# Study of many-body quantum phenomena in the ruthenium-oxides by ARPES

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*University of British Columbia*
*Vancouver, B.C.*

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S. Wang
F. Cao
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M. Plate
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J. Mottershead

**Nicholas Ingle**

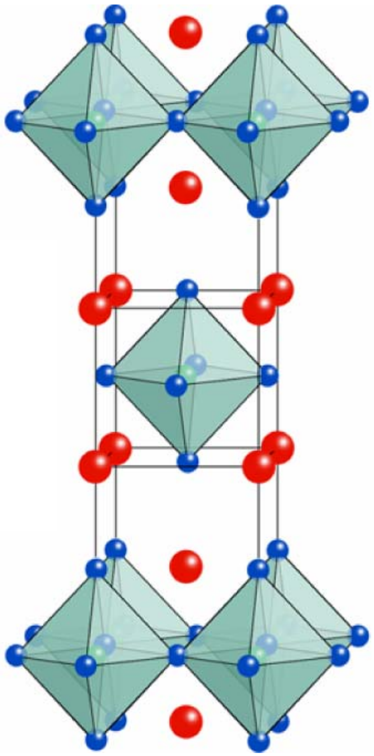
# Outline

- ▶ Electronic structure of **complex systems**
- ▶ State-of-the-Art **ARPES:** the essentials
- ▶ **$Sr_2RuO_4$**
  - ● **Introduction**
    - Interesting properties and open issues
    - Fermi surface controversy
  - ● **Experimental results**
    - **Bulk & surface** electronic structure
    - Surface **Ferromagnetism ?**
- ▶ Outlook and conclusions

# Collaborators

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

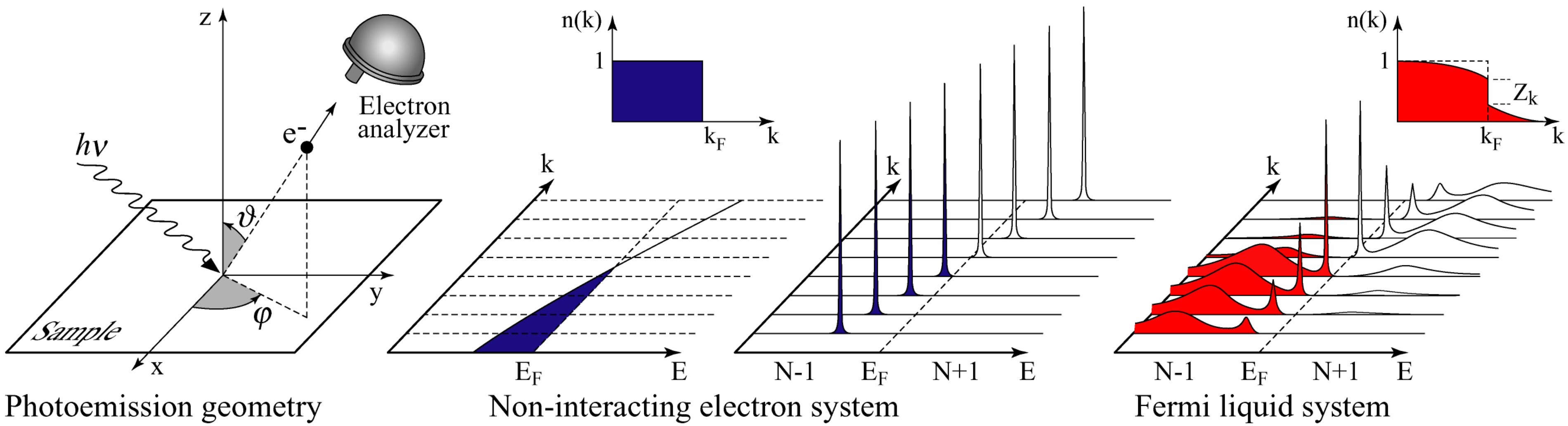

- **Band Structure Calculations (NRL, Washington):**
  I.I. Mazin, D.J. Singh



- **Samples:**
  - **$Sr_2RuO_4$**
    S. Nakatsuji, T. Kimura, Y. Tokura, Z.Q. Mao, Y. Maeno
  - **$Sr_3Ru_2O_7$**
    R.S. Perry, A.P.Mackenzie, Y. Maeno
  - **$Tl_2Ba_2CuO_{6+\delta}$**
    D. Peets, D.A. Bonn, R. Liang, W.N. Hardy

# ARPES: The One-Particle Spectral Function

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




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

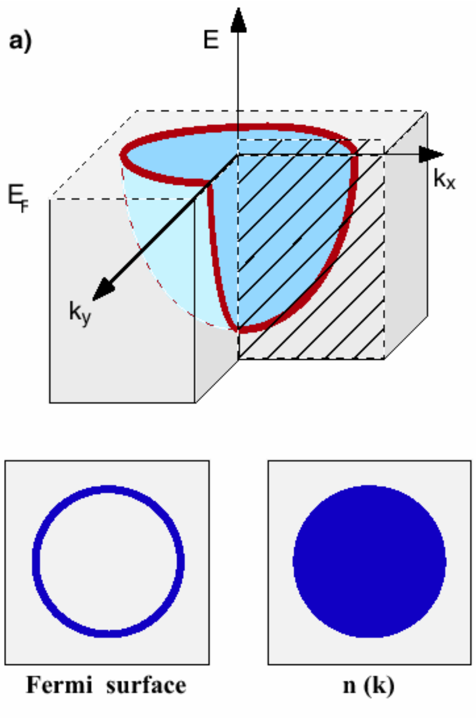
**Single-particle spectral function**

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

$\Sigma(\mathbf{k},w)$ **: the "self-energy" captures the effects of interactions**

# Understanding the Solid State: Electrons in Reciprocal Space

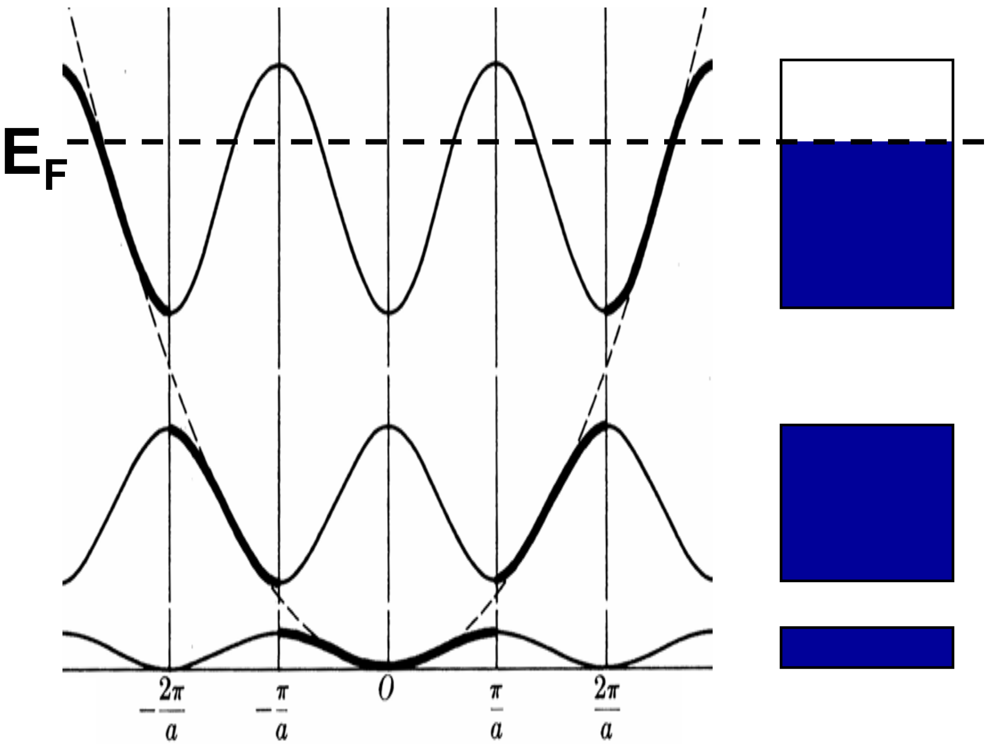
Many **properties** of a solids are determined by **electrons near $E_F$** (**conductivity**, **magnetoresistance**, **superconductivity**, **magnetism**)




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

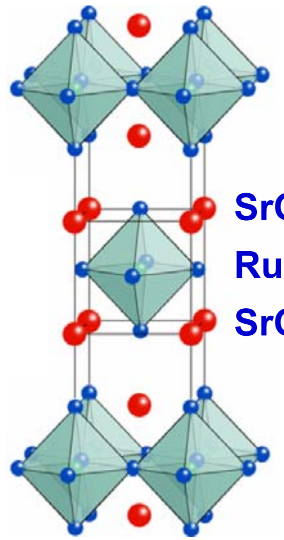
**Allowed electronic states**

Repeated-zone scheme



# $Sr_2RuO_4$: basic properties

**2D perovskite**

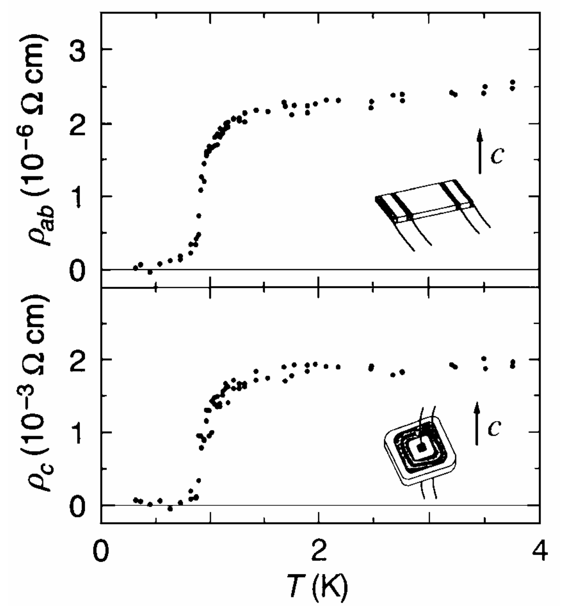



## Unconventional superconductivity

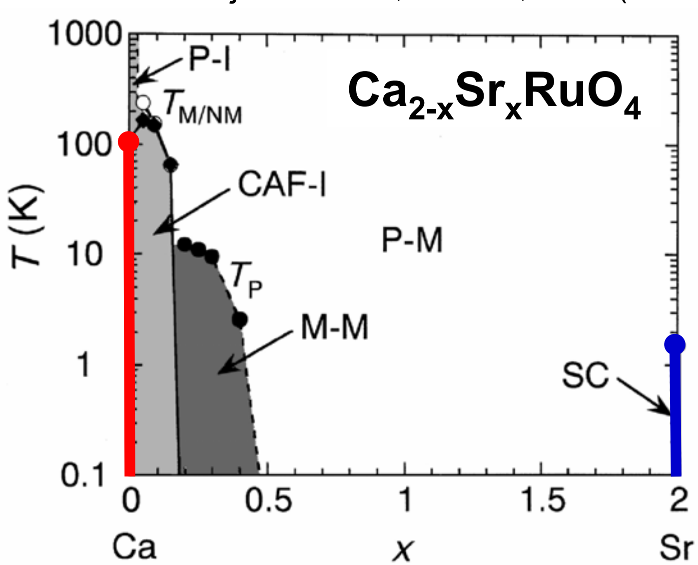
- Pairing mechanism ?
- Order parameter ?
- FM-AF fluctuations ?

