Recent ARPES Results from 4d & 5d TMOs ($\boxed{Sr_2RhO_4,}$ Sr_2IrO_4)

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Effect of the Octahedra Rotation on the Electronic Structure of Sr_2RhO_4

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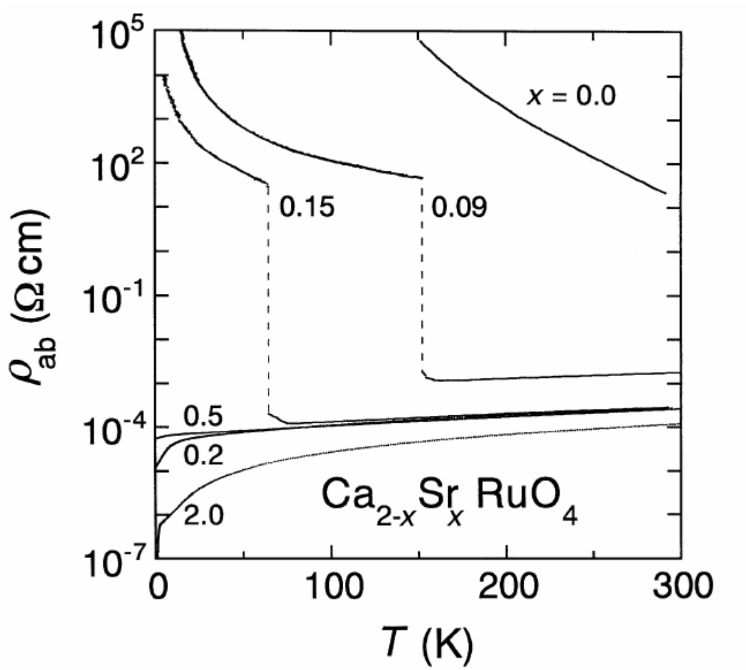
B. J. Kim, et al., PRL, **97**, 106401 (2006).

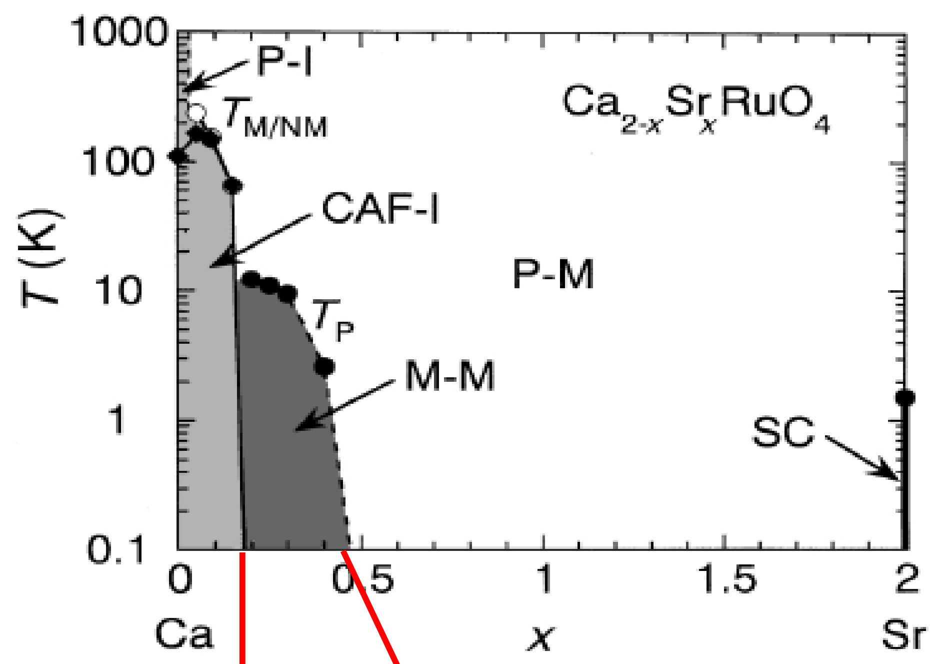
Outline

- Background - $(Sr,Ca)_2RuO_4$
- ARPES data from Sr_2RhO_4 – Missing d_{xy} Fermi Surface
- Comparison with Band Calculation
- Summary – Octahedra Rotation Effect on the Electronic Structure

