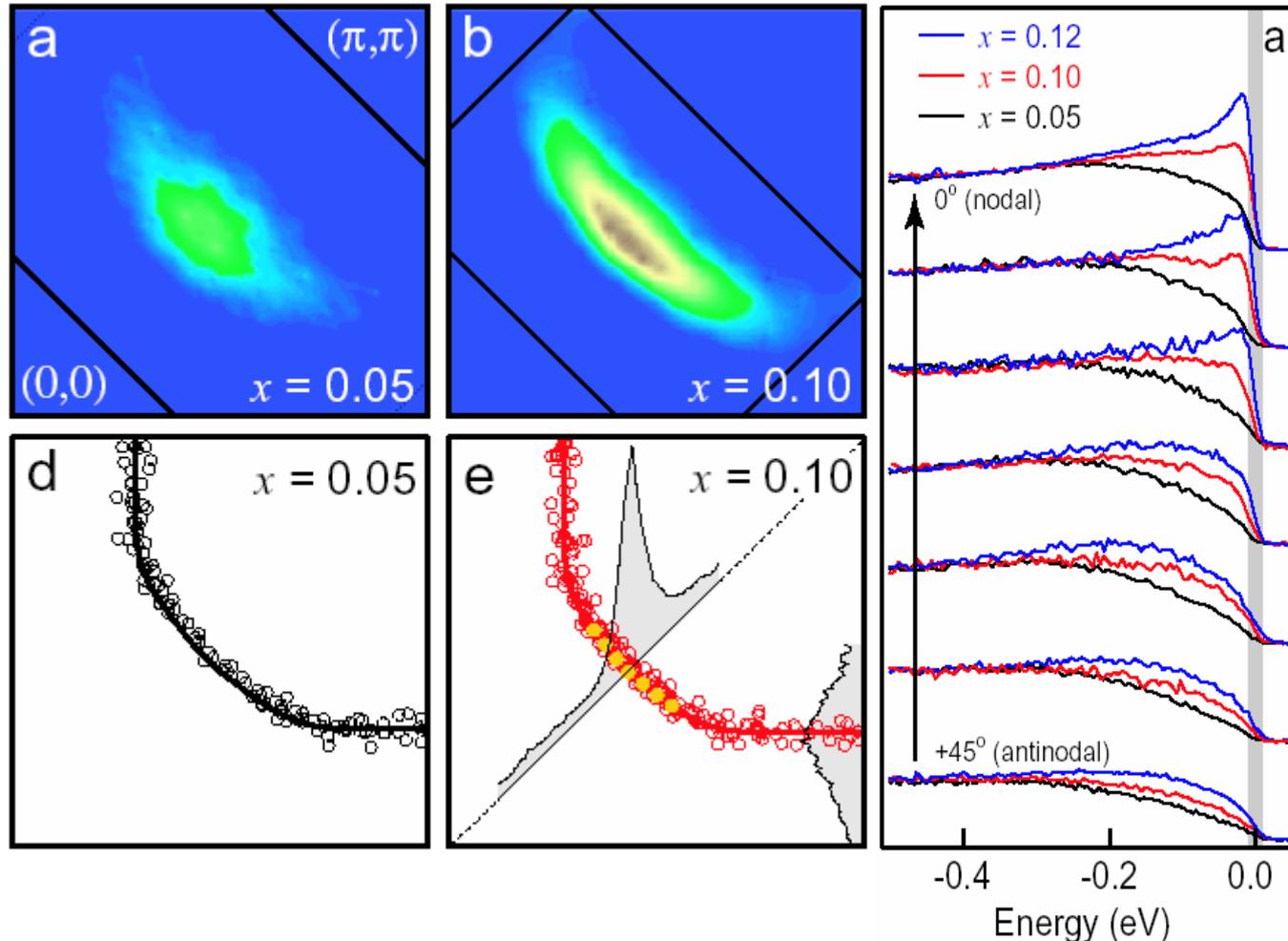
FS and Pseudogap in Underdoped Cuprates

ARPES on $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$

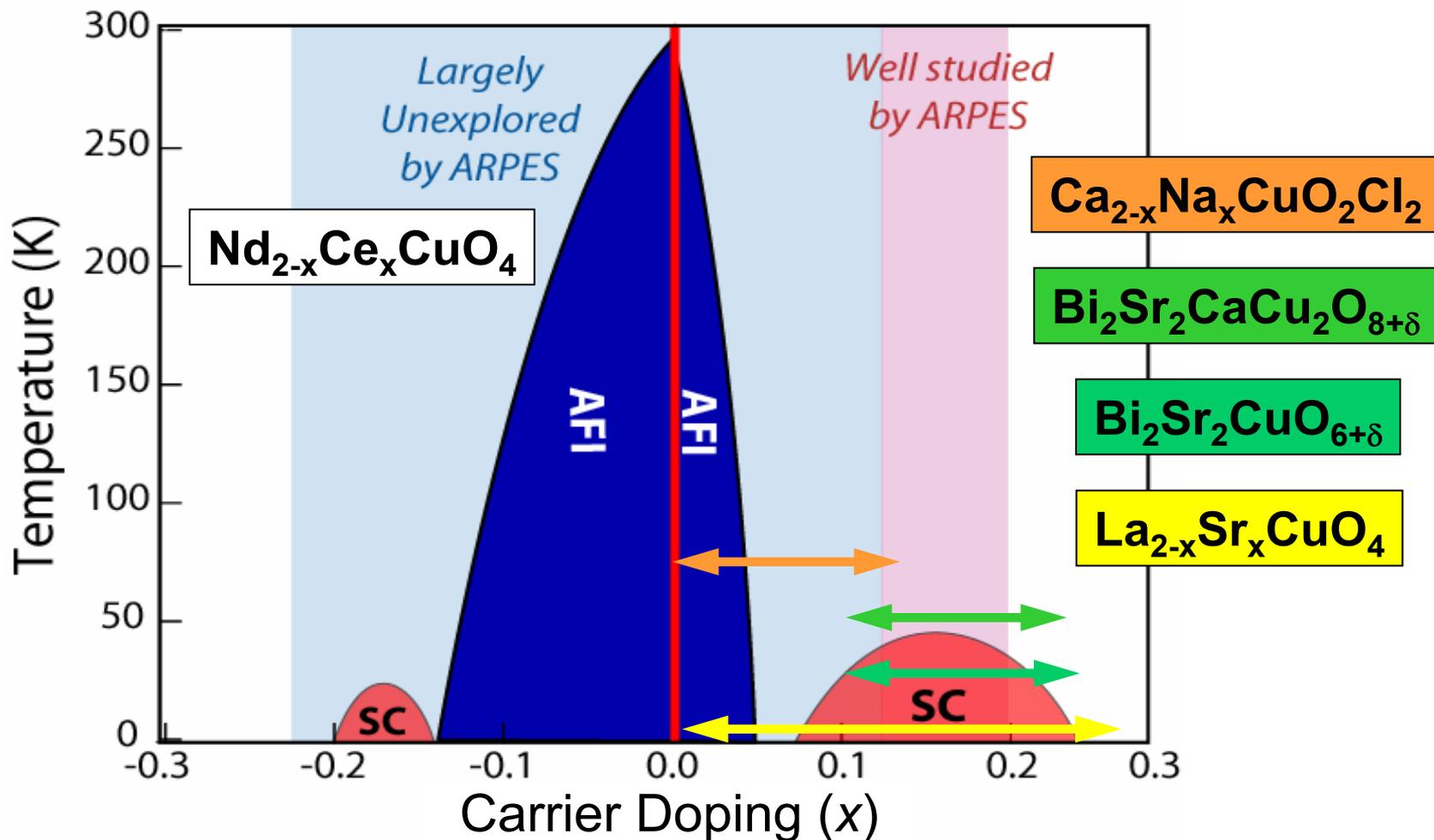


FS and Pseudogap in Underdoped Cuprates

ARPES on $\text{Ca}_{2-x}\text{Na}_x\text{CuO}_2\text{Cl}_2$

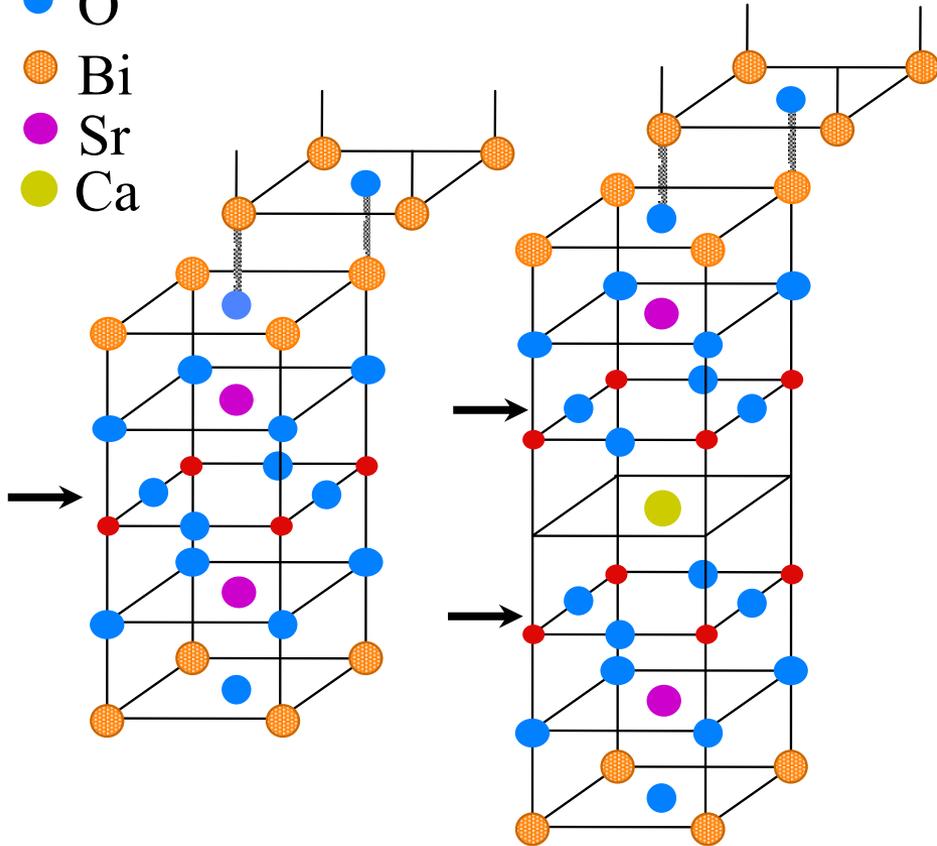


High-Temperature Superconductors



Bilayer Splitting in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

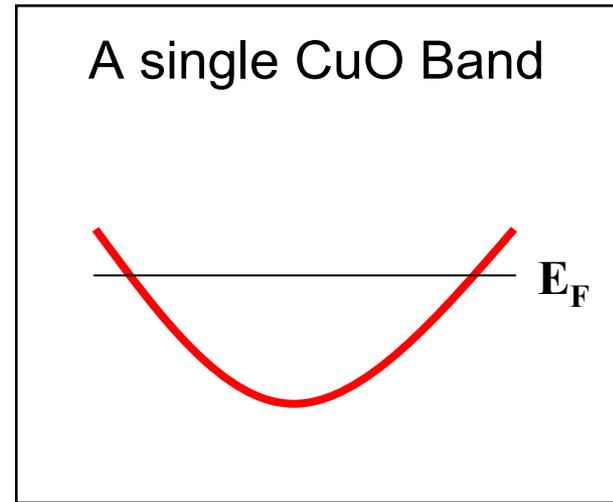
- Cu
- O
- Bi
- Sr
- Ca



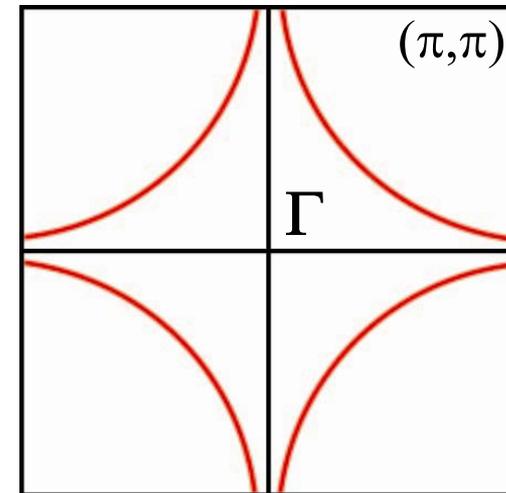
Bi2201



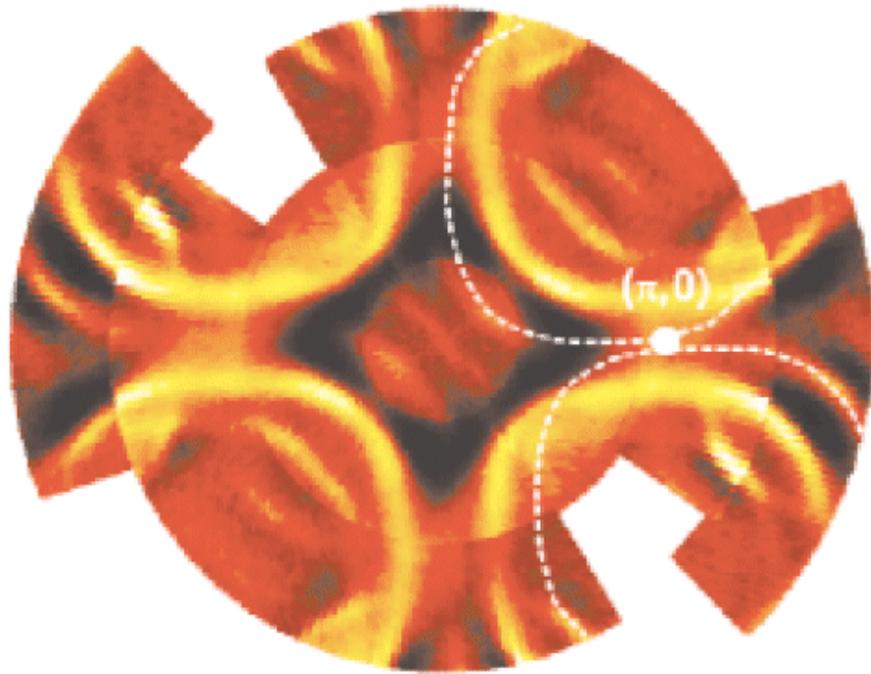
Bi2212



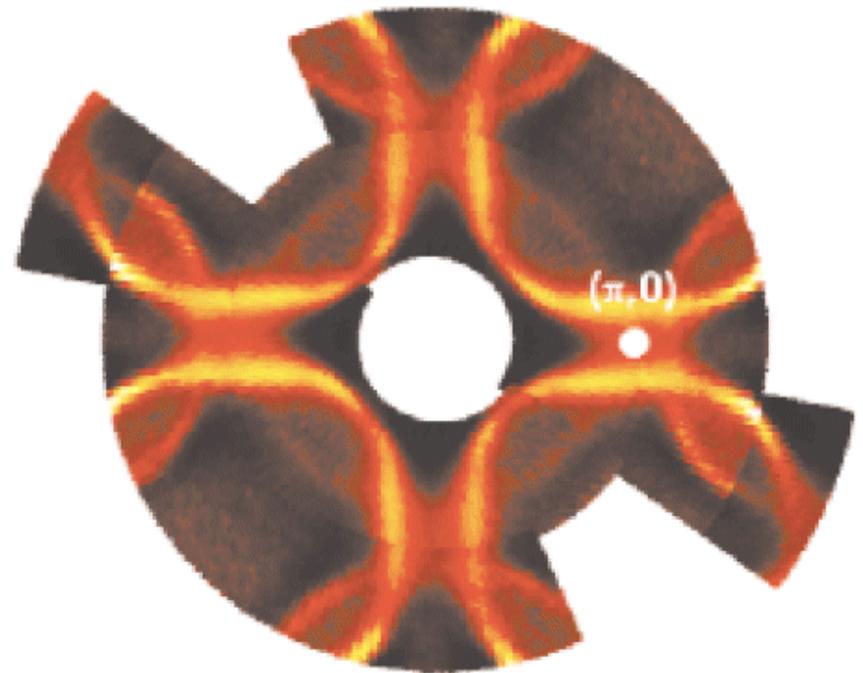
One FS Sheet



Bilayer Splitting in $\text{Pb-Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$



Pristine Bi2212

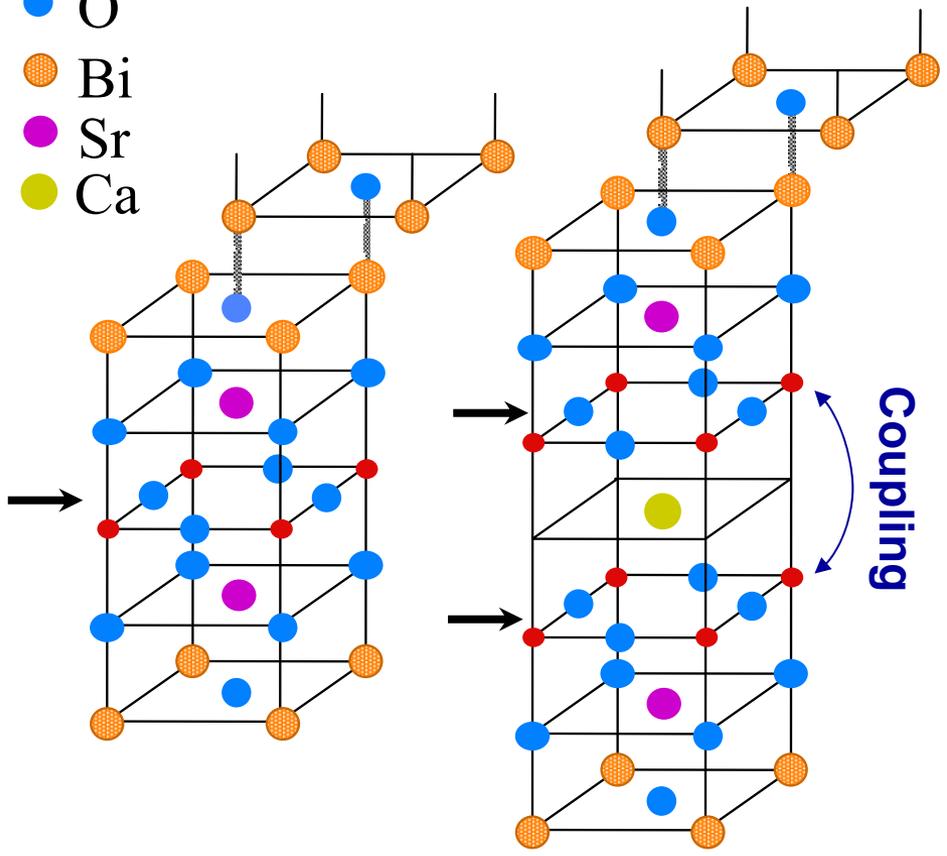


