# State-of-the-Art ARPES: Momentum-Space Microscopy of $Sr_2RuO_4$ and Bi2212

**Andrea Damascelli**

*Department of Physics & Astronomy*

*University of British Columbia*

*Vancouver, B.C.*

# Group: ARPES on Complex Systems

S. Wang
B. Lau
S. Hossain
J. Mottershead
K. Ajdari
A. Damascelli

Advanced Materials & Process Engineering Laboratory

# Previous Collaborators

- **ARPES at Stanford:**

  K.M. Shen, D.H. Lu, D.L. Feng, N.P. Armitage, F. Ronning, C. Kim, **Z.-X. Shen**

- **Band Structure Calculations (NRL, Washington):**

  I.I. Mazin, D.J. Singh

- **Samples:**
  - **$Sr_2RuO_4$**

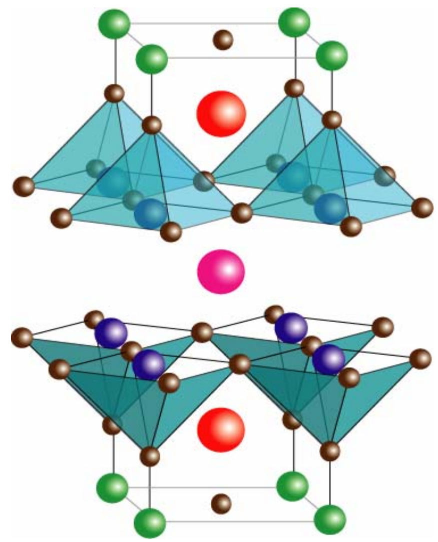
    S. Nakatsuji, T. Kimura, Y. Tokura, Z.Q. Mao, Y. Maeno
  - **$Bi_2Sr_2CaCu_2O_{8+\delta}$**

    H. Eisaki, R. Yoshizaki, J.-i. Shimoyama, K. Kishio, G.D. Gu, S. Oh, A. Andrus, J. O'Donnell, J.N. Eckstein
  - $YBa_2Cu_3O_{7-\delta}$

    D.A. Bonn, R. Liang, W.N. Hardy, A.I. Rykov, S. Tajima
  - $Nd_{2-x}Ce_xCuO_4$

    Y. Onose, Y. Taguchi, Y. Tokura; P.K. Mang, N. Kaneko, M. Greven
  - $Ca_{2-x}Na_xCu_2O_2Cl_2$

    L.L. Miller, T. Sasagawa, Y. Kohsaka, H. Takagi

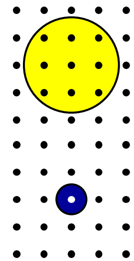


# Outline

- ▶ Electronic structure of **complex systems**
- ▶ State-of-the-Art **ARPES:** the essentials
- ▶ ARPES on **$Sr_2RuO_4$**
  - **Bulk** & **surface** electronic structure
  - Surface **Ferromagnetism**?
- ▶ ARPES on **$Bi_2Sr_2CaCu_2O_{8+\delta}$**
  - **Bilayer splitting** of the electronic structure
  - Signatures of **superfluid density**
- ▶ Conclusions and discussion

# Strongly Correlated Electron Systems

**d - f**
**open shells materials**

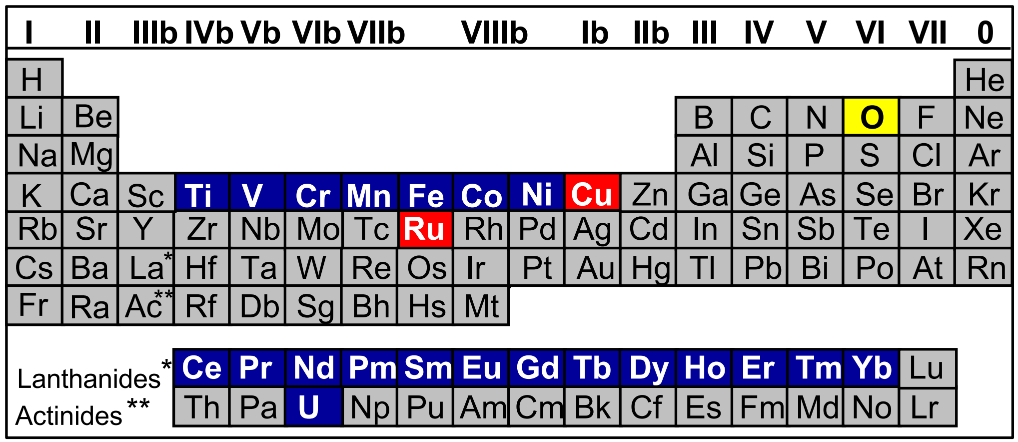


**U<<W**
**Charge fluctuations**

**U>>W**
**Spin fluctuations**

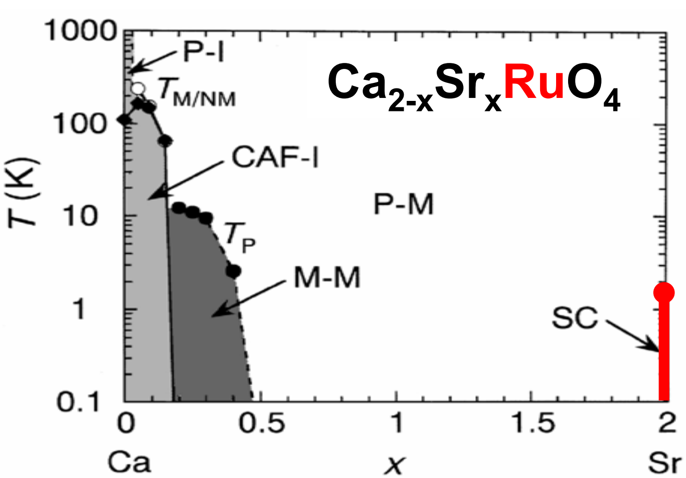
## Control parameters

**Bandwidth (U/W)**
**Band filling**
**Dimensionality**

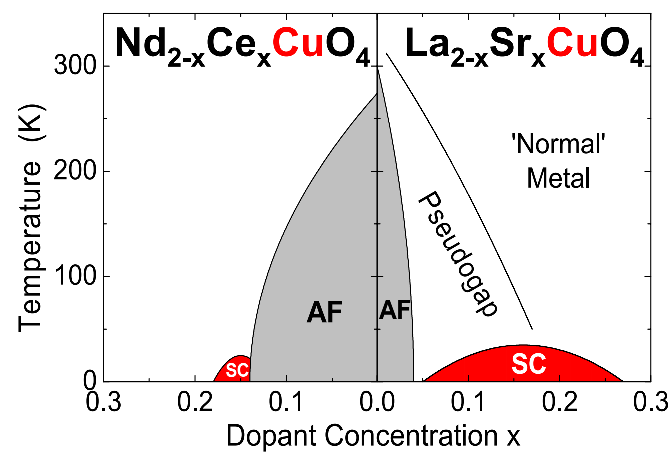



## Degrees of freedom

**Charge / Spin**
**Orbital**
**Lattice**




- **Kondo**
- **Mott-Hubbard**
- **Heavy Fermions**
- **Unconventional SC**
- **Spin-charge order**
- **Colossal MR**



# Probing the Low-Electronic Structure

**Understand the**
**macroscopic electronic properties**

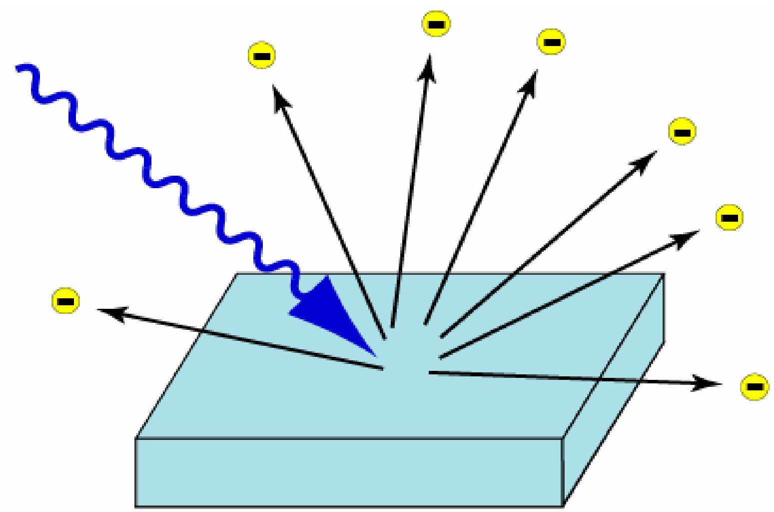
⬇

**Study the low-energy electronic excitations**

⬇

**Angle-Resolved PhotoElectron Spectroscopy**

---



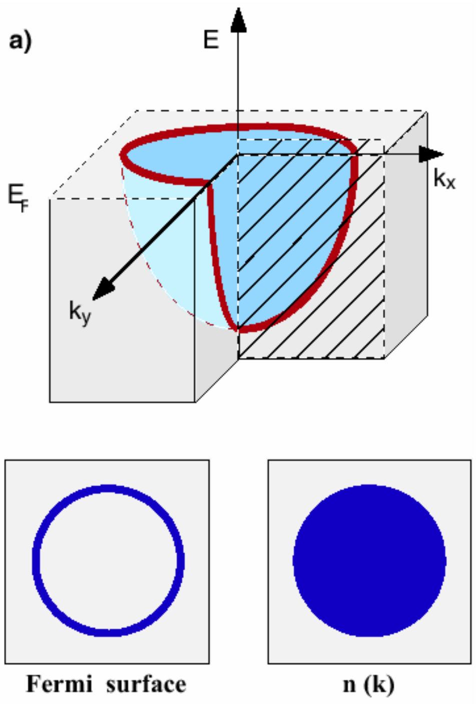
**The Photoelectric Effect**

**FIRST EXPERIMENTAL EVIDENCE FOR QUANTIZATION OF LIGHT!**

**Velocity and direction of the electrons in the solid**

# Understanding the Solid State: Electrons in Reciprocal Space

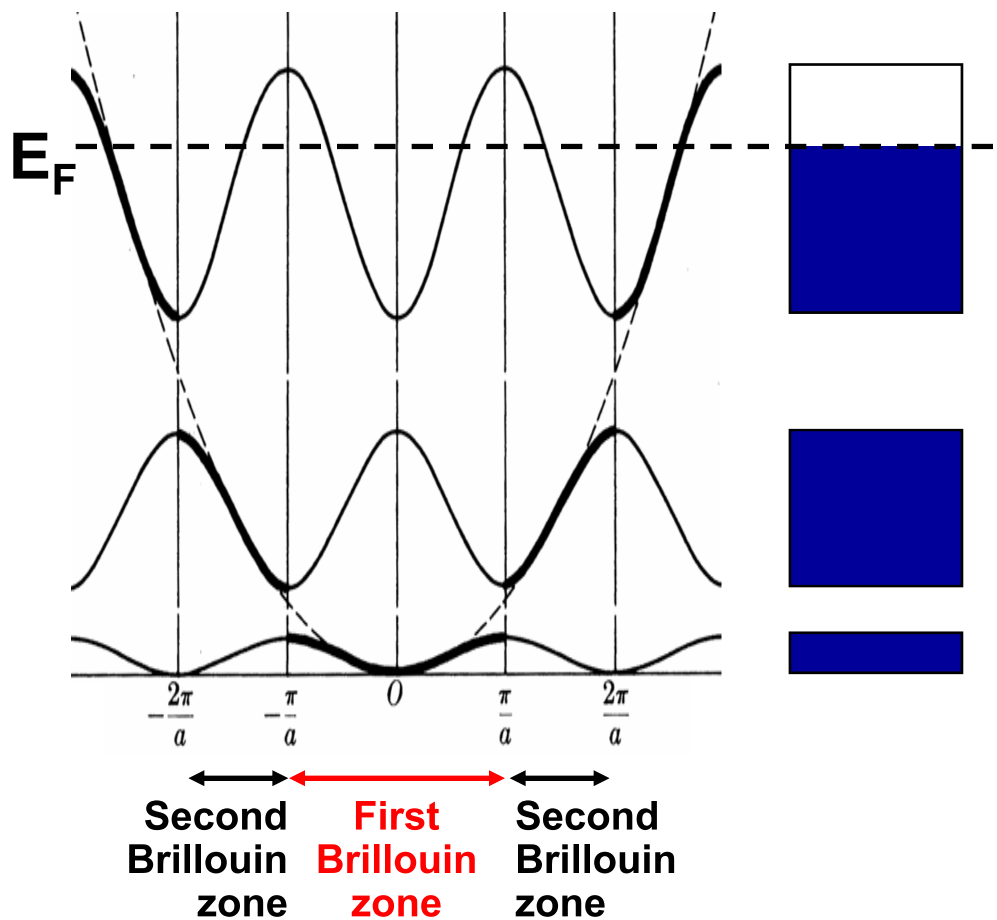
**Many properties of a solids are determined by electrons near $E_F$ (conductivity, magnetoresistance, superconductivity, magnetism)**




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

**Allowed electronic states**

Repeated-zone scheme



# Interaction effects between electrons : "Many-body Physics"

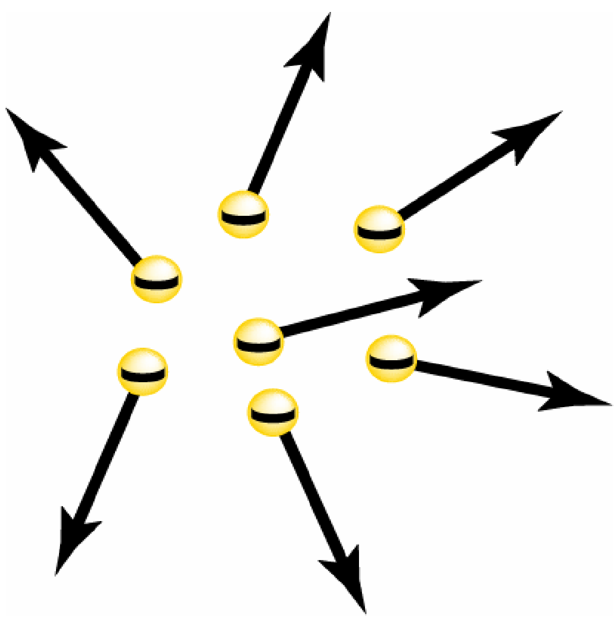
**Many-body effects are due to the interactions between the electrons and each other, or with other excitations inside the crystal :**

1) A "many-body" problem : intrinsically hard to calculate and understand

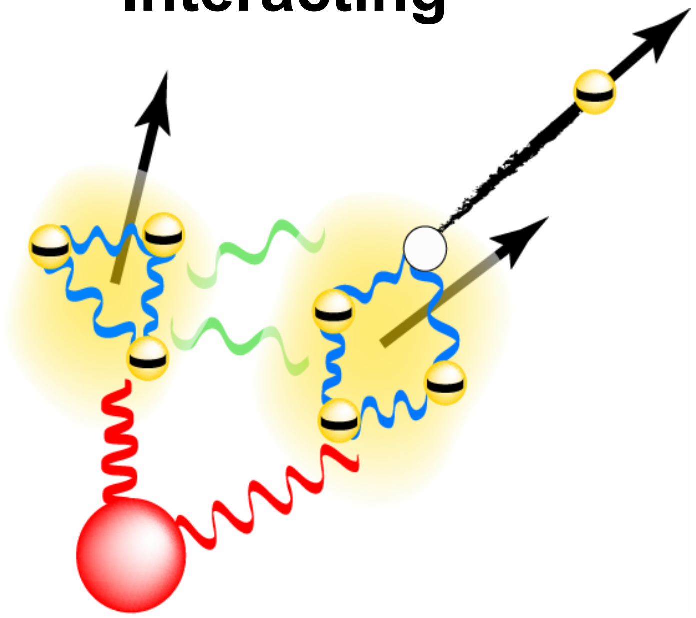
2) Responsible for many surprising phenomena :