Phase diagram of $Ca_{2-x}Sr_xRuO_4$

S. Nakatsuji et al, Phys. Rev. Lett. 84, 2666 (2000).

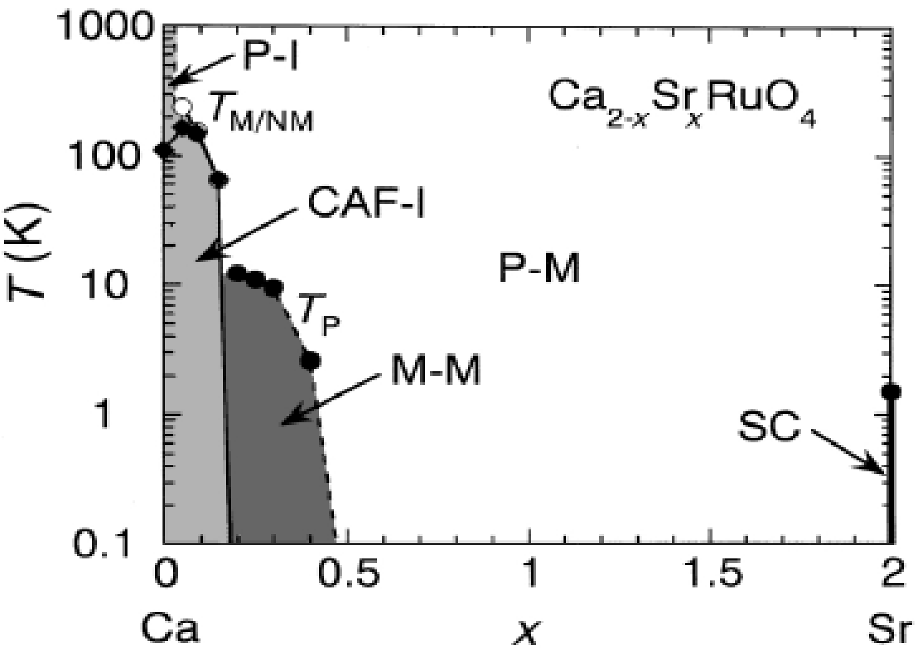


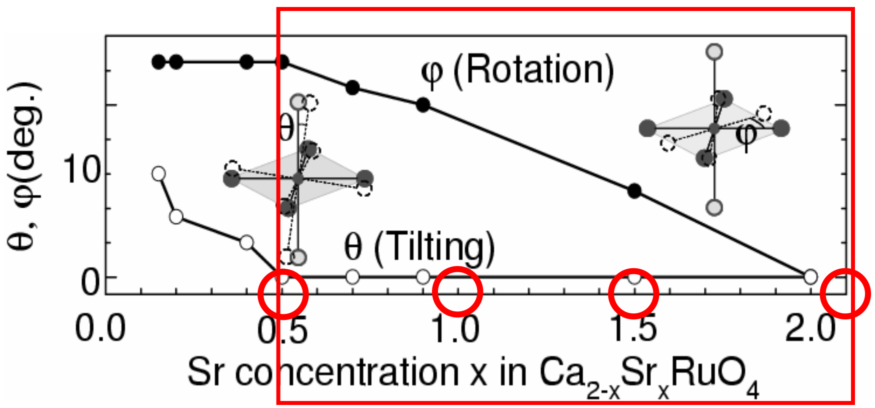


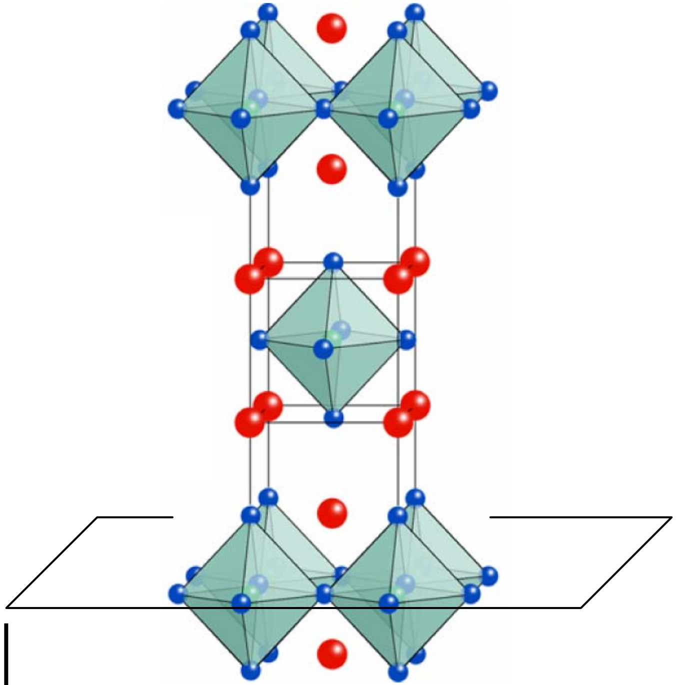
Mott transition

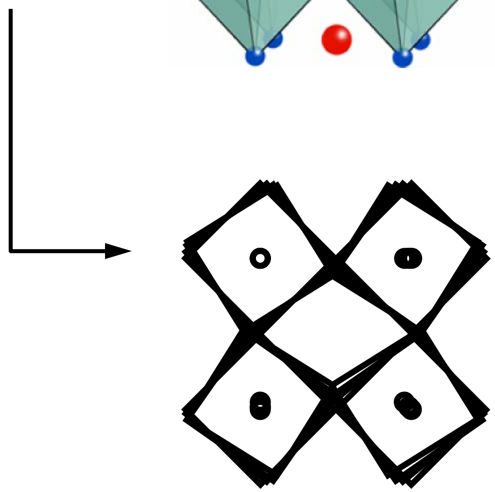
Orbital Selective Mott Transition (OSMT

Structural distortion of $Ca_{2-x}Sr_xRuO_4$









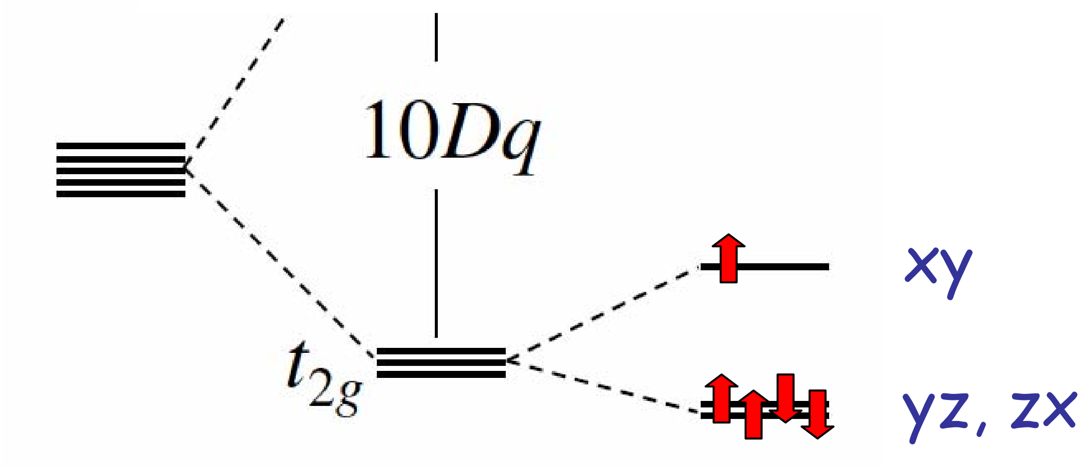
Various ground states are realized by structural distortions.

4*d* transition-metal oxide

- Large spatial extent of 4*d* orbitals
  - →large bandwidth, large 10*Dq*.
  - →tends to be weakly-correlated.
- Low-spin configuration is expected.

$Ca_{2-x}Sr_xRuO_4$

Sr_2RhO_4



Rotation of Octahedra

Rotation brings about:

- Doubling of the unit cell
- Decrease of M-O-M bond angle

which cause:

- Band folding
- Bandwidth narrowing

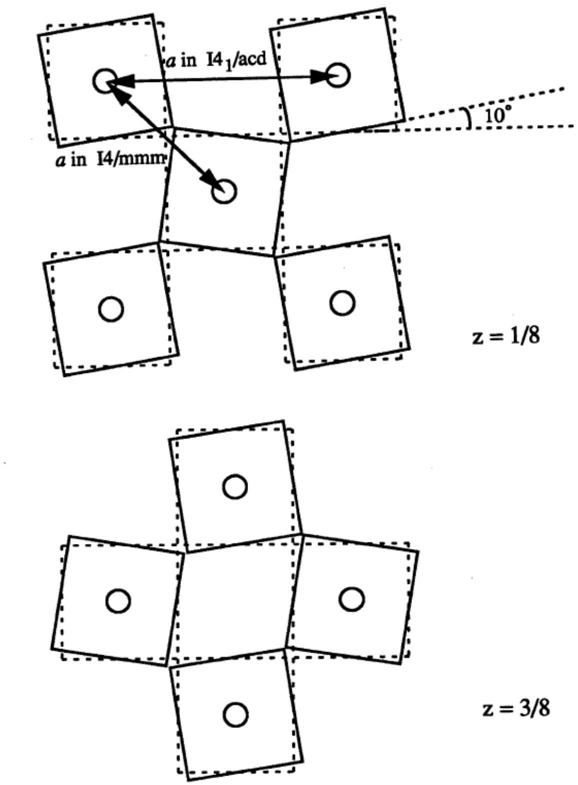
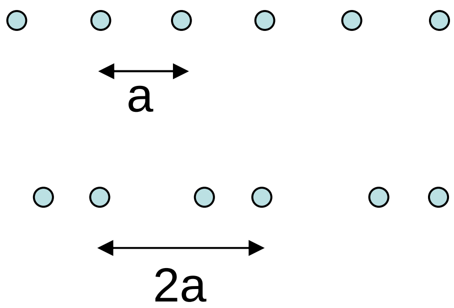
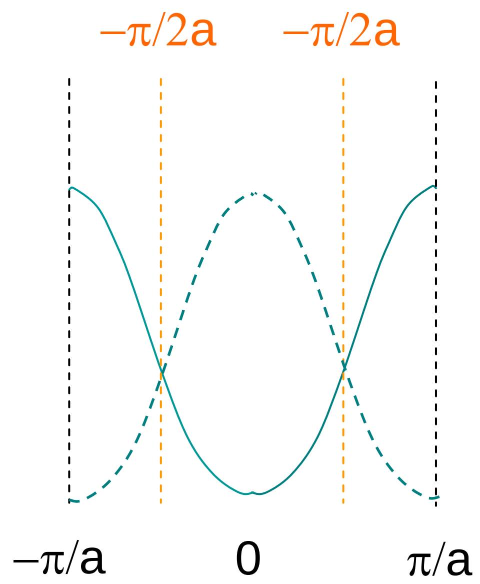


Fig. 1. Structure diagram of the Sr_2RhO_4 with $I4_1/acd$ sp group showing the RhO_6 octahedra rotation at $z = 1/8$ and z 3/8 in ref. 4. The dotted lines shows the structure of Sr_2Ru with I4/mmm space group.

