

The electronic structure of layered ruthenates from Angle-Resolved Photoemission Spectroscopy

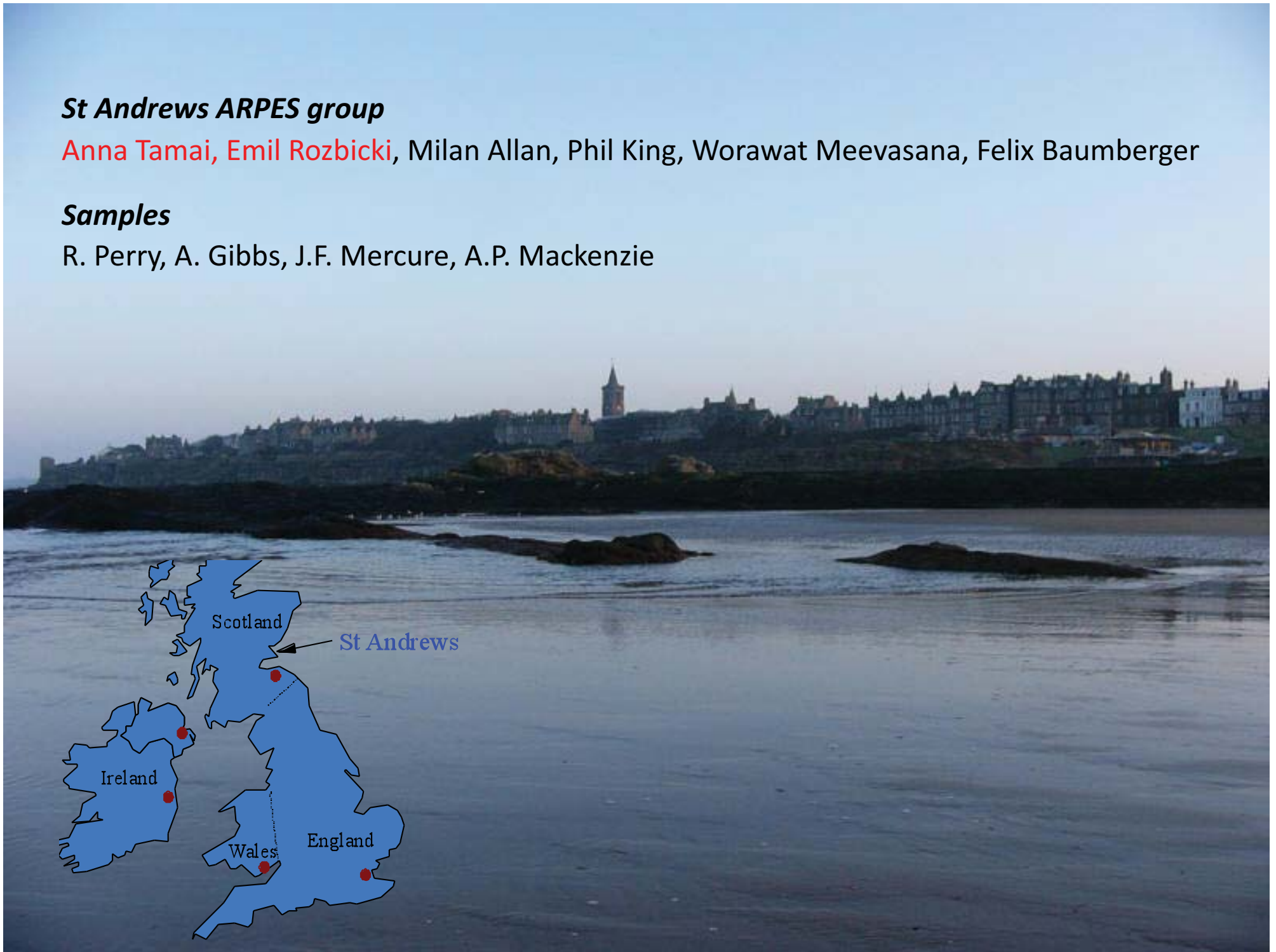
Felix Baumberger, University of St. Andrews

St Andrews ARPES group

Anna Tamai, Emil Rozbicki, Milan Allan, Phil King, Worawat Meevasana, Felix Baumberger

Samples

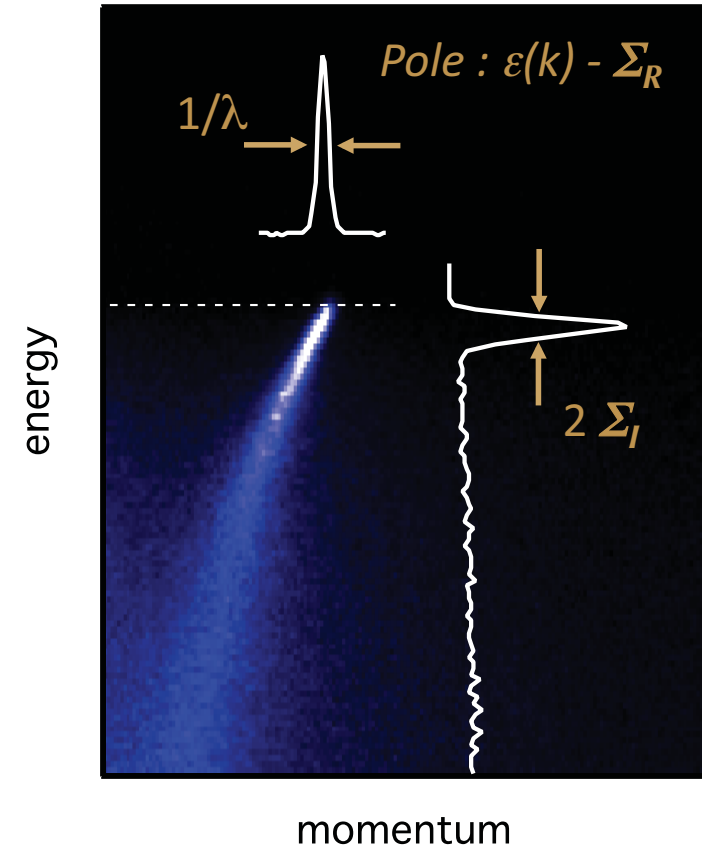
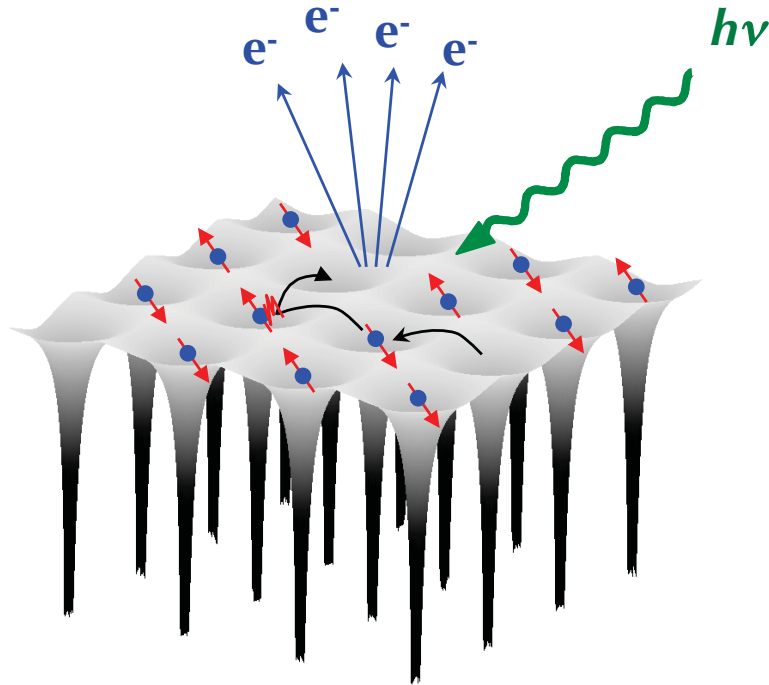
R. Perry, A. Gibbs, J.F. Mercure, A.P. Mackenzie