***Superconductivity, Magnetism, Density Waves, ....***

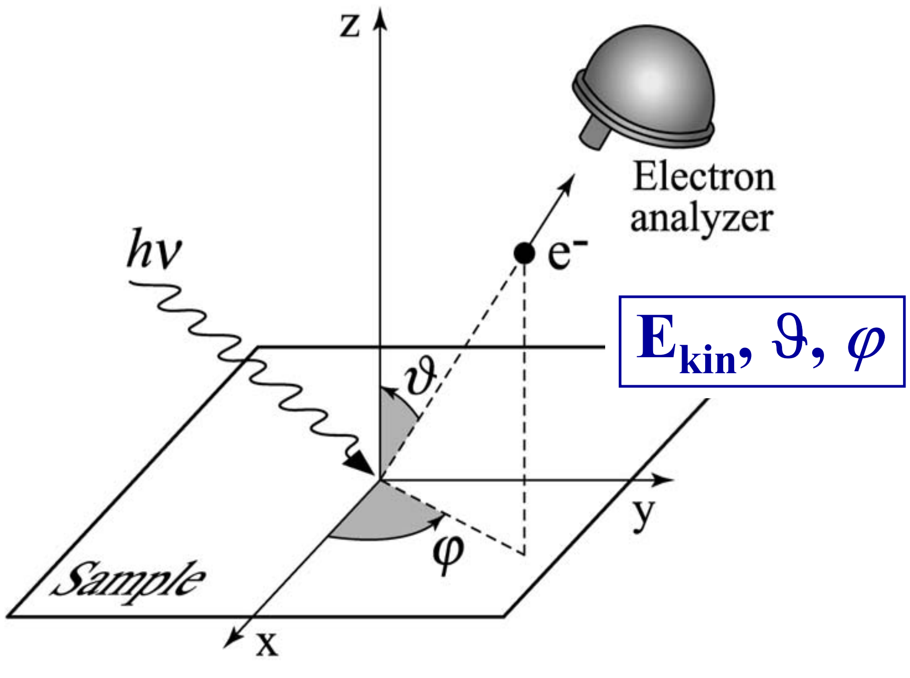
## Non-Interacting



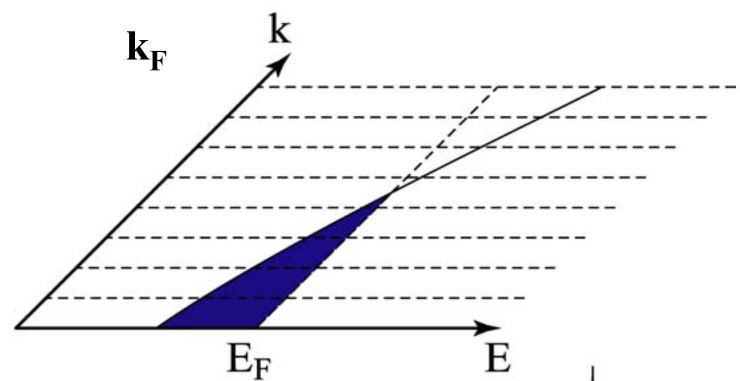
## Interacting

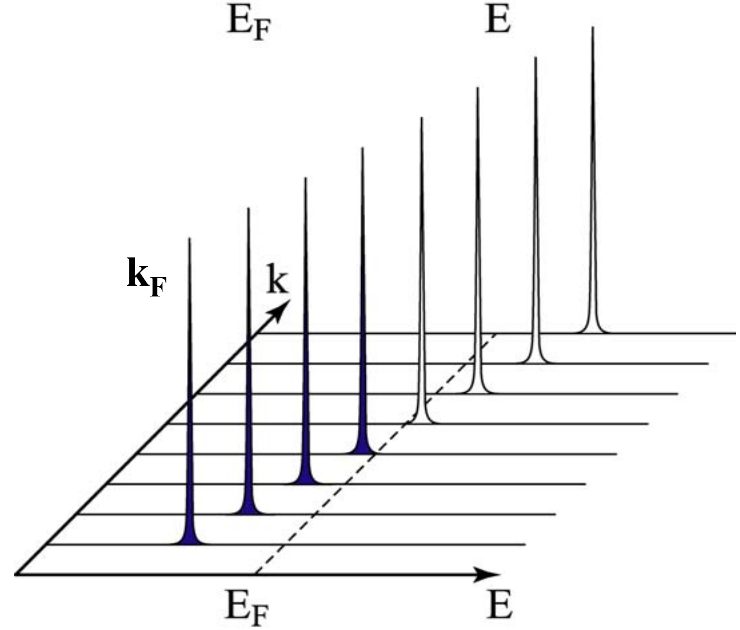


# Angle-Resolved Photoemission Spectroscopy




## Electrons in Reciprocal Space



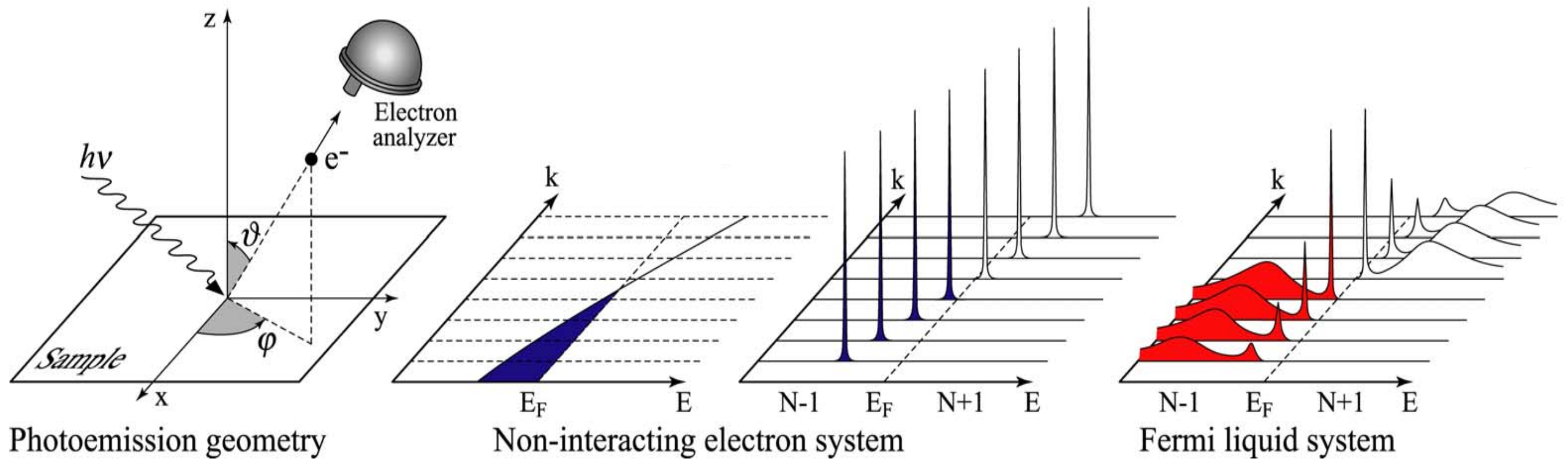

**Energy Conservation**

$$E_{kin} = h\nu - \phi - |E_B|$$

**Momentum Conservation**

$$\mathbf{p}_{\|} = \hbar \mathbf{k}_{\|} = \sqrt{2mE_{kin}} \cdot \sin\vartheta$$

# Angle-Resolved Photoemission Spectroscopy



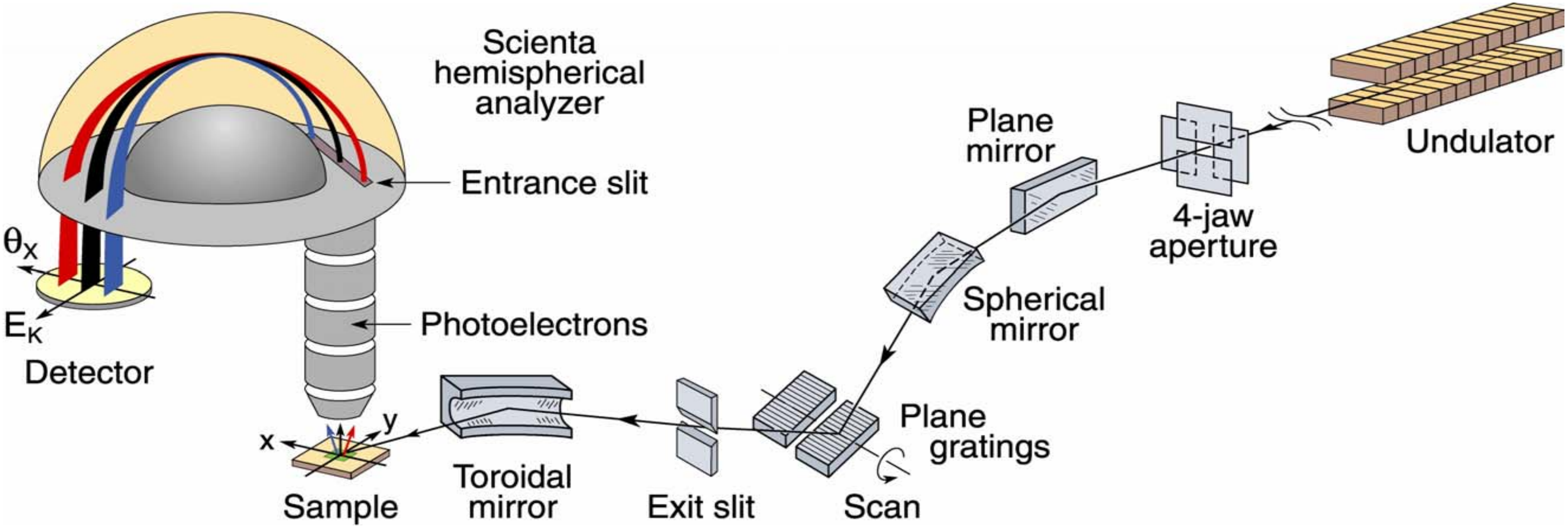

**Photoemission intensity**: $I(k,\omega)=I_0\,|M(k,\omega)|^2 f(\omega)\,A(k,\omega)$

**Single-particle spectral function**

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

**$\Sigma(k,\omega)$ : the "self-energy" - captures the effects of interactions**

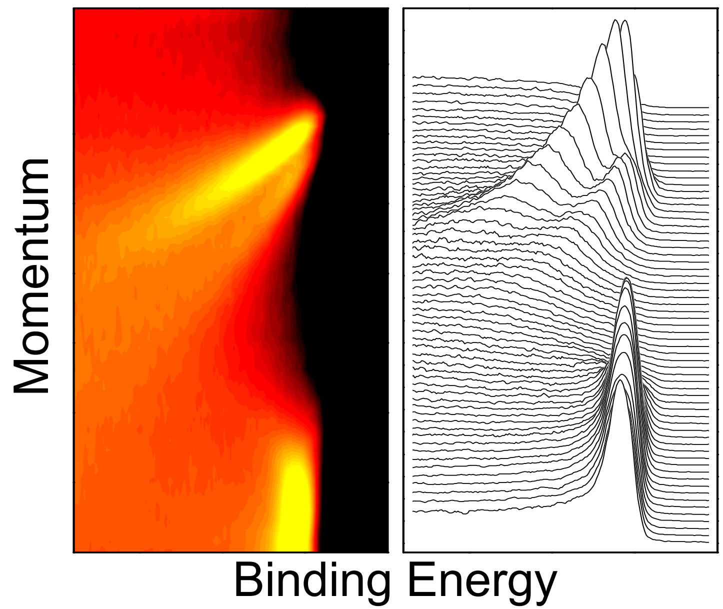
# Angle-Resolved Photoemission Spectroscopy




## Parallel multi-angle recording

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

| | *ΔE (meV)* | *Δθ* |
|---|---|---|
| **past** | *20-40* | *2°* |
| **now** | *2-10* | *0.2°* |

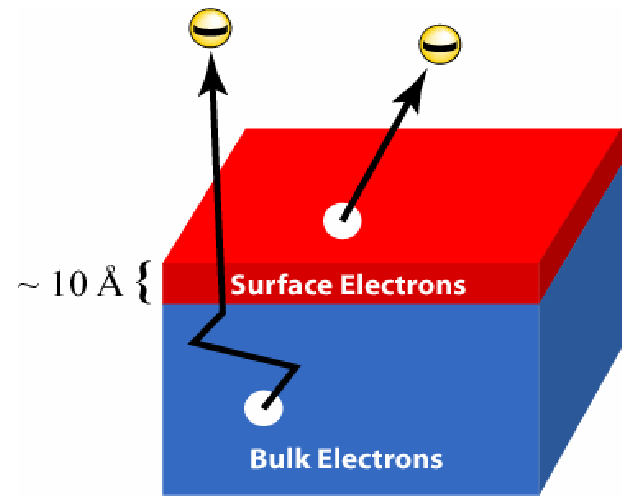


# ARPES: advantages and limitations

## Advantages

- **Direct information about electronic states!**
- Straightforward comparison with theory - little or no modelling.
- High-resolution information about **BOTH energy** and **momentum**
- **Surface-sensitive probe**
- Sensitive to “many-body” effects
- Can be applied to small samples (100 μm x 100 μm x 10 nm)

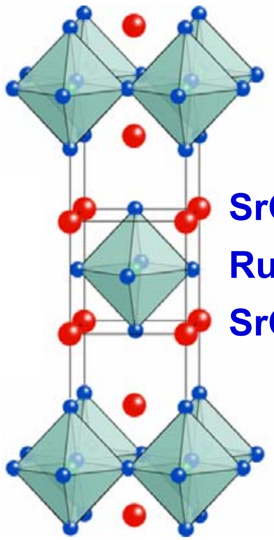
## Limitations




- **Not bulk sensitive**
- Requires clean, atomically flat surfaces in **ultra-high vacuum**
- Cannot be studied as a function of pressure or magnetic field

# $Sr_2RuO_4$: basic properties

**2D perovskite**

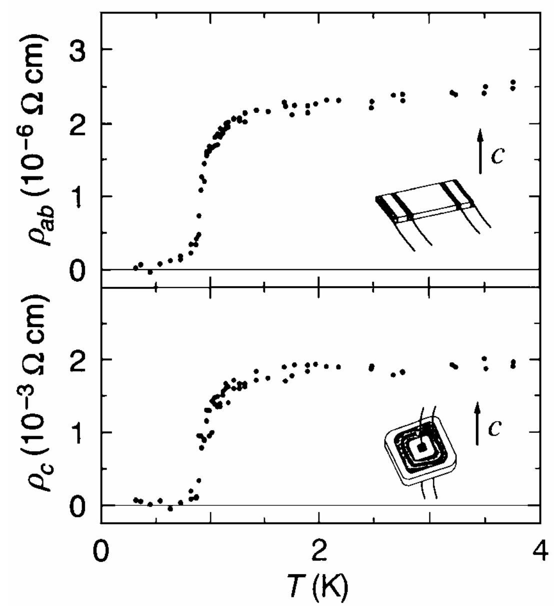



**Unconventional superconductivity**

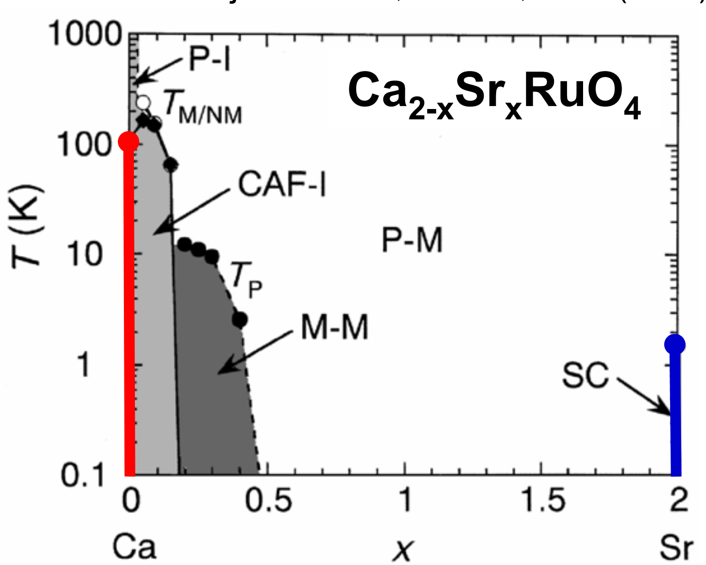
- Pairing mechanism ?
- Order parameter ?
- FM-AF fluctuations ?