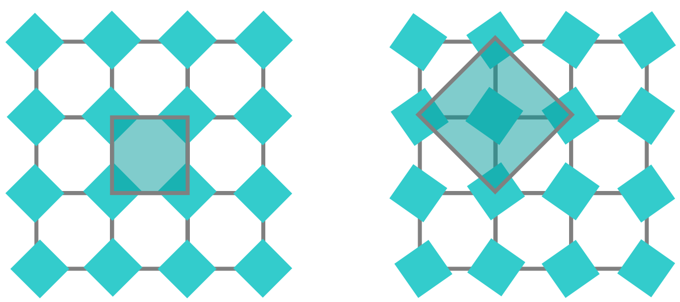
Unit cell doubling and band folding

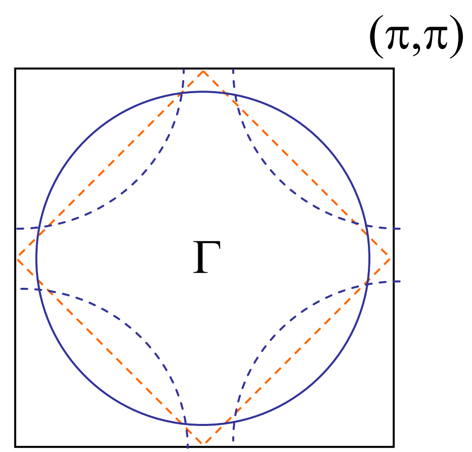
1D





2D





Band width narrowing

Octahedra rotation

↓

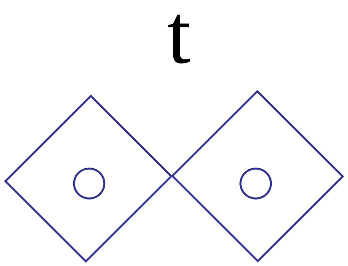
Decrease of M-O-M bond angle

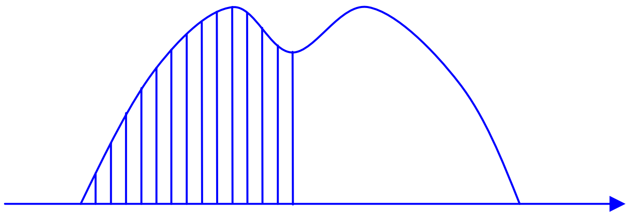
↓

Decrease in hopping energy *t*

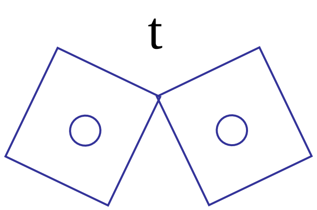
↓

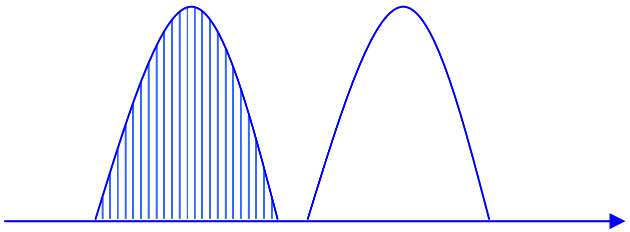
Increase in *U/t*





Metal, small *U/W*

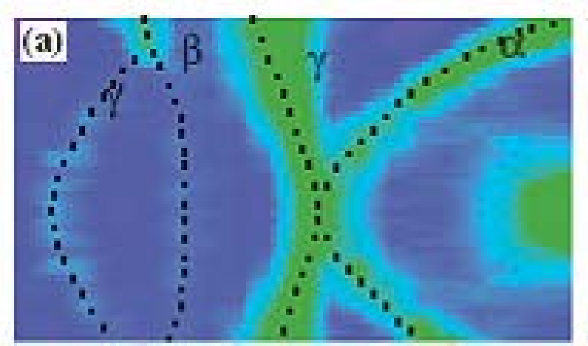




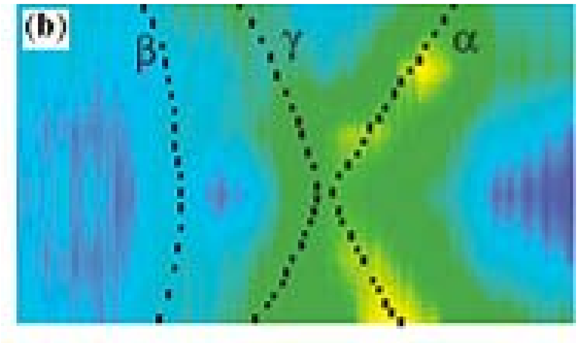
Insulator, large *U/W*

ARPES data on Ca-doped SRO

S.-C. Wang et al. PRL 93,177007 (2004)



Sr_2RuO_4

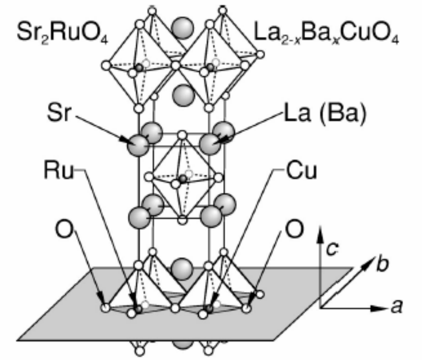


$Ca_{1.5}Sr_{0.5}RuO_4$

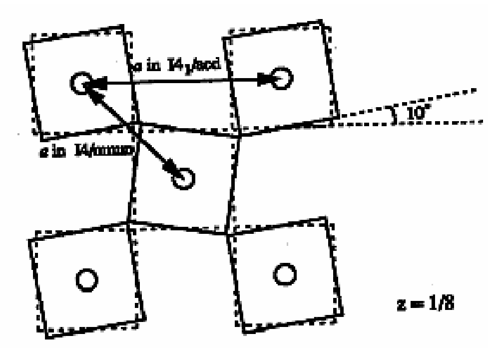
ARPES signal is generally broad and weak.

Sr_2RhO_4

- Share same crystal structure with Sr_2RuO_4.
- 5 electrons in 4*d* orbitals.
- Rotation angle ~ 10º.
- No supeconductivity.