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

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




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



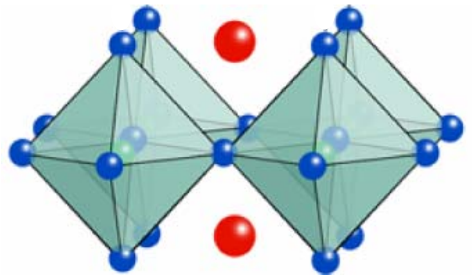

**Lattice-magnetism interplay**
**Orbital degrees of freedom**

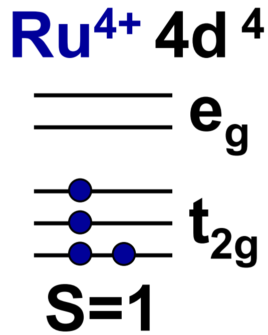
$Sr_2RuO_4$ : 2D **Fermi Liquid** ($\rho_c/\rho_{ab}$=850)

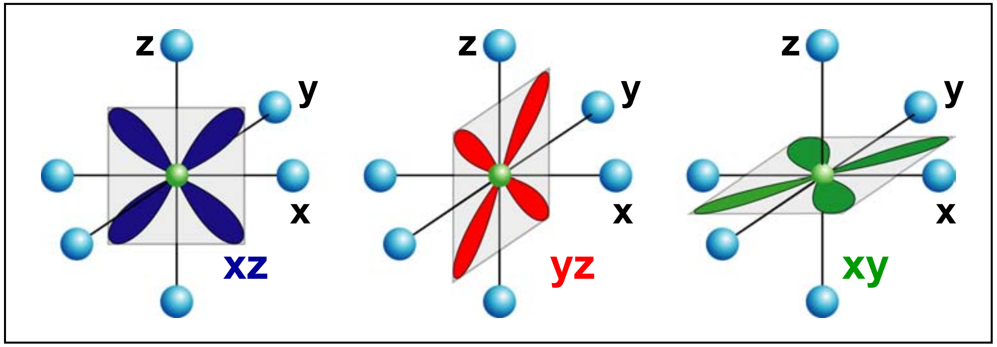
$Ca_2RuO_4$ : insulating **Anti-FerroMagnet**

$SrRuO_3$ : metallic **FerroMagnet**

# Low-Energy Electronic structure of $Sr_2RuO_4$

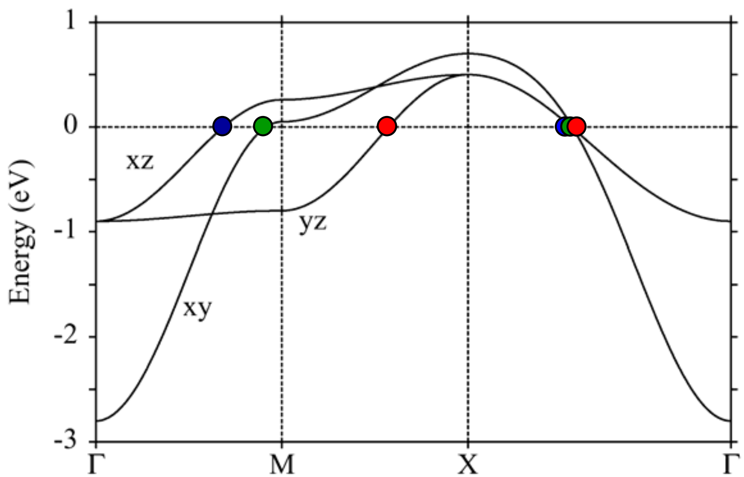




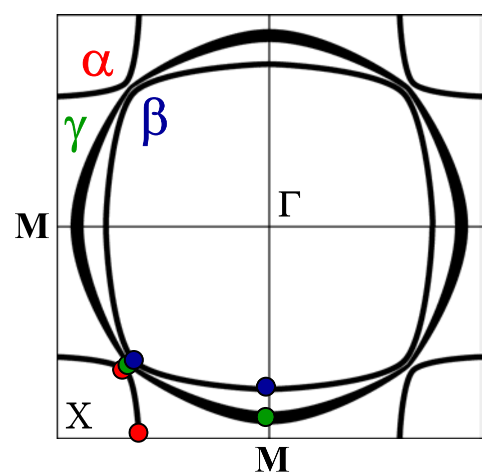




▶ Band structure calculation: **3 $t_{2g}$** bands crossing $\mathbf{E_F}$

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




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

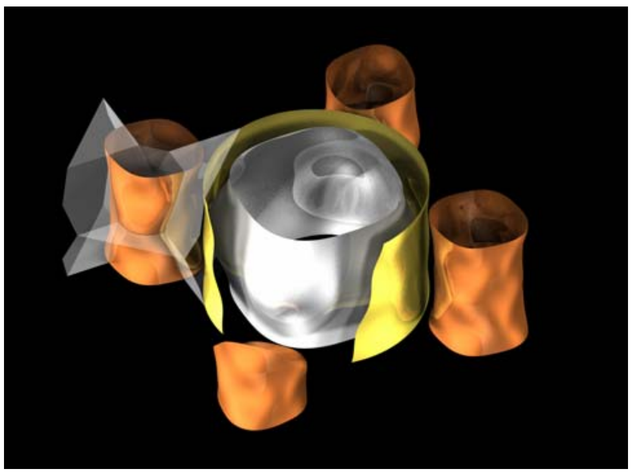



I.I. Mazin *et al*, PRL **79**, 733 (1997)

# Fermi Surface Topology of $Sr_2RuO_4$

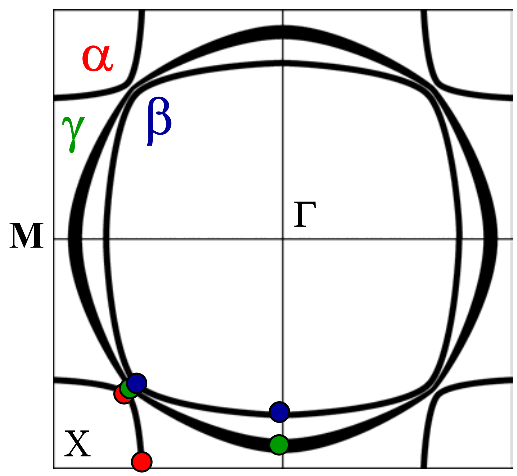
▶ **Early ARPES results gave a different topology**

**de Haas-van Alphen**



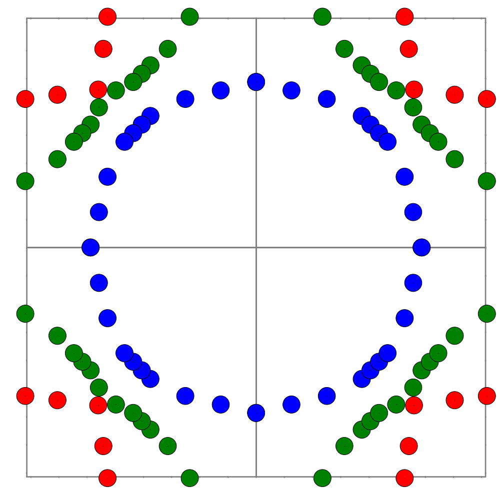
A.P. Mackenzie *et al.*, PRL **76**, 3786 (1996)
C. Bergemann *et al.*, PRL **84**, 2662 (2000)

**LDA**




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

**ARPES**

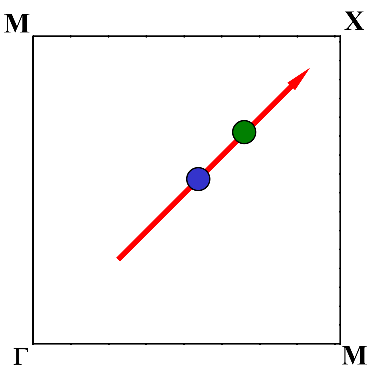


T.Yokoya *et al.*, PRB **54**, 13311 (1996)
D.H. Lu *et al.*, PRL **76**, 4845 (1996)

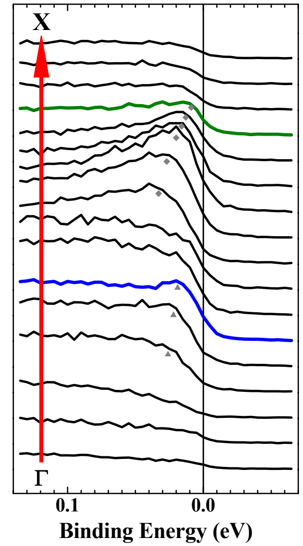
**Reliability of ARPES ??**

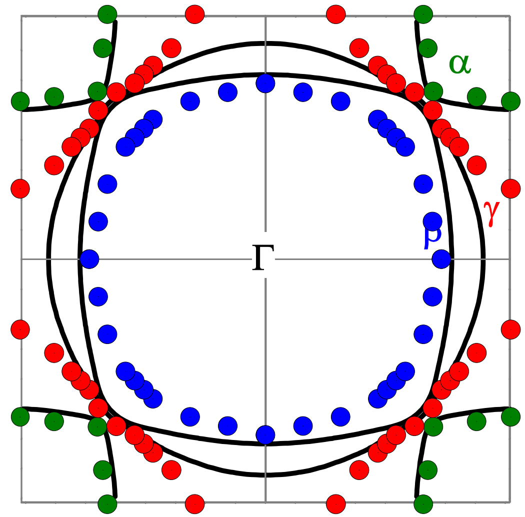
# Fermi Surface Topology of $Sr_2RuO_4$

## *ARPES : circa 1996*



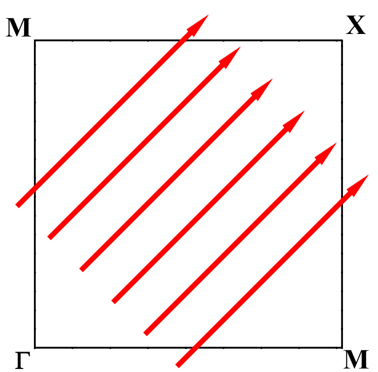

D.H. Lu *et al.*, PRL **76**, 4845 (1996)