Pb-doped Bi2212

A.A. Kordyuk, M.S. Golden, et al., PRL 89, 077003 (2002)

Bilayer Splitting in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

- Cu
- O
- Bi
- Sr
- Ca

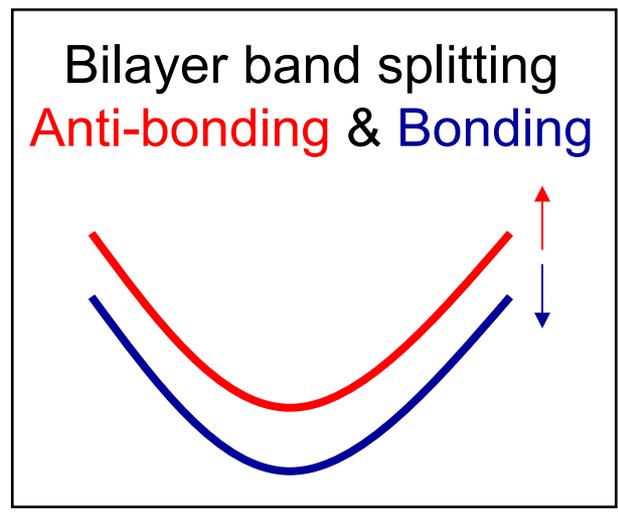


$\text{Bi}_2\text{Sr}_2\text{Cu}_1\text{O}_{6+\delta}$

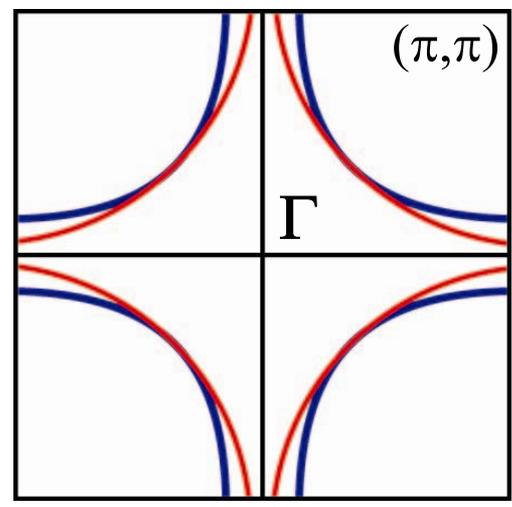
Bi2201

$\text{Bi}_2\text{Sr}_2\text{Ca}_1\text{Cu}_2\text{O}_{8+\delta}$

Bi2212

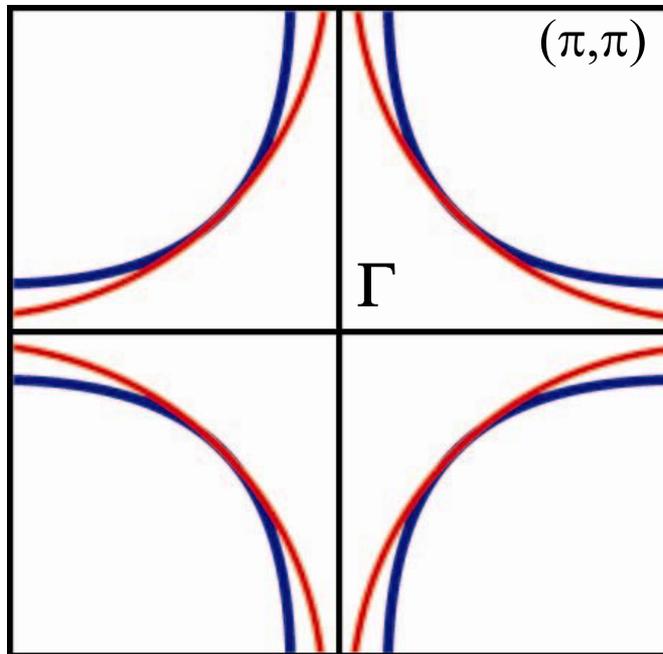


Two FS Sheets



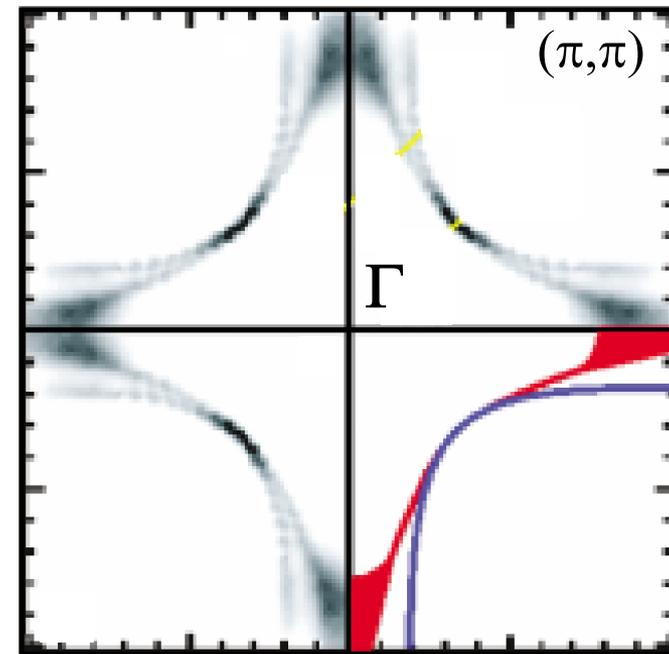
Bilayer Splitting in $\text{Pb-Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

**FS with
bilayer splitting**



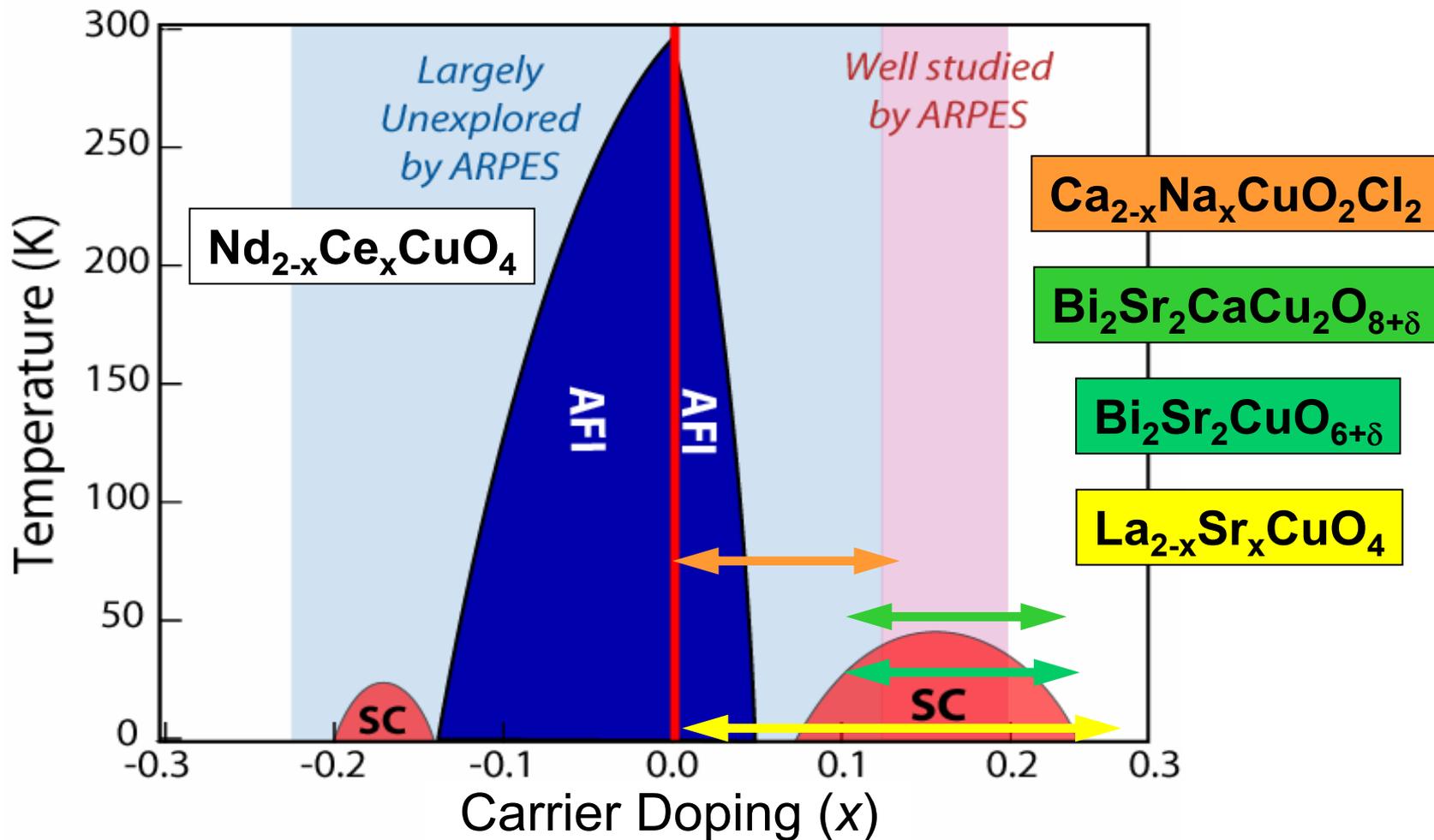
A. I. Liechtenstein *et al.*, PRB **54**, 12505 (1996)

**Overdoped Bi2212
Normal state**



P.V. Bogdanov *et al.*, PRL **89**, 167002 (2002)