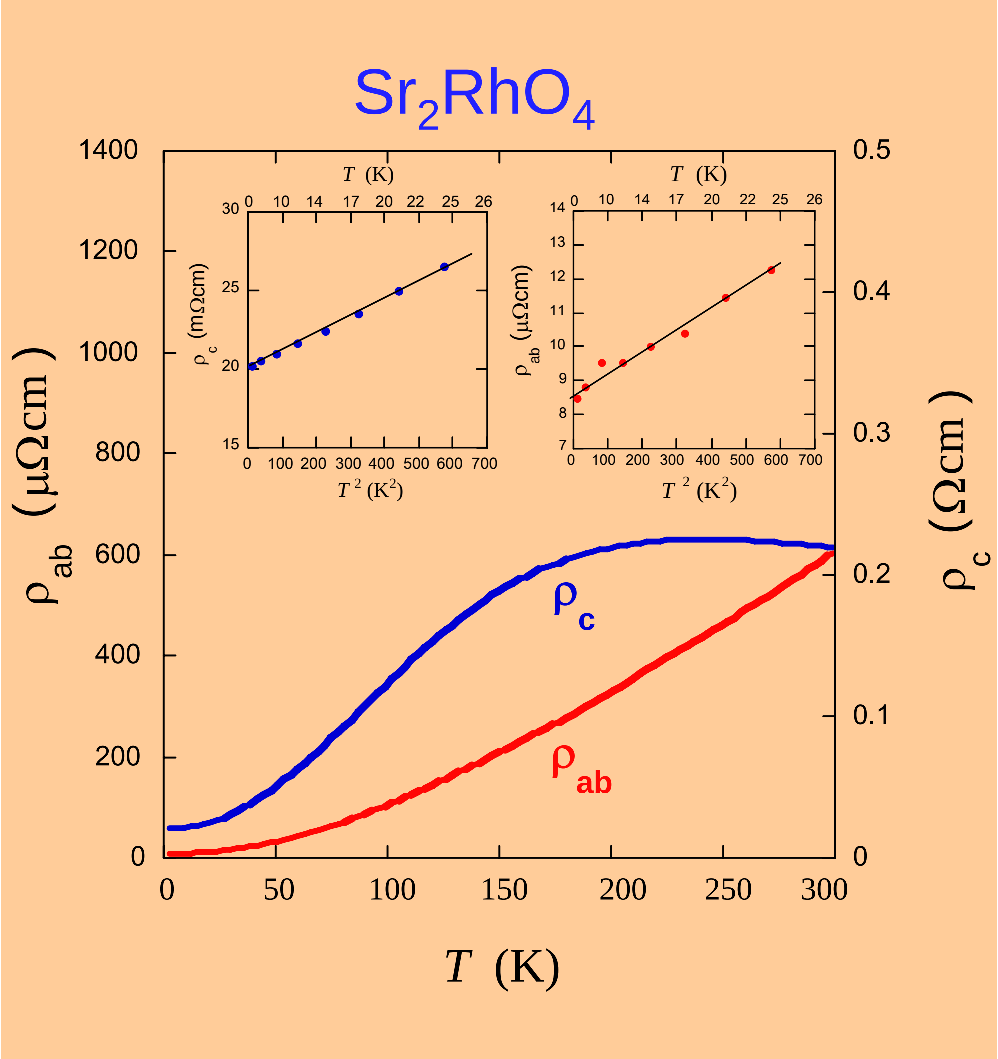


Sr_2RhO_4 presents an opportunity to study the effect of rotation without "disorder".



Electrical resistivity

Similar to $\rho(T)$ in Sr_2RuO_4



- Large anisotropy

  ρ_c / ρ_{ab} (3K) = 2400

- T^2- dependence

  Fitting with $\rho = \rho_0 + AT^2$

  $\rho_{ab}(T)$ $\rho_0 = 8.6\ \mu\Omega\text{cm}$, $A_{ab} = 6.26\times10^{-3}\ \mu\Omega\text{cm/K}^2$

  $\rho_c(T)$ $\rho_0 = 20.1\ \text{m}\Omega\text{cm}$, $A_c = 10.55\ \mu\Omega\text{cm/K}^2$

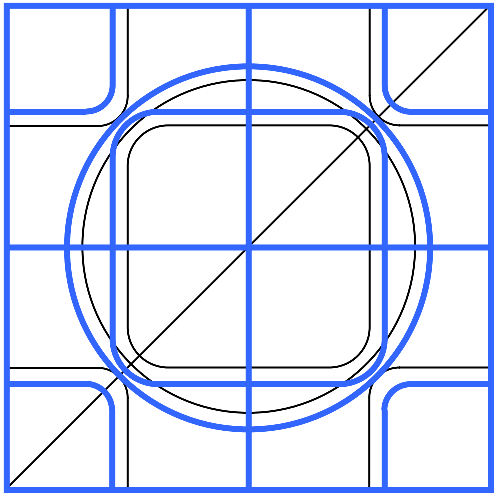
- Below ~250 K, ρ_c decreases with lowering temperature.

- No superconducting transition was observed down to 36 mK.

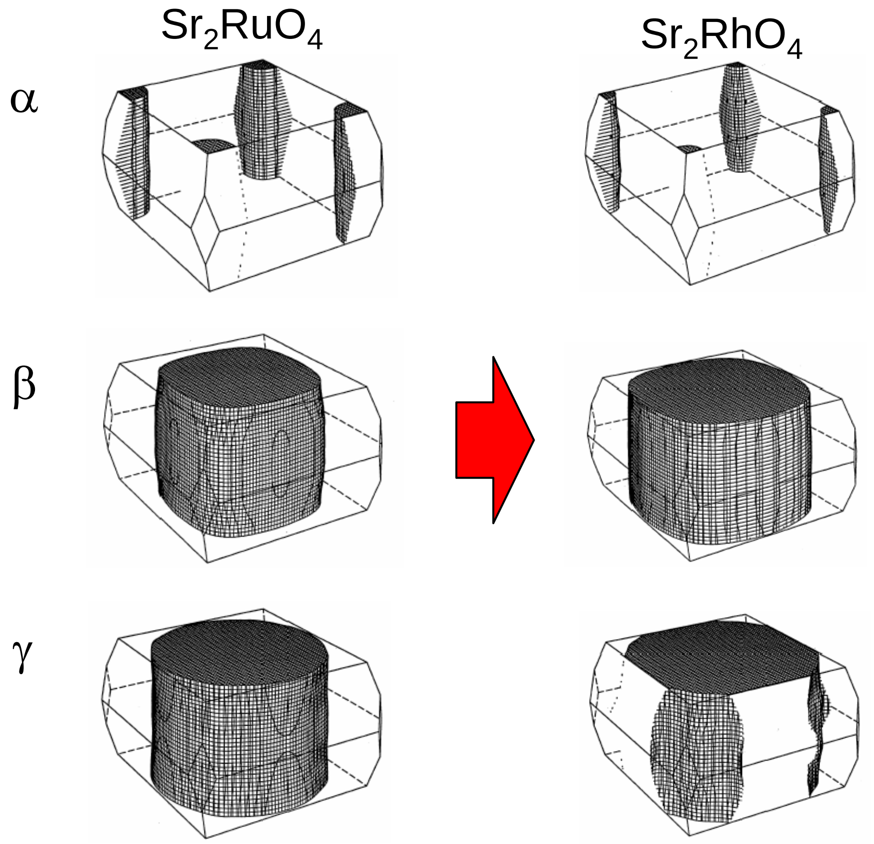
Sr_2RhO_4 is a two-dimensional Fermi liquid.