Content

1. Introduction
2. Van Hove singularities and strong correlations in $\text{Sr}_3\text{Ru}_2\text{O}_7$
3. **k**-dependent mass renormalization in Sr_2RuO_4

ARPES : a probe of interactions



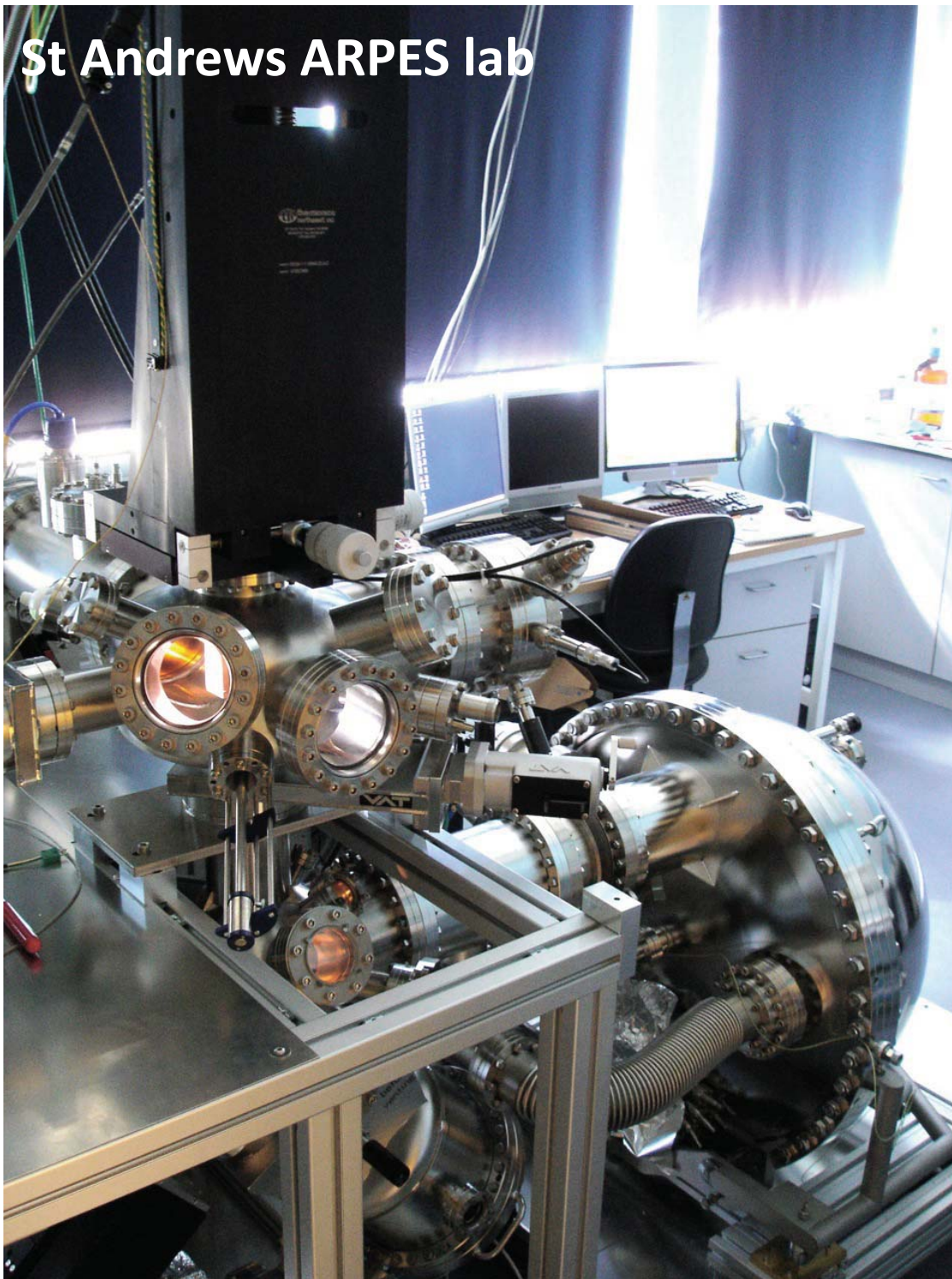
$$A(k, \omega) = \frac{1}{\pi} \frac{Z_k \Sigma_I}{(\omega - \epsilon(k) - \Sigma_R)^2 + (\Sigma_I)^2} + (1 - Z_k) A_{inc}$$

Z_k : renormalization constant (weight of QP pole)