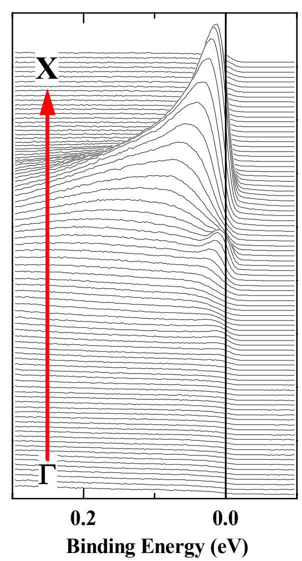



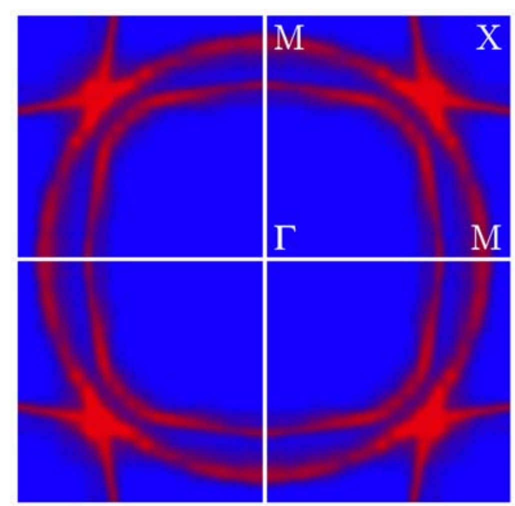

D.J. Singh, PRB **52**, 1358 (1995)

## *ARPES : present day*



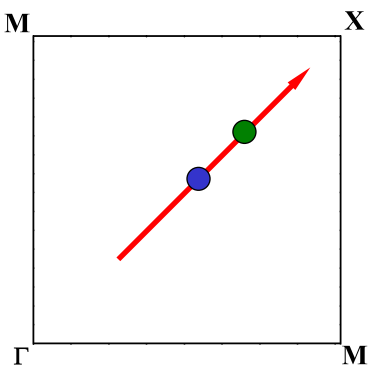

A. Damascelli *et al.*, PRL **85**, 5194 (2000)



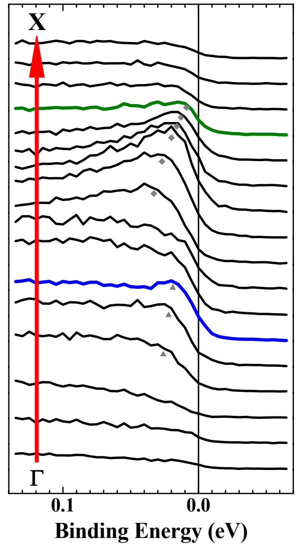



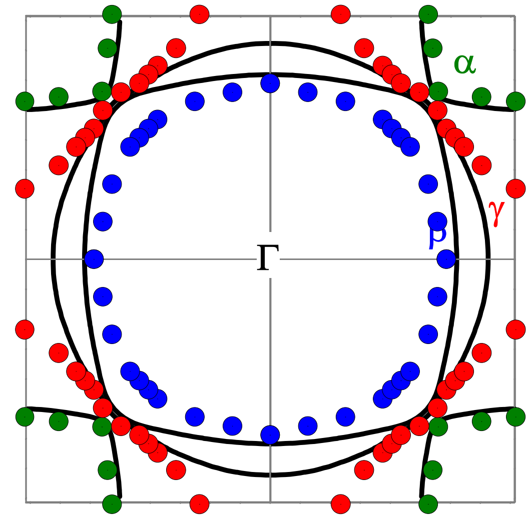
# Fermi Surface Topology of $Sr_2RuO_4$

## ***ARPES : circa 1996***



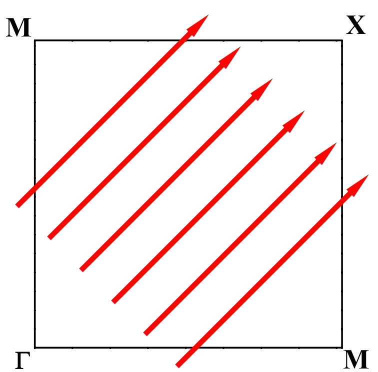

D.H. Lu *et al.*, PRL **76**, 4845 (1996)



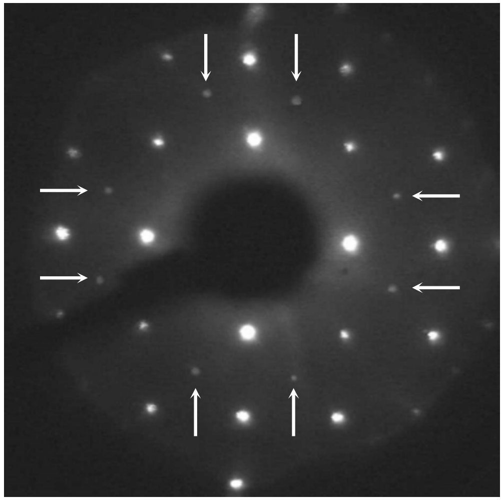

D.J. Singh, PRB **52**, 1358 (1995)

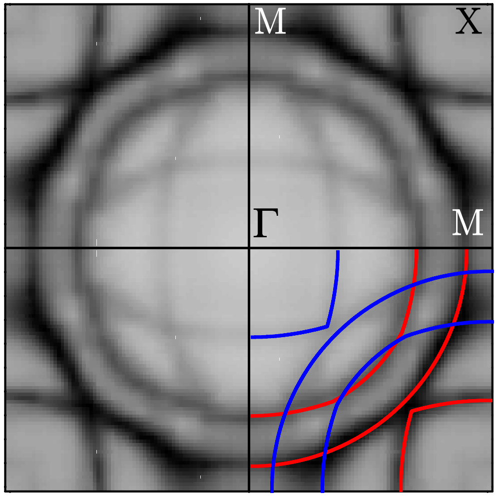
## ***ARPES : present day***



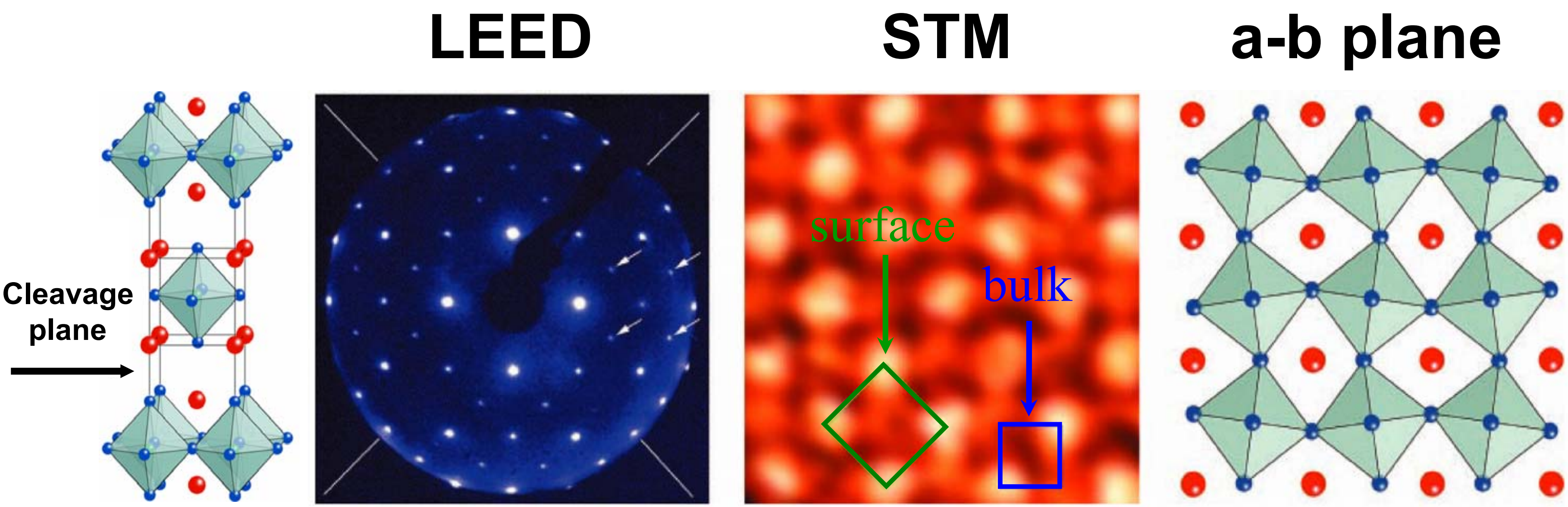

A. Damascelli *et al.*, PRL **85**, 5194 (2000)

**Surface instability** ↔ **Band folding**





# Surface reconstruction of cleaved $Sr_2RuO_4$



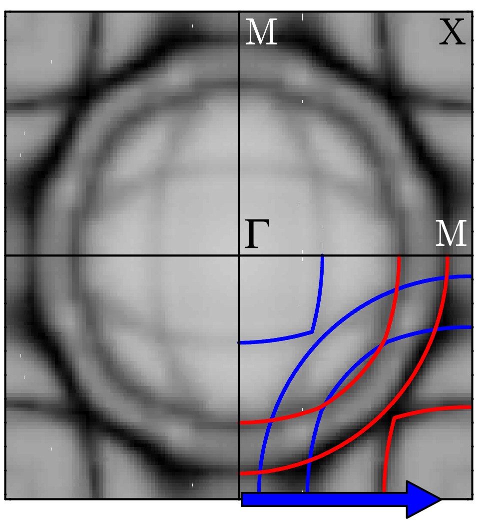

R. Matzdorf *et al.*, Science **289**, 746 (2000)

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

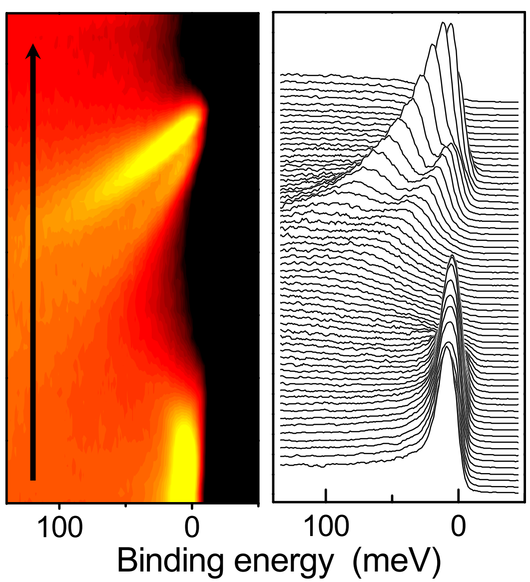
# Surface electronic structure of $Sr_2RuO_4$