High-Temperature Superconductors



High-Temperature Superconductors: Bi2212

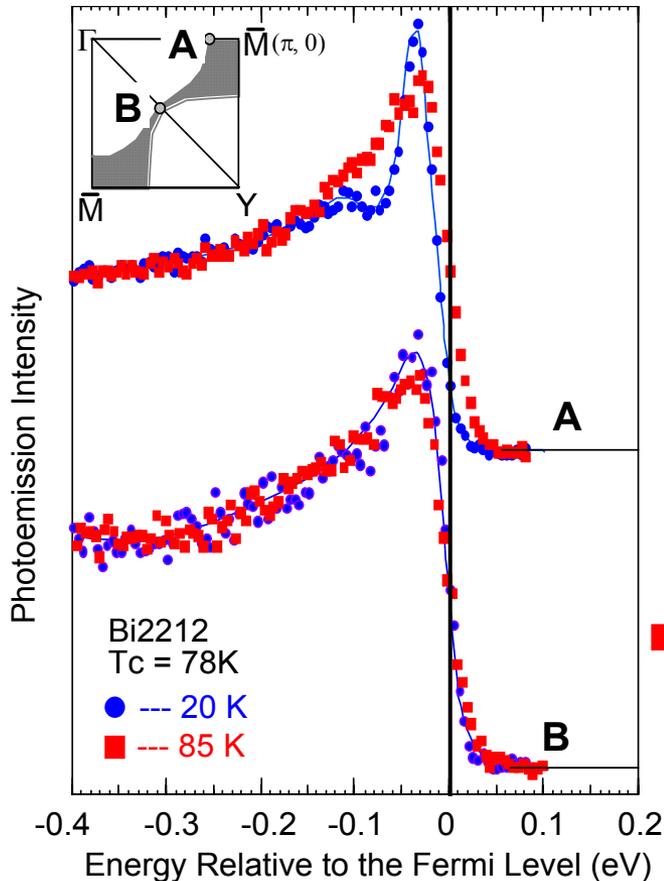
VOLUME 70, NUMBER 10

PHYSICAL REVIEW LETTERS

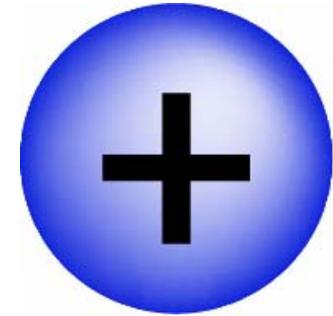
8 MARCH 1993

Anomalous Large Gap Anisotropy in the a - b Plane of $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

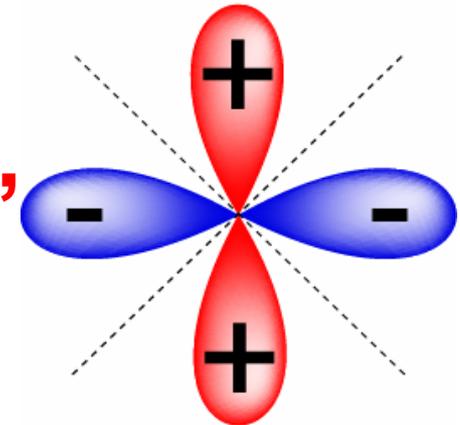
Z.-X. Shen,^{(1),(2)} D. S. Dessau,^{(1),(2)} B. O. Wells,^{(1),(2),(a)} D. M. King,⁽²⁾ W. E. Spicer,⁽²⁾ A. J. Arko,⁽³⁾
D. Marshall,⁽²⁾ L. W. Lombardo,⁽¹⁾ A. Kapitulnik,⁽¹⁾ P. Dickinson,⁽¹⁾ S. Doniach,⁽¹⁾ J. DiCarlo,^{(1),(2)}
A. G. Loeser,^{(1),(2)} and C. H. Park^{(1),(2)}



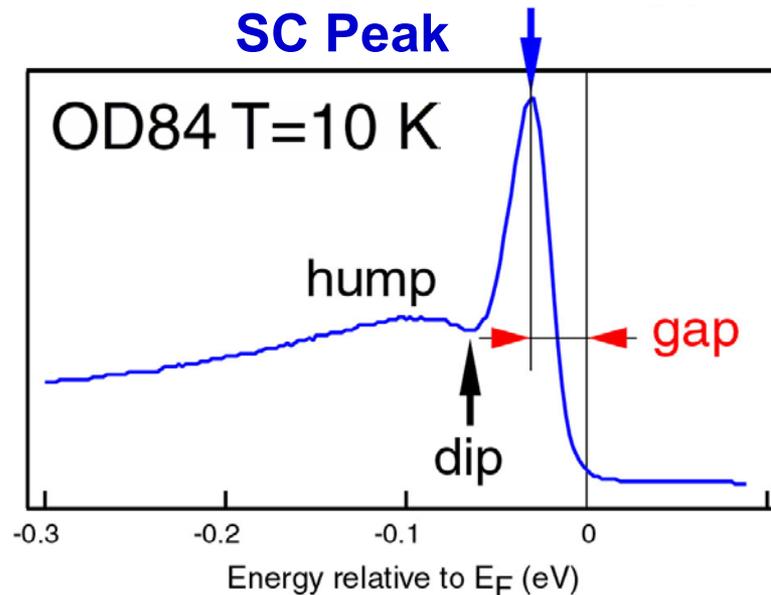
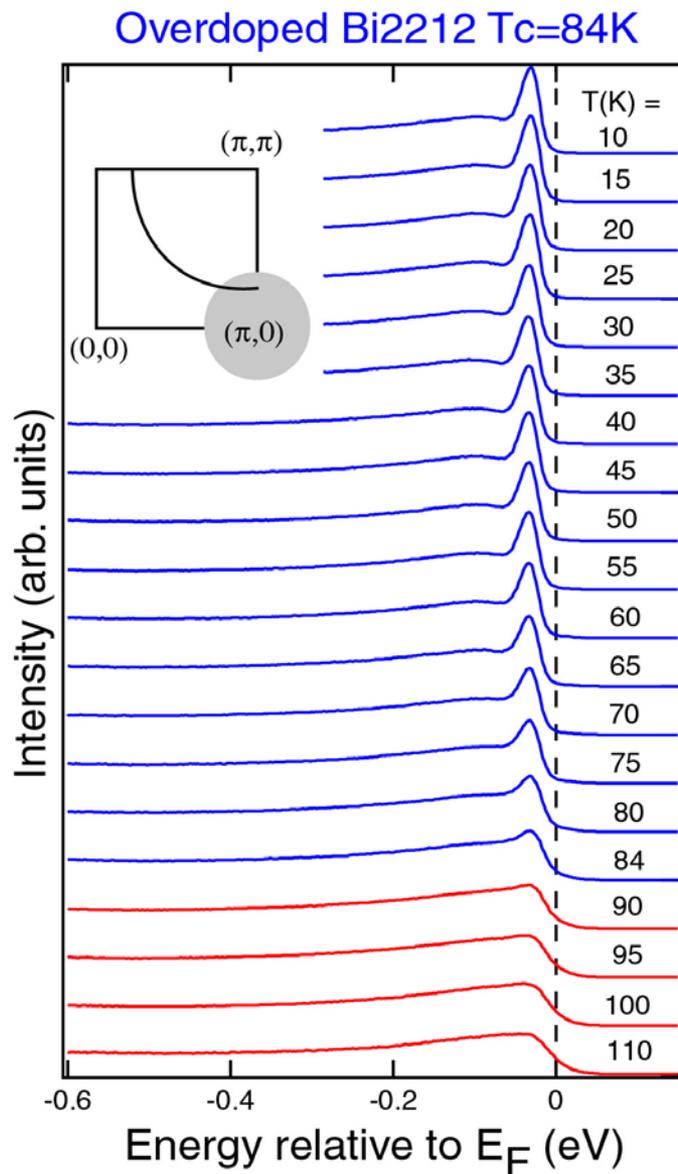
“s-wave”



“d-wave”



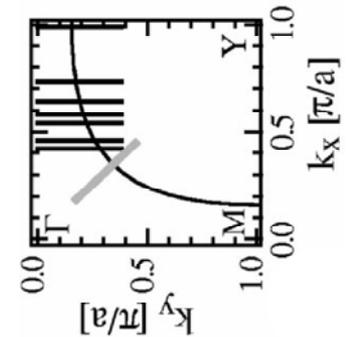
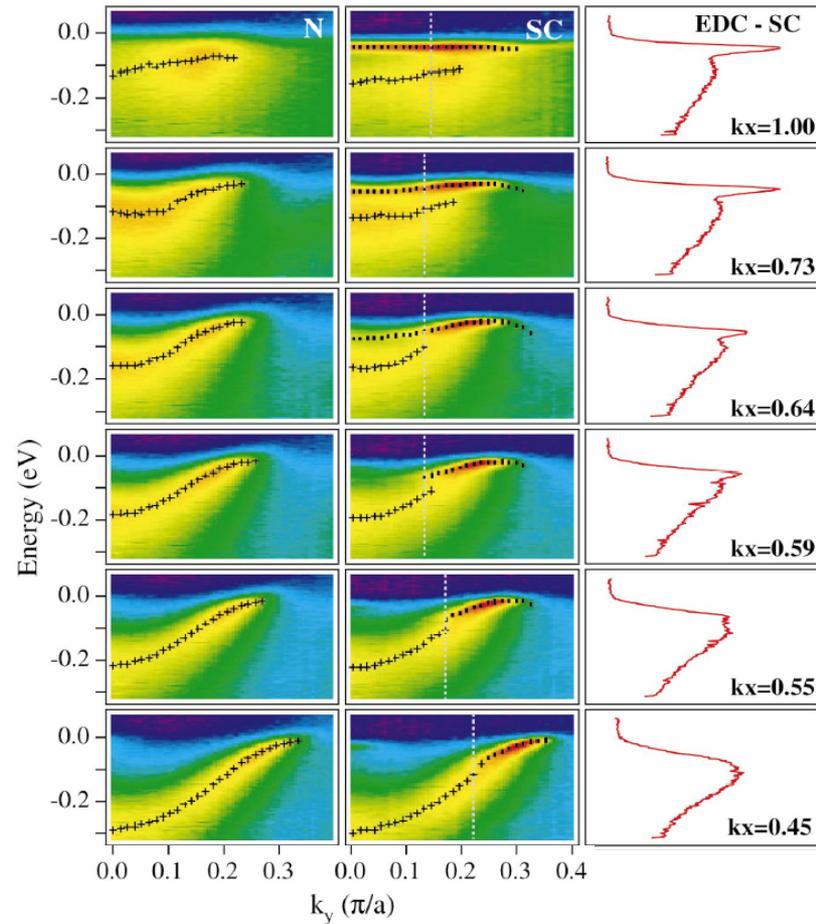
SC signatures from ARPES on $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$



Pairing
d-wave SC Gap
Phase coherence



Many Body effects in the Quasiparticle Dispersion

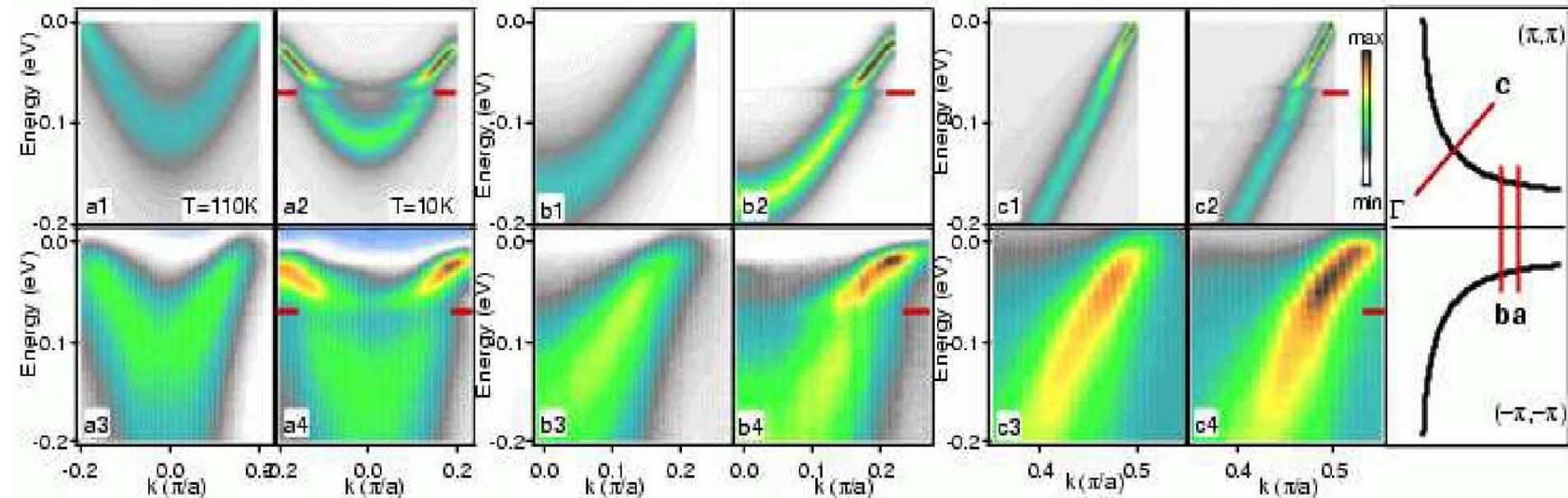


Kaminski et al.,
PRL 86, 1070 (2001)

Mechanism for High- T_c { **Magnetic fluctuations ?**
Electron-phonon coupling ?