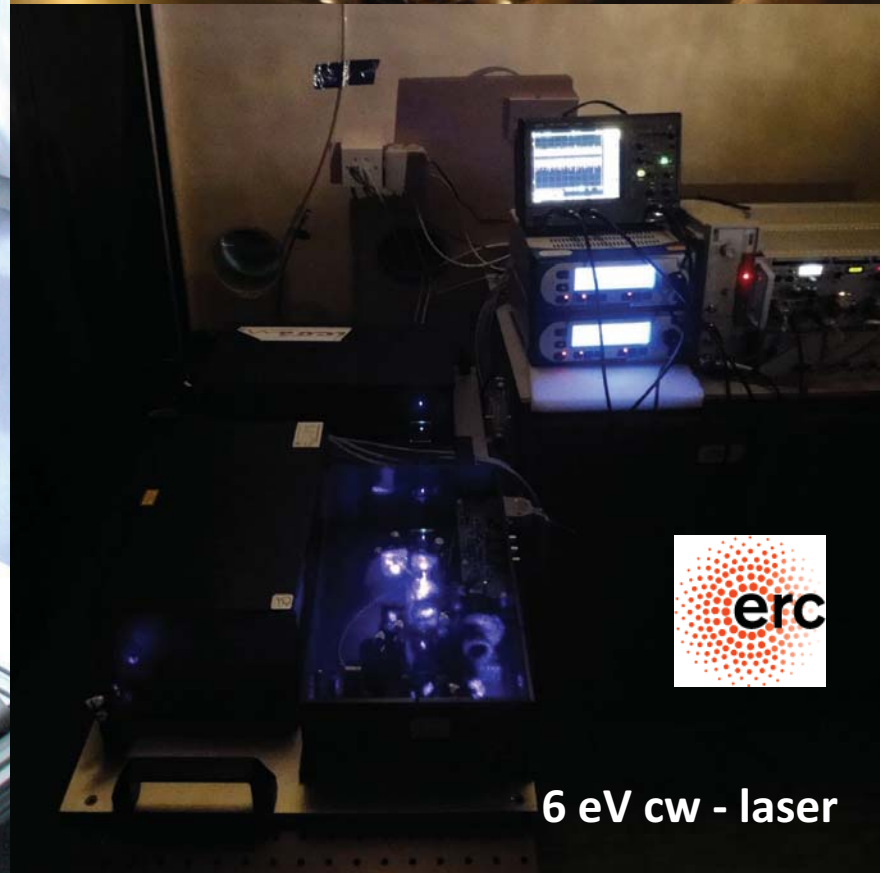
Σ_I : inverse lifetime

Σ_R : energy shift of pole

St Andrews ARPES lab

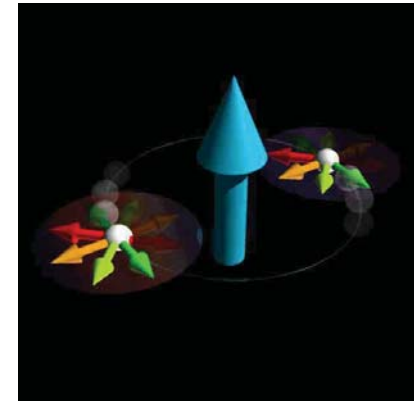
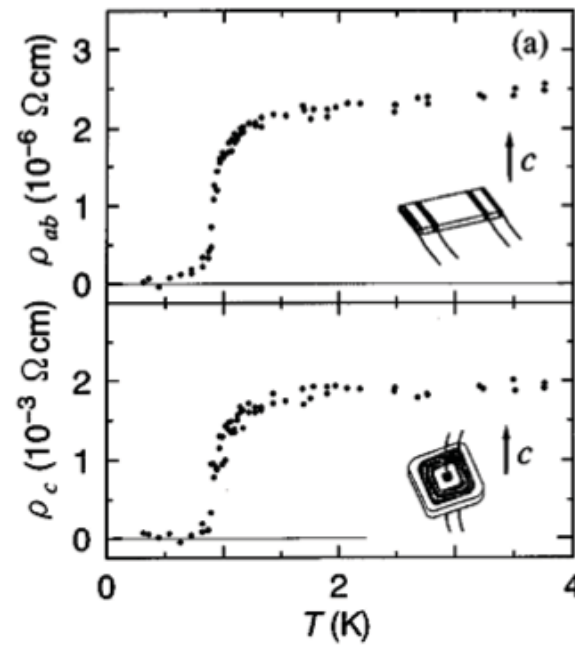
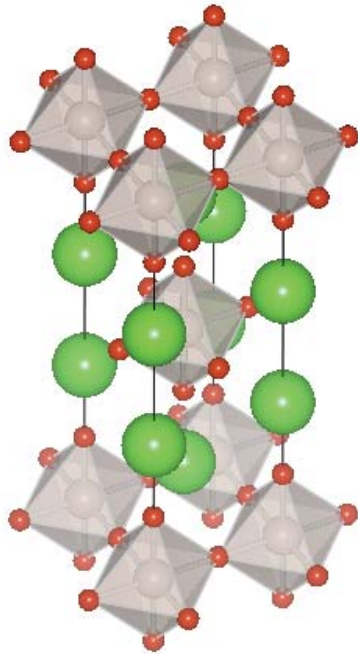


sub - 4 K 6 axis goniometer



6 eV cw - laser

1994 : Superconductivity in Sr_2RuO_4

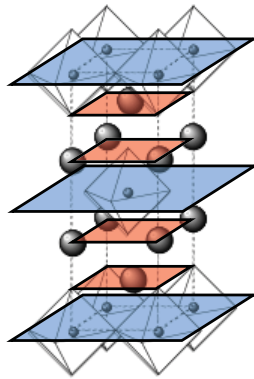


Mackenzie and Maeno, RMP **75**, 657
Ishida, PRB **56**, 505
Nelson *et al.* Science **306**, 1151
Rice and Sigrist JPCM **7**, L643

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

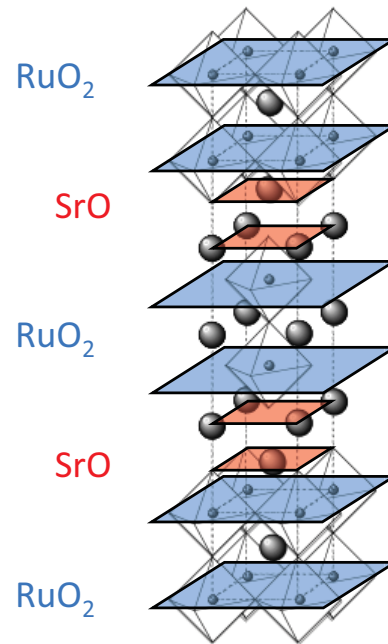
The bilayer ruthenate $\text{Sr}_3\text{Ru}_2\text{O}_7$

Sr_2RuO_4 , $n = 1$



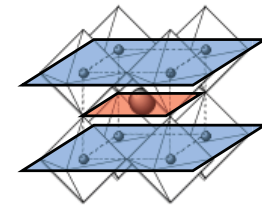
Fermi liquid with p-wave
superconducting ground
state, $T_c = 1.5$ K

$\text{Sr}_3\text{Ru}_2\text{O}_7$, $n = 2$



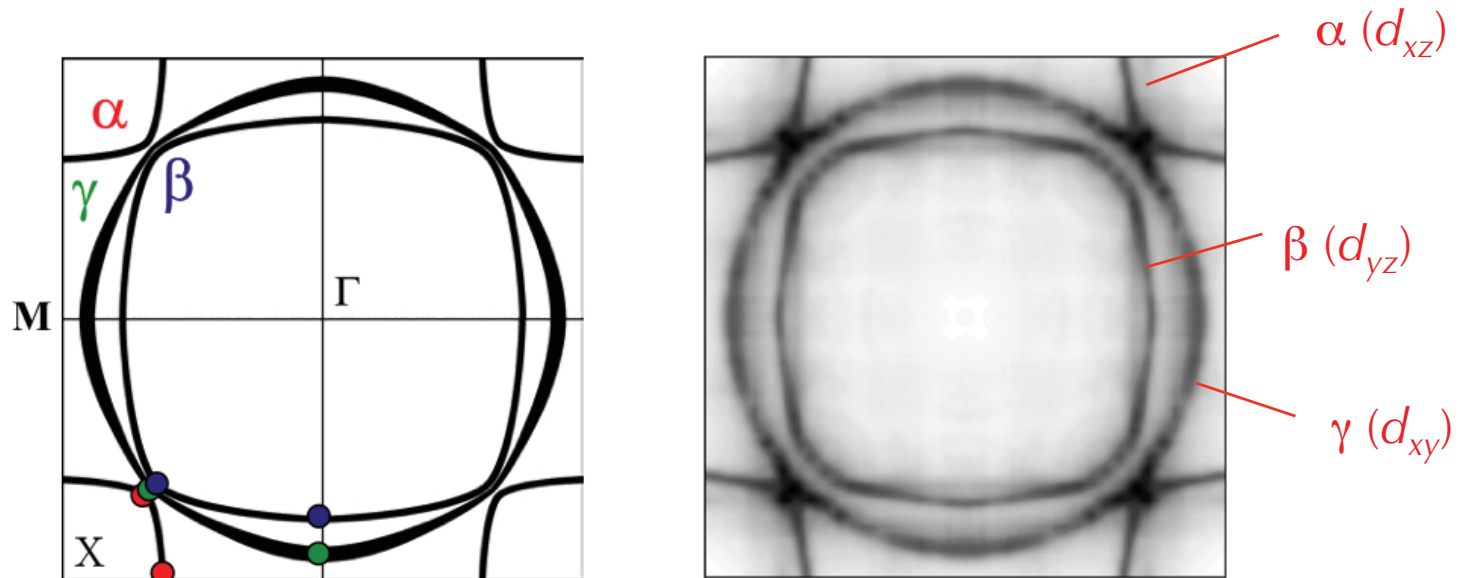
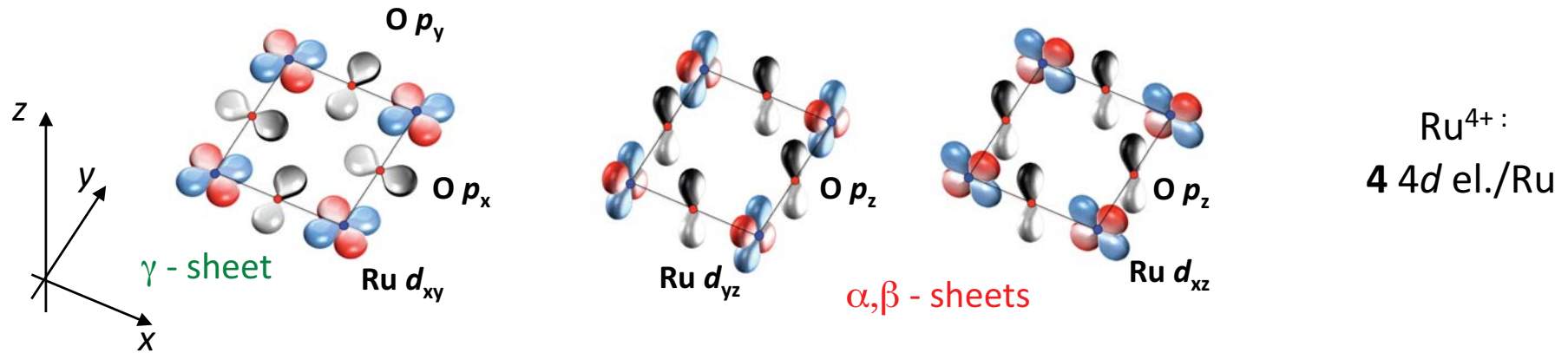
Strongly enhanced paramagnet