Rice & Sigrist, JPCM **7**, L643 (1995)

Maeno *et al.*, Nature **372**, 532 (1994)




Nakatsuji & Maeno, PRL **84**, 2666 (2000)



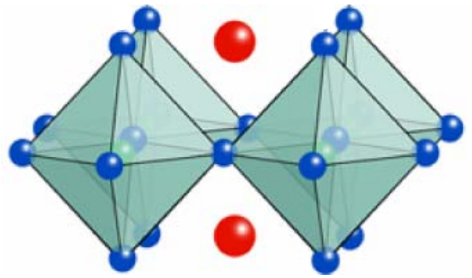

**Lattice-magnetism interplay**
**Orbital degrees of freedom**

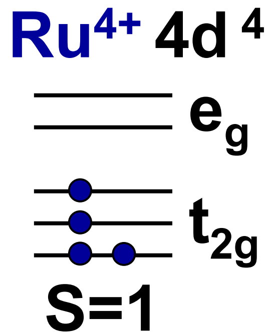
**$Sr_2RuO_4$** : 2D **Fermi Liquid** ($\rho_c/\rho_{ab}$=850)

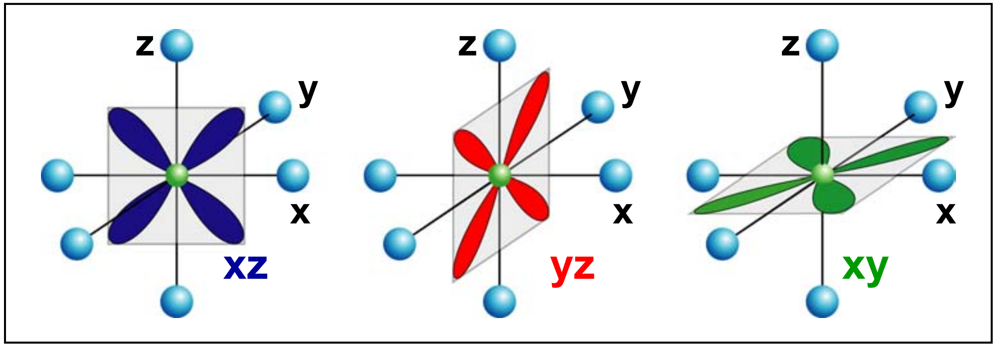
**$Ca_2RuO_4$** : insulating **Anti-FerroMagnet**

**$SrRuO_3$** : metallic **FerroMagnet**

# Low-Energy Electronic structure of $Sr_2RuO_4$

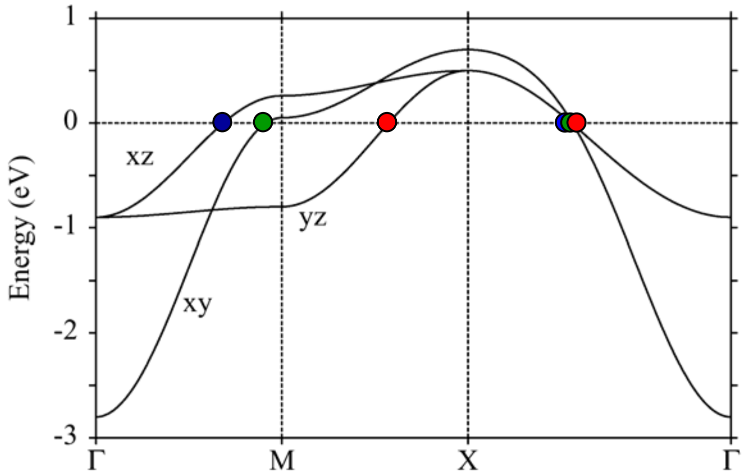




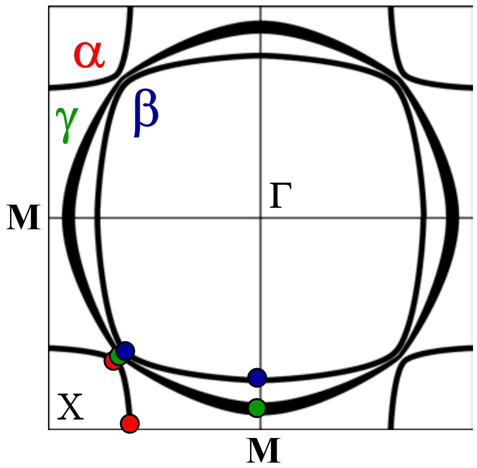




▶ Band structure calculation: **3 $t_{2g}$** bands crossing $\mathbf{E_F}$

→ 3 sheets of FS { $\alpha$ (hole-like); $\beta$ and $\gamma$ (electron-like)



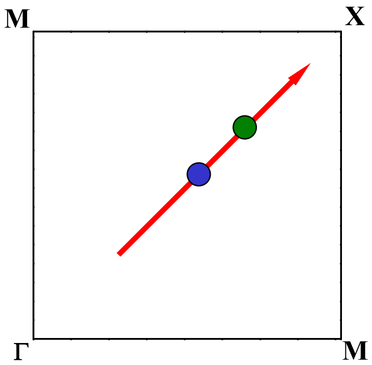

A. Liebsch *et al*, PRL **84**, 1591 (2000)



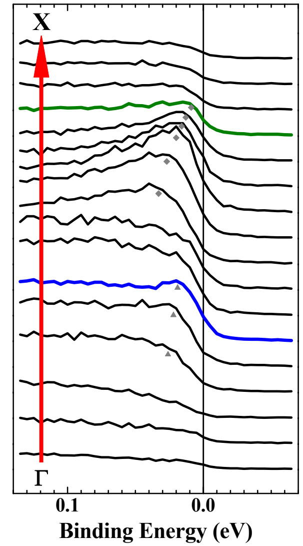

I.I. Mazin *et al*, PRL **79**, 733 (1997)

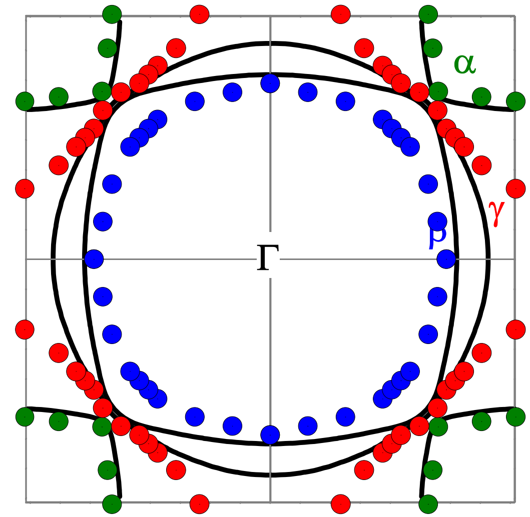
# Fermi Surface Topology of $Sr_2RuO_4$

## *ARPES : circa 1996*




D.H. Lu *et al.*, PRL **76**, 4845 (1996)

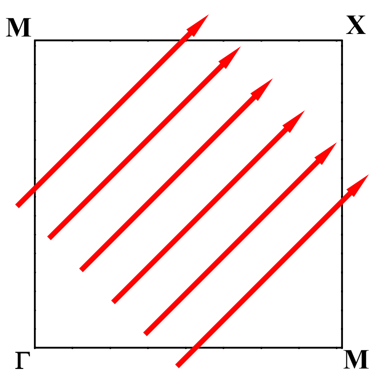


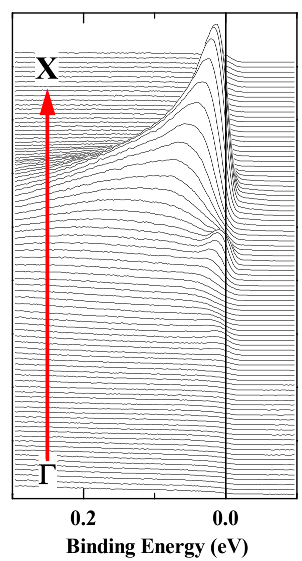

D.J. Singh, PRB **52**, 1358 (1995)

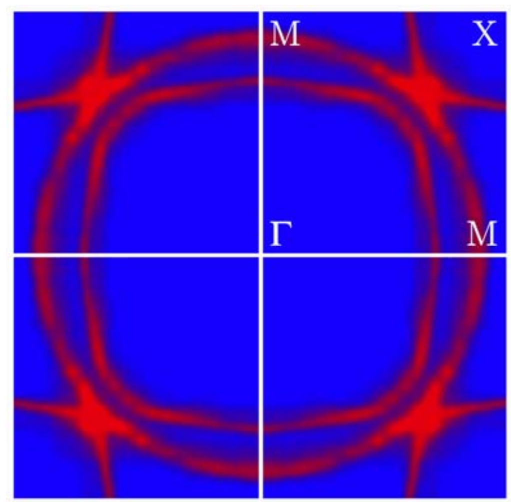
---

## *ARPES : present day*



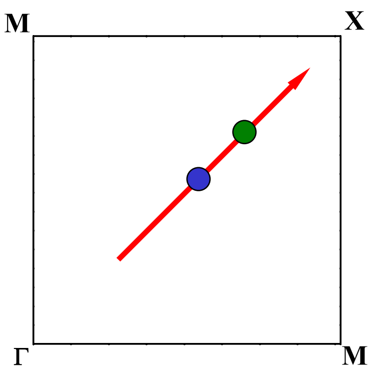

A. Damascelli *et al.*, PRL **85**, 5194 (2000)



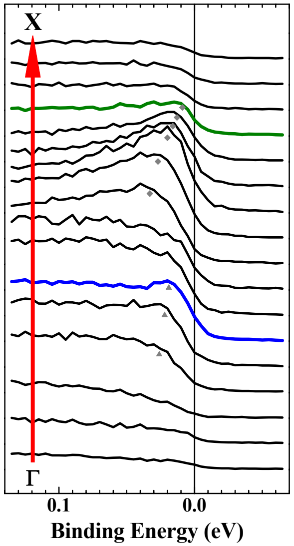



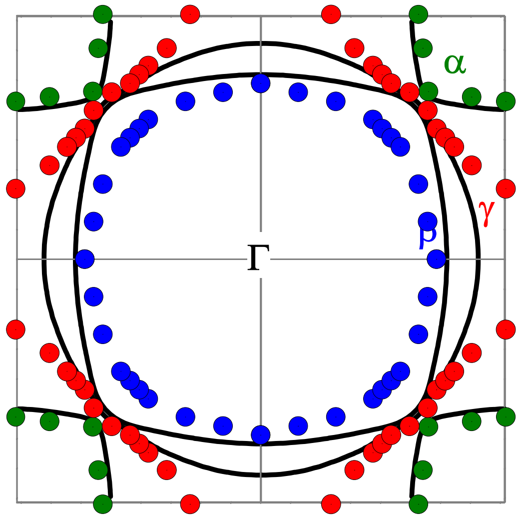
# Fermi Surface Topology of $Sr_2RuO_4$

## *ARPES : circa 1996*



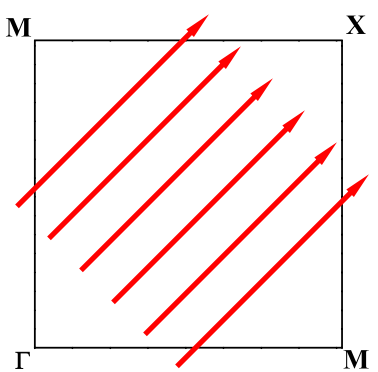

D.H. Lu *et al.*, PRL **76**, 4845 (1996)



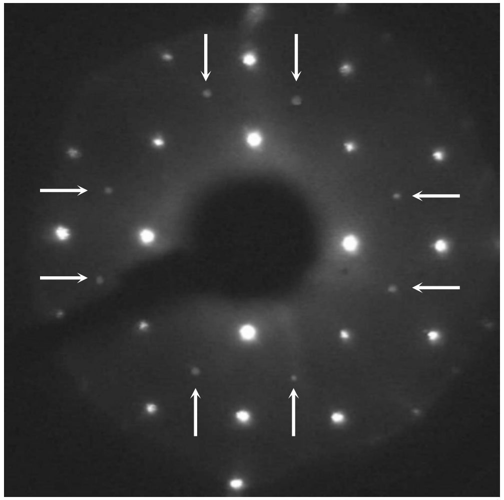

D.J. Singh, PRB **52**, 1358 (1995)