Many Body effects in the Quasiparticle Dispersion

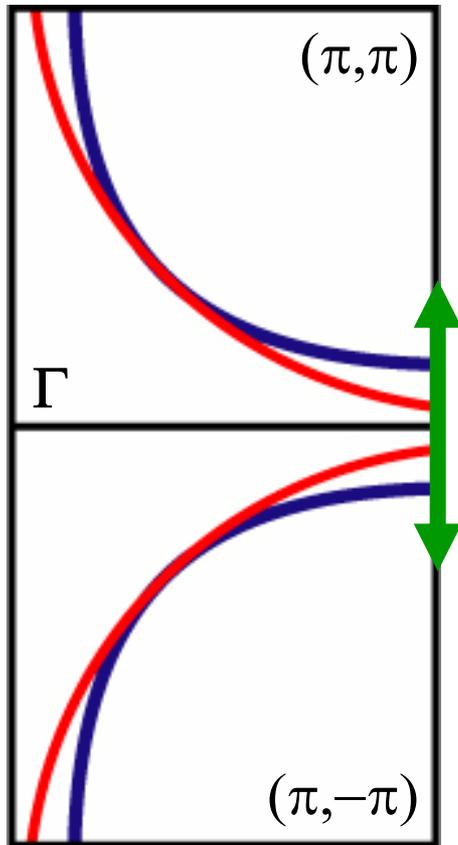
Cuk, Devereaux, Shen, et al., PRL (2004)



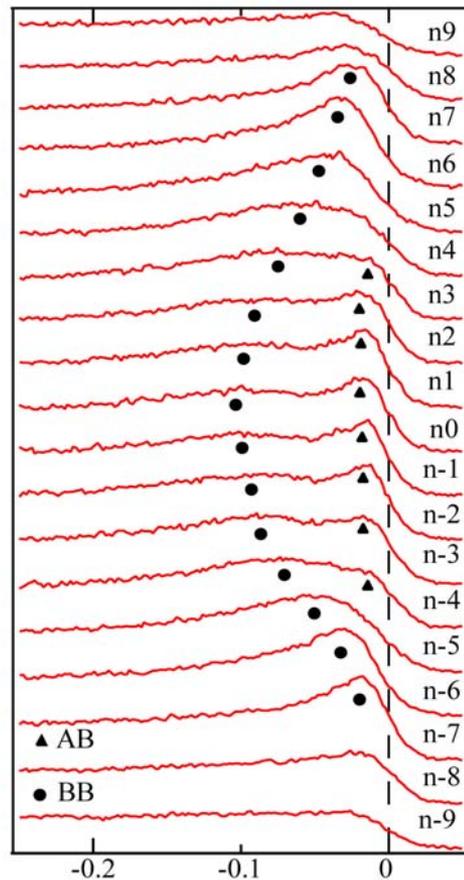
Mechanism for High- T_c { **Magnetic fluctuations ?**
Electron-phonon coupling ?

Bilayer Splitting in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$

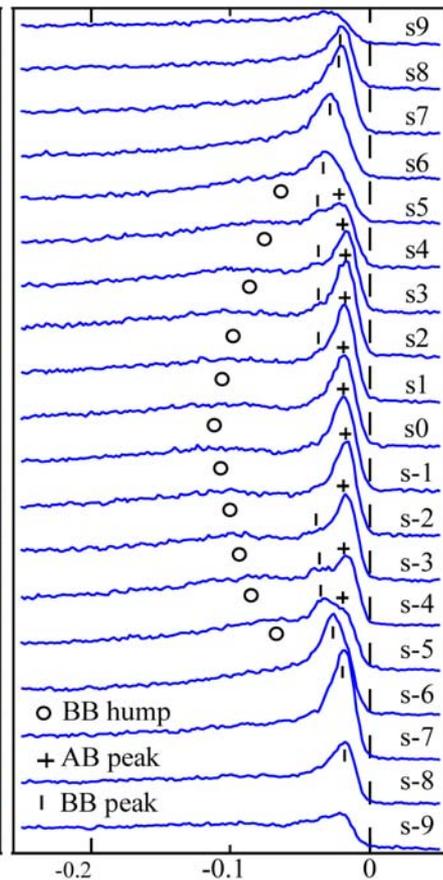
**Bilayer Split
Fermi Surface**



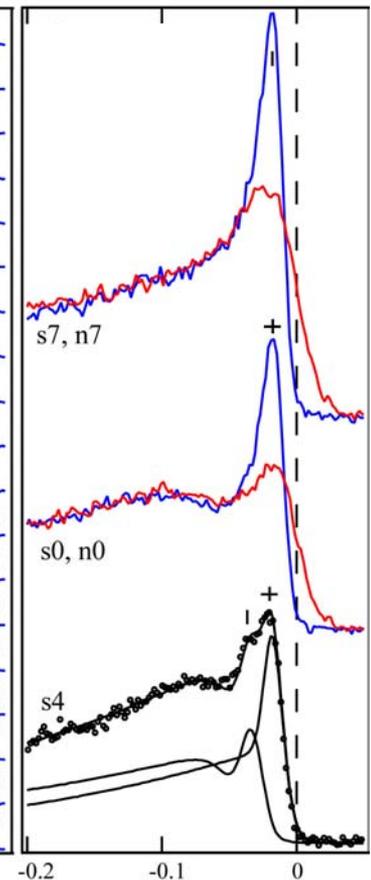
**Normal State
T=90K**



**SC State
T=10K**



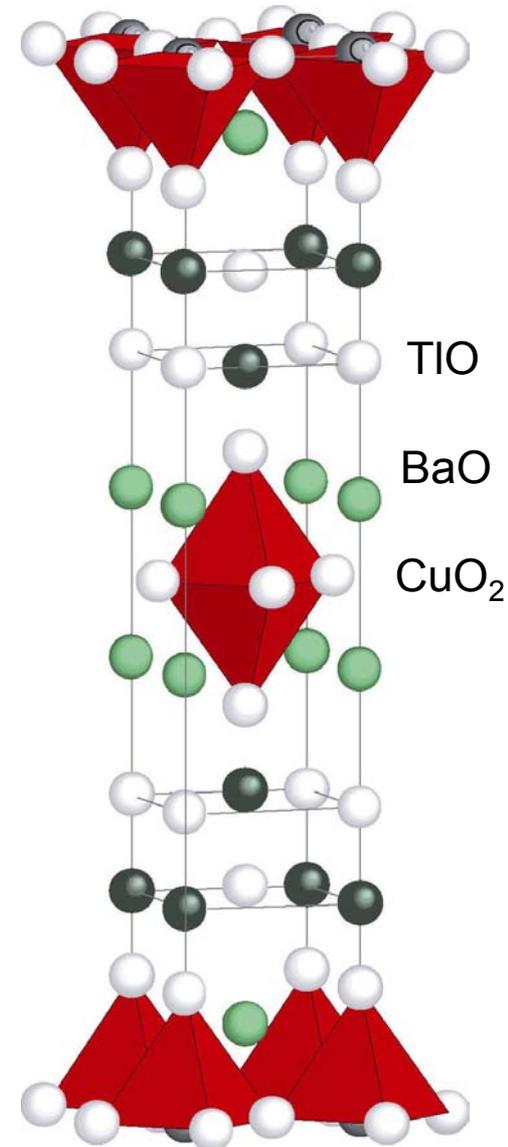
**Normal & SC
State Data**



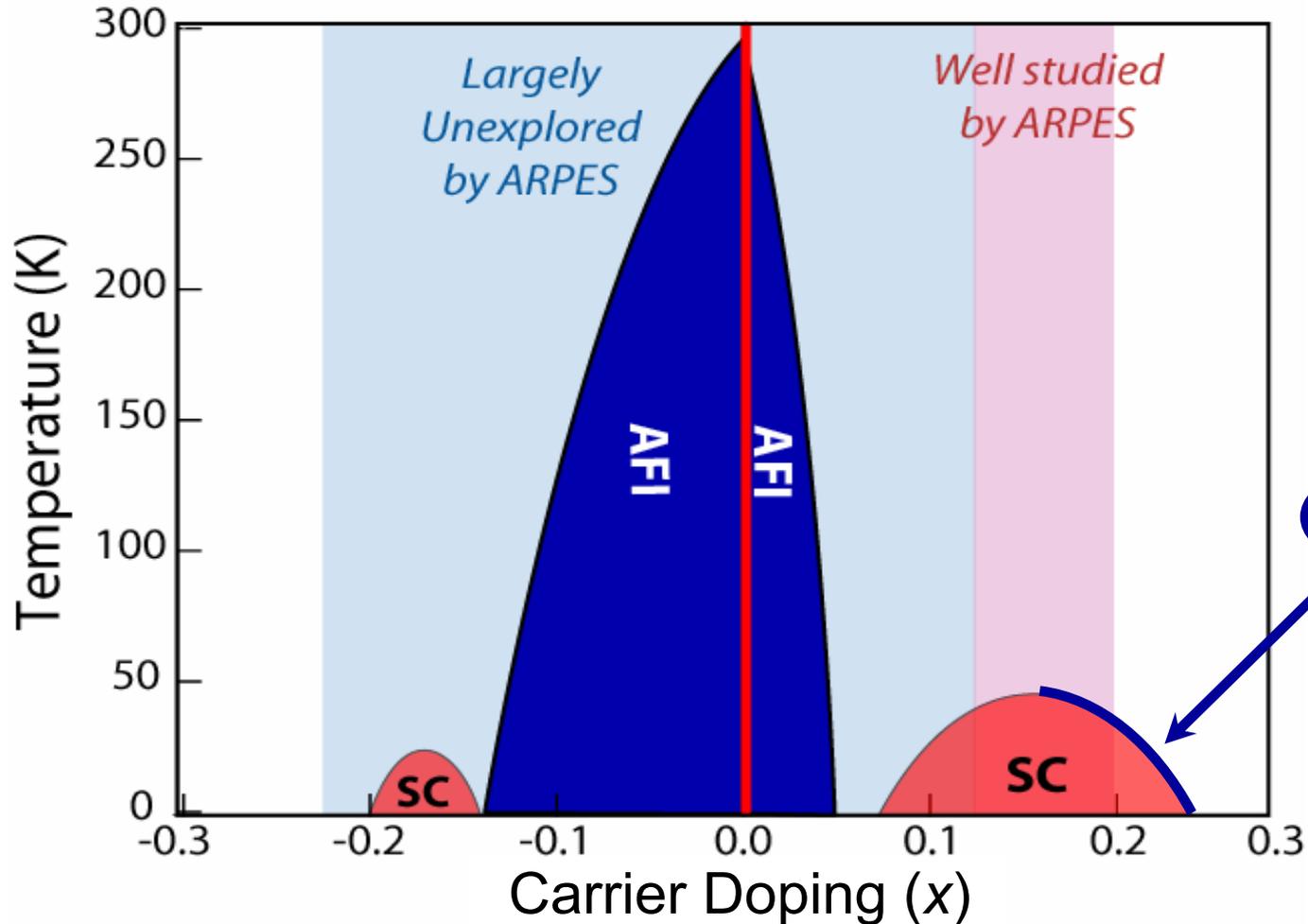
Why $Tl_2Ba_2CuO_{6+\delta}$?

$Tl_2Ba_2CuO_{6+\delta}$: ideal HTSC material

- Single CuO_2 plane material
- Very high transition: $T_c(\text{opt})=93\text{K}$
- No additional CuO chains
- No structural distortions
- Low cation disorder (T/O structure)
- $d_{x^2-y^2}$ SC gap (Tsuei et al., Nature 1997)
- (π,π) resonant mode (He et al., Science 2002)
- FS from AMRO (Hussey et al., Nature 2003)



ARPES on $\text{Ti}_2\text{Ba}_2\text{CuO}_{6+\delta}$



Paring mechanism?

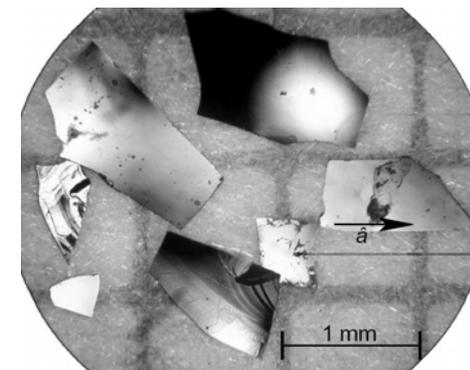
Quantum criticality?

Orthorhombic $Tl_2Ba_2CuO_{6+\delta}$

- High-quality single crystals:

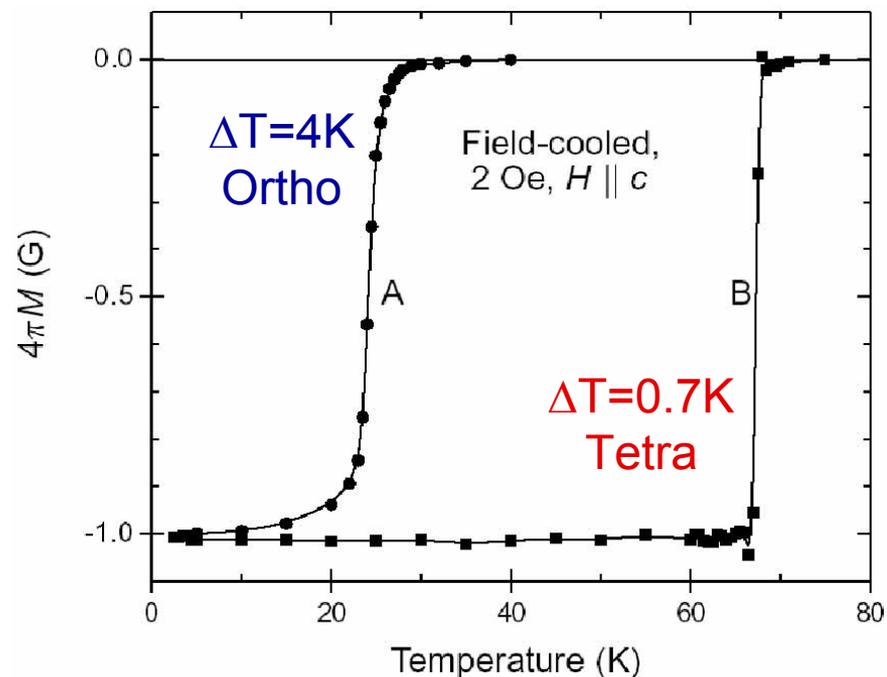
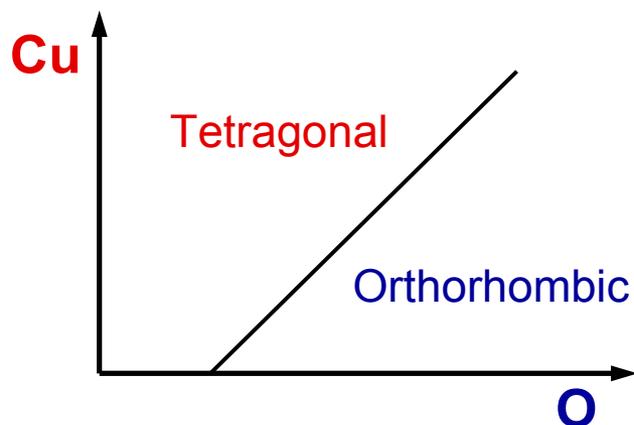
Orthorhombic Tl2201 grown by self-flux method