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

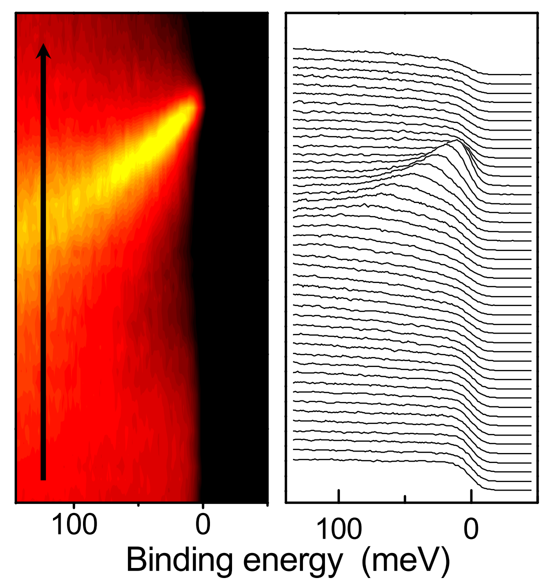
**$E_F$ mapping ±10 meV**




**Cold cleave T=10 K**



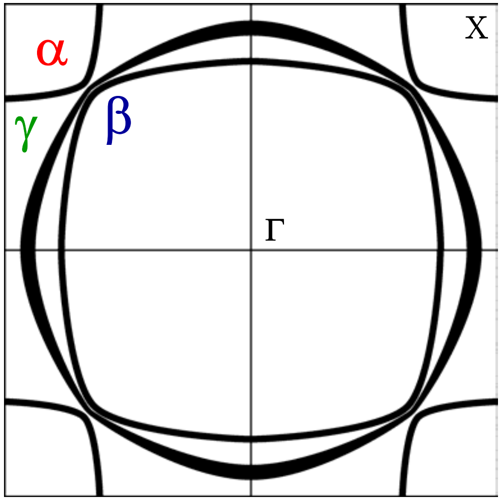

**Hot cleave T=180 K**



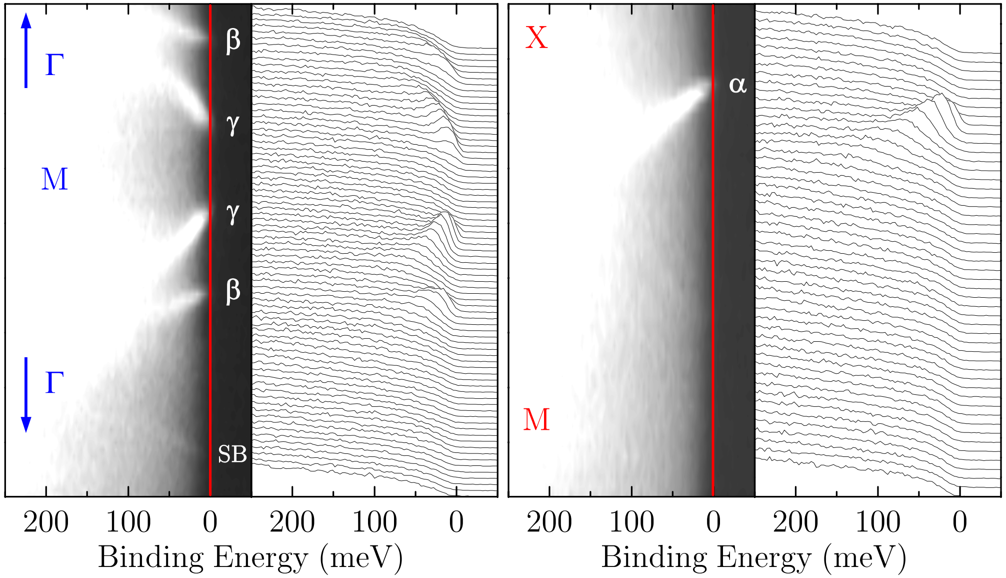
# Bulk electronic structure of $Sr_2RuO_4$

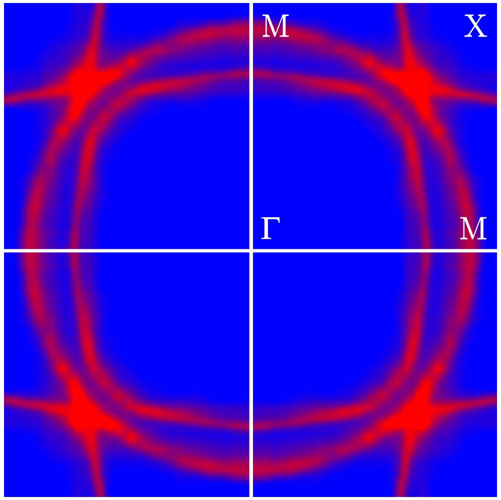
**What do we learn about the bulk electronic structure?**

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




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



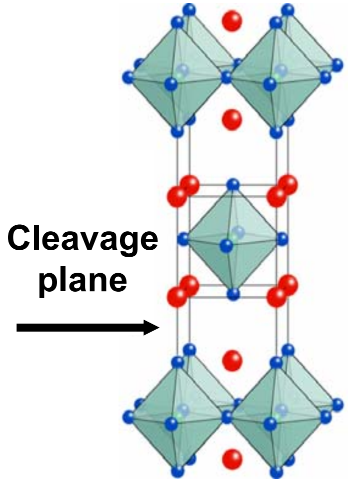

$Sr_2RuO_4$ cleaved at 180 K

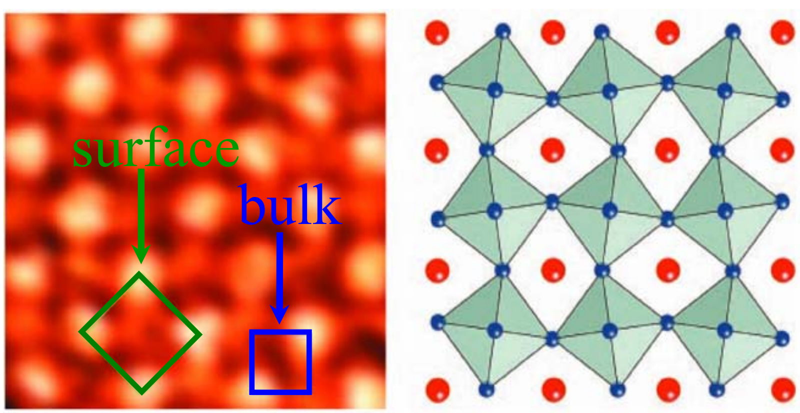
T= 10 K  hν=28 eV

# Surface reconstruction of cleaved $Sr_2RuO_4$

## STM topography

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




**T-dependent cleavage plane?**

## STM spectroscopy

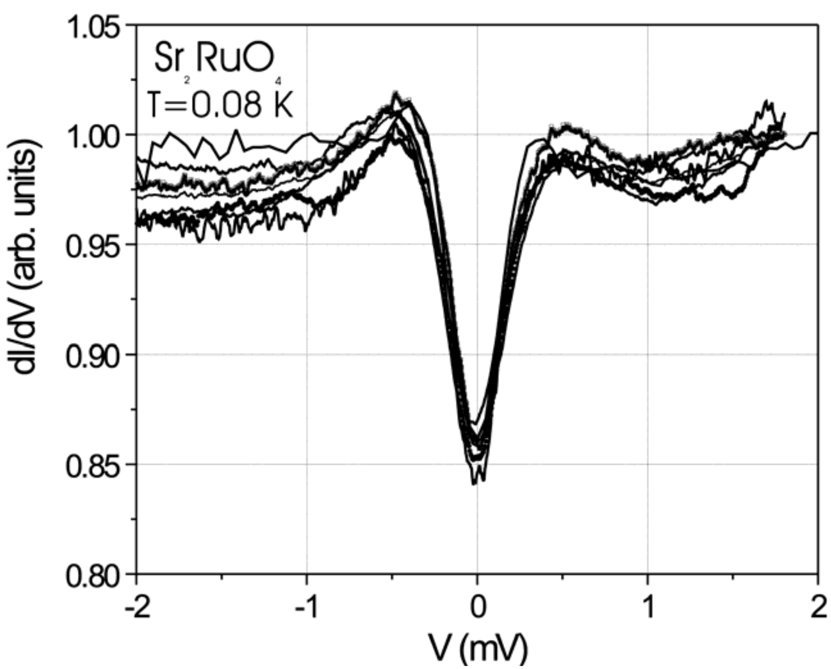
M.D. Upward *et al.*, PRB **65**, 220512 (2002)