SrRuO_3 , $n = \infty$



Itinerant ferromagnet, non-
FL fractional power law
conductivity

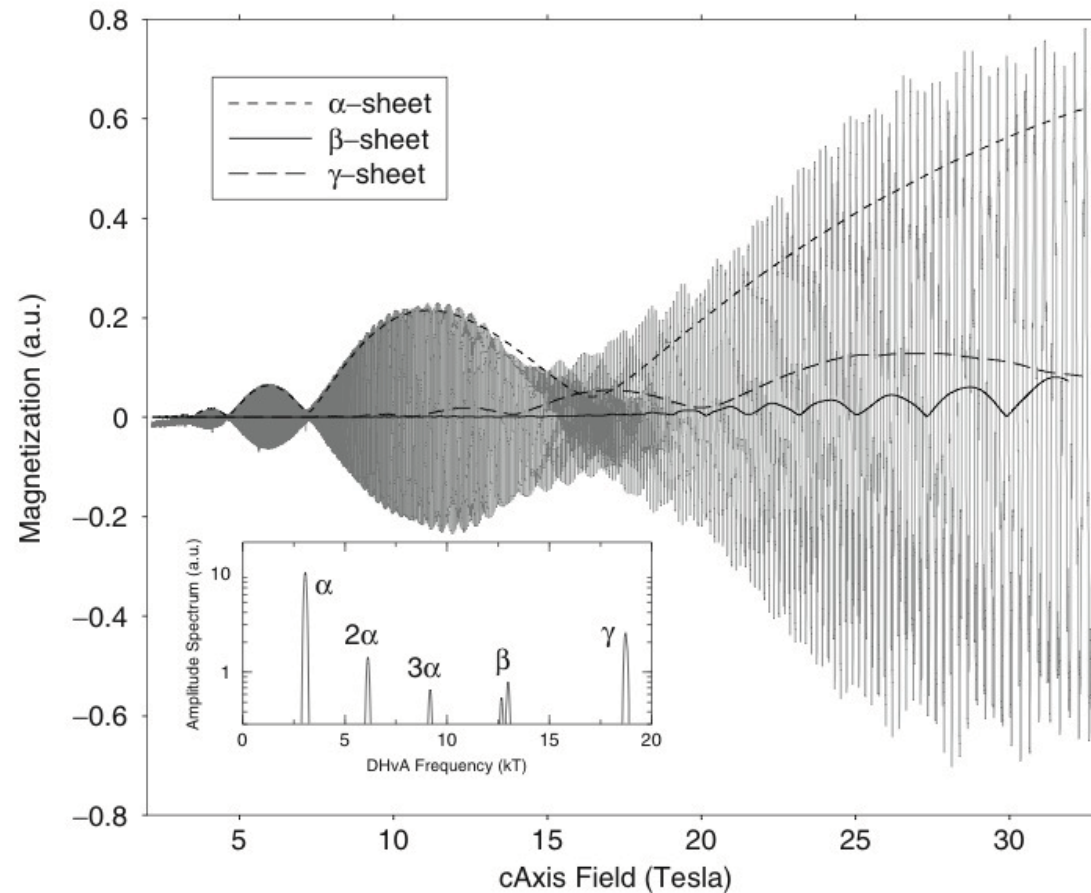
Relevant Orbitals in Ruthenates



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

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

Sr_2RuO_4 - normal state: a model Fermi liquid

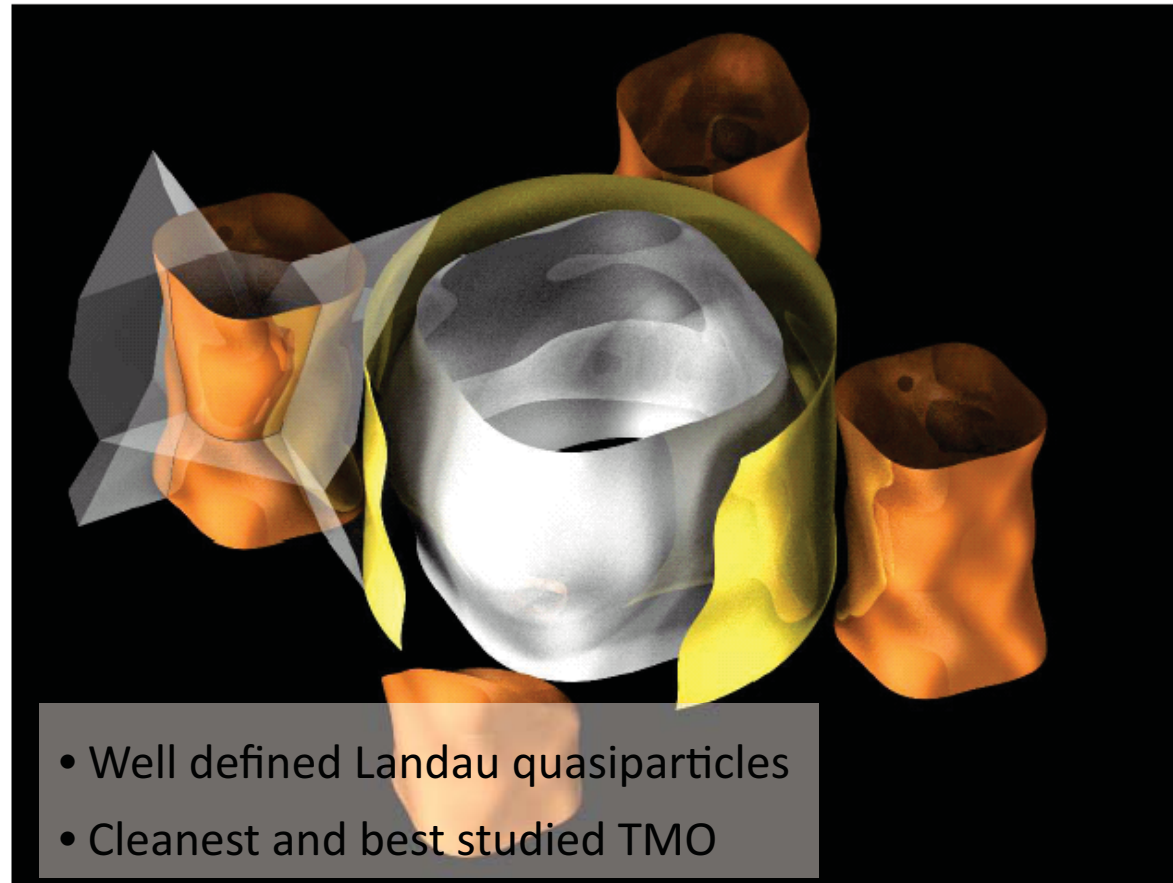


Mackenzie *et al.* PRL **76**, 3786

Bergemann *et al.* PRL **84**, 2662