Expected FS of Sr_2RhO_4

FS of Sr_2RhO_4



By doping one electron: (rigid-band model)



Hase *et al*. J. of solid state chemistry **123**,186 (1996)

We expect basically similar FS topology in Sr_2RhO_4

ARPES measurements

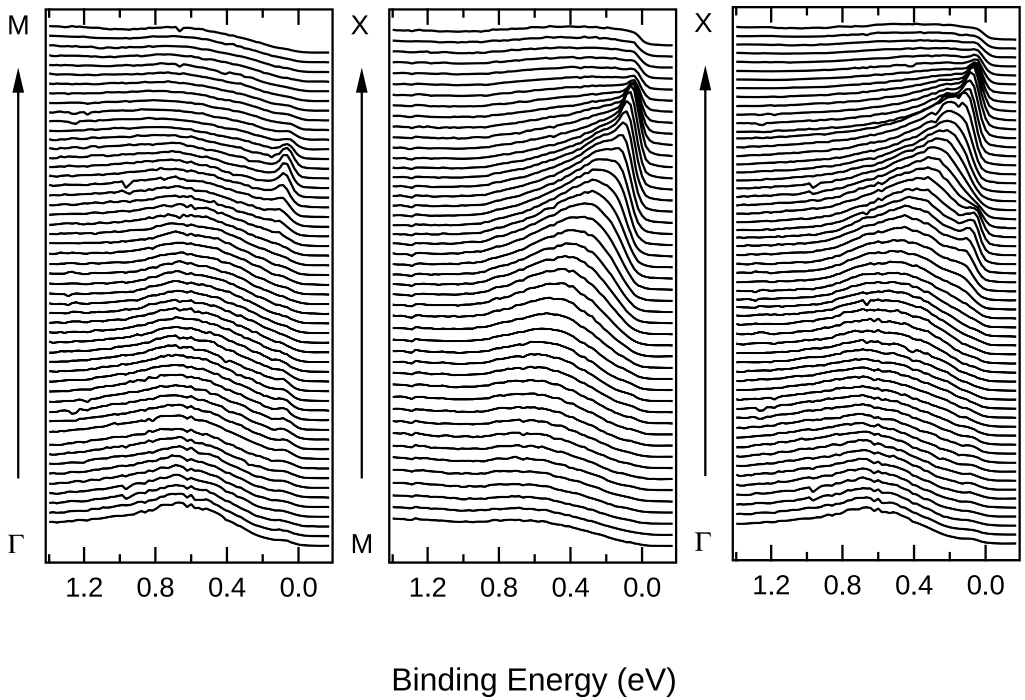
High energy ARPES

- ALS BL 7
- Analyzer : Scienta 100
- Temperature : 40K
- Total Energy Resolution : 40 meV
- Angular Resolution : 0.25º
- Photon energy : 85 eV
- Sample cleaved *in situ*

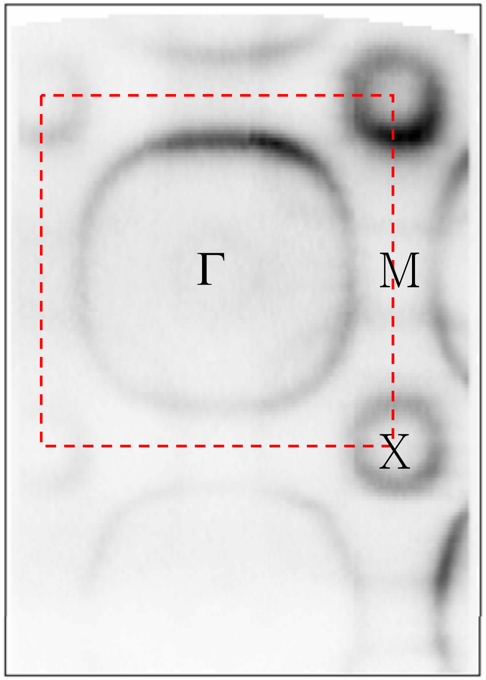
low energy ARPES

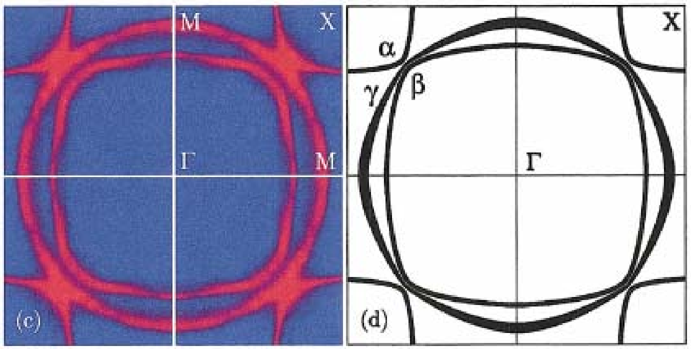
- SSRL BL
- Analyzer : Scienta 2002
- Temperature : 20K
- Total Energy Resolution : 40 meV
- Angular Resolution : 0.25º
- Photon energy : 20 eV
- Sample cleaved *in situ*

FS of Sr_2RhO_4



Fermi Surface Mapping





Sr_2RuO_4 cleaved at 180 K
T= 10 K hv=28 eV

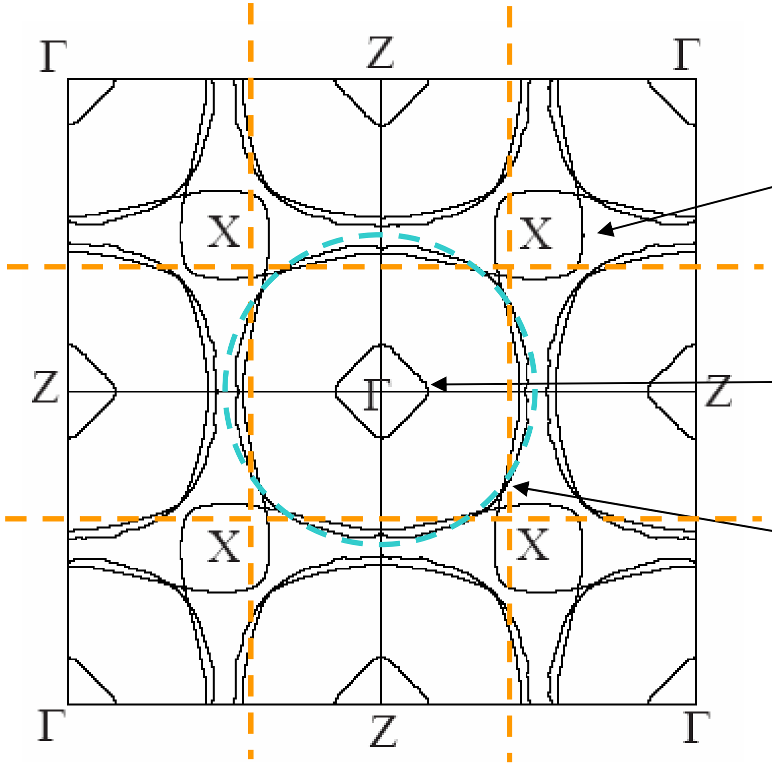
Local-density-approximation
band-structure calculation

Missing *xy*-band(g)
FS in Sr_2RhO_4!

B.J. Kim et al.