DOS suppression within 500 μV

Gap closes for T>1.5K ; B>700G

$2\Delta_{max} / kT_C \sim 8.0$

**Opening of a SC gap**



# Surface Ferromagnetism?

**Surface Reconstruction ⟷ Surface Ferromagnetism**

R. Matzdorf *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?**

↓

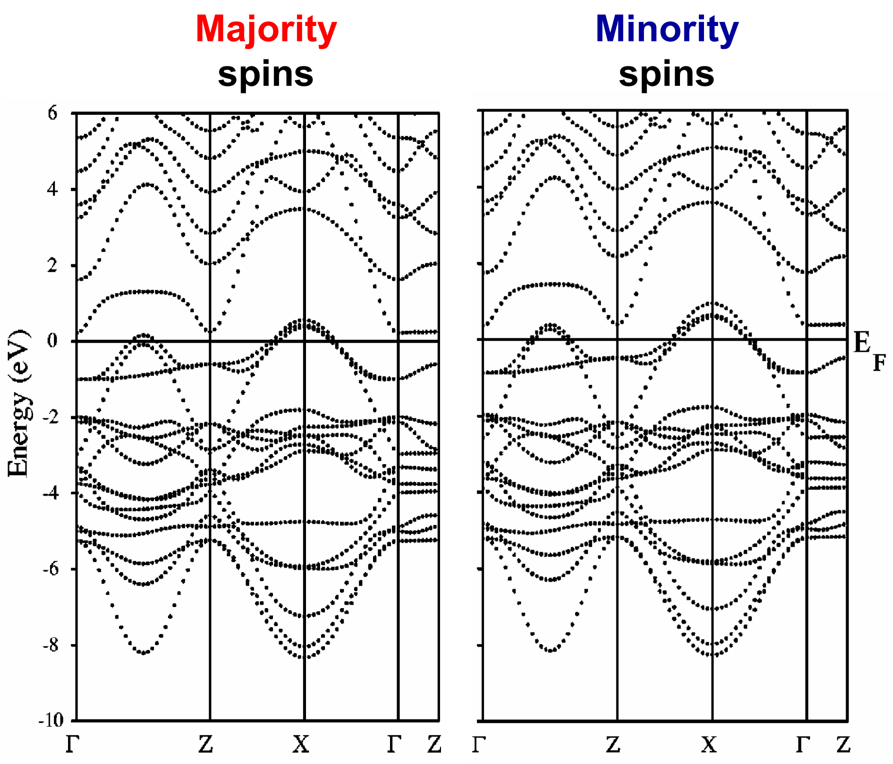
**Pairing mechanism of SC**

# Surface Ferromagnetism?

## Surface Reconstruction ⟷ Surface Ferromagnetism

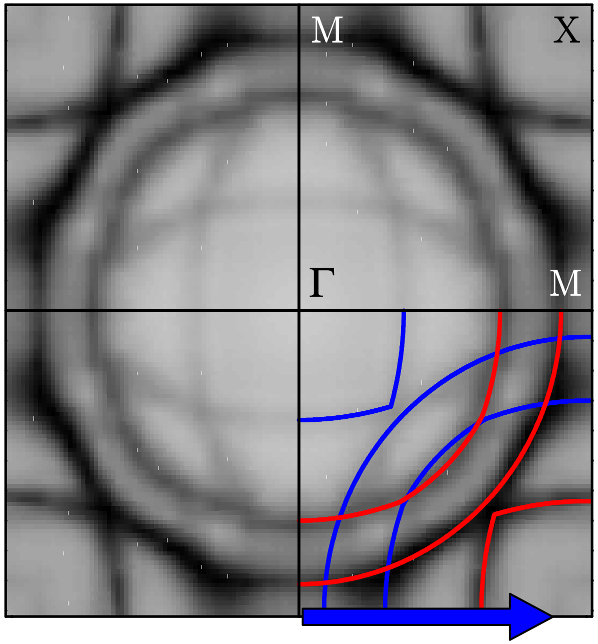
R. Matzdorf *et al.*, Science **289**, 746 (2000)

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



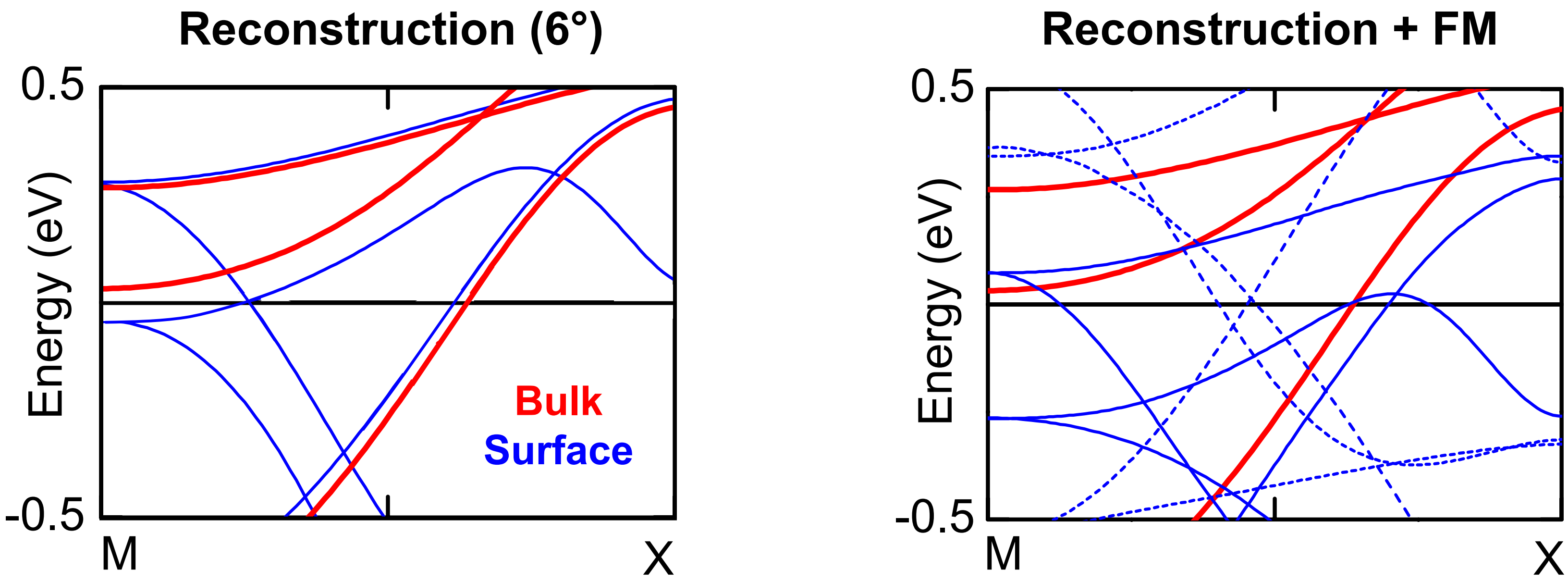

P.K. de Boer *et al.*, PRB **59**, 9894 (1999)

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



# Surface Ferromagnetism?

## Band structure results




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

# ARPES studies on $Sr_2RuO_4$

VOLUME 92, NUMBER 13 PHYSICAL REVIEW LETTERS week ending 2 APRIL 2004

## Quasiparticle Line Shape of $Sr_2RuO_4$ and Its Relation to Anisotropic Transport

S.-C. Wang,[1] H.-B. Yang,[1] A. K. P. Sekharan,[1] H. Ding,[1] J. R. Engelbrecht,[1] X. Dai,[1,*] Z. Wang,[1] A. Kaminski,[2] T. Valla,[3] T. Kidd,[3] A.V. Fedorov,[3,†] and P. D. Johnson[3]

VOLUME 93, NUMBER 11 PHYSICAL REVIEW LETTERS week ending 10 SEPTEMBER 2004

## Kink in the Dispersion of Layered Strontium Ruthenates

Y. Aiura,[1,*] Y. Yoshida,[1,2] I. Hase,[1] S. I. Ikeda,[1] M. Higashiguchi,[3] X. Y. Cui,[3] K. Shimada,[4] H. Namatame,[4] M. Taniguchi,[3,4] and H. Bando[1]

PHYSICAL REVIEW B **70**, 060506(R) (2004)

## Technique for bulk Fermiology by photoemission applied to layered ruthenates

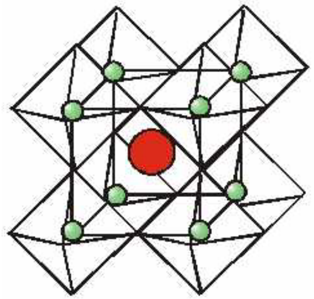
A. Sekiyama,[1] S. Kasai,[1] M. Tsunekawa,[1] Y. Ishida,[1] M. Sing,[1,2] A. Irizawa,[1] A. Yamasaki,[1] S. Imada,[1] T. Muro,[3] Y. Saitoh,[3,4] Y. Ōnuki,[5] T. Kimura,[6,*] Y. Tokura,[6] and S. Suga[1]

## Fermi surface topology of $Ca_{1.5}Sr_{0.5}RuO_4$ determined by ARPES

S.-C. Wang,[1] H.-B. Yang,[1] A.K.P. Sekharan,[1] S. Souma,[2] H. Matsui,[2] T. Sato,[2] T. Takahashi,[2] Chenxi Lu,[3] Jiandi Zhang,[3] R. Jin,[4] D. Mandrus,[4] E.W. Plummer,[4] Z. Wang,[1] and H. Ding[1]

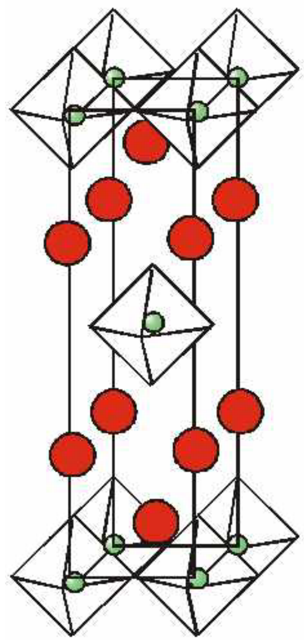
# The layered ruthenates $Sr_{n+1}Ru_nO_{3n+1}$

$SrRuO_3$:
3D itinerant
ferromagnet

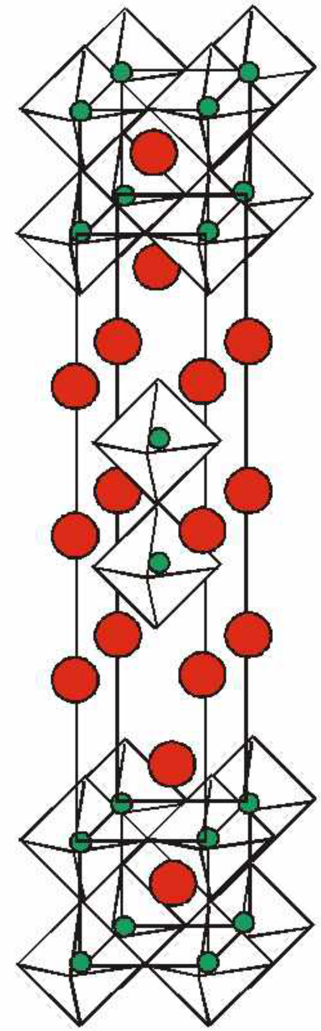


n=∞

$Sr_2RuO_4$: highly
2D Fermi liquid
and unconventional
superconductor.
Pauli paramagnet.