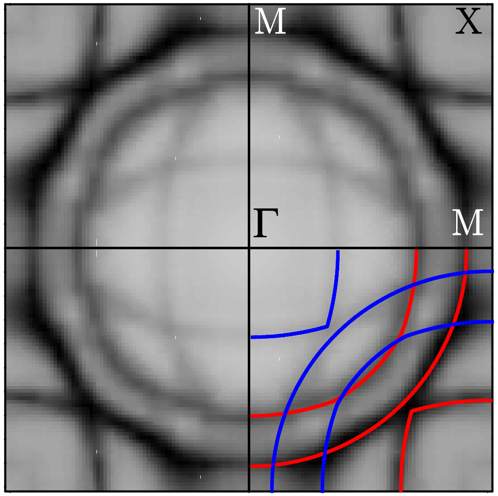
## *ARPES : present day*



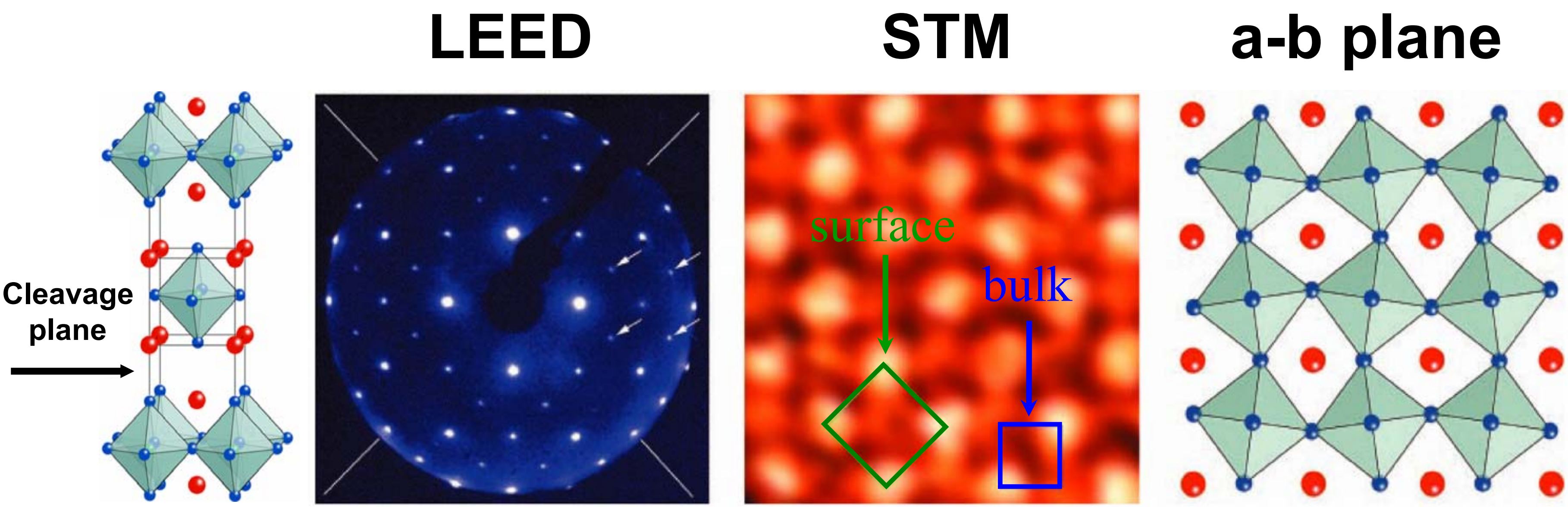

A. Damascelli *et al.*, PRL **85**, 5194 (2000)

**Surface instability** ⟷ **Band folding**





# Surface reconstruction of cleaved $Sr_2RuO_4$

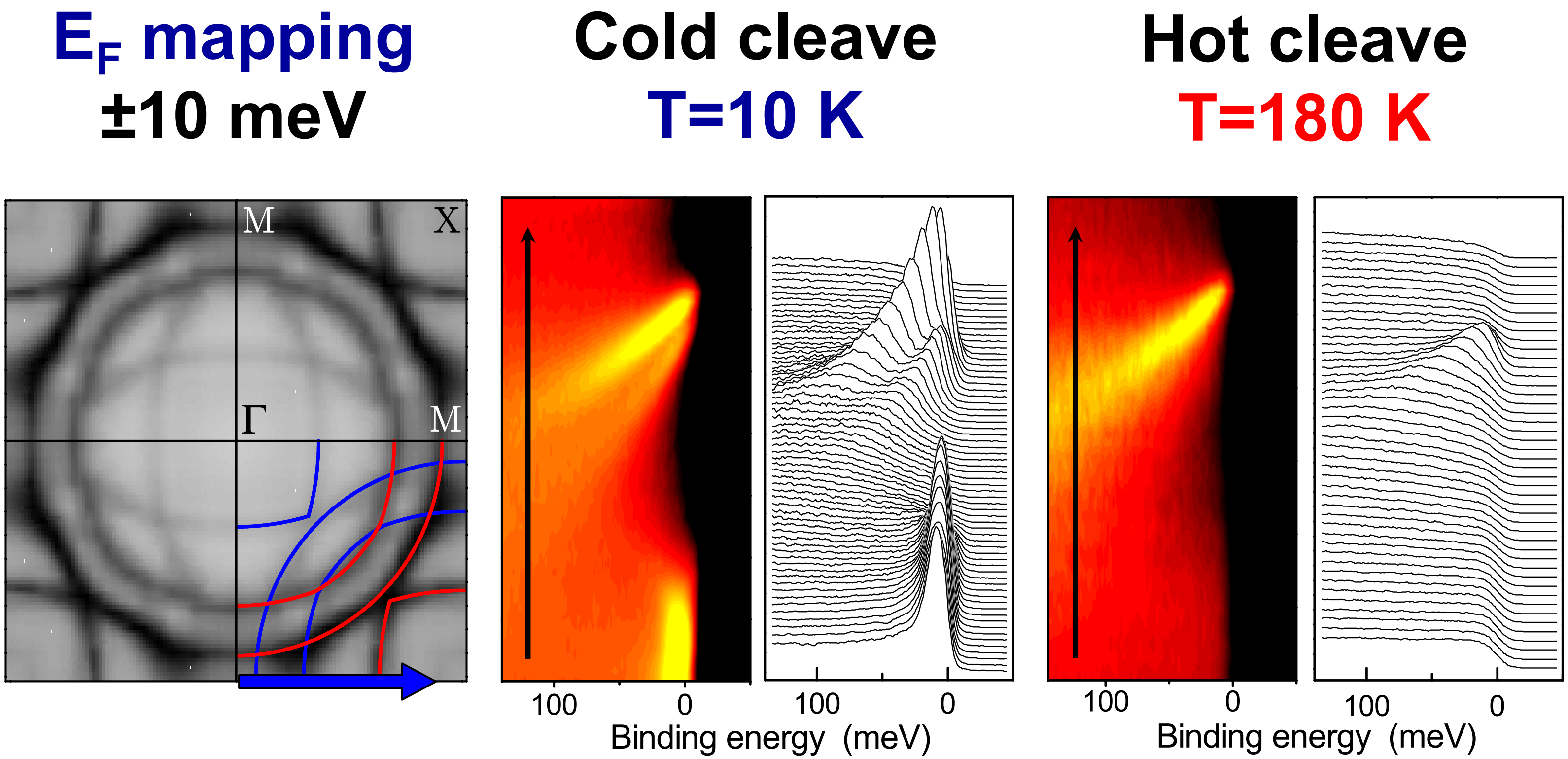



R. Matzdorf *et al.*, Science **289**, 746 (2000)

**Rotation of the $RuO_6$ octahedra around the c axis (9°)**

# Surface electronic structure of $Sr_2RuO_4$

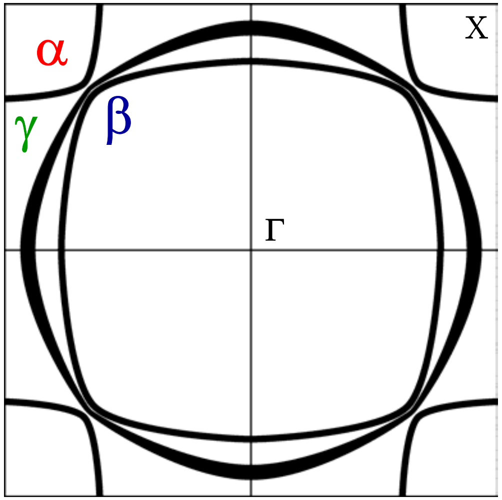
On samples cleaved at **180 K** the **surface**-related features are **suppressed**



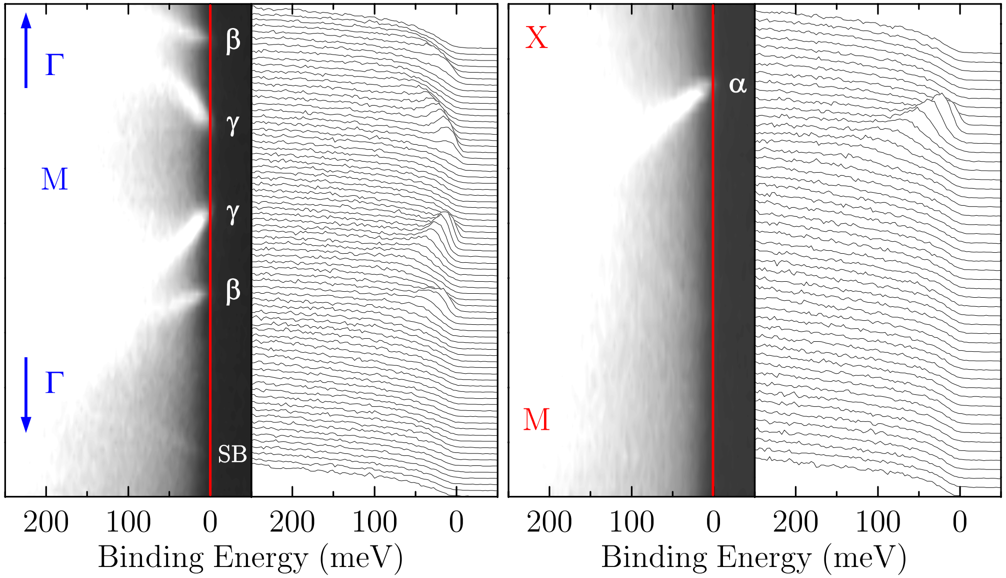
# Bulk electronic structure of $Sr_2RuO_4$

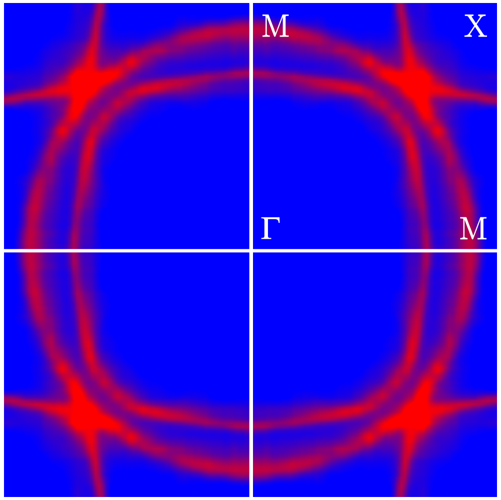
**What do we learn about the bulk electronic structure?**

- **FS topology**
- **Fermi velocity**
- **Effective mass**




I.I. Mazin *et al.*, PRL **79**, 733 (1997)

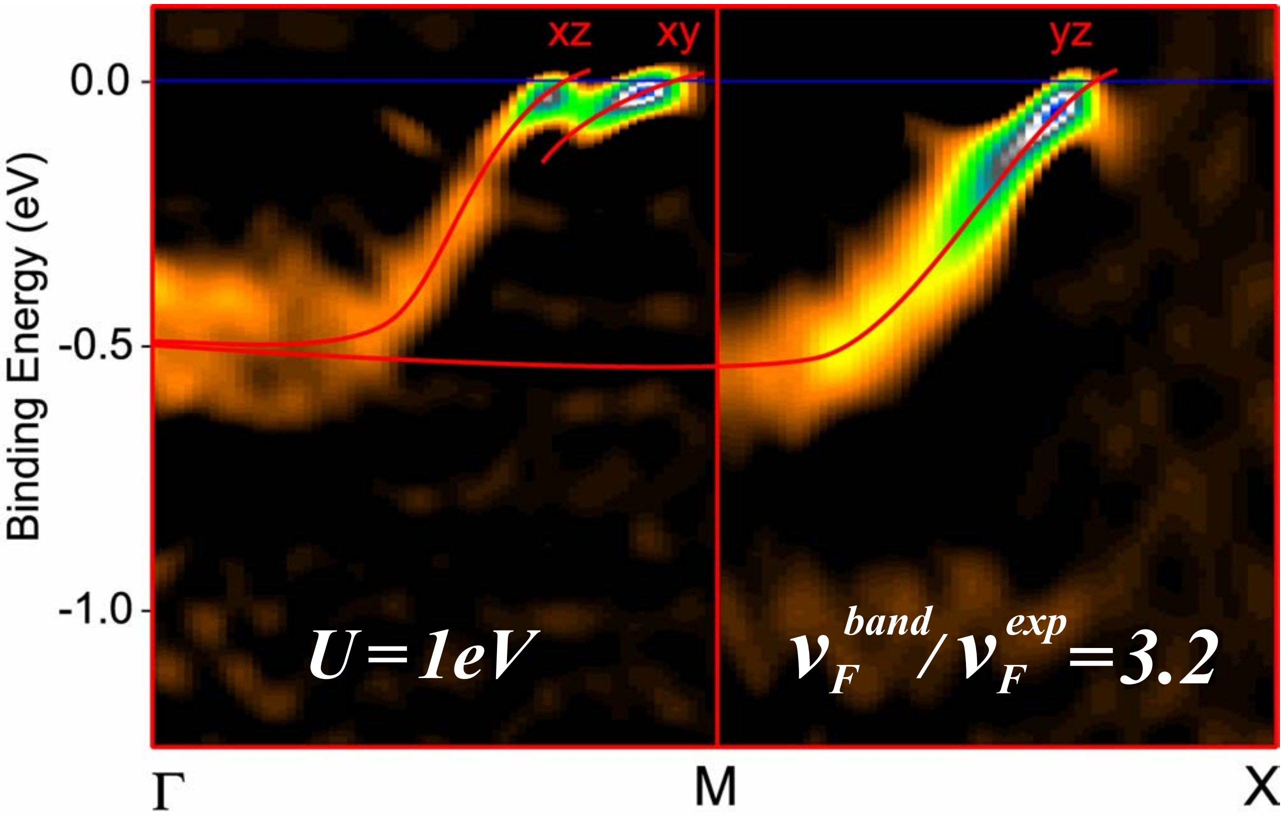



$Sr_2RuO_4$ cleaved at 180 K

T= 10 K hν=28 eV

# Dispersion of the bulk electronic bands




**Experiment compares well with LDA+U calculations**

A. Liebsch & A. Lichtenstein, PRL **84**, 1591 (2000)

# Surface Ferromagnetism?

**Surface Reconstruction ⟷ Surface Ferromagnetism**

R. Matzdorf, Z. Fang, et al., Science **289**, 746 (2000)

**First principle calculations**

**FM surface**

Exchange splitting: **500 meV**

Magnetic moment: **1.0 $\mu_B$/Ru**

Z. Fang & K. Terakura, PRB **64**, 20509 (2001)

**Coexistence of SC and FM on the surface?**

⇩

**Pairing mechanism of SC**

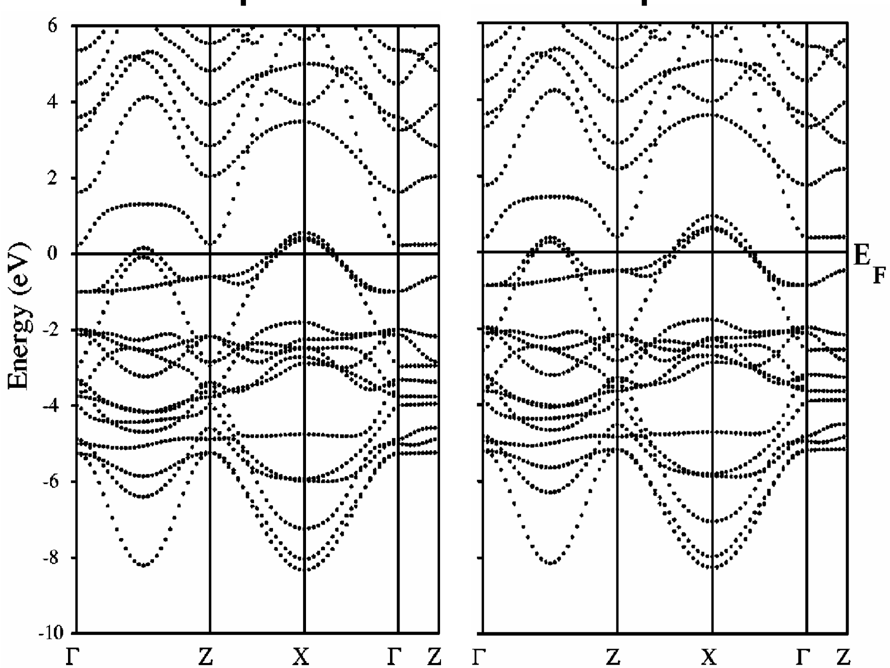
# Surface Ferromagnetism?

**Surface Reconstruction ⟷ Surface Ferromagnetism**

R. Matzdorf, Z. Fang, et al., Science **289**, 746 (2000)

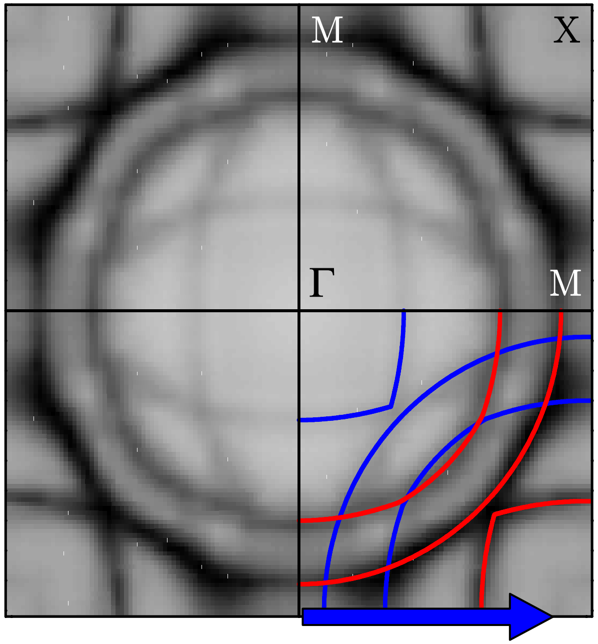
**Spin-split Fermi-level crossings of the electronic bands in $Sr_2RuO_4$**

**Majority spins** **Minority spins**




P.K. de Boer *et al.*, PRB **59**, 9894 (1999)

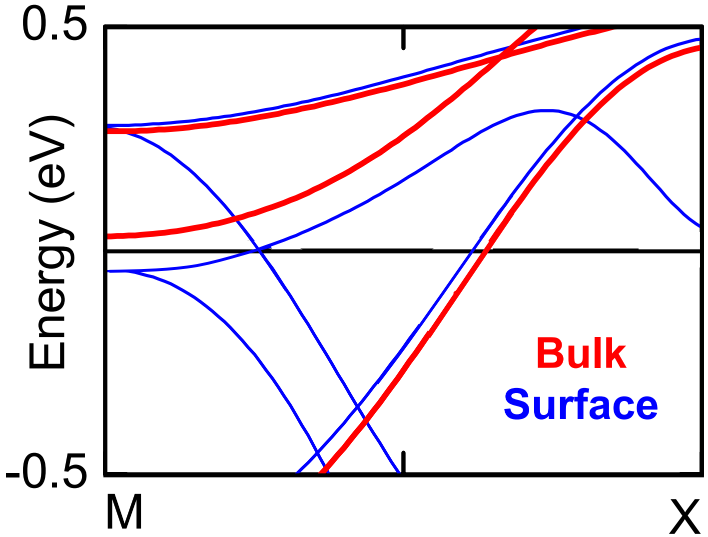
**Where to look for spin-split electronic bands in $Sr_2RuO_4$?**



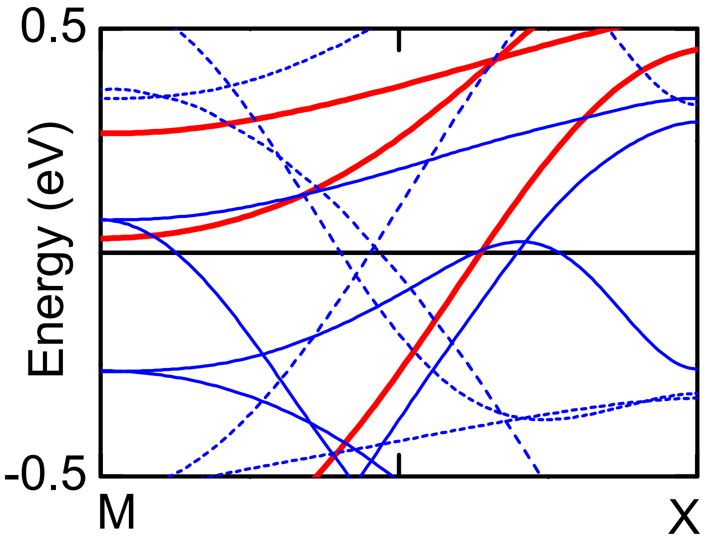
# Evidence for surface FM ?