Bergemann *et al.* Adv. Phys. **52**, 639

Sr_2RuO_4 - normal state: a model Fermi liquid

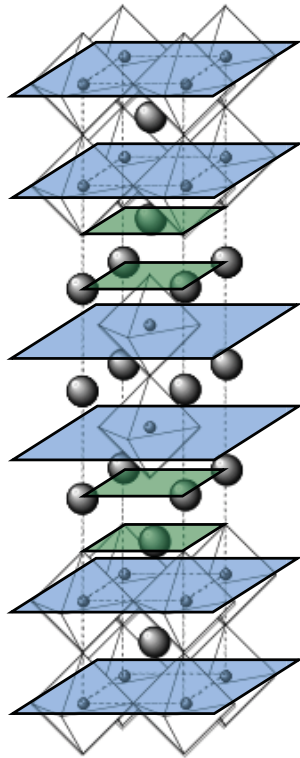


Mackenzie *et al.* PRL **76**, 3786

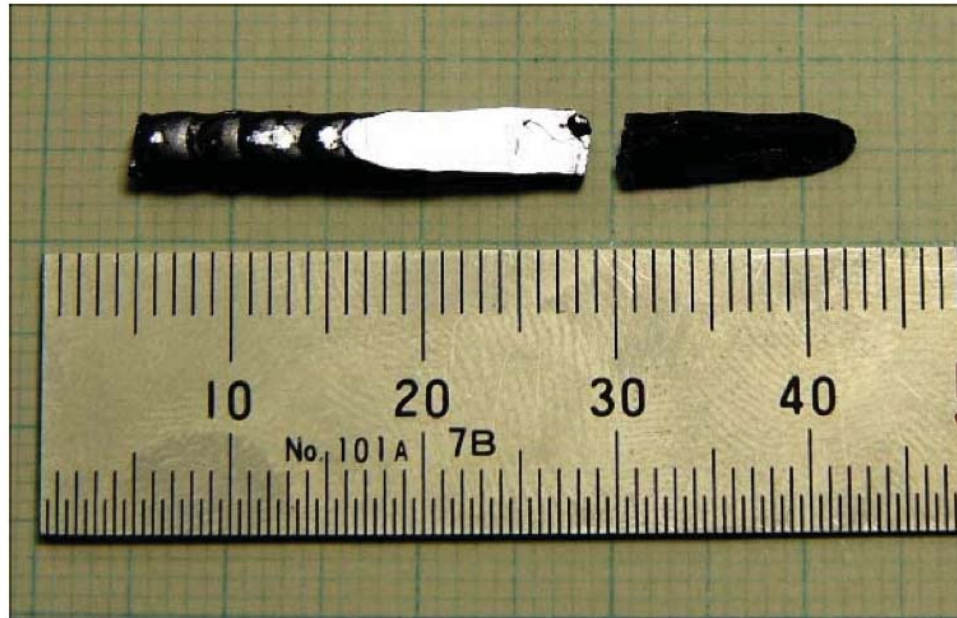
Bergemann *et al.* PRL **84**, 2662

Bergemann *et al.* Adv. Phys. **52**, 639

The bilayer strontium-ruthenate $\text{Sr}_3\text{Ru}_2\text{O}_7$

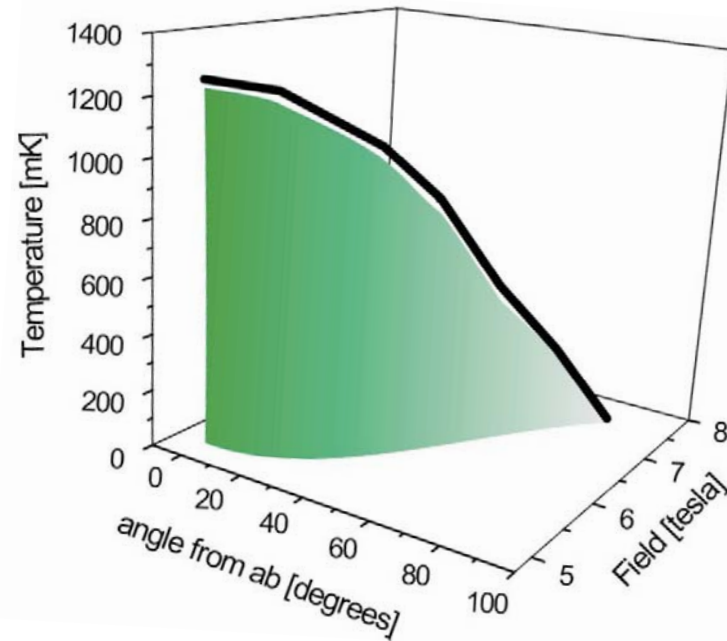
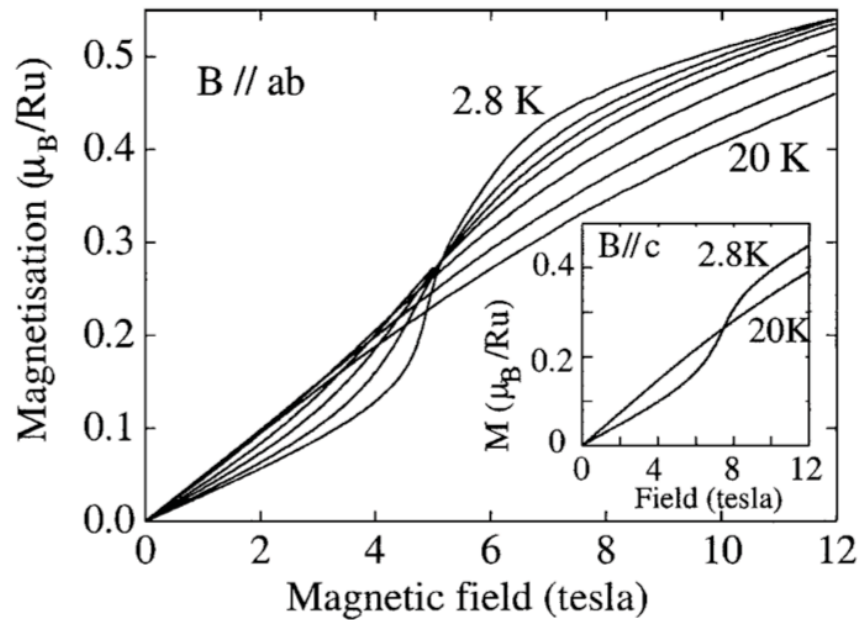