LDA calculation

WITHOUT distortion (rotation of octahedra)



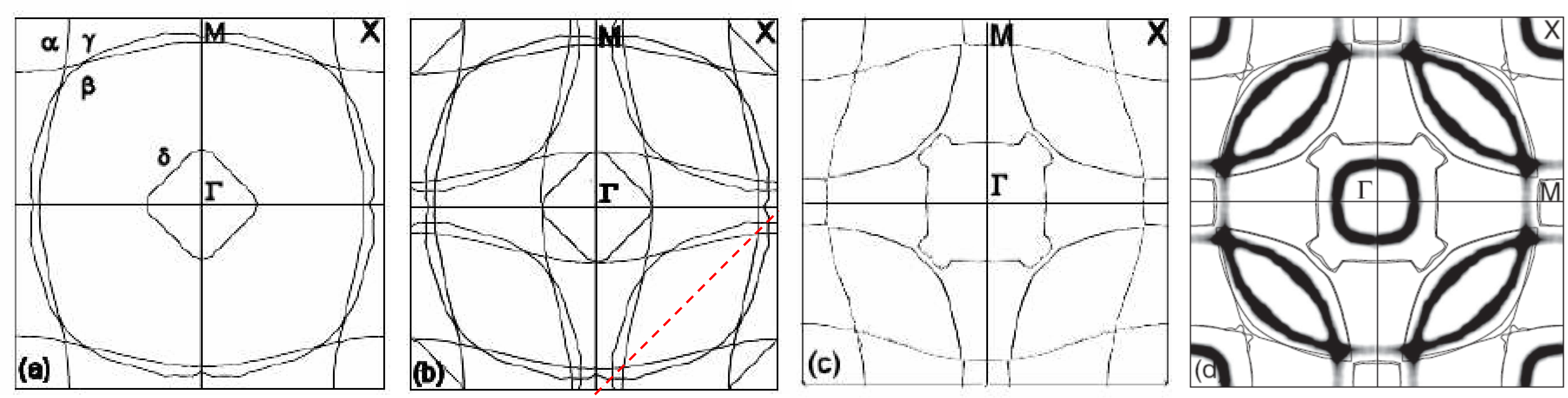
a hole pocket formed by *xz/yz* orbital band. (α)

an electron pocket formed by x^2-y^2 orbital band. (δ)

two electron pockets formed by *xy* (γ) and *yz,zx* band (β)

Occupation :	α	94.8%
	β	66.8%
	γ	72.5%
	δ	7.1%

Effects of the rotational distortion



undistorted

undistorted
+band folding

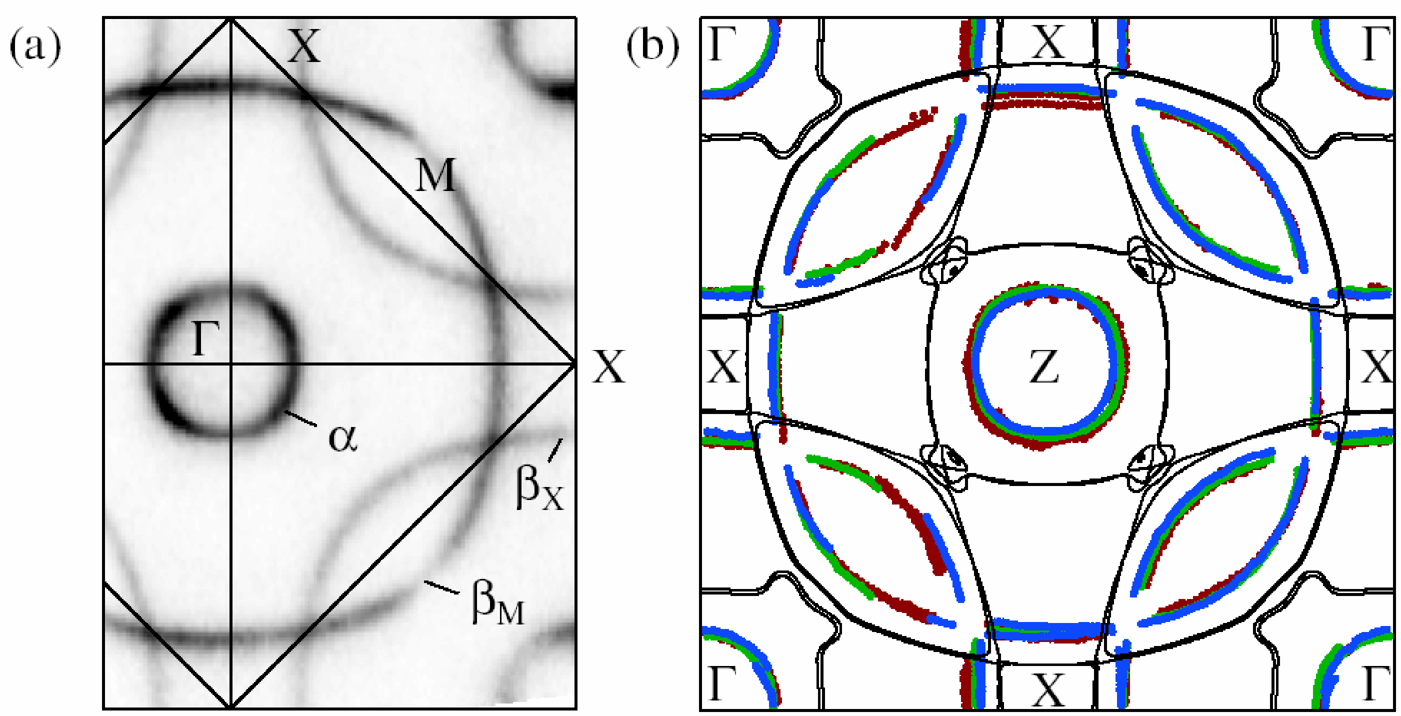
distorted

exp and calc.

LDA calculation shows disappearance of *xy*-FS (γ) and x^2-y^2 FS (δ).

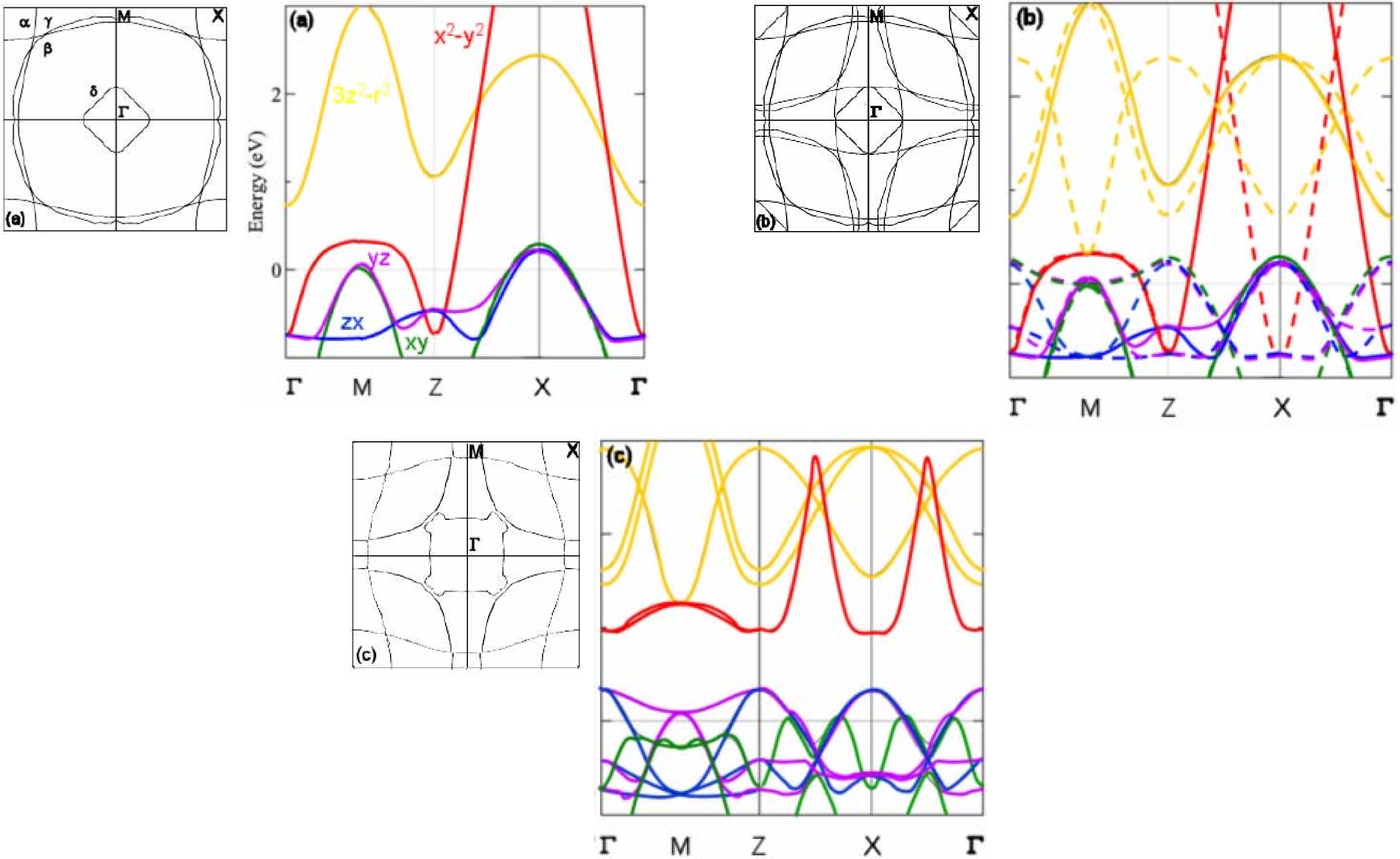
B. J. Kim, et al., PRL, **97**, 106401 (2006).