D. Peets, Ruixing Liang, D.A. Bonn, W.N. Hardy



Tetragonal ($a=3.865\text{\AA}$; $c=23.247\text{\AA}$)

Orthorhombic ($a=5.458\text{\AA}$; $b=5.485$; $c=23.201\text{\AA}$)



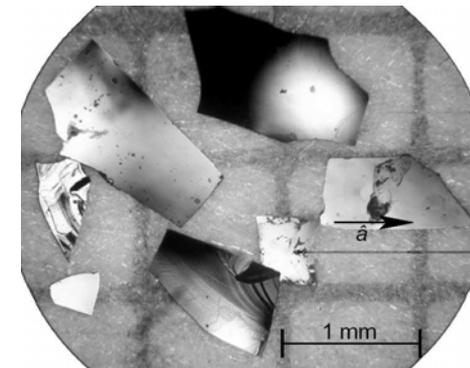
Ortho as-grown $Tl_{1.88}Ba_2Cu_{1.11}O_{6+\delta}$

Orthorhombic $Tl_2Ba_2CuO_{6+\delta}$

- High-quality single crystals:

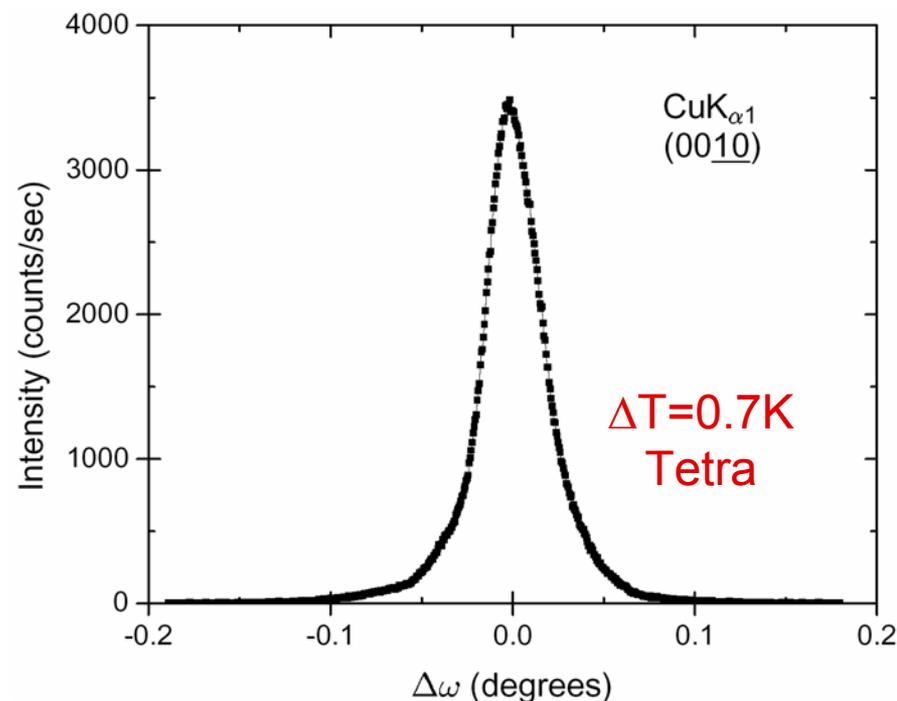
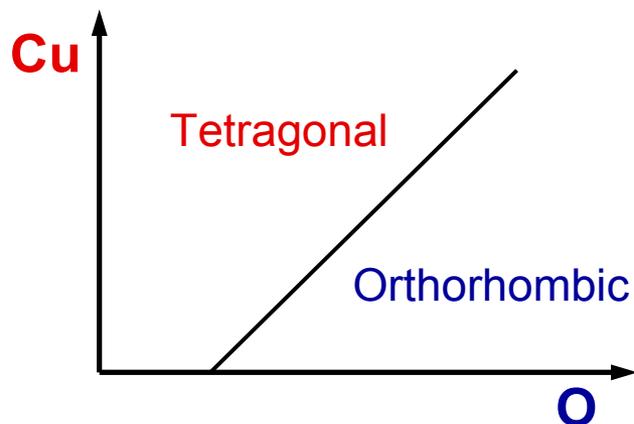
Orthorhombic $Tl2201$ grown by self-flux method

D. Peets, Ruixing Liang, D.A. Bonn, W.N. Hardy



Tetragonal ($a=3.865\text{\AA}$; $c=23.247\text{\AA}$)

Orthorhombic ($a=5.458\text{\AA}$; $b=5.485$; $c=23.201\text{\AA}$)



Ortho as-grown $Tl_{1.88}Ba_2Cu_{1.11}O_{6+\delta}$

Peets et al., cond-mat/0211028

Swiss Light Source – SIS Beamline

- **ARPES Experiments:**

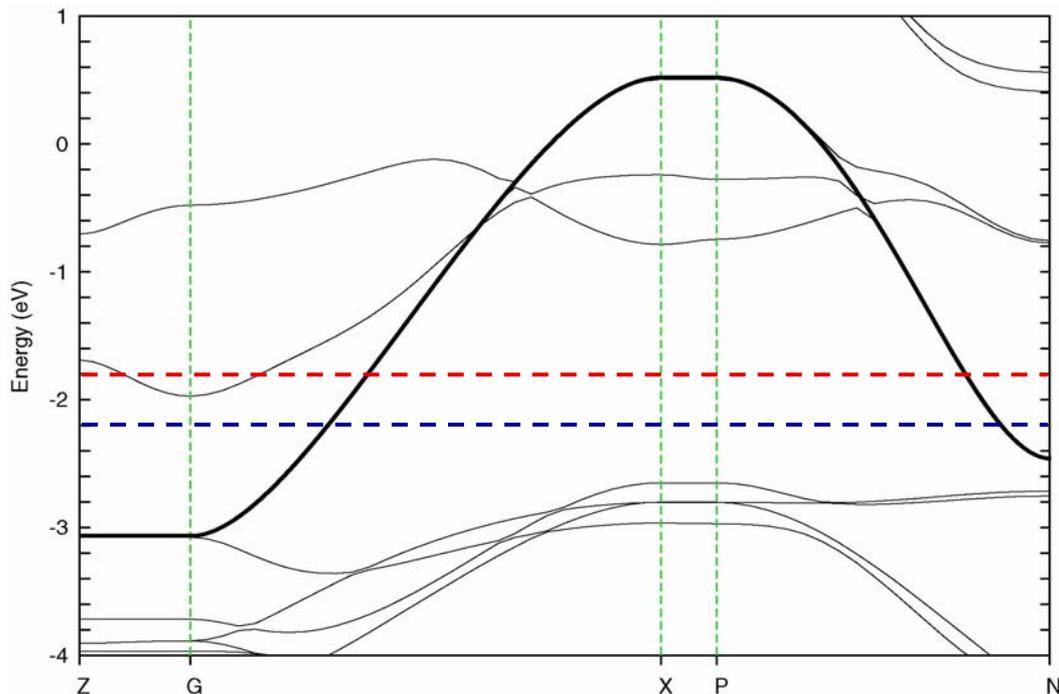
- **Surface and Interface Spectroscopy Beamline**

S. Chiuzbaian, M. Falub, M. Shi, **L. Patthey**



- **Twin Undulator**
- **Monochromator**
 - Energy Range: 10-800 eV
 - Polarization: circular/planar
- **ARPES**
 - Detector: SES2002
 - $E/\Delta E > 10^4$; $\Delta k = 0.3^\circ$
 - Low T: 10-300K
 - spot size: $20 \times 20 \mu\text{m}^2$
- **Spin resolved ARPES**

Tl2201: Low energy electronic structure

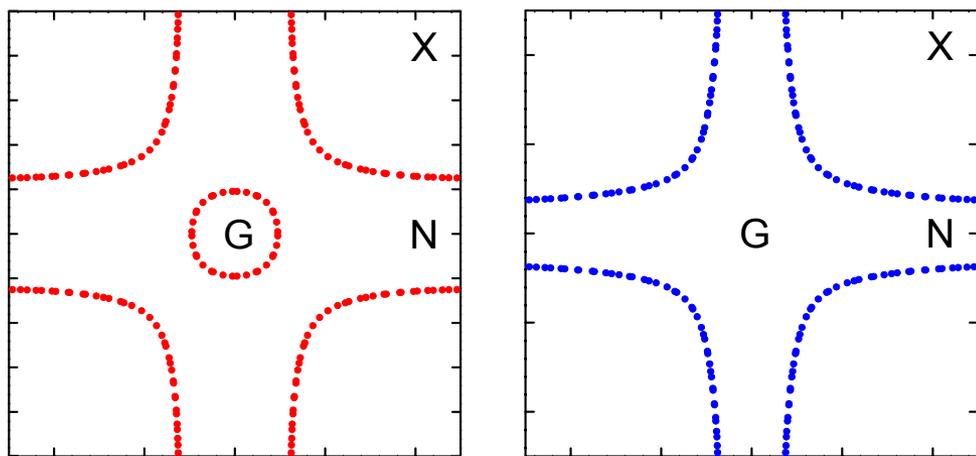


Tl³⁺:Ba²⁺:Cu²⁺:O²⁻ in ratios 2:2:1:6

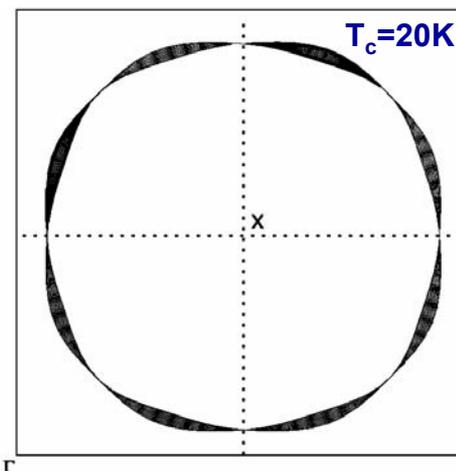
Charge Transfer Insulator

- Short TI-O distance
→ CuO band not 1/2 filled
- Cu-Tl substitution
→ Additional hole-doping

Tl2201: Optimally Doped SC

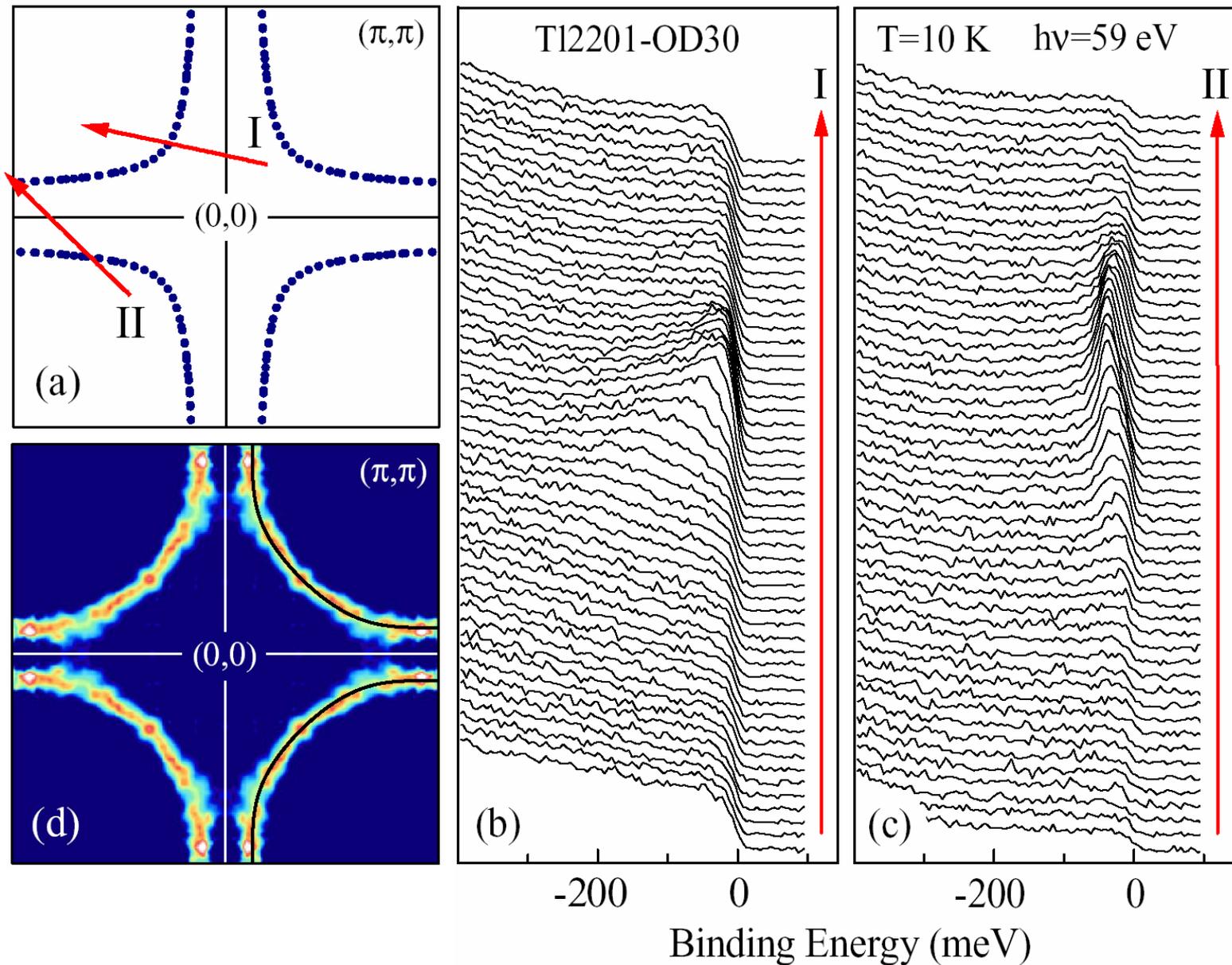


Elfimov (2004)