R. Perry and Y. Maeno, *Journal of Crystal Growth* **271** (2004) 134.



High purity samples
Residual in-plane resistivity $< 0.5 \mu\Omega\text{cm}$

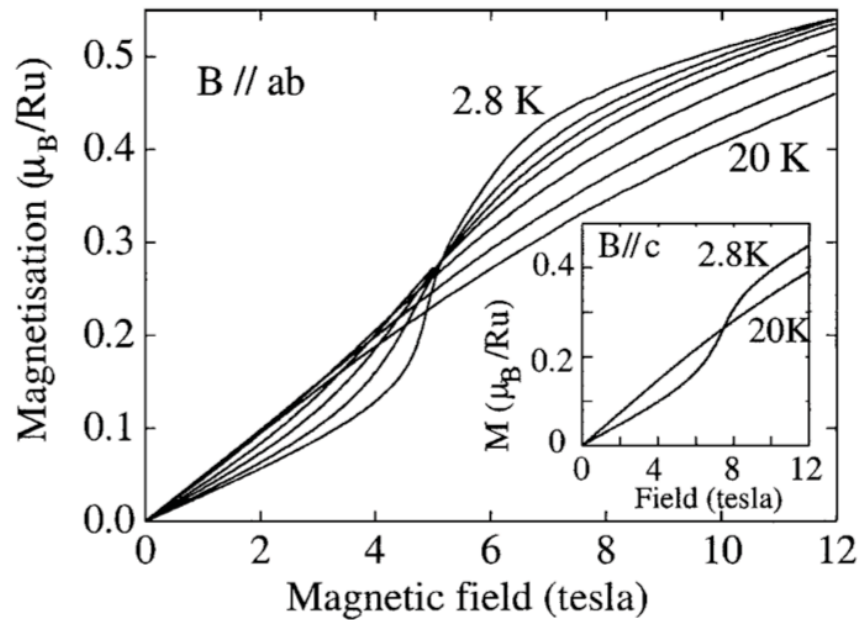
Metamagnetic transition in $\text{Sr}_3\text{Ru}_2\text{O}_7$



R.S. Perry, et al., PRL **86**, 2661 (2001)

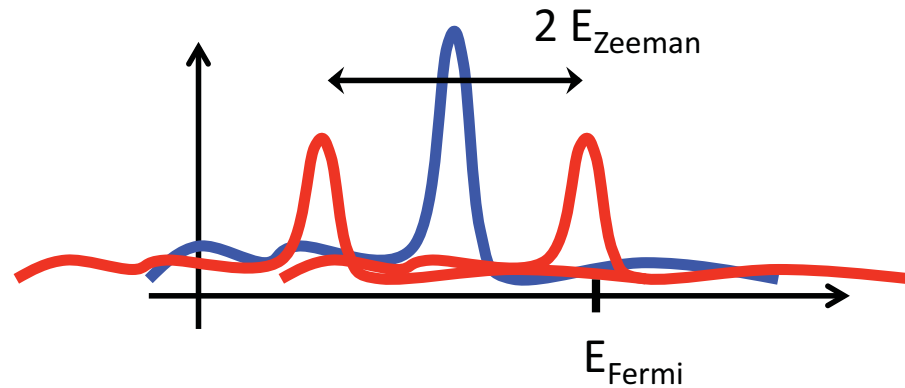
S.A. Grigera et al., PRB **67**, 214427 (2003)

Metamagnetic transition



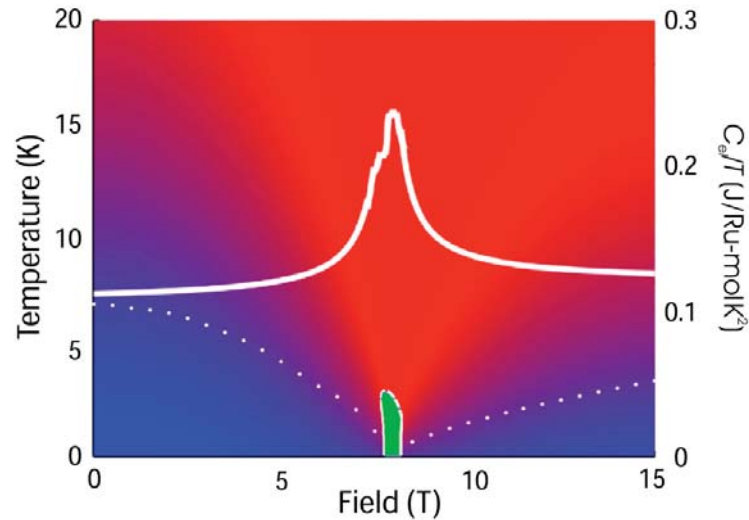
Stoner enhancement :

$$\frac{\chi}{\chi_0} = \frac{1}{1 - \rho(0) \times const}$$



Wohlfarth and Rhodes '62
Binz and Sigrist '04

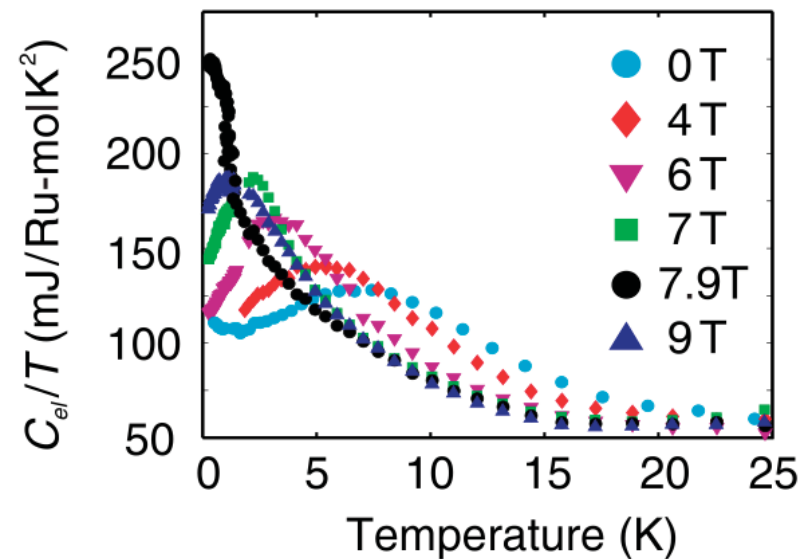
Quantum criticality



Suppression of single energy scale of ≈ 2 meV

Non – Fermi liquid behavior :

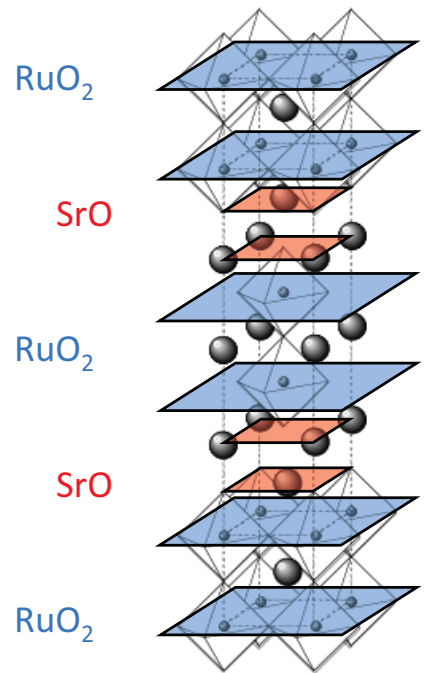
- T – linear resistivity
- Logarithmic divergence of specific heat