Other's result



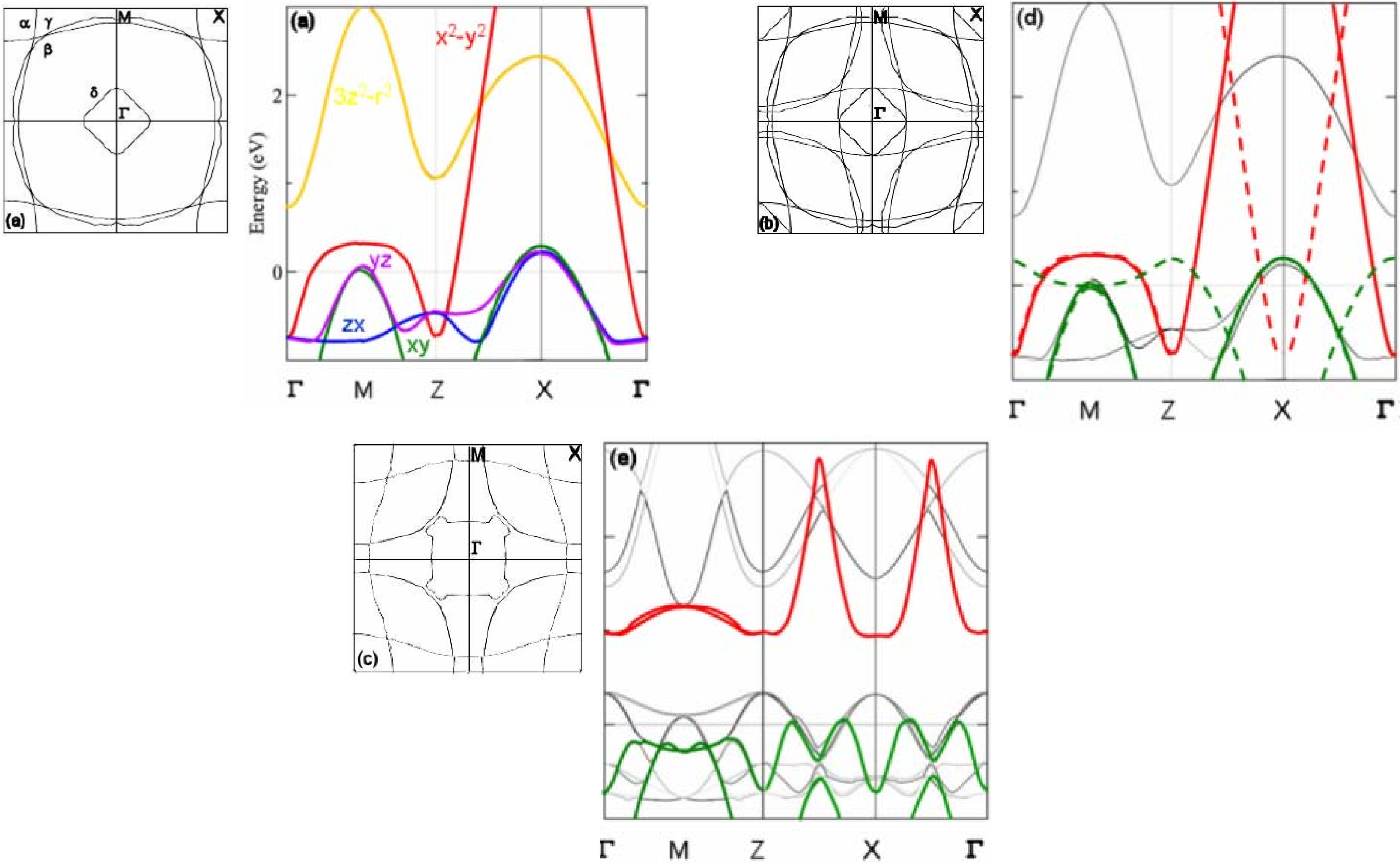
F. Baumberger et al., PRL **96, 246402** (2006)

Effects of the rotational distortion



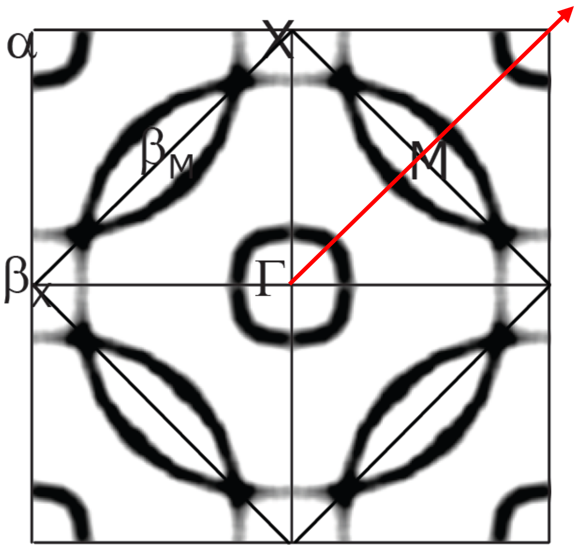
B. J. Kim, et al., PRL, **97**, 106401 (2006).