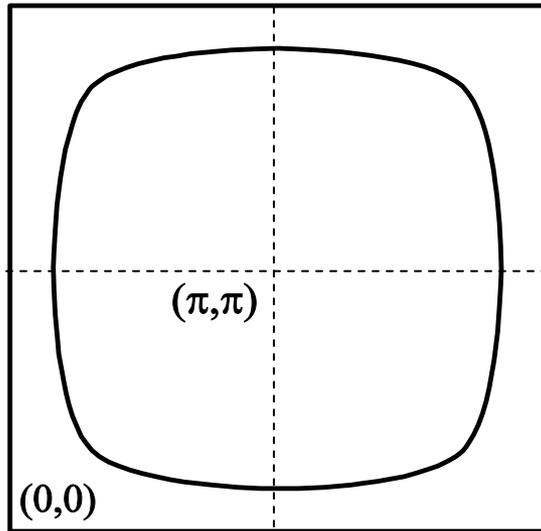
Hussey et al, Nature **425**, 814 (2004)

Tl2201 : ARPES Results

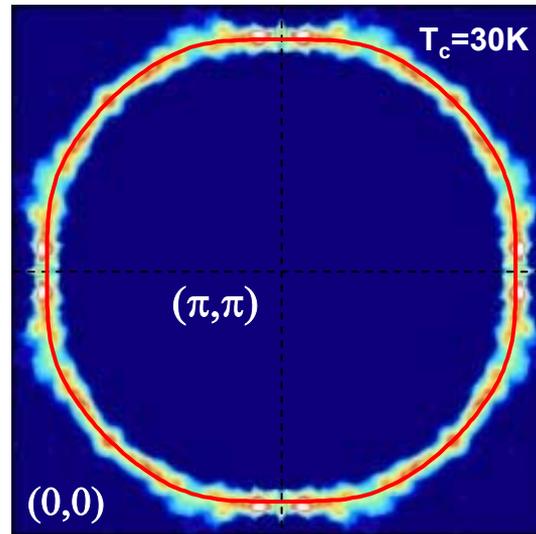


TI2201 : Fermi Surface Volume

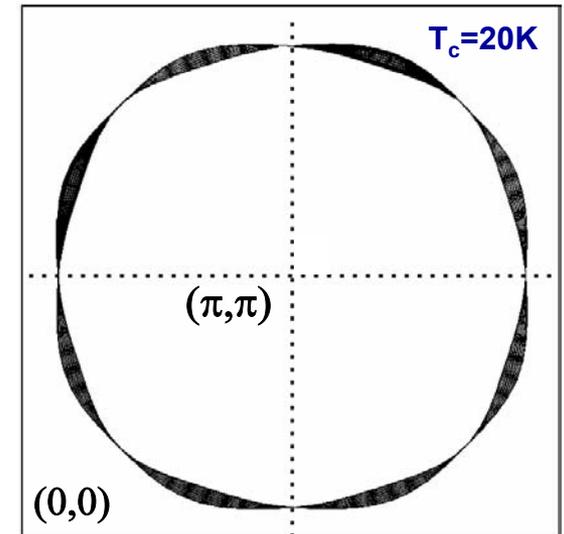
LDA



ARPES



AMRO



Hussey et al, Nature **425**, 814 (2004)

Hole FS volume

63%

$p=0.26/\text{Cu}$

63%

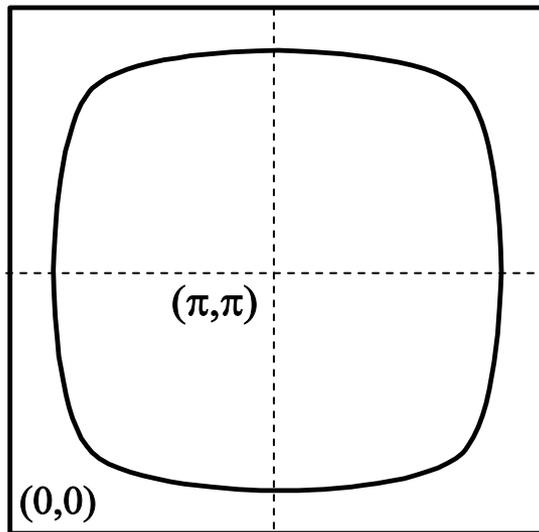
$p=0.26/\text{Cu}$

62%

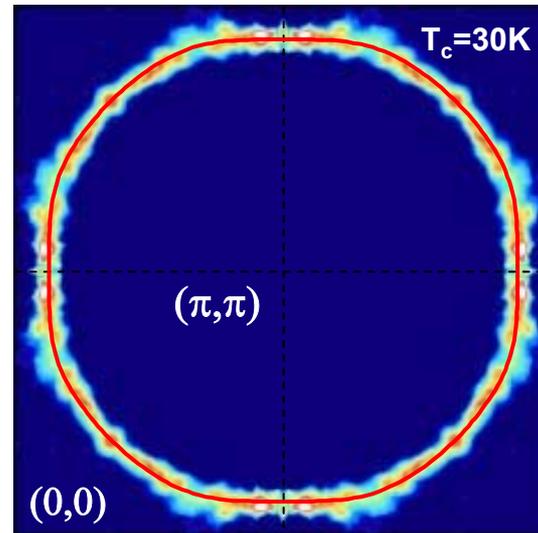
$p=0.24/\text{Cu}$

TI2201 : Fermi Surface Volume

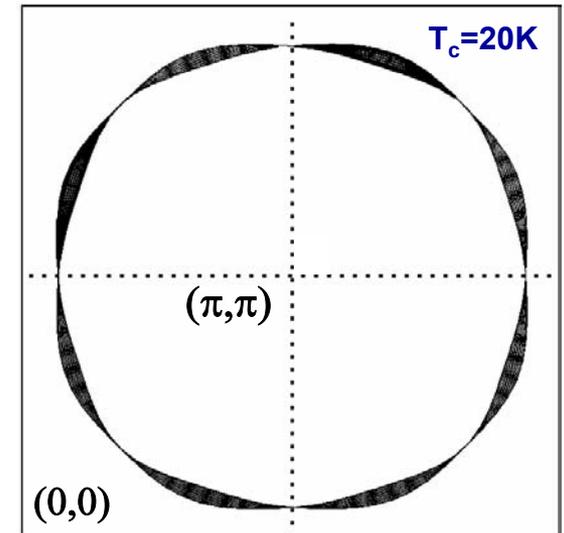
LDA



ARPES



AMRO

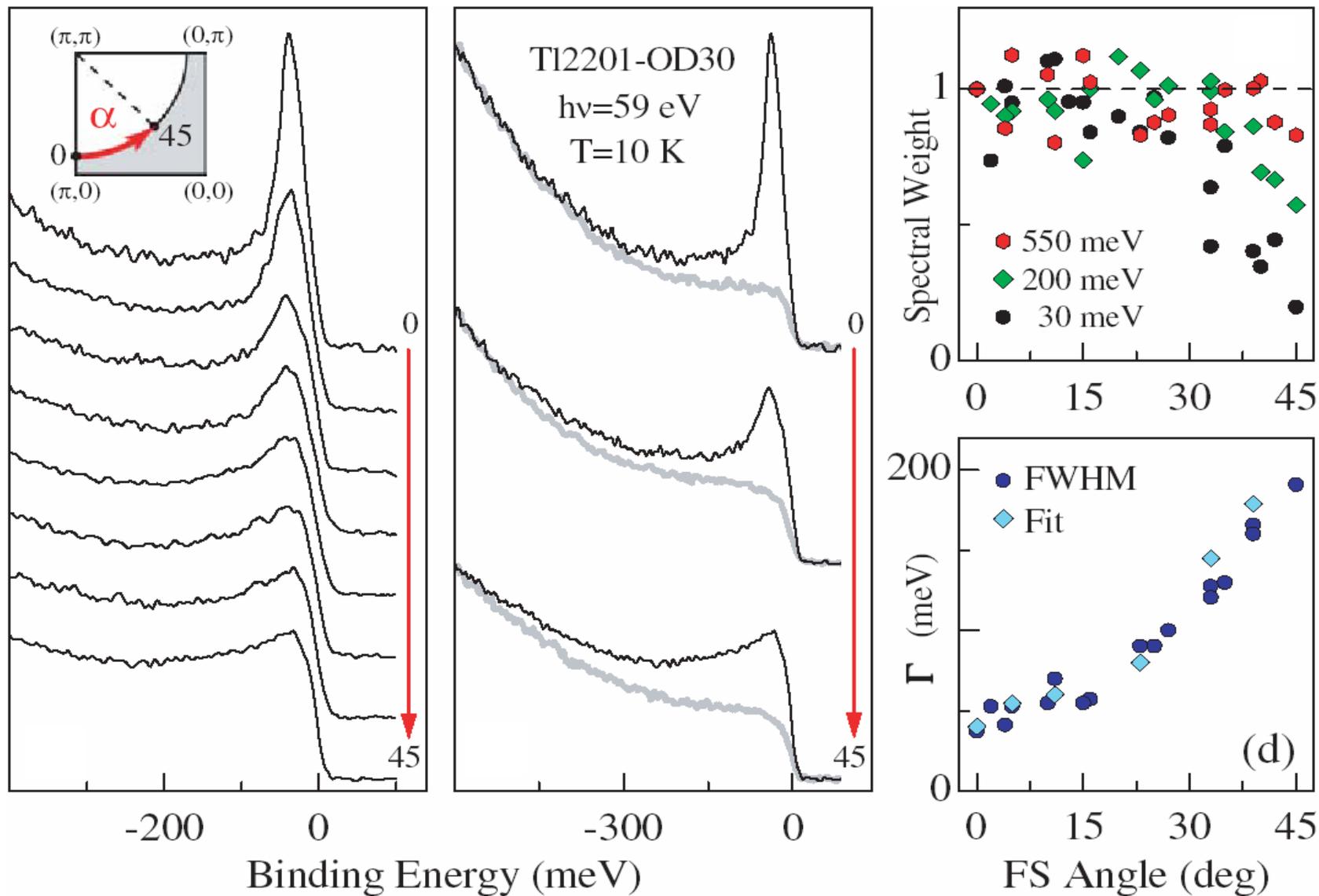


Hussey et al, Nature **425**, 814 (2004)

Tight binding FS fit

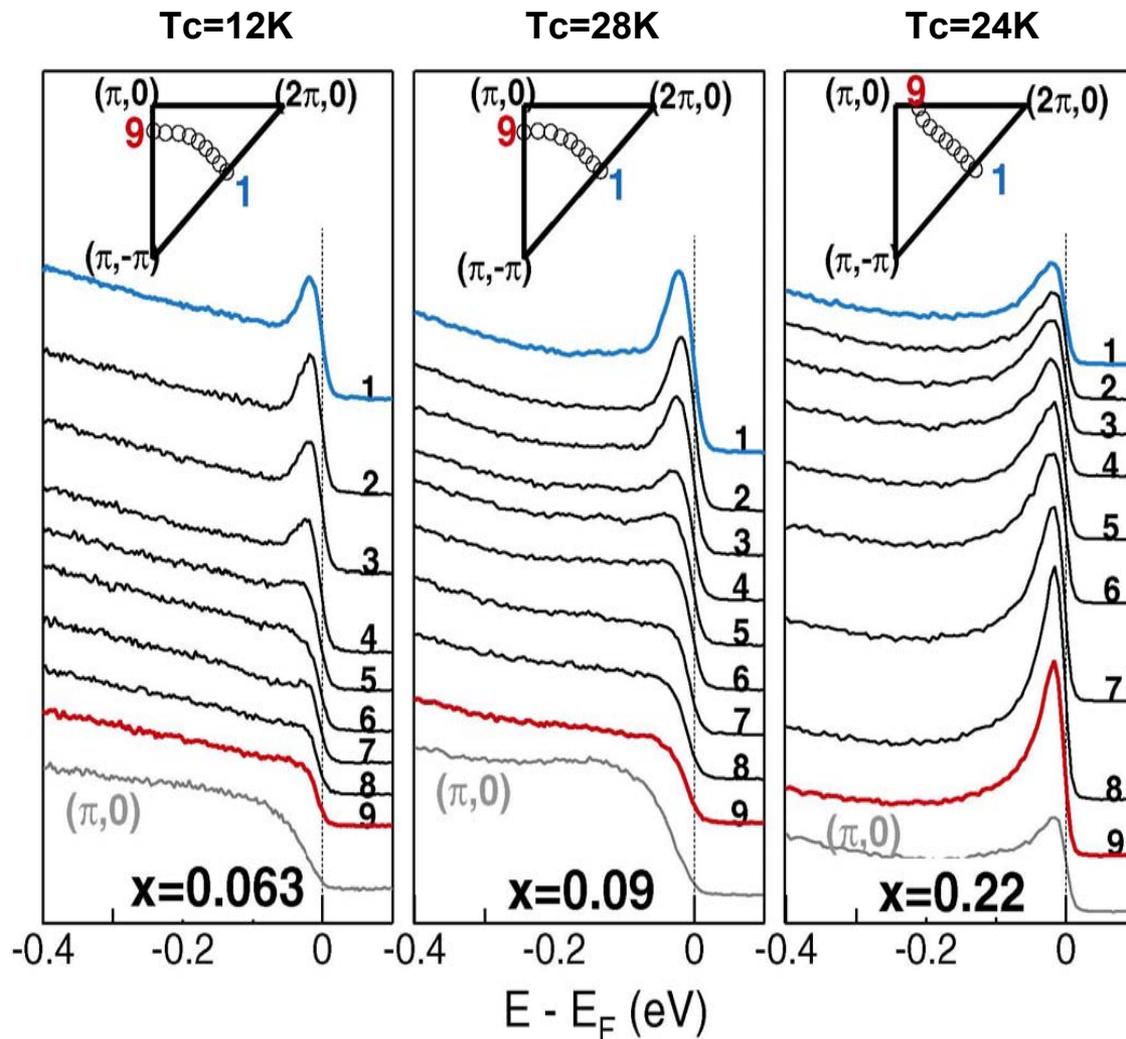
$$\begin{aligned}\epsilon_{\mathbf{k}} = & \mu + \frac{t_1}{2} (\cos k_x + \cos k_y) + t_2 \cos k_x \cos k_y + \frac{t_3}{2} (\cos 2k_x + \cos 2k_y) \\ & + \frac{t_4}{2} (\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) + t_5 \cos 2k_x \cos 2k_y\end{aligned}$$