## Band structure results

Reconstruction (6°)

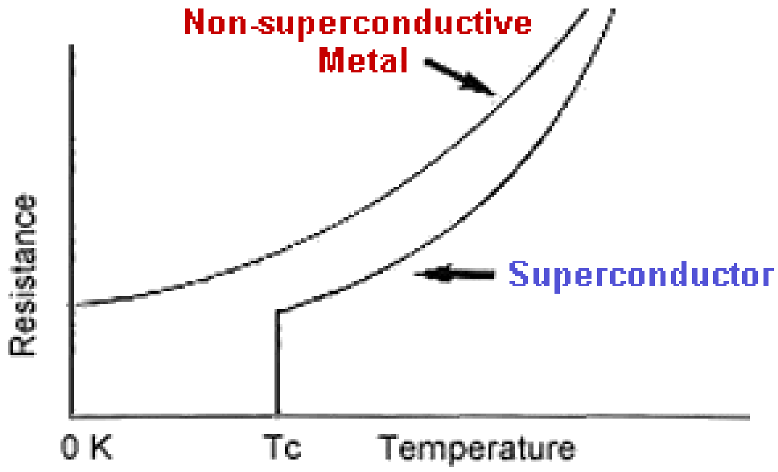


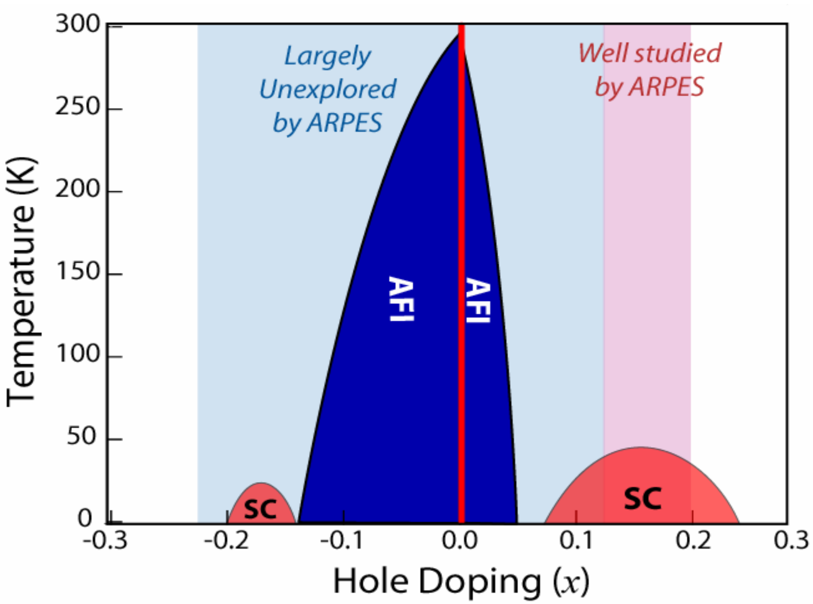

Reconstruction + FM

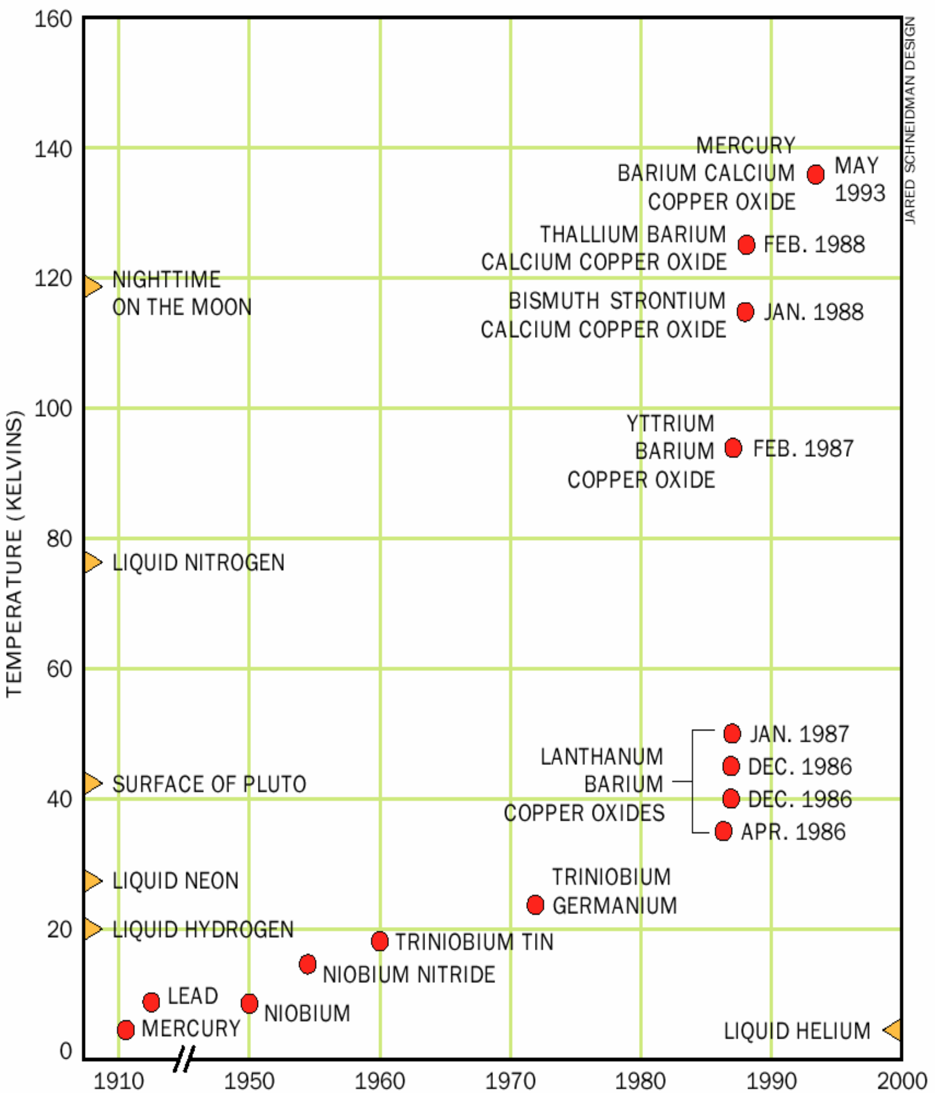



K.M. Shen, A. Damascelli *et al*., PRB **64**, 180502(R) (2001)

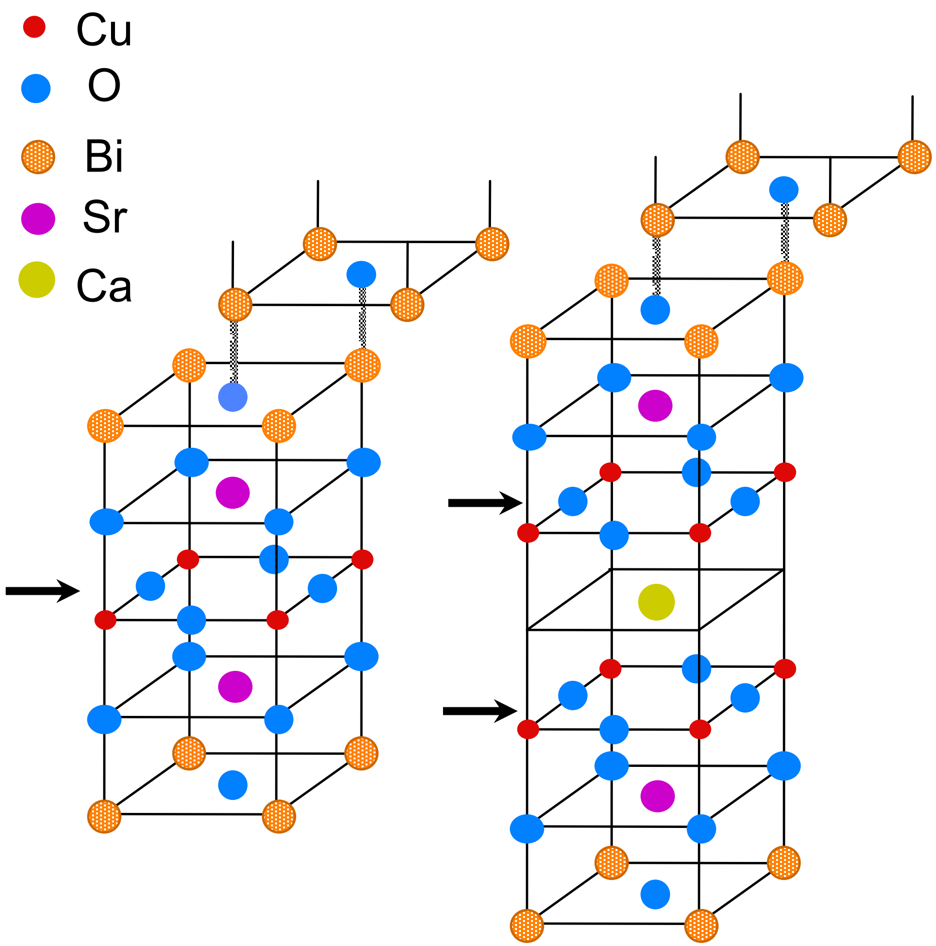
# High-Tc Superconductivity



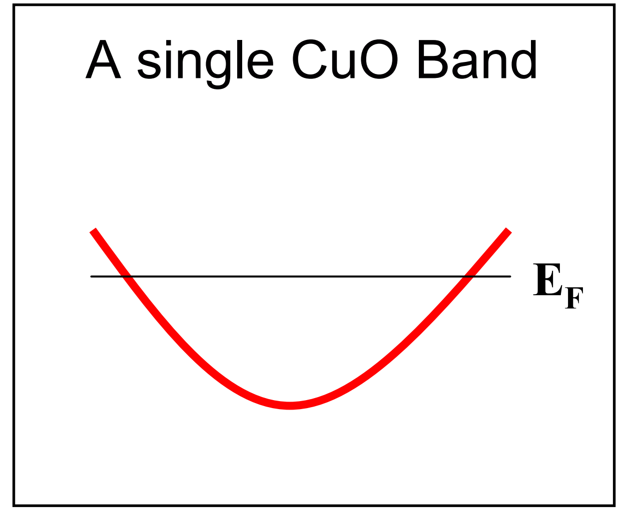



# Bilayer Splitting in $Bi_2Sr_2CaCu_2O_{8+\delta}$

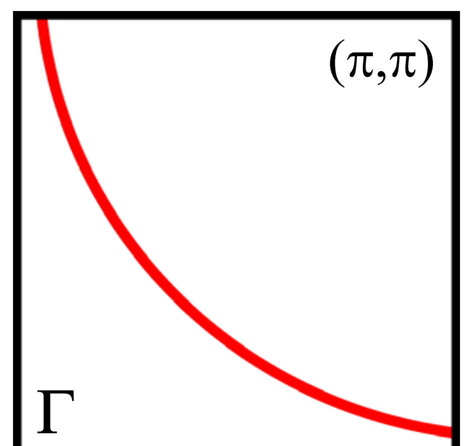



**$Bi_2Sr_2CuO_{6+\delta}$** **$Bi_2Sr_2CaCu_2O_{8+\delta}$**

**Bi2201** **Bi2212**

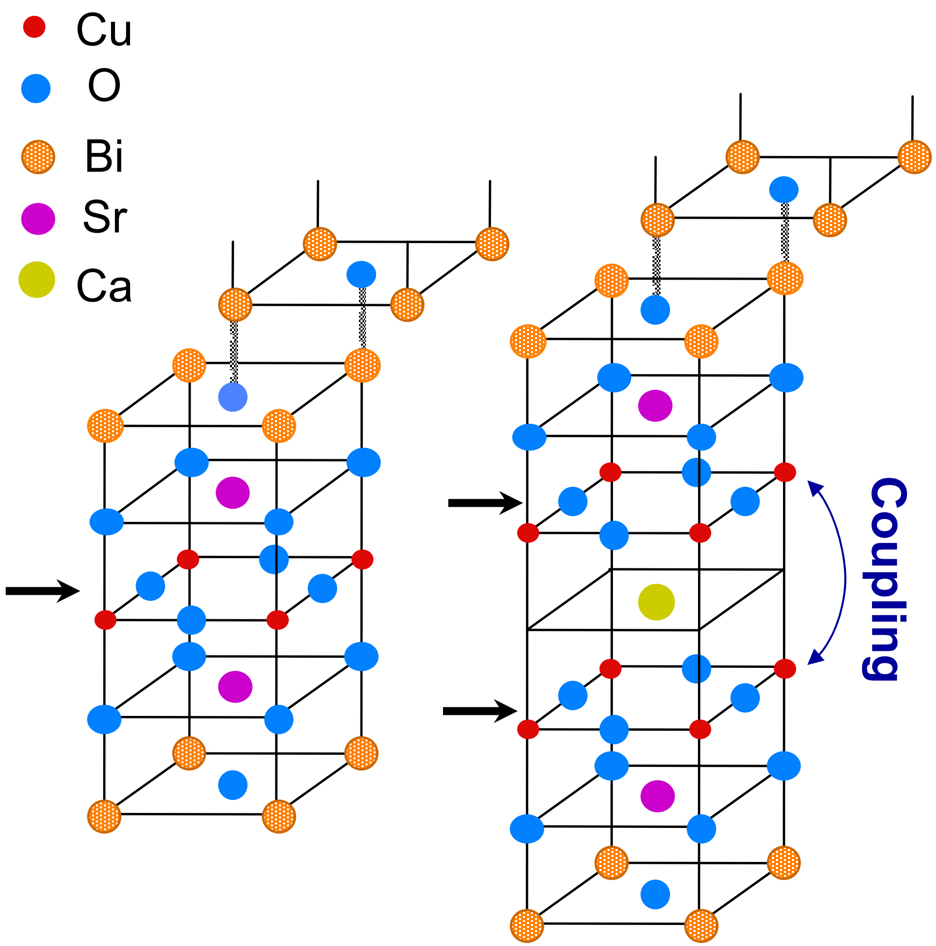



One FS Sheet



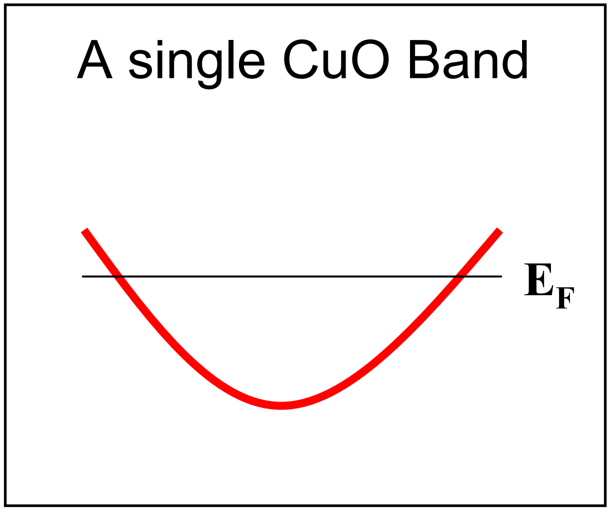

Liechtenstein *et al.*, PRB **54**, 12505 (1996)