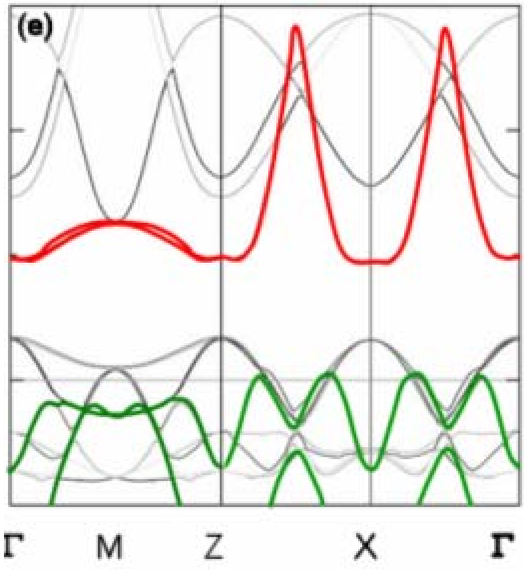
Effects of the rotational distortion

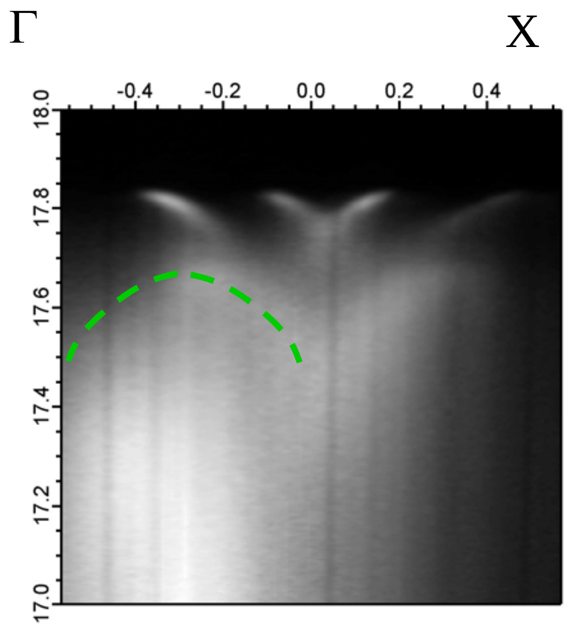


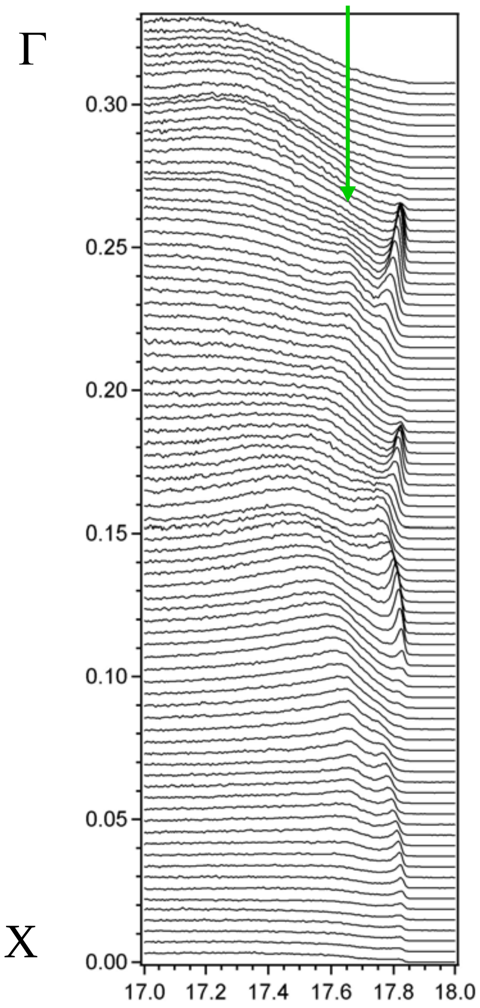
B. J. Kim, et al., PRL, **97**, 106401 (2006).

xy-Band



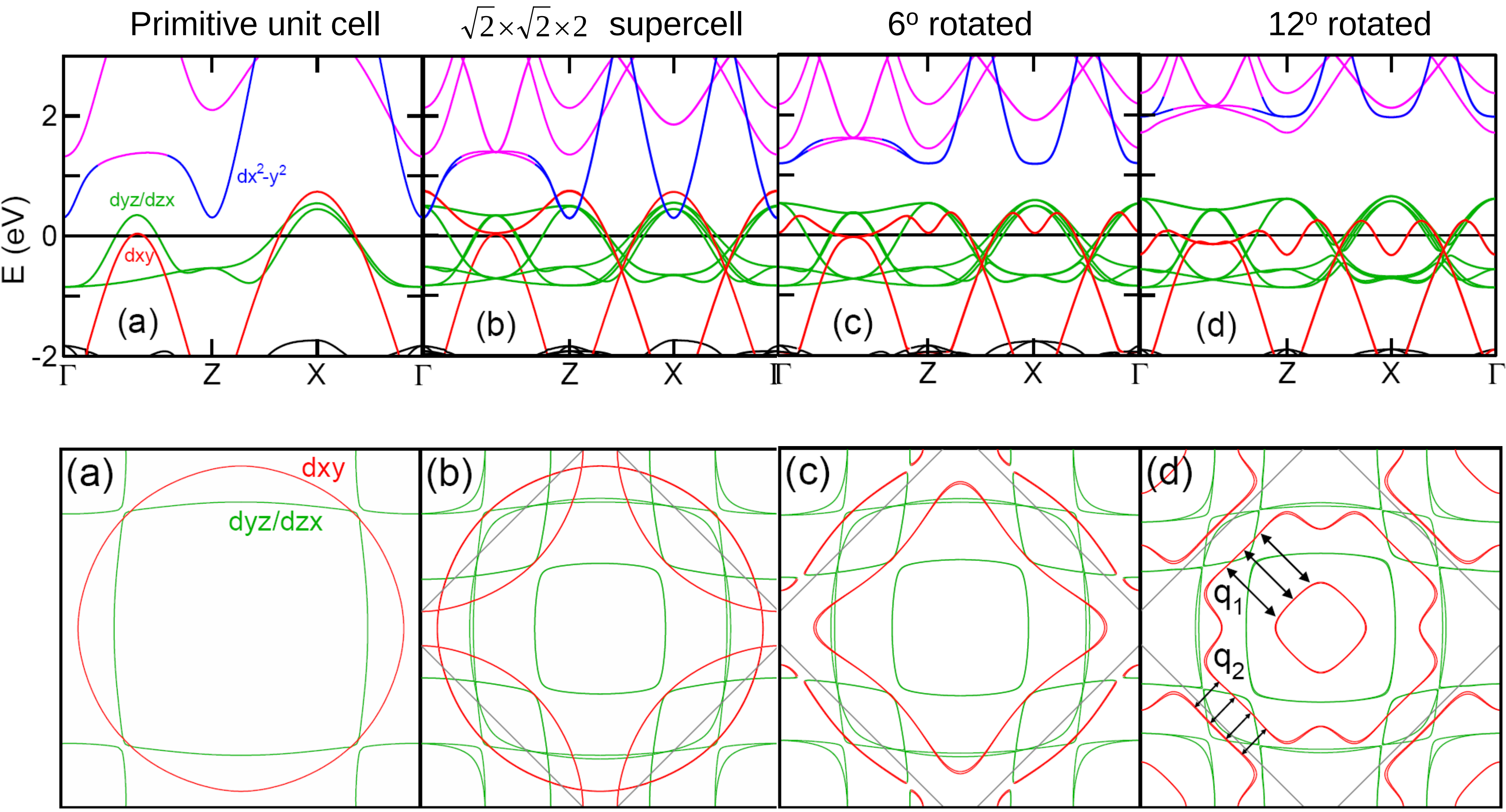






Observation of *xy*-band sunken under E_f

What about $(Ca,Sr)_2RuO_4$? - LDA



E. Ko, et al., to appear in PRL

Summary – Sr_2RhO_4

- Rotation of the octahedra leads to hybridization of *xy* and x^2-y^2 bands.

- Hybridization of *xy* and x^2-y^2 bands results in:
  (1) transfer of electrons from *yz/zx* to *xy* band and
  (2) disappearance of the *xy* Fermi surface.

- e_g states play vital role in determining electronic structures near E_f, and therefore should be included in the theoretical models that deals with 4*d* TMOs.