Tl2201: Lineshape evolution



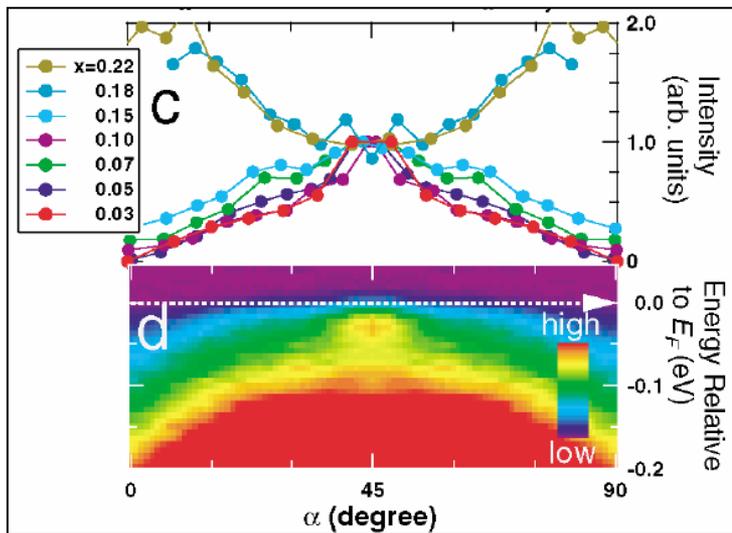
$Tl_2Ba_2CuO_{6+\delta}$: Lineshape evolution

LSCO



$Tl_2Ba_2CuO_{6+\delta}$: Lineshape evolution

Integrated Spectral Weight

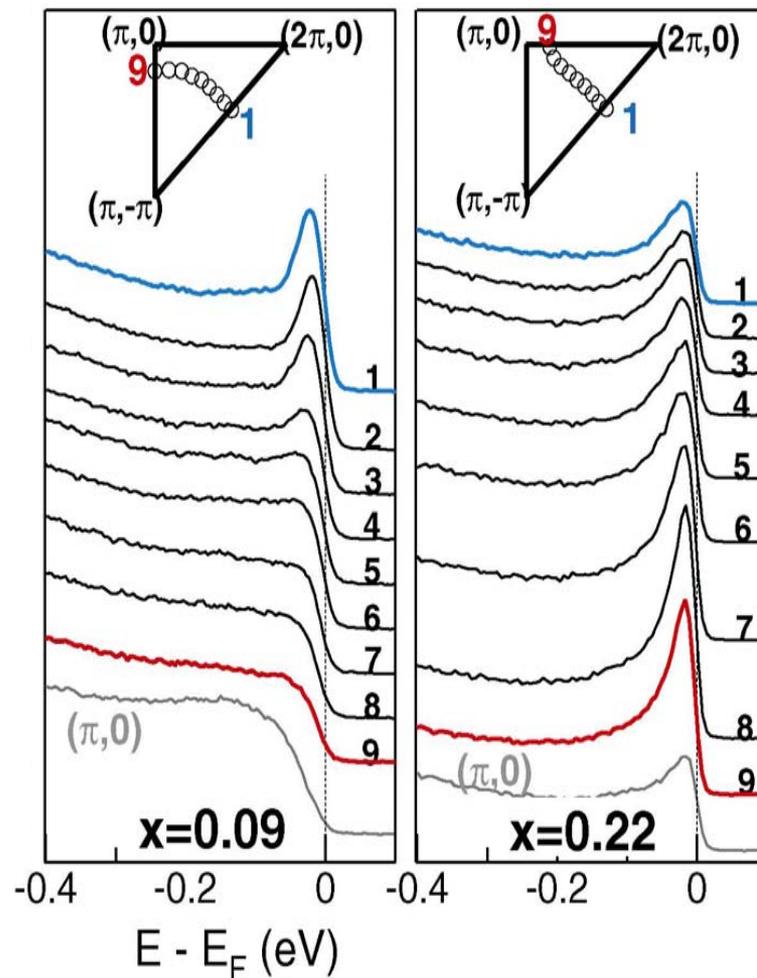


T. Yoshida et al., PRL **91**, 027001 (2003)

LSCO

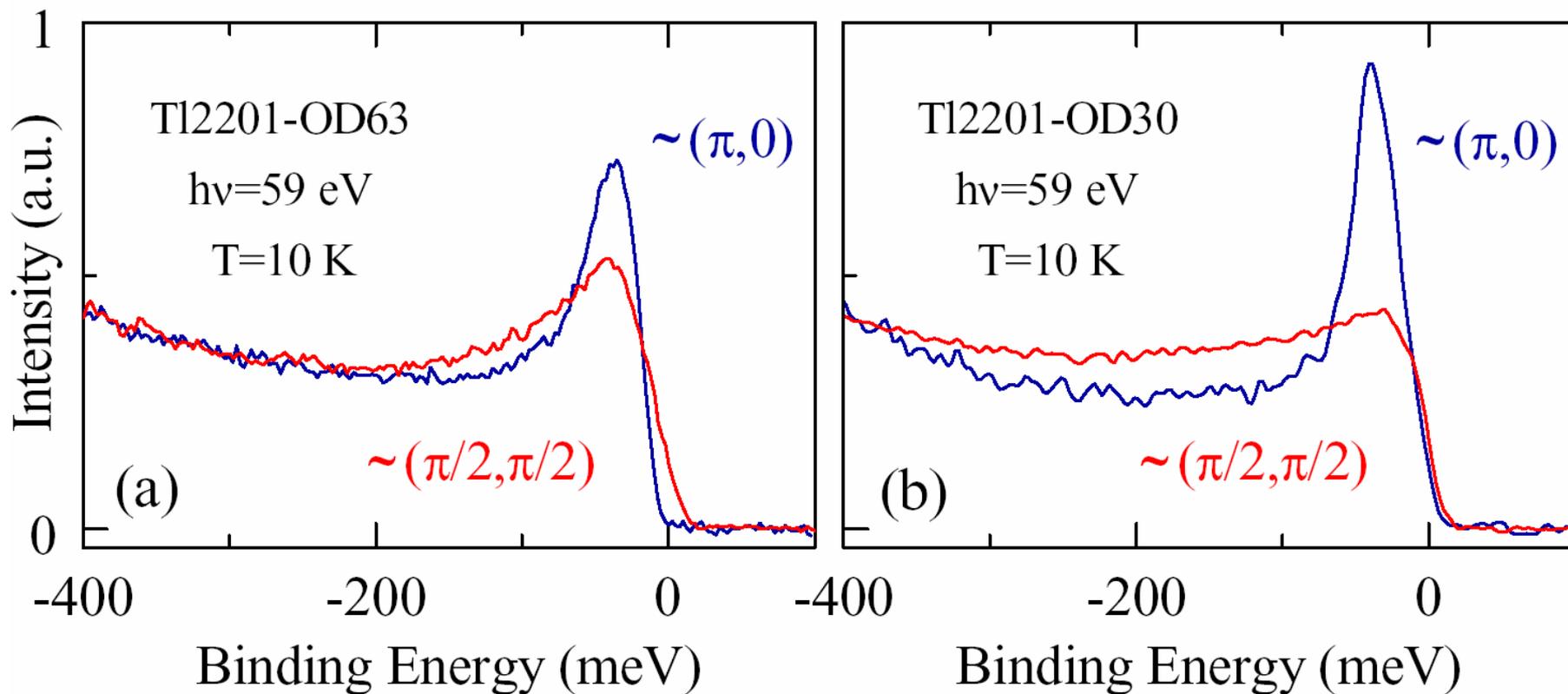
$T_c=28K$

$T_c=24K$

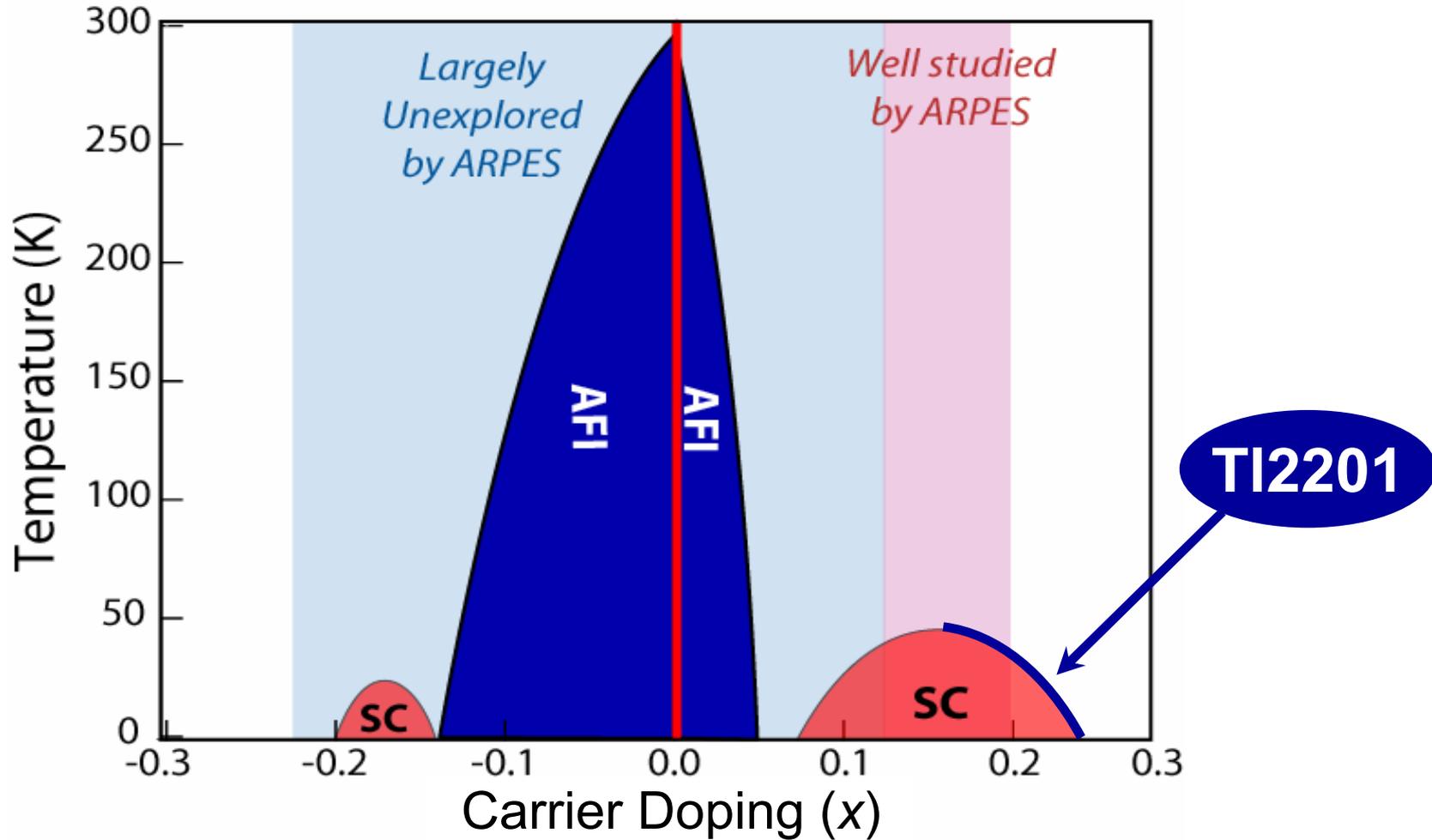


X.J. Zhou et al., PRL **92**, 187001 (2004)

$\text{Ti}_2\text{Ba}_2\text{CuO}_{6+\delta}$: ARPES Results



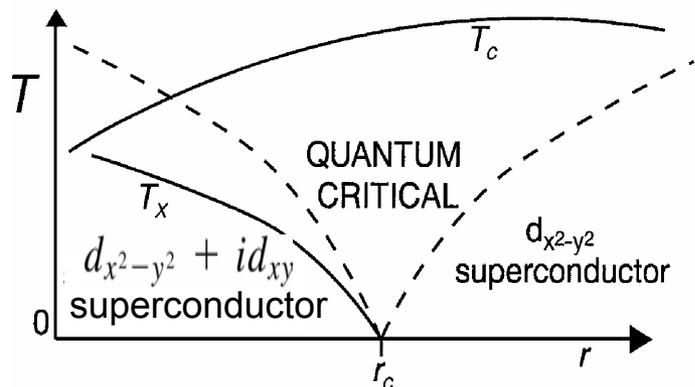
ARPES on $\text{Ti}_2\text{Ba}_2\text{CuO}_{6+\delta}$



Paring mechanism?

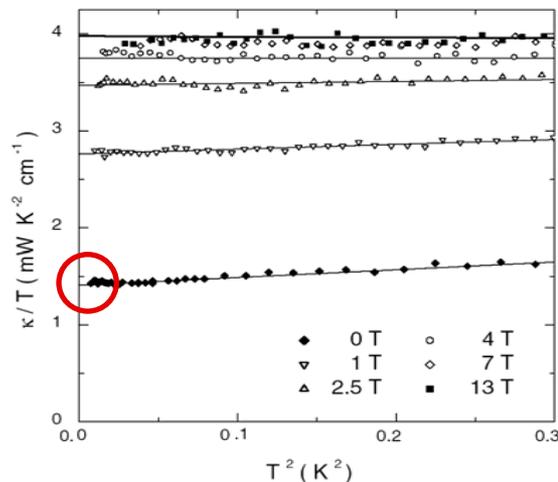
Quantum criticality?