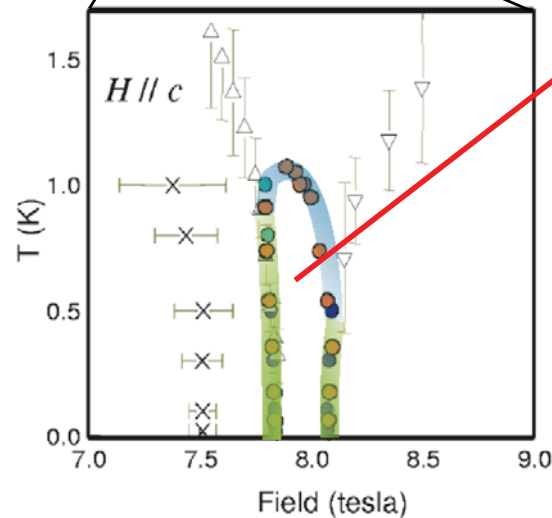
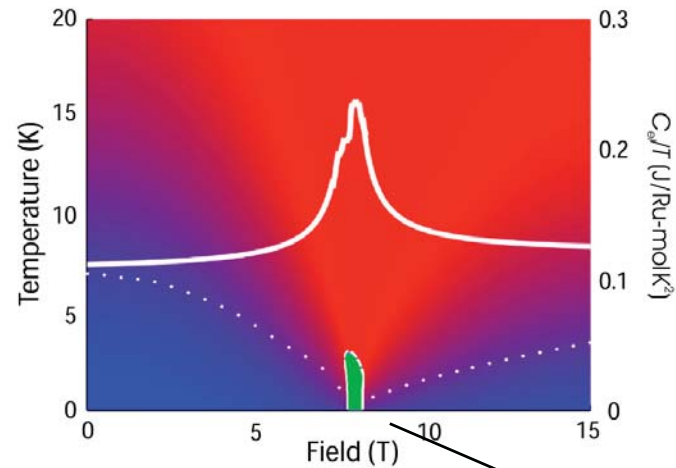
S. A. Grigera, et al., Science **294** 329 (2001)
R.A. Borzi et al. Science **315**, 214 (2007)
A.W. Rost et al. Science **325**, 1360 (2009)
A.W. Rost et al. PNAS (2011)

A.W. Rost et al. PNAS (2011)

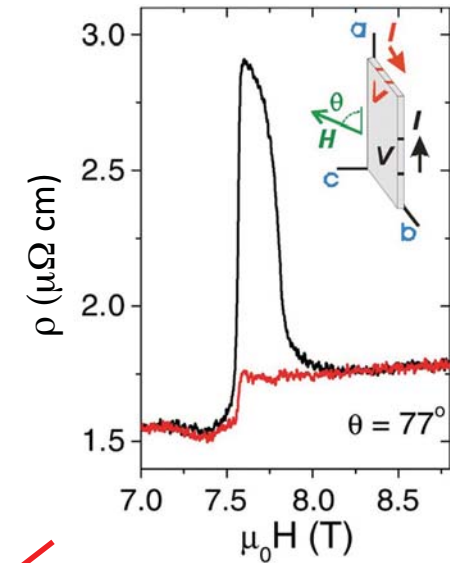
Nematic phase in $\text{Sr}_3\text{Ru}_2\text{O}_7$



C_4 symmetry



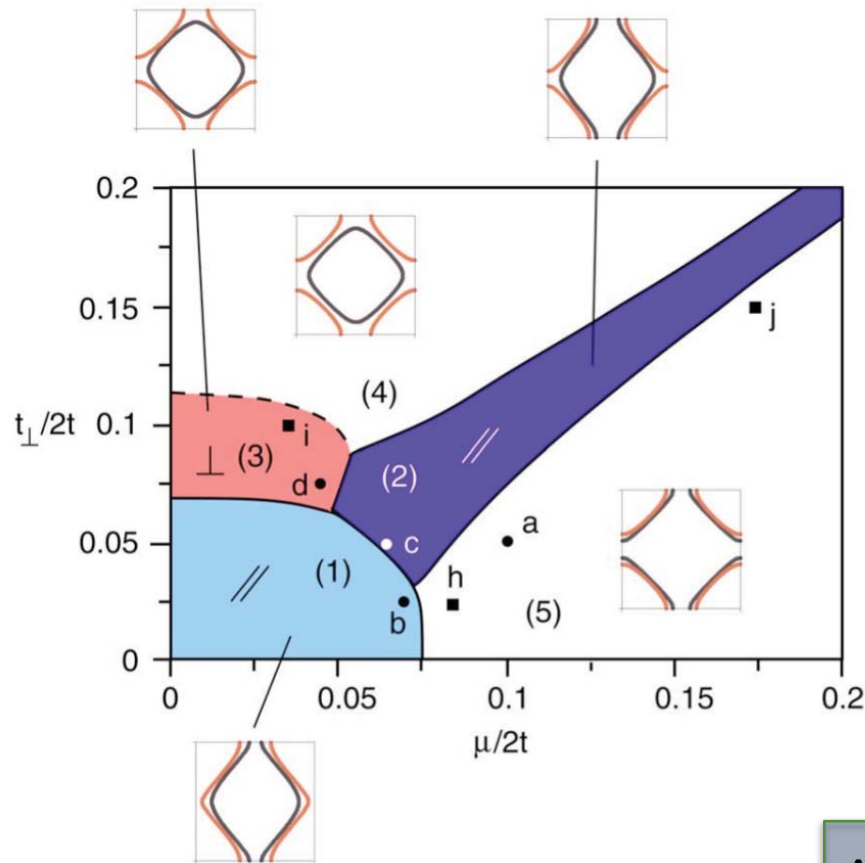
C_4 symmetry



2-fold symmetry

- S.A. Grigera, et al, Science **306**, 1154 (2004)
- R.A. Borzi et al. Science **315**, 214 (2007)
- A.W. Rost et al. Science **325**, 1360 (2009)

Recent theoretical work



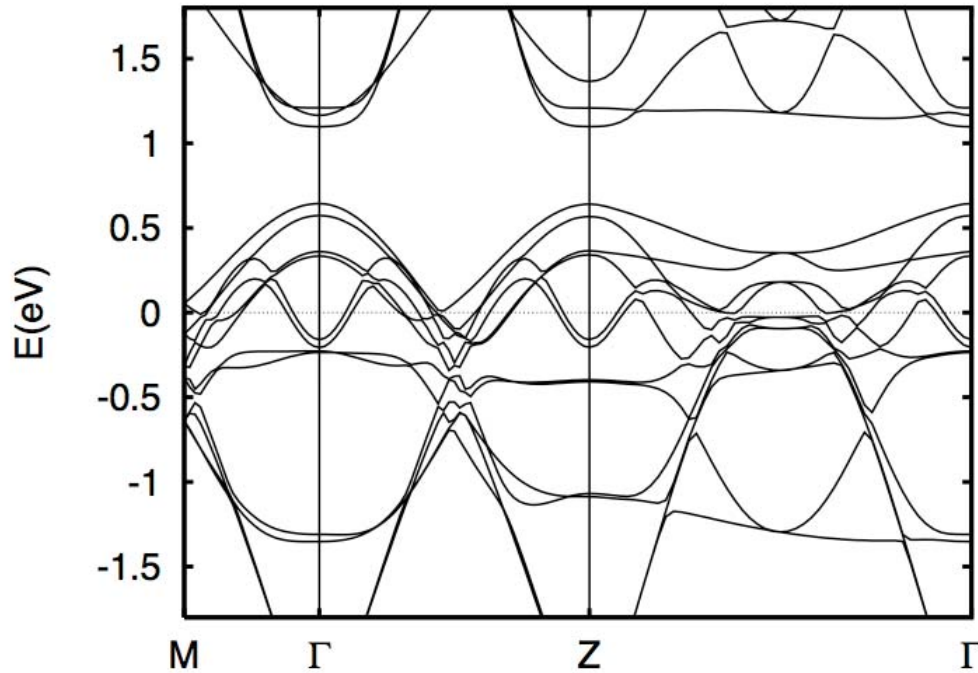
Microscopic models based on hypothetical band structure :