# Bilayer Splitting in $Bi_2Sr_2CaCu_2O_{8+\delta}$

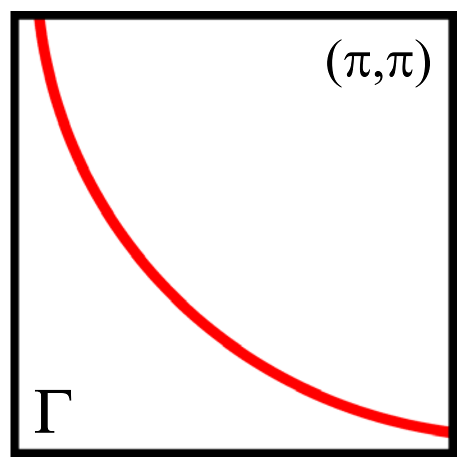



**$Bi_2Sr_2CuO_{6+\delta}$** **$Bi_2Sr_2CaCu_2O_{8+\delta}$**

**Bi2201** **Bi2212**

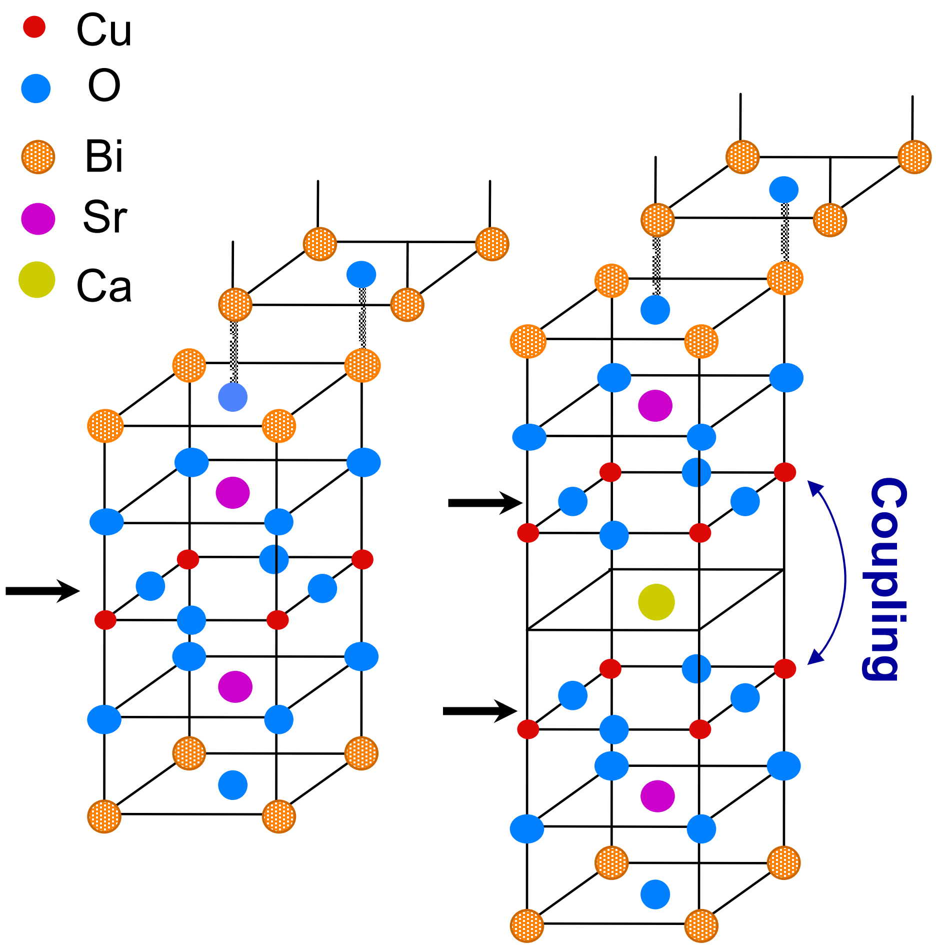



One FS Sheet



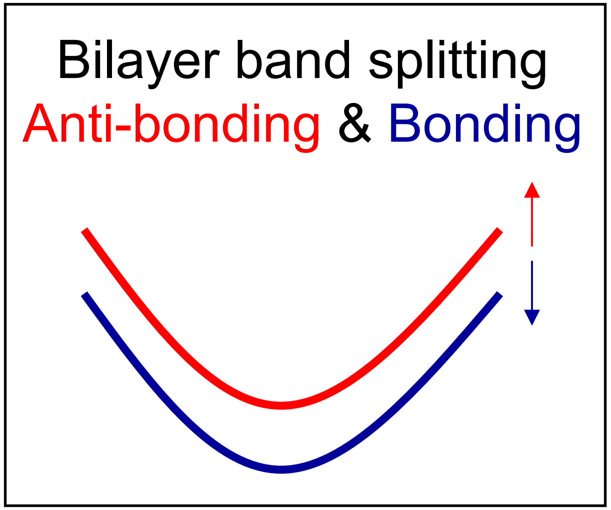

Liechtenstein *et al*., PRB **54**, 12505 (1996)

# Bilayer Splitting in $Bi_2Sr_2CaCu_2O_{8+\delta}$

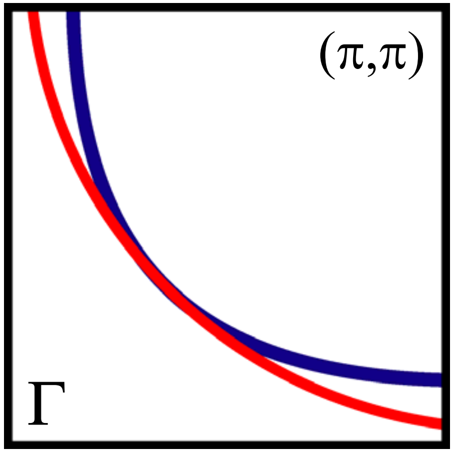



$Bi_2Sr_2CuO_{6+\delta}$ — **Bi2201**

$Bi_2Sr_2CaCu_2O_{8+\delta}$ — **Bi2212**



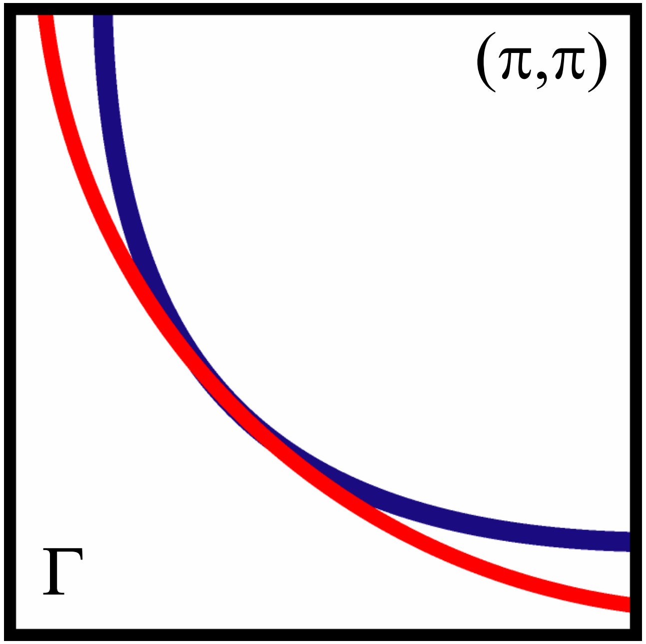

Fermi Surface with bilayer splitting



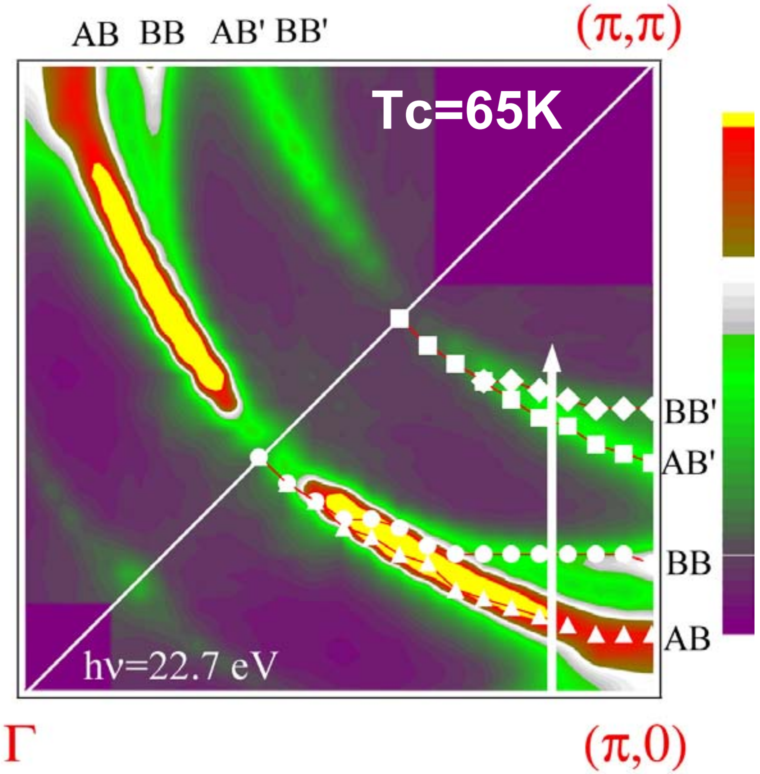

Liechtenstein *et al.*, PRB **54**, 12505 (1996)

# Bilayer Splitting in $Bi_2Sr_2CaCu_2O_{8+\delta}$

**Fermi Surface with bilayer splitting**



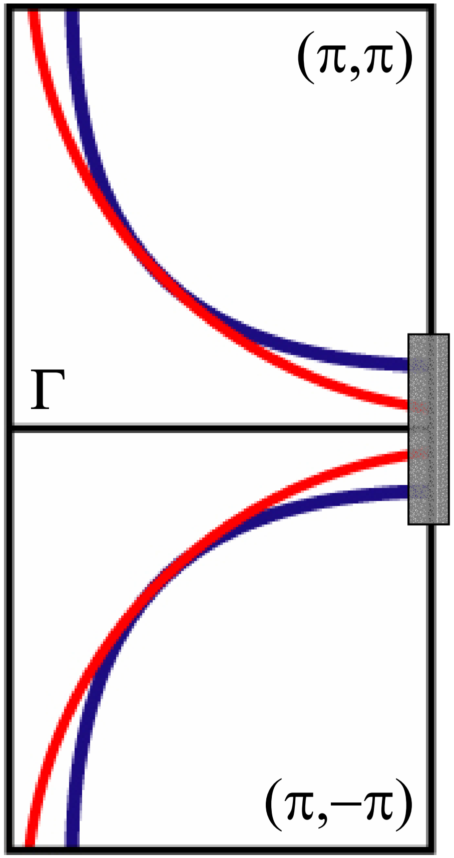

**Overdoped Bi2212 Normal state**



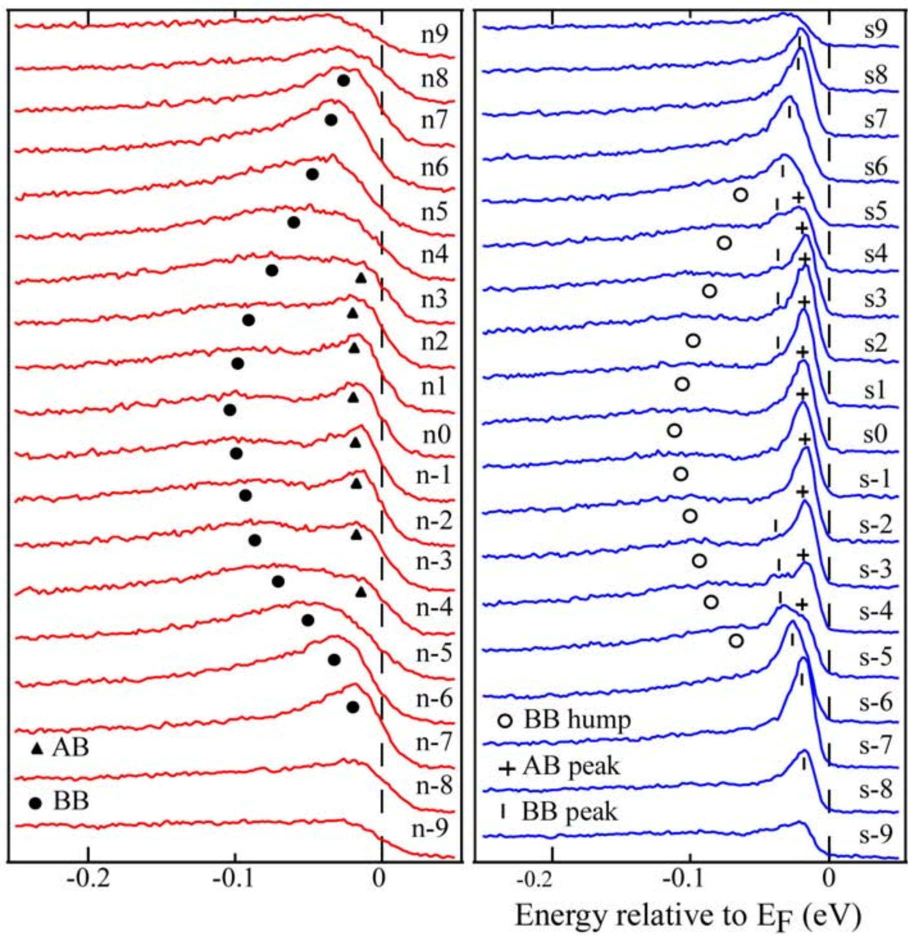

Feng, Damascelli *et al.*, PRL **86**, 5550 (2001)

# Bilayer Splitting in $Bi_2Sr_2CaCu_2O_{8+\delta}$

**Bilayer Split Fermi Surface**



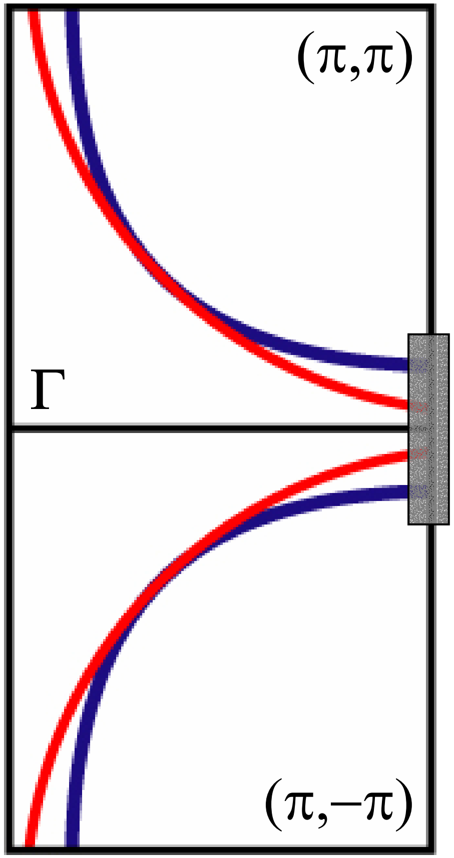

**Normal State T=90K** | **SC State T=10K**



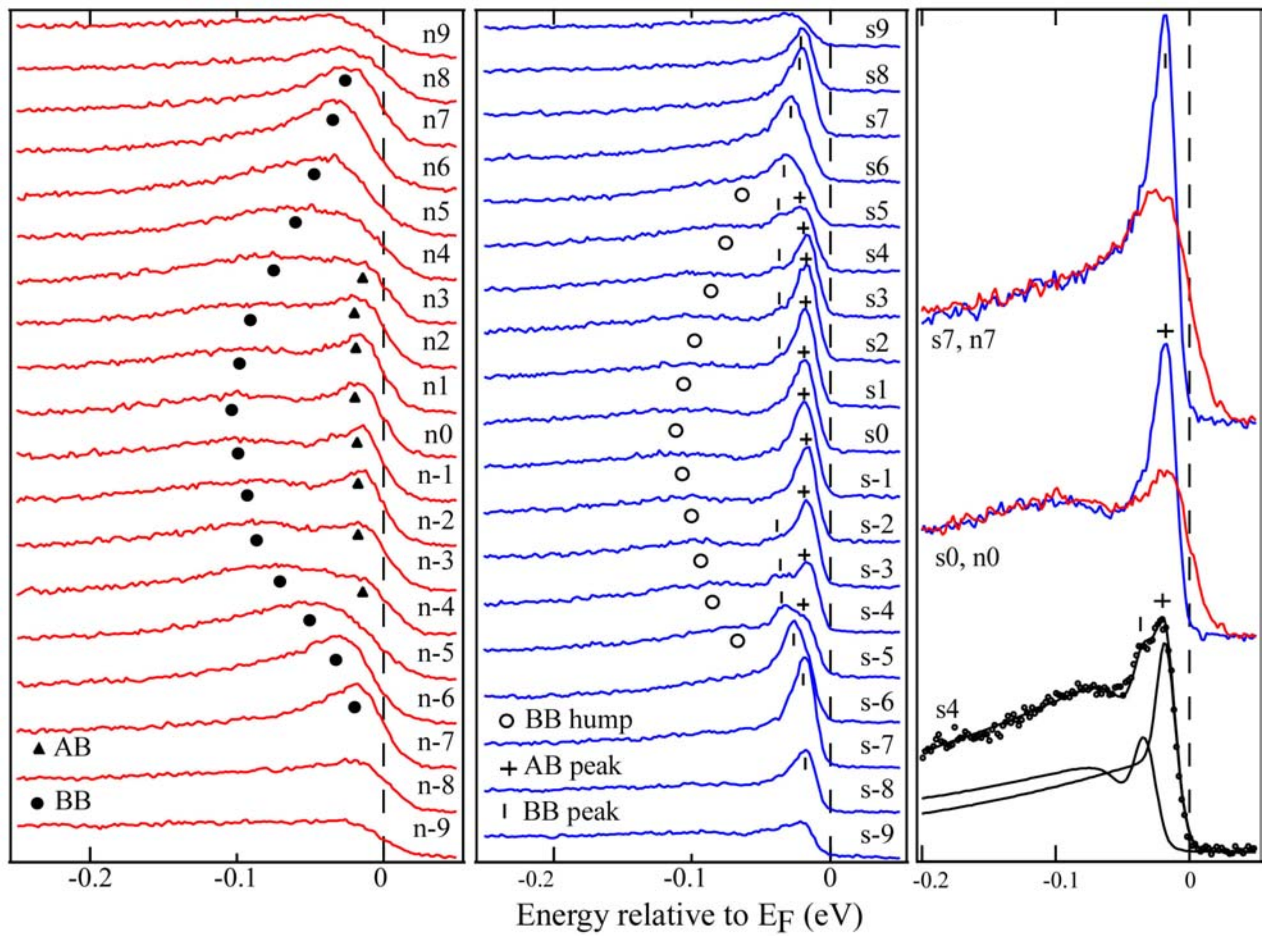

Feng, Damascelli *et al.*, PRL **86**, 5550 (2001)