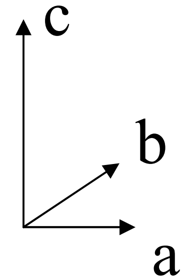


n=1



n=2

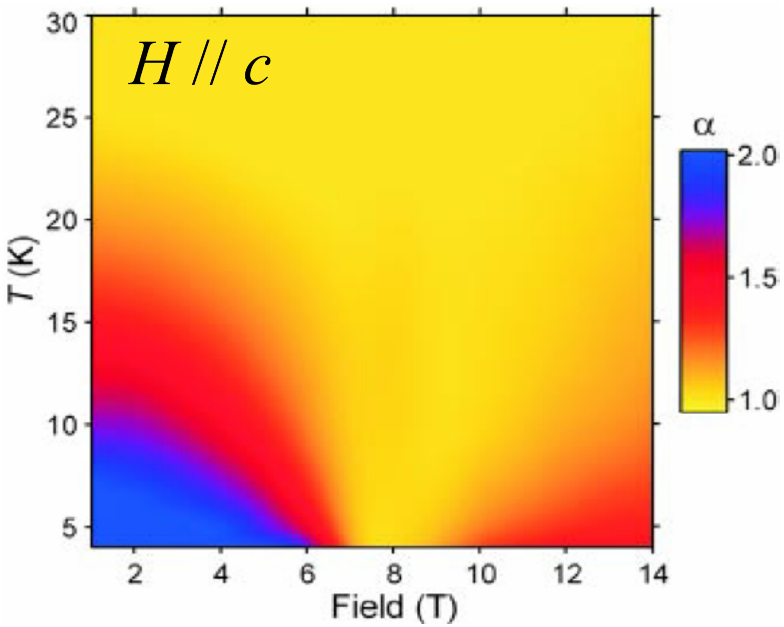
$Sr_3Ru_2O_7$:
intermediate
properties
expected

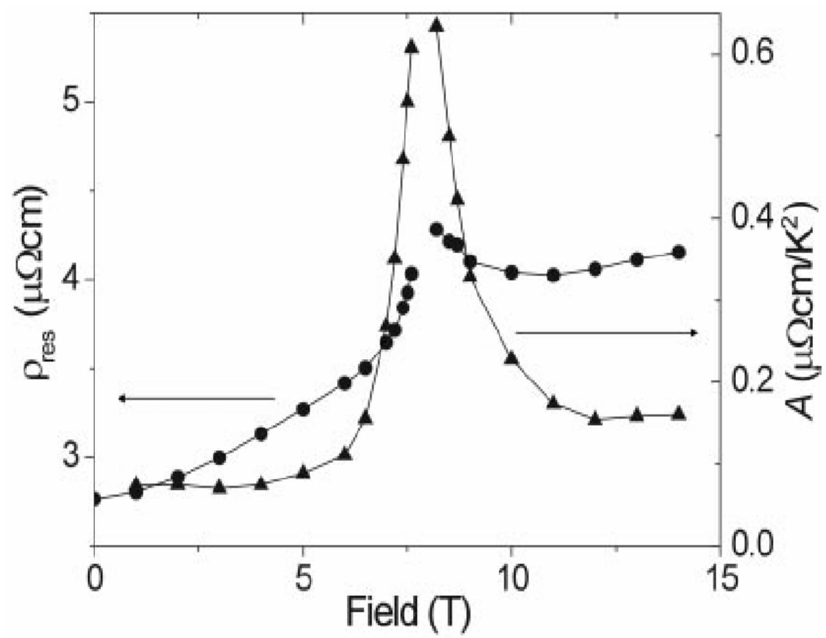


# Transport studies of the QC phase diagram of $Sr_3Ru_2O_7$

Anomalous power-laws in the resistivity: $\rho=\rho_0+AT^\alpha$

Diverging *A* coefficient as the metamagnetic transition is approached : $\rho=\rho_0+AT^2$

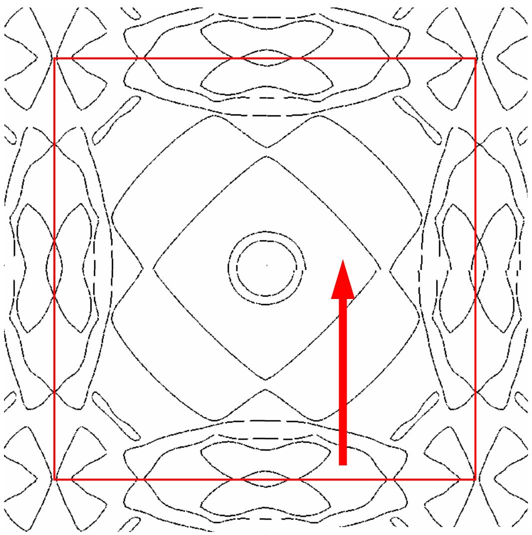



S.A.Grigera et al, Science **294**, 329 (2001)

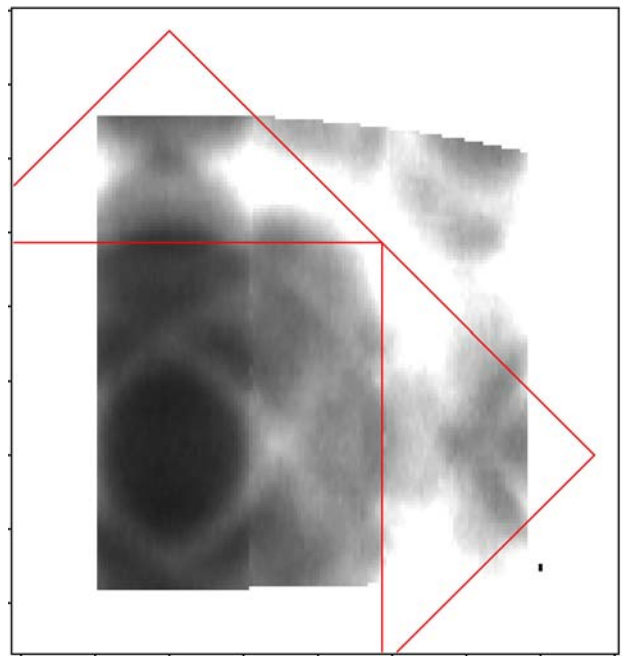
# ARPES studies on $Sr_3Ru_2O_7$

Band structure calculations



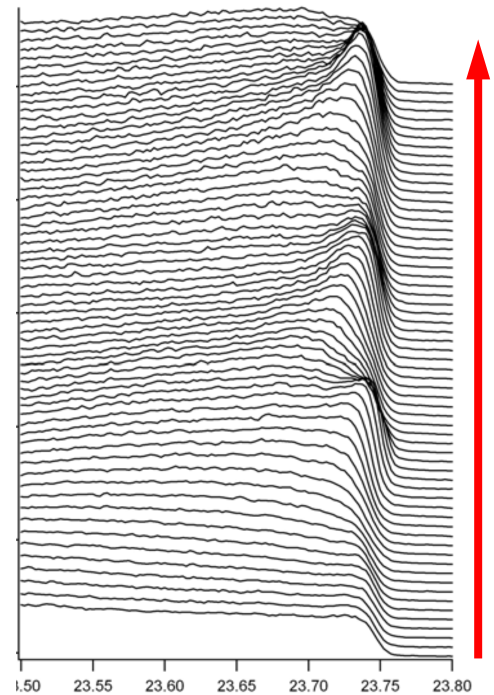
D.J. Singh and I.I. Mazin
PRB **63**, 165101 (2001)

ARPES - FS



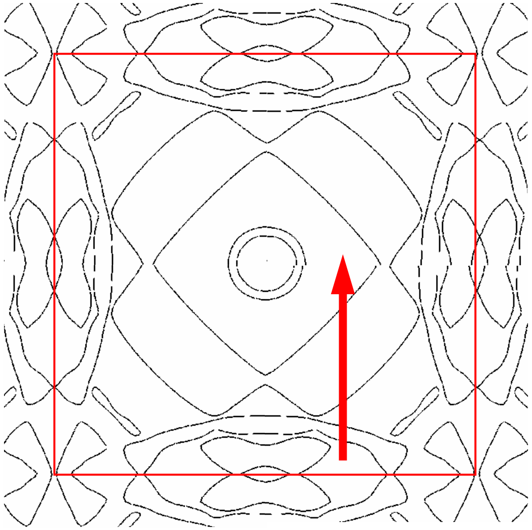
S.Hossain, F. Baumberger

ARPES - EDC



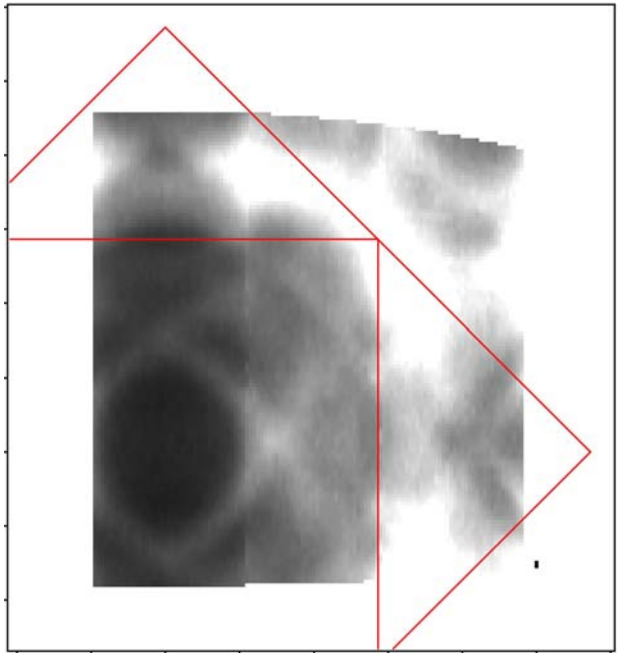
# ARPES studies on $Sr_3Ru_2O_7$

Band structure calculations



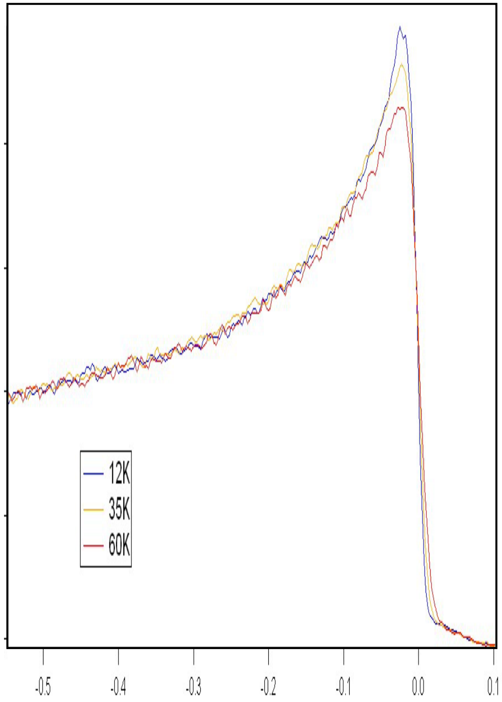
D.J. Singh and I.I. Mazin
PRB **63**, 165101 (2001)