TI2201: SC gap symmetry

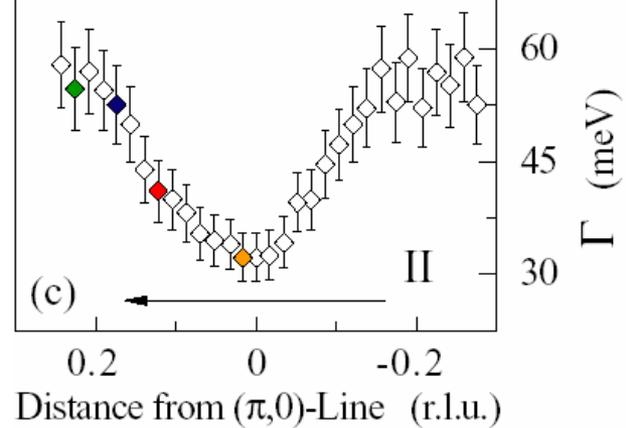
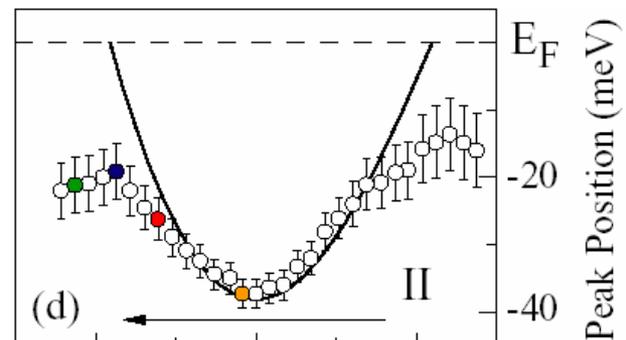
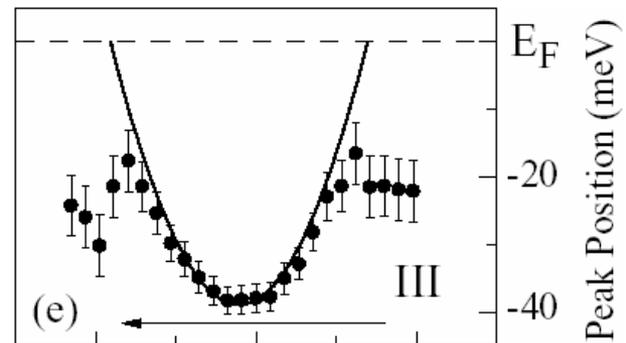
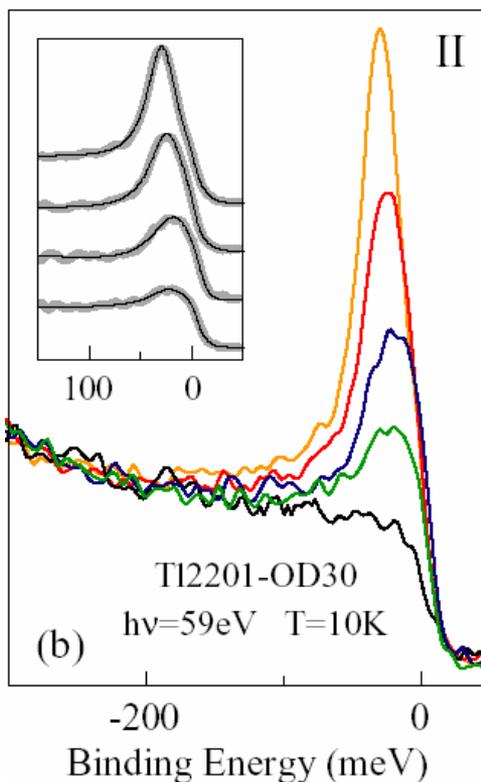
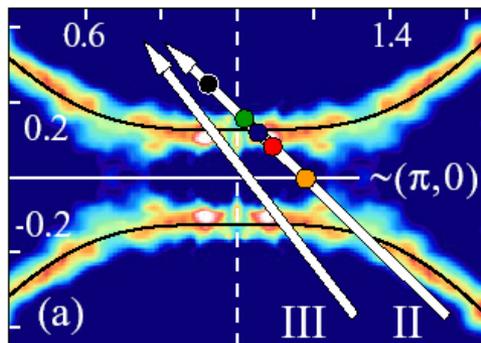


Vojta, Zhang, Sachdev, PRL 2000

Large residual linear term in heat conductivity

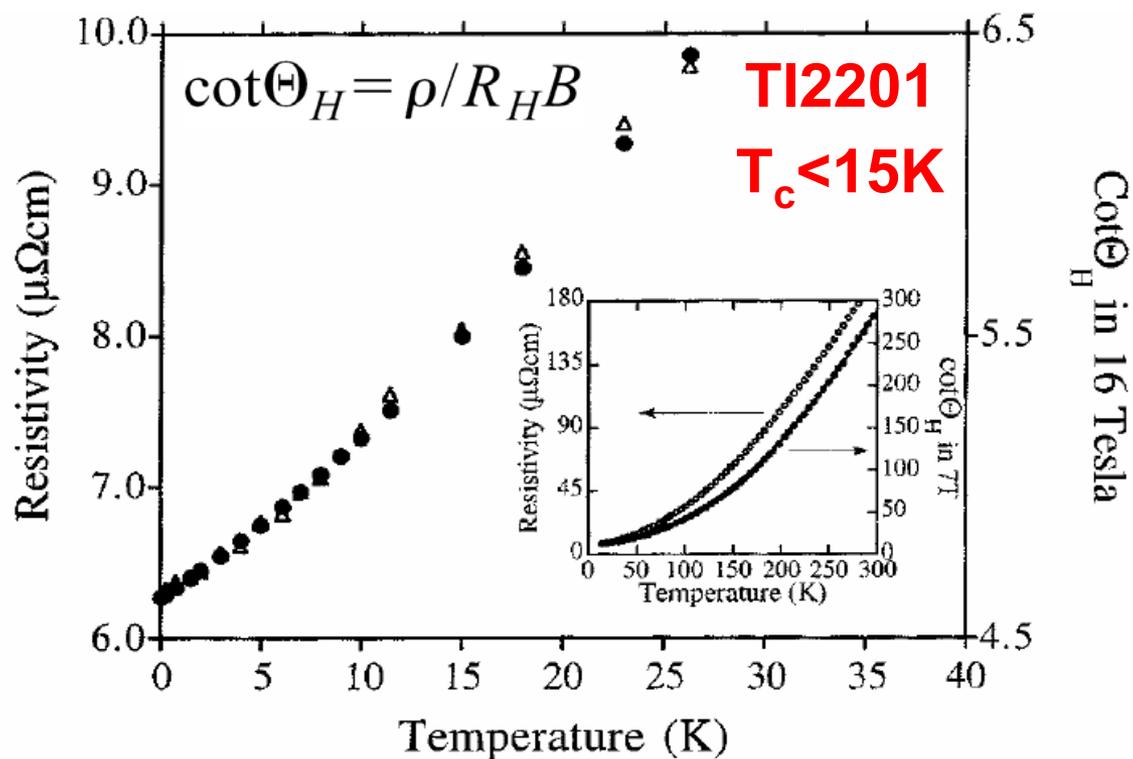


Proust et al., PRL 2002



TI2201: Momentum Dependent Scattering?

Electronic scattering appears
isotropic in overdoped cuprates



A. Mackenzie *et al.*, PRB **53**, 5848 (1996)

Residual k_z -dispersion

Forward scattering

TI2201: Small Angle Scattering?

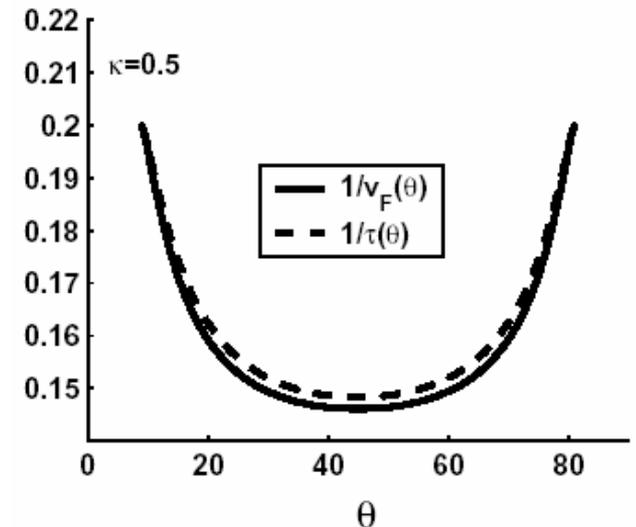
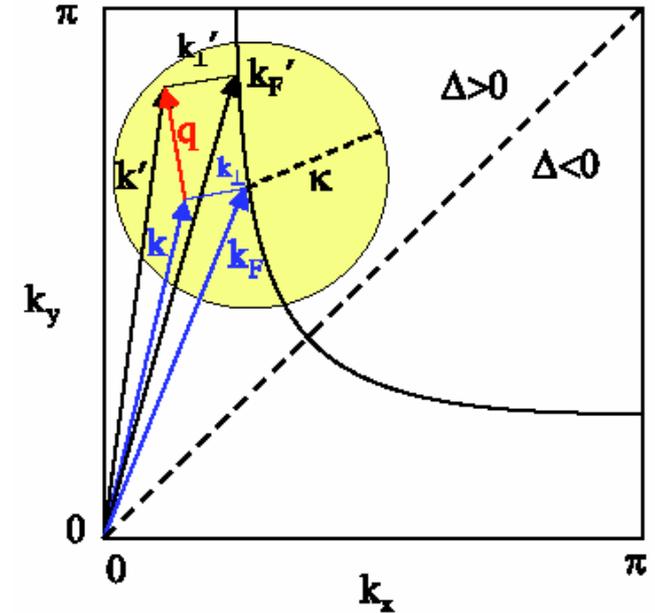
$$\underline{\Sigma}_{tot} = \underline{\Sigma}_{el,f} + \underline{\Sigma}_{el,u} + \underline{\Sigma}_{inel}$$

$$V(r) = V_0 e^{-\kappa r}$$

$$V_{\mathbf{k}\mathbf{k}'} = \frac{2\pi\kappa V_0}{((\mathbf{k} - \mathbf{k}')^2 + \kappa^2)^{3/2}}$$

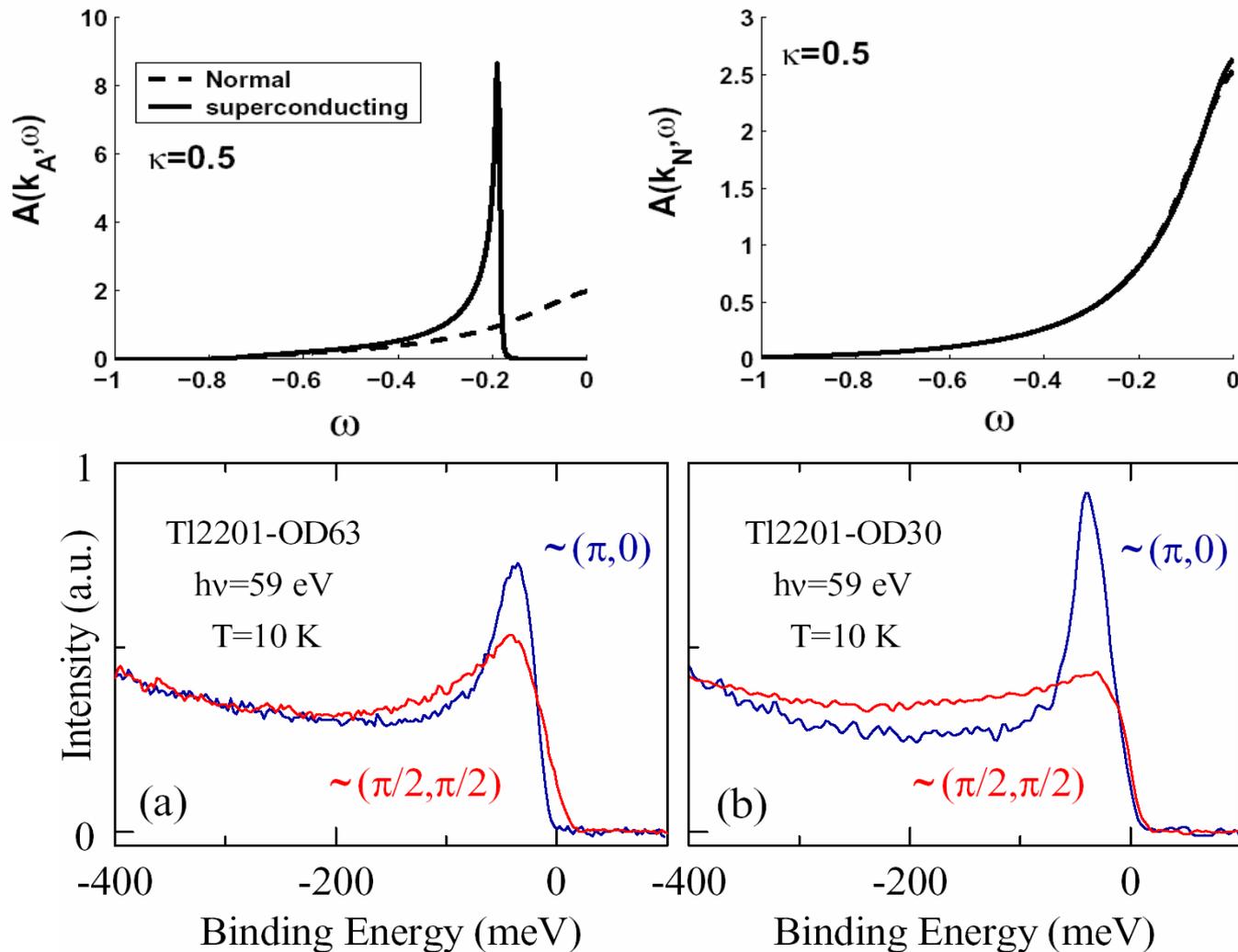
$$\Sigma(\mathbf{k}, \omega) = n_I \sum_{k'} |V_{\mathbf{k}\mathbf{k}'}|^2 G^0(\mathbf{k}', \omega)$$

$$-\Sigma''(\mathbf{k}_F, 0) \equiv \Gamma_0(\mathbf{k}_F) = \frac{3\pi n_i V_0^2}{8|v_F(\mathbf{k}_F)|\kappa^3}$$



Tl2201: Small Angle Scattering?

Small Angle Scattering: strong T-dependence at $(\pi, 0)$



ARPES on TI2201: Conclusions