# Bilayer Splitting in $Bi_2Sr_2CaCu_2O_{8+\delta}$

**Bilayer Split Fermi Surface**

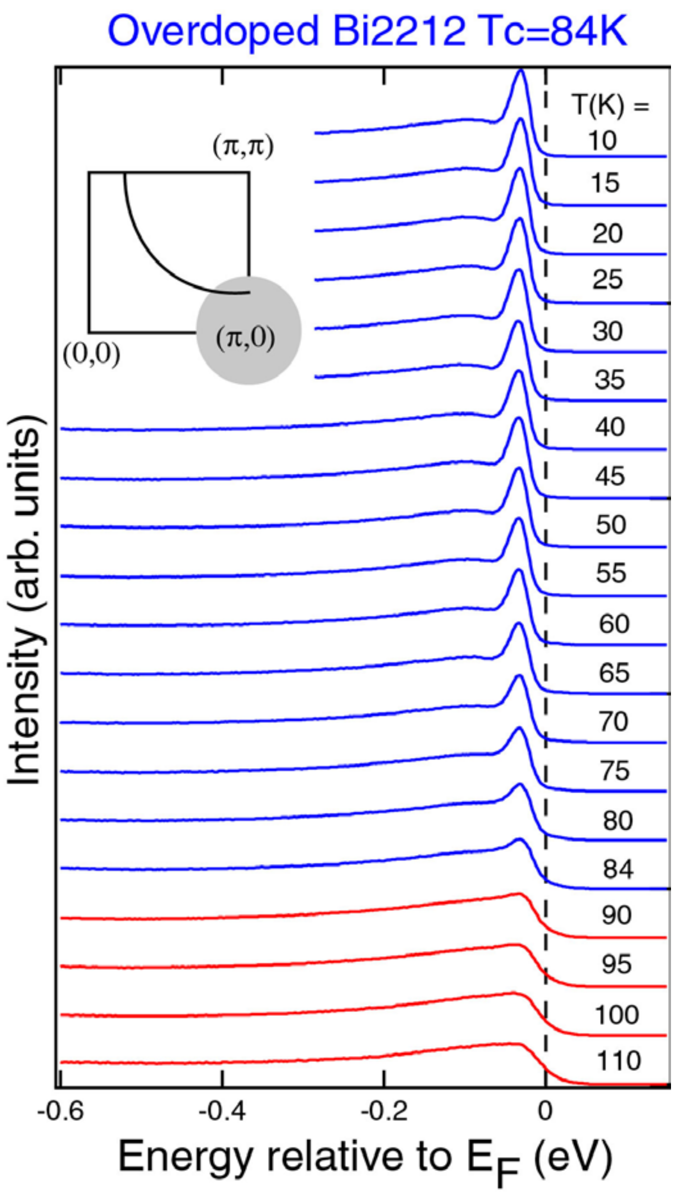


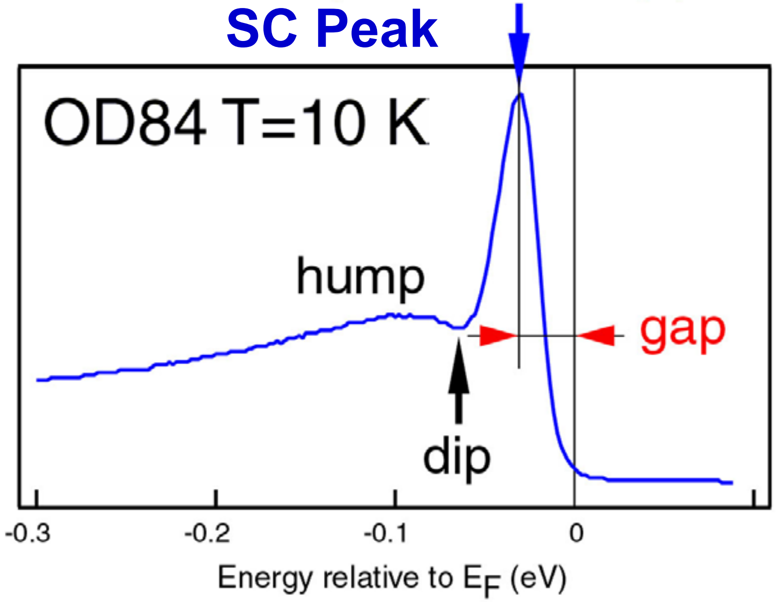

**Normal State T=90K** | **SC State T=10K** | **Normal & SC State Data**




Feng, Damascelli *et al.*, PRL **86**, 5550 (2001)

# SC signatures from ARPES on $Bi_2Sr_2CaCu_2O_{8+\delta}$



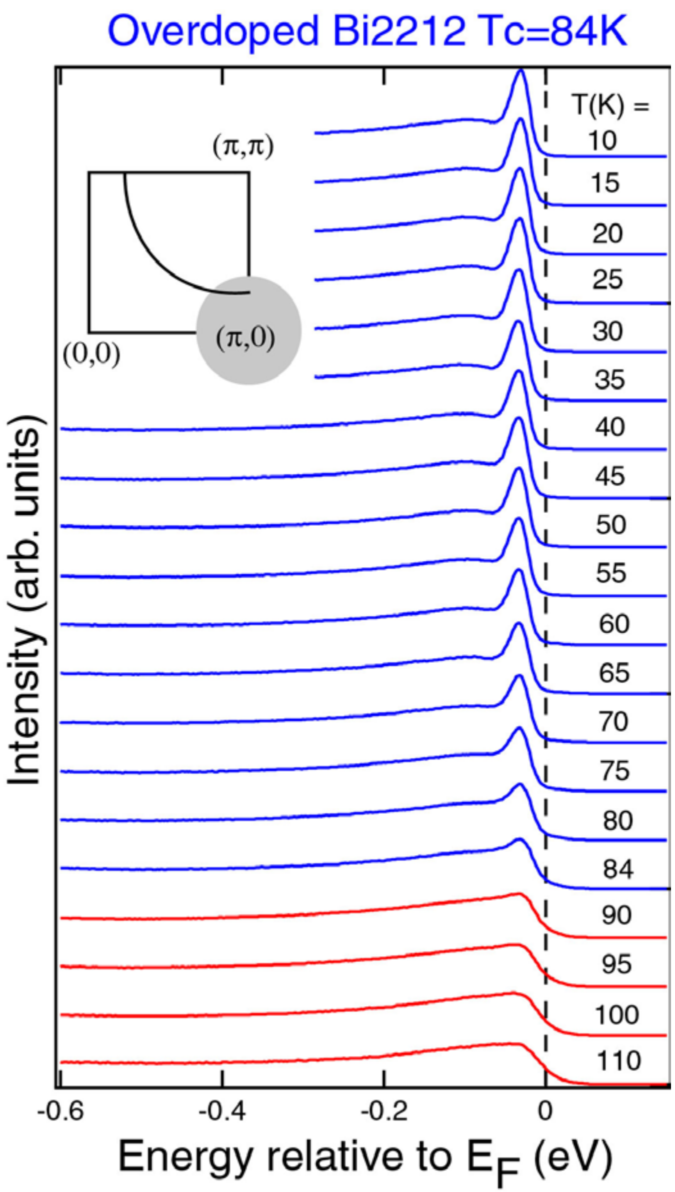

**Pairing**

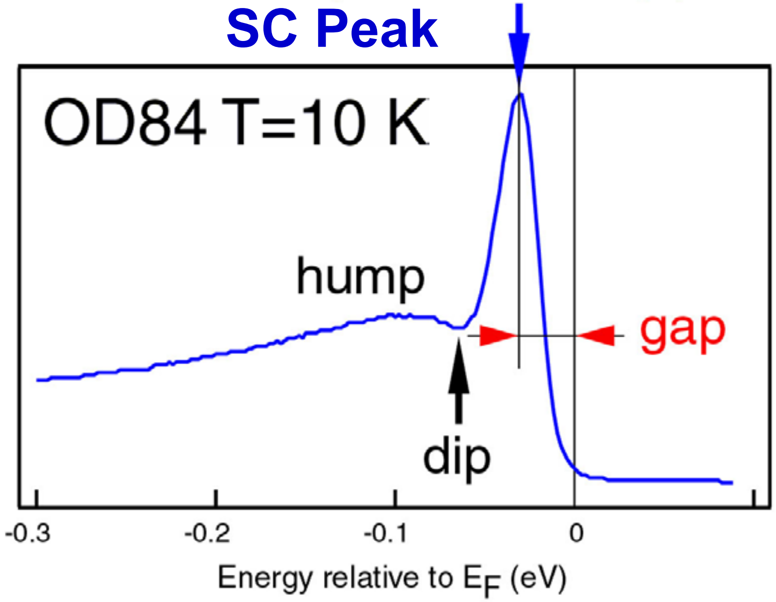
**d-wave SC Gap**

**Phase coherence** ?

Feng, Damascelli *et al.*, Science **289**, 277 (2000)

# SC signatures from ARPES on $Bi_2Sr_2CaCu_2O_{8+\delta}$



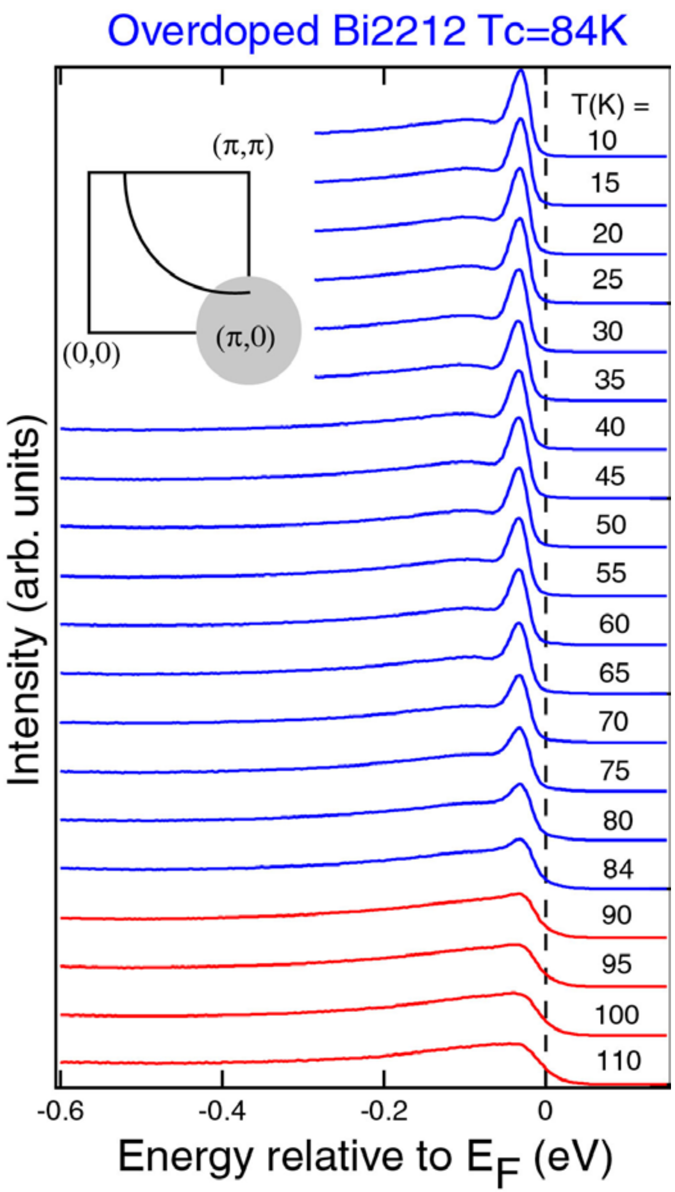



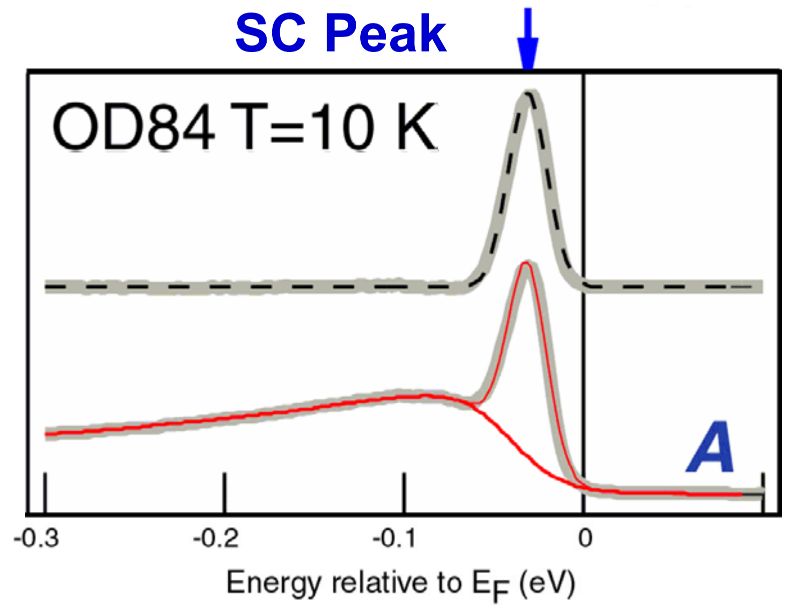

**Pairing**
**d-wave SC Gap**

**Phase coherence**
**Coherent QP weight**

Feng, Damascelli *et al.*, Science **289**, 277 (2000)