ARPES - FS



S.Hossain, F. Baumberger

ARPES - EDC



# ARPES studies on $(Ca,Sr)_{n+1}Ru_nO_{3n+1}$

VOLUME 92, NUMBER 13 PHYSICAL REVIEW LETTERS week ending 2 APRIL 2004

**Quasiparticle Line Shape of $Sr_2RuO_4$ and Its Relation to Anisotropic Transport**

S.-C. Wang,[1] H.-B. Yang,[1] A. K. P. Sekharan,[1] H. Ding,[1] J. R. Engelbrecht,[1] X. Dai,[1,*] Z. Wang,[1] A. Kaminski,[2] T. Valla,[3] T. Kidd,[3] A.V. Fedorov,[3,†] and P. D. Johnson[3]

VOLUME 93, NUMBER 11 PHYSICAL REVIEW LETTERS week ending 10 SEPTEMBER 2004

**Kink in the Dispersion of Layered Strontium Ruthenates**

Y. Aiura,[1,*] Y. Yoshida,[1,2] I. Hase,[1] S. I. Ikeda,[1] M. Higashiguchi,[3] X. Y. Cui,[3] K. Shimada,[4] H. Namatame,[4] M. Taniguchi,[3,4] and H. Bando[1]

PHYSICAL REVIEW B **70**, 060506(R) (2004)

**Technique for bulk Fermiology by photoemission applied to layered ruthenates**

A. Sekiyama,[1] S. Kasai,[1] M. Tsunekawa,[1] Y. Ishida,[1] M. Sing,[1,2] A. Irizawa,[1] A. Yamasaki,[1] S. Imada,[1] T. Muro,[3] Y. Saitoh,[3,4] Y. Ōnuki,[5] T. Kimura,[6,*] Y. Tokura,[6] and S. Suga[1]

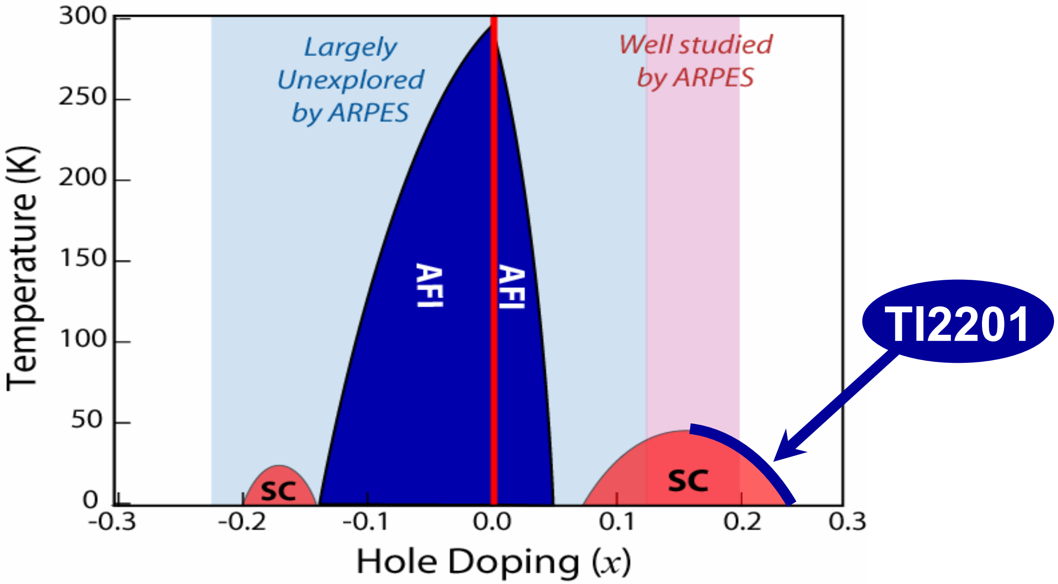
**Fermi surface topology of $Ca_{1.5}Sr_{0.5}RuO_4$ determined by ARPES**

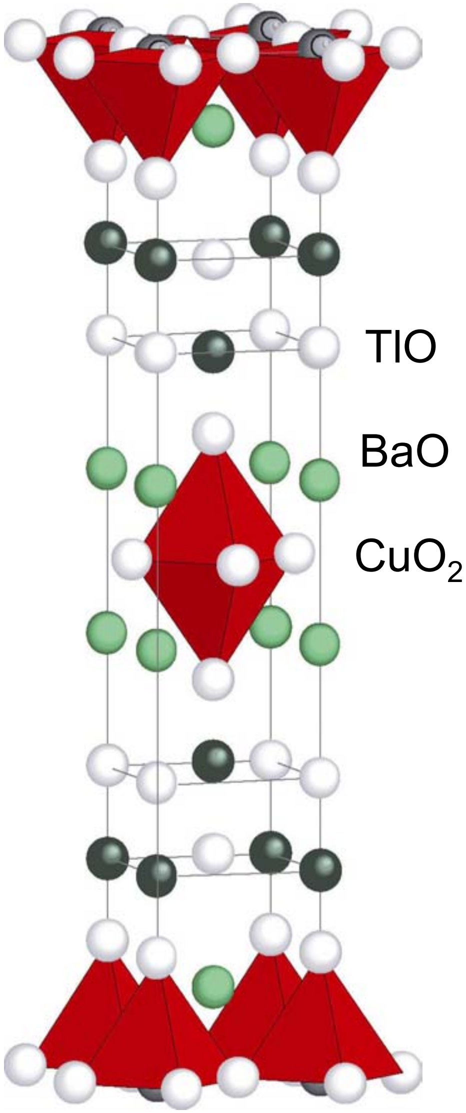
S.-C. Wang,[1] H.-B. Yang,[1] A.K.P. Sekharan,[1] S. Souma,[2] H. Matsui,[2] T. Sato,[2] T. Takahashi,[2] Chenxi Lu,[3] Jiandi Zhang,[3] R. Jin,[4] D. Mandrus,[4] E.W. Plummer,[4] Z. Wang,[1] and H. Ding[1]

# ARPES on $Tl_2Ba_2CuO_{6+\delta}$ ?

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

- Single $CuO_2$ plane material
- Very high transition: $T_c$(opt)=93K
- No additional CuO chains
- No structural distortions
- Low cation disorder (T/O structure)



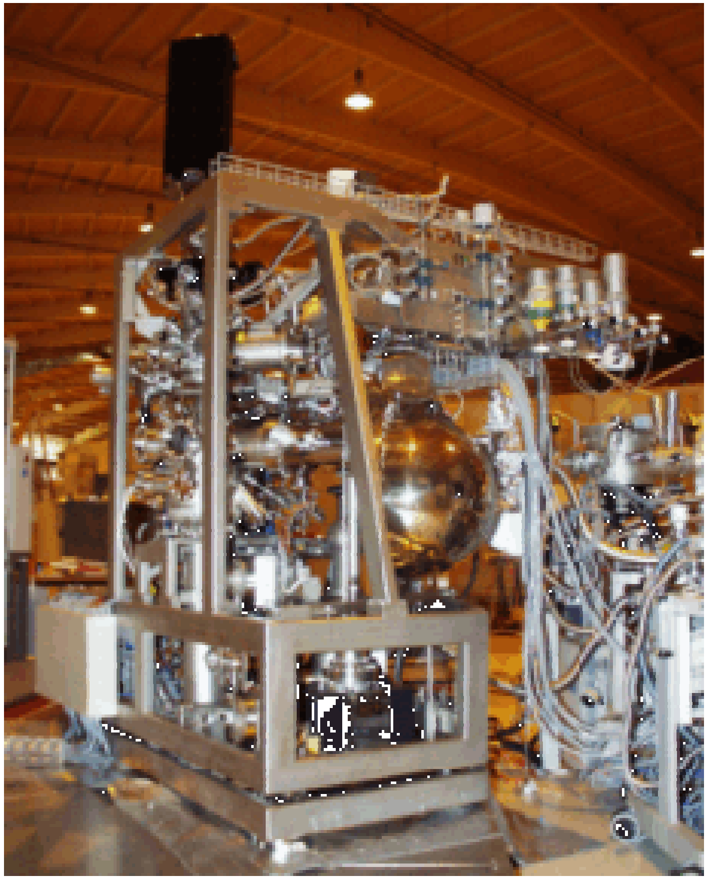

D. Peets, R. Liang
D. Bonn, W. Hardy

# Swiss Light Source – SIS Beamline

- **ARPES Experiments:**

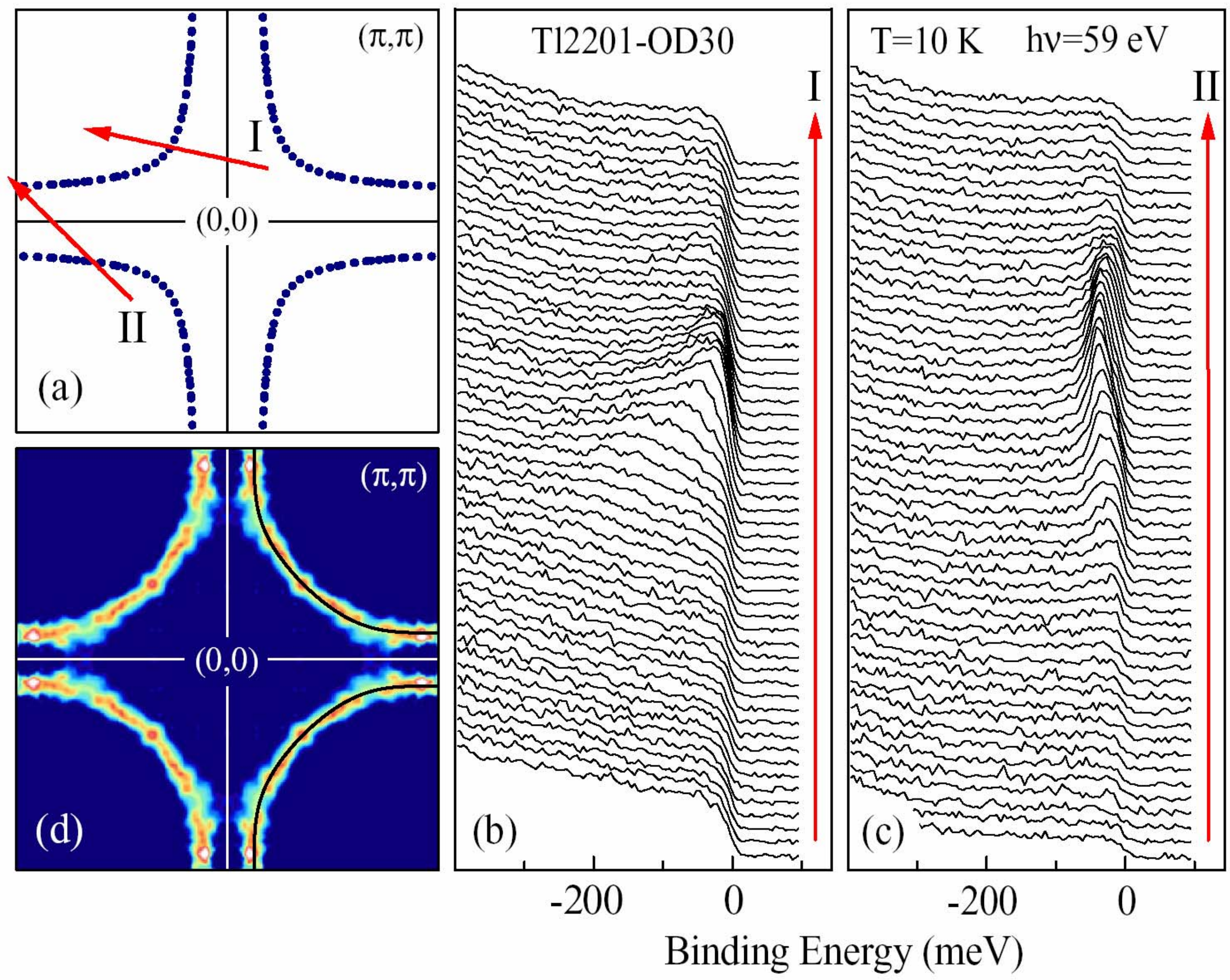
**Surface and Interface Spectroscopy Beamline**