Binz and Sigrist, Europhysics Letters **65** 816 (2004)
 Puetter *et al.*, PRB **76**, 235112 (2007)
 Kee and Kim, PRB **71**, 184402 (2005)
 Binz *et al.*, PRL **96** 196406 (2006)
 Raghu *et al.*, PRB, **79** 214402 (2009)
 Berridge, *et al.*, PRL **102** 136404 (2009)
 Lee and Wu, PRB **80**, 104438 (2009)
 Yamase, PRB **80**, 115102 (2009)
 Adachi and Sigrist, PRB **80**, 155123 (2009)
 Fischer and Sigrist, PRB **81**, 064435 (2010)
 Puetter *et al.*, PRB **81**, 081105(R) (2010)
 Fradkin, Kivelson *et al.*, Ann. Rev. Cond. Mat. Phys. **1** (153) (2010)
 Piefke, Lechermann, arXiv:1102.0781
 Berridge *et al.*, arXiv:1011.3733
 Yamase *et al.* PRL **108**, 186405 (2012)

Assumptions:

- Extremely narrow bands
- vHs on the Zeeman energy scale (≈ 1 meV)

Bilayer band structure



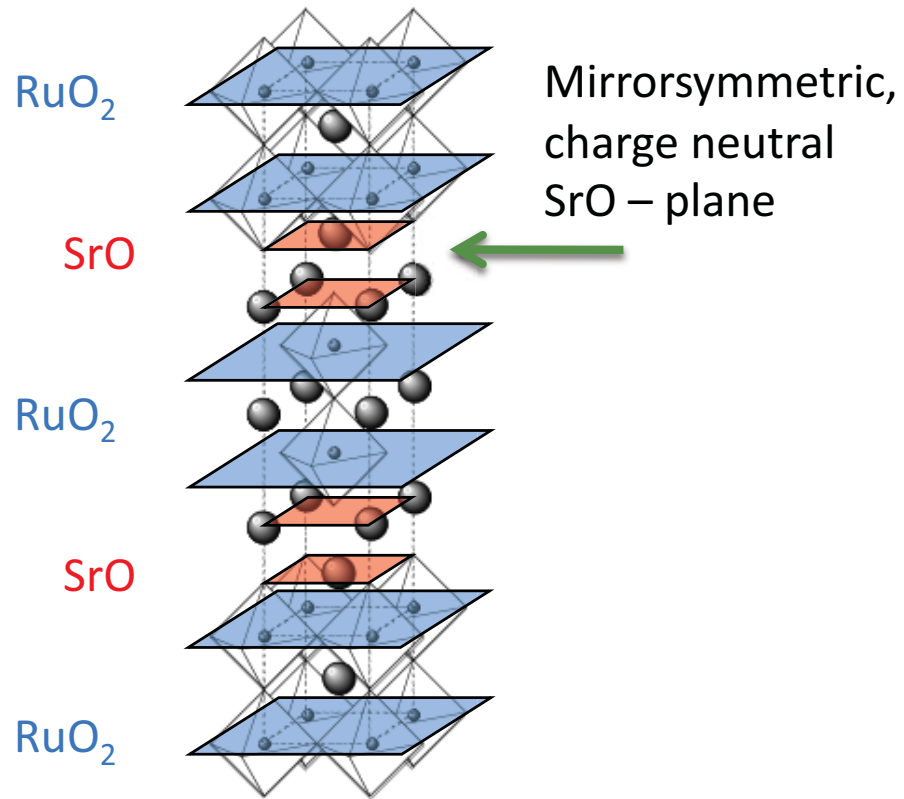
LDA band width ≈ 2.5 eV
3 orders of magnitude larger than assumed
vHs energy

LDA – DOS ≈ 4.5 states/eV/Ru
Almost identical to Sr_2RuO_4 (4.1 states/eV/Ru)

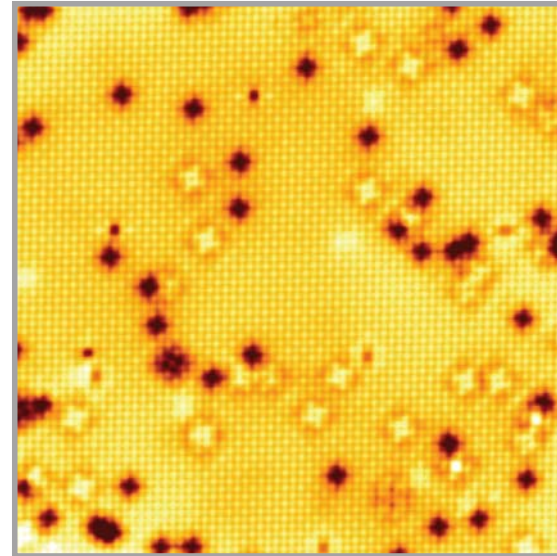
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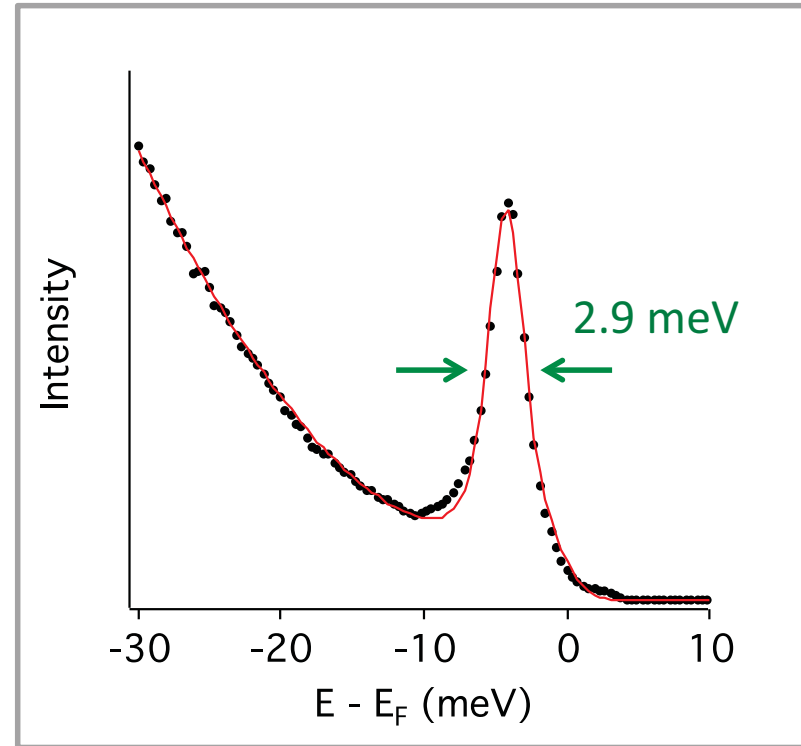