# SC signatures from ARPES on $Bi_2Sr_2CaCu_2O_{8+\delta}$




**Pairing**

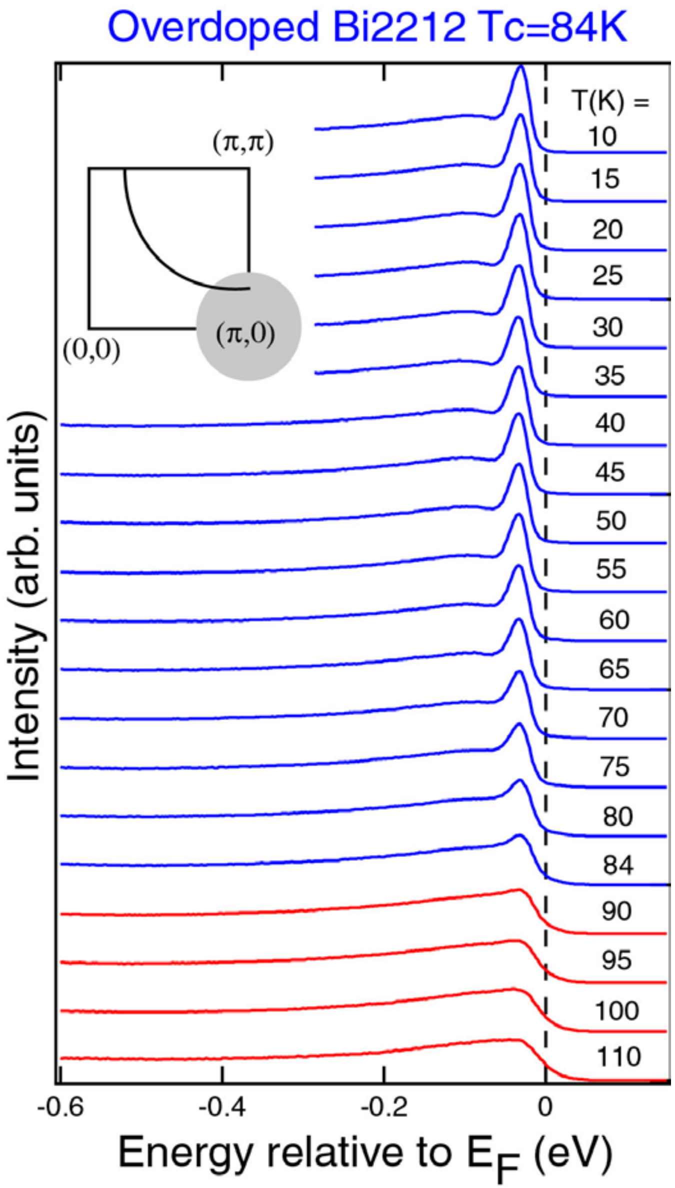
**d-wave SC Gap**

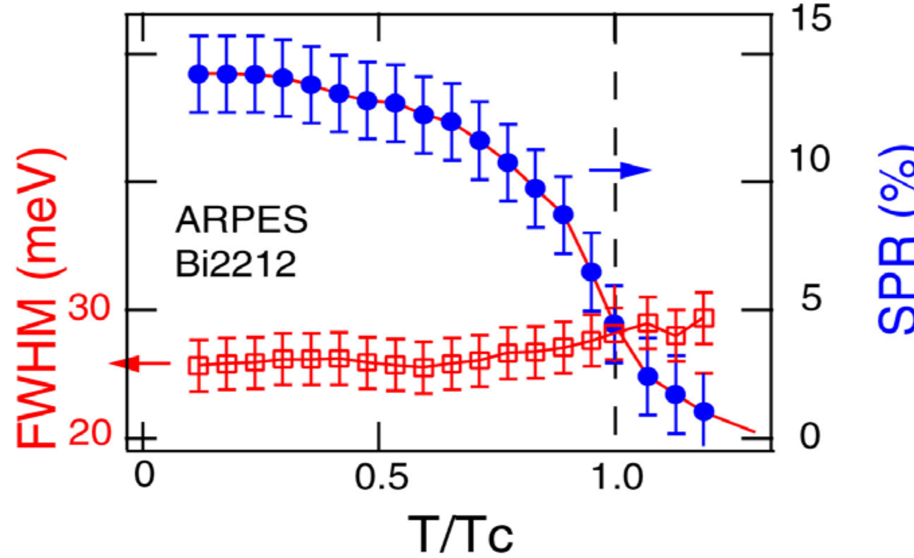
**Phase coherence**

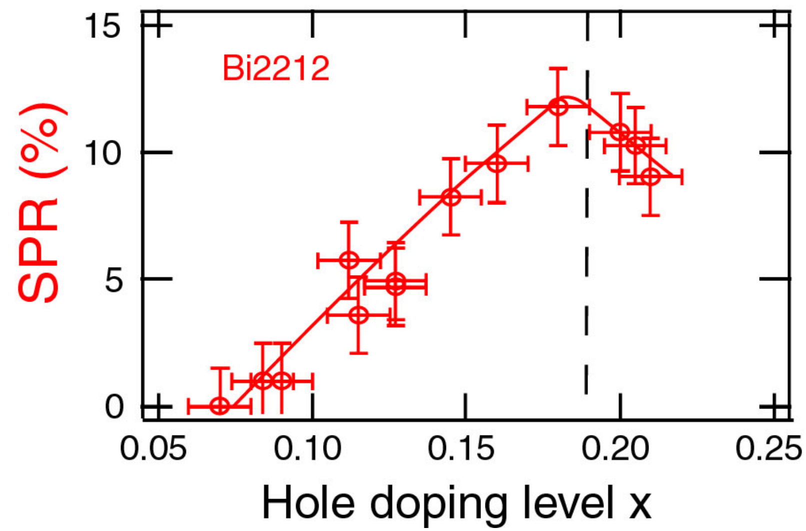
**Coherent QP weight**

Feng, Damascelli *et al.*, Science **289**, 277 (2000)

# SC signatures from ARPES on $Bi_2Sr_2CaCu_2O_{8+\delta}$

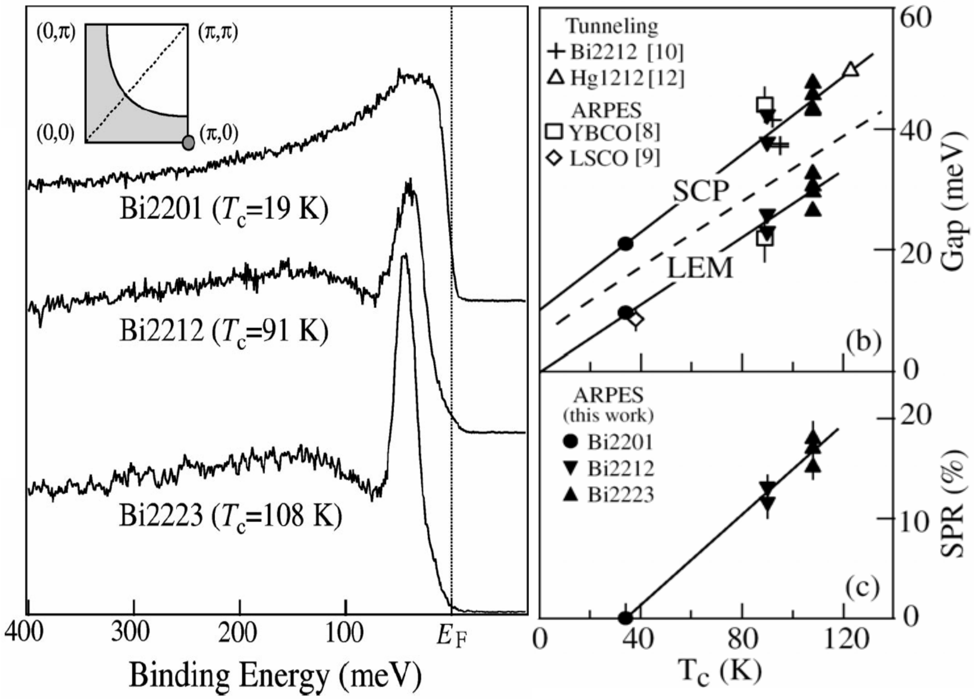



Feng, Damascelli *et al.*, Science **289**, 277 (2000)

# SC signatures from ARPES on Bi-Cuprates

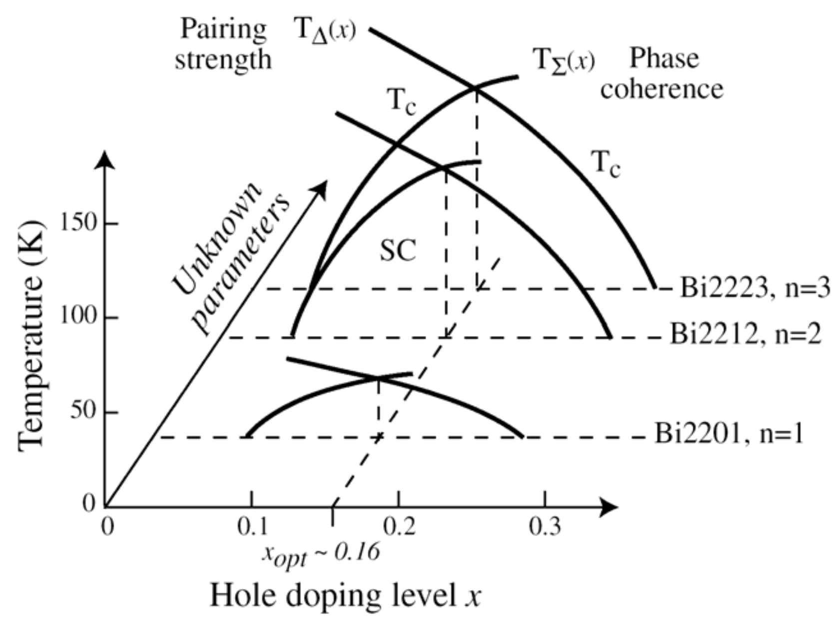



$$\Delta_{0,\mathrm{opt}} \propto T_{c,\mathrm{opt}}$$

$$\rho_{s,\mathrm{opt}} \propto T_{c,\mathrm{opt}}$$

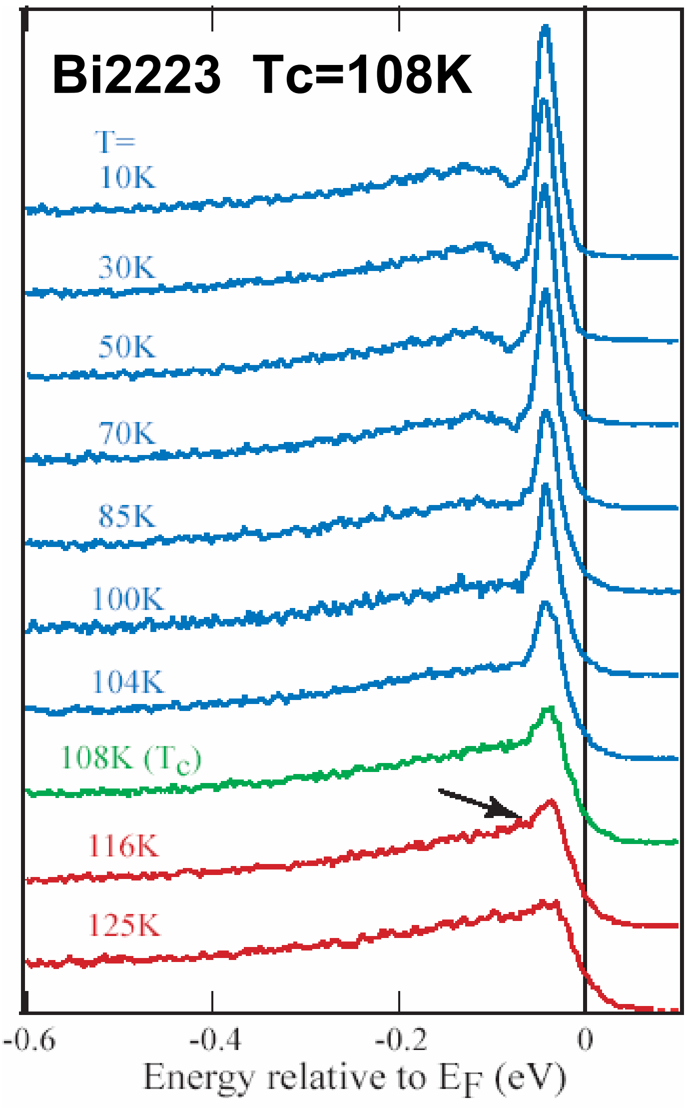
$$T_c = \min(T_\Delta, T_\Sigma)$$

$$T_\Delta(x_{\mathrm{opt}}) = T_\Sigma(x_{\mathrm{opt}}) = T_{c,\mathrm{opt}}$$




Feng, Damascelli *et al.*, PRL **88**, 107001 (2002)

# Electronic Structure of Bi2223: Superconducting Peak




## Coherent transition

**Well defined Quasi Particles may be formed only at large doping and/or below Tc**

Feng, Damascelli *et al.*, PRL **88**, 107001 (2002)

## QP lifetime catastrophe

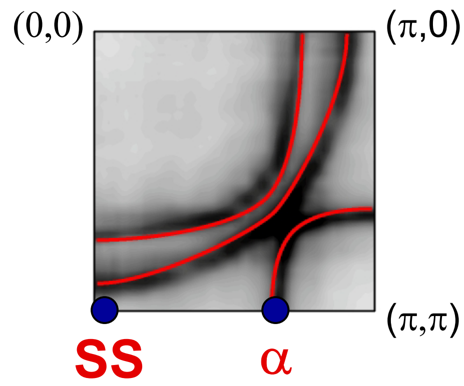
**The coherence factor Z does not vanish above Tc**

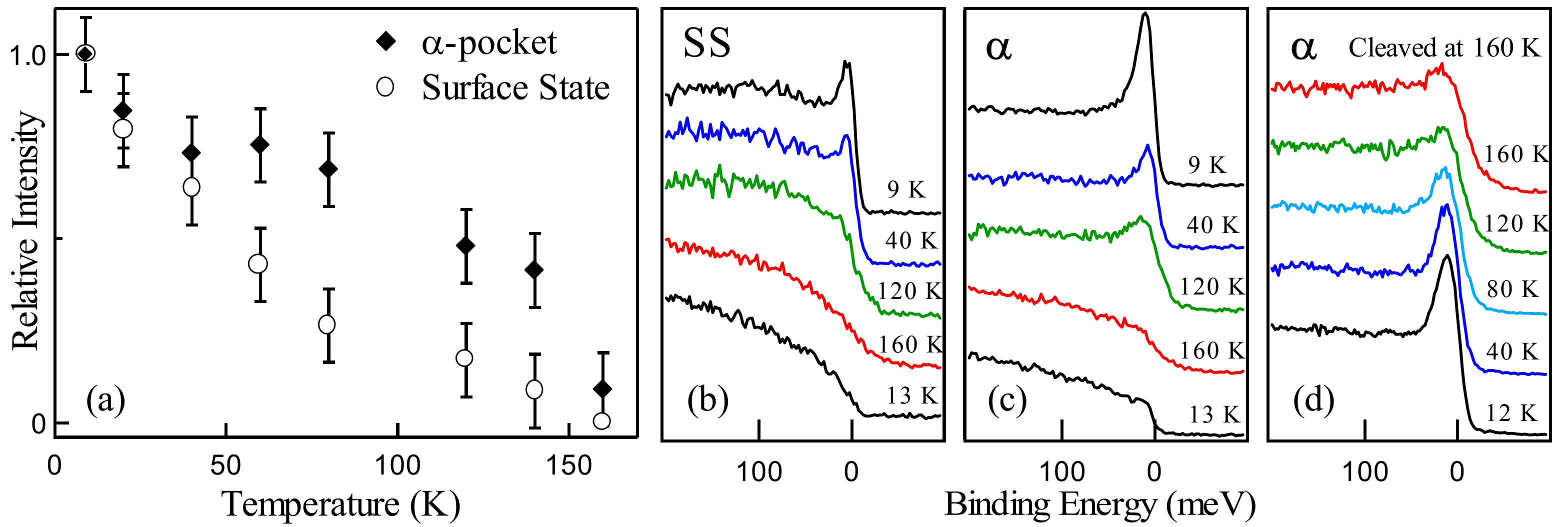
**is the reduction of lifetime that broadens the QP out of existence**

Norman *et al.*, PRB **63**, 140508 (2001)

# 2D-3D Crossover in $Sr_2RuO_4$ at T=130K ?

## Temperature dependence along the M-X cut




A. Damascelli *et al.*, JESRP **114-116**, 641 (2001)

# Conclusions

## ARPES results from complex systems

- **Bands and FS in unprecedented detail**
- **Fermi velocity and effective mass**
- **Superconducting (d-wave) gap**
- **Many-body effects (superfluid density)**
- **Surface FM (nanostructured materials)**

➡ **ARPES is a powerful tool for the study of the electronic structure of complex systems**

---

**For a review article see:**

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

**For additional material see:**

www.physics.ubc.ca/~QuantMat/ARPES.html