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



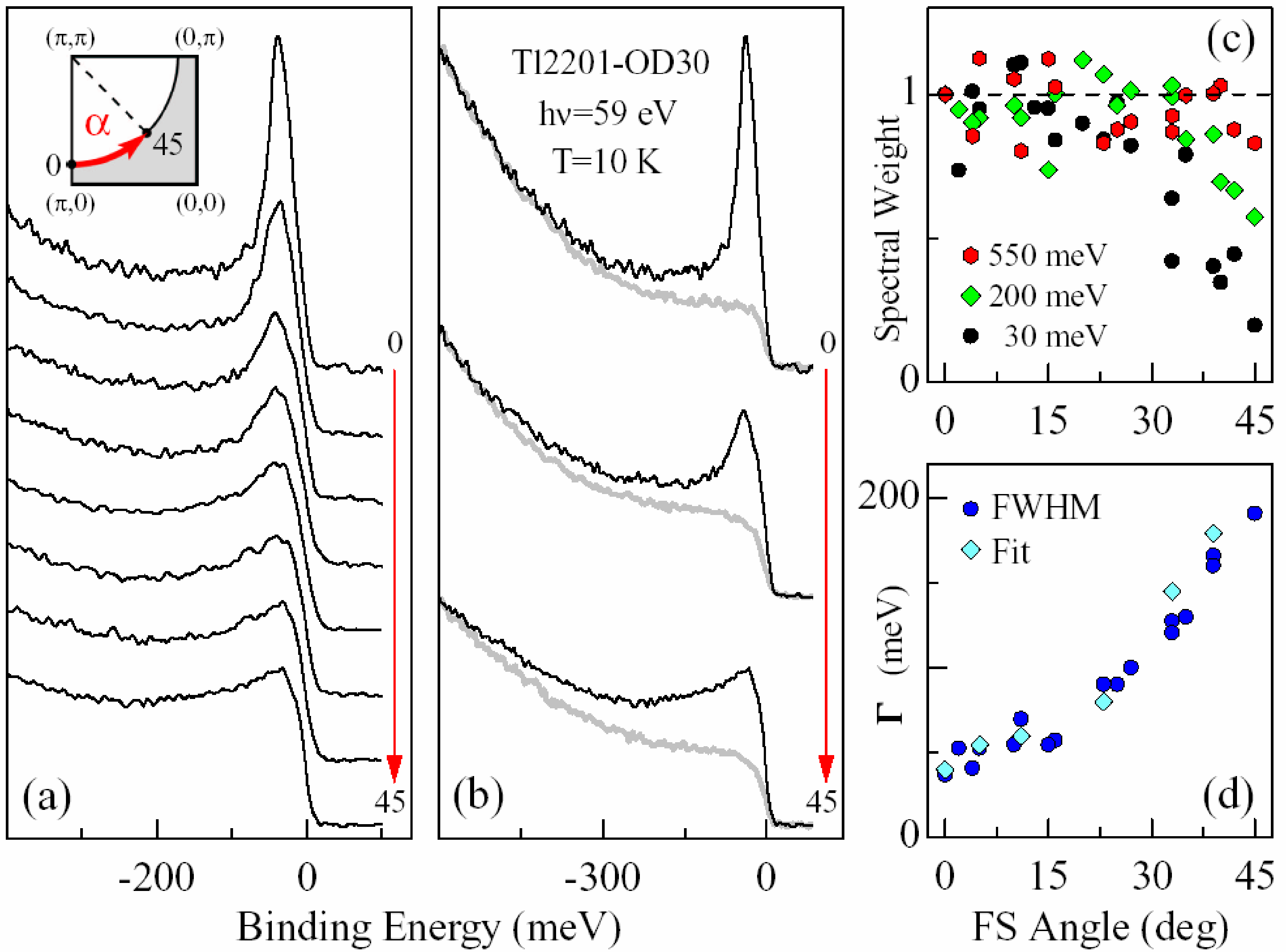
- **Twin Undulator**
- **HR Monochromator**
  - Energy Range: 10-800 eV
  - Polarization: circular/planar
- **ARPES**
  - Detector: SES2002
  - $E/\Delta E > 10^4$ ; $\Delta k = 0.3^o$
  - Low T: 10-300K
  - spot size: 20x20 $\mu m^2$
- **Spin resolved ARPES**

# $Tl_2Ba_2CuO_{6+\delta}$ : ARPES Results



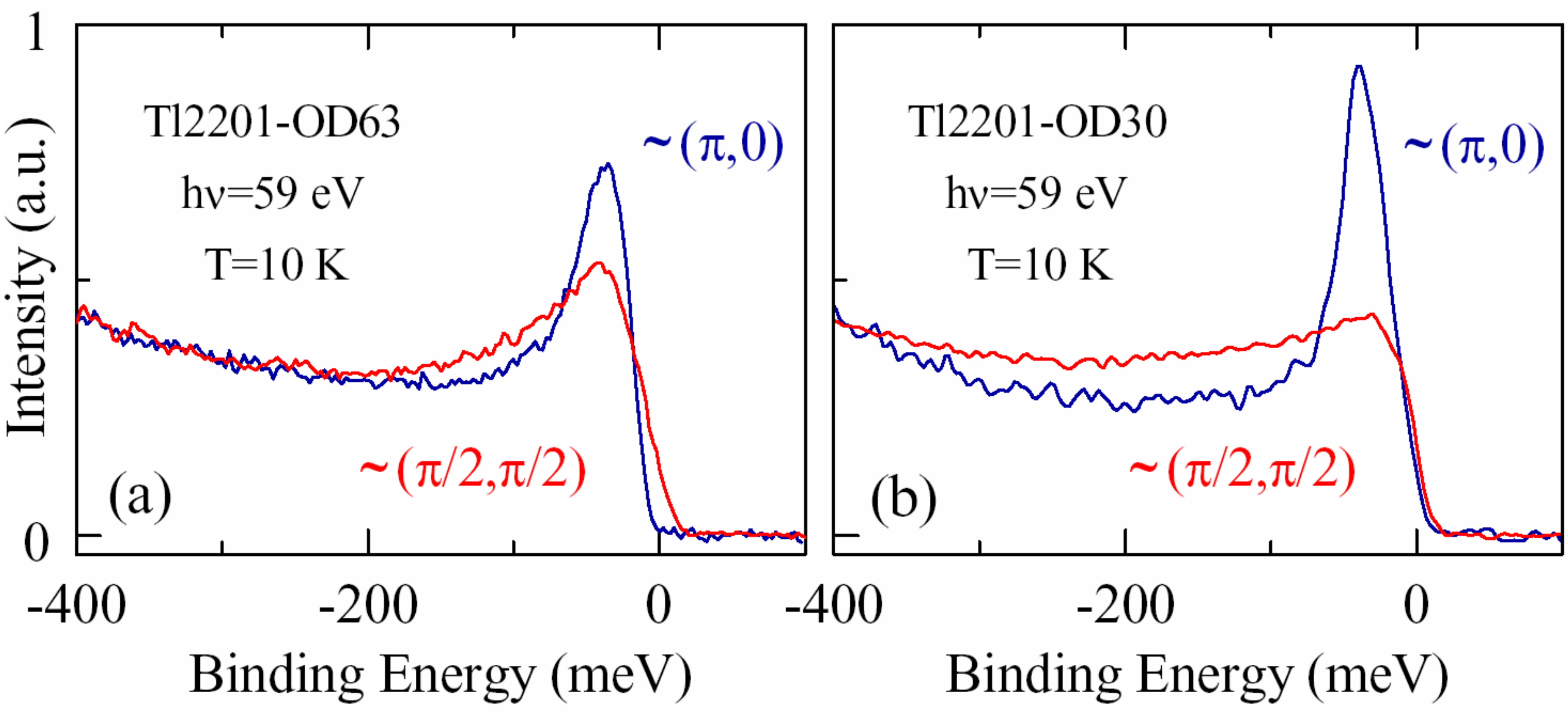

M. Platé, J. Mottershead, A. Damascelli, et al., cond-mat/0503117

# $Tl_2Ba_2CuO_{6+\delta}$ : ARPES Results




M. Platé, J. Mottershead, A. Damascelli, et al., cond-mat/0503117

# $Tl_2Ba_2CuO_{6+\delta}$ : ARPES Results




M. Platé, J. Mottershead, A. Damascelli, et al., cond-mat/0503117

# Conclusions

## ARPES results from $Sr_2RuO_4$

- **Bulk** and **surface** electronic structure
- **FS** topology in unprecedented detail
- Fermi **velocity** and **effective mass**
- Investigate the issue of **surface FM**

Feedback to microscopic models
Quantify the spin/charge correlation effects

Films/interfaces $Sr_3Ru_2O_7$ $Tl_2Ba_2CuO_{6+\delta}$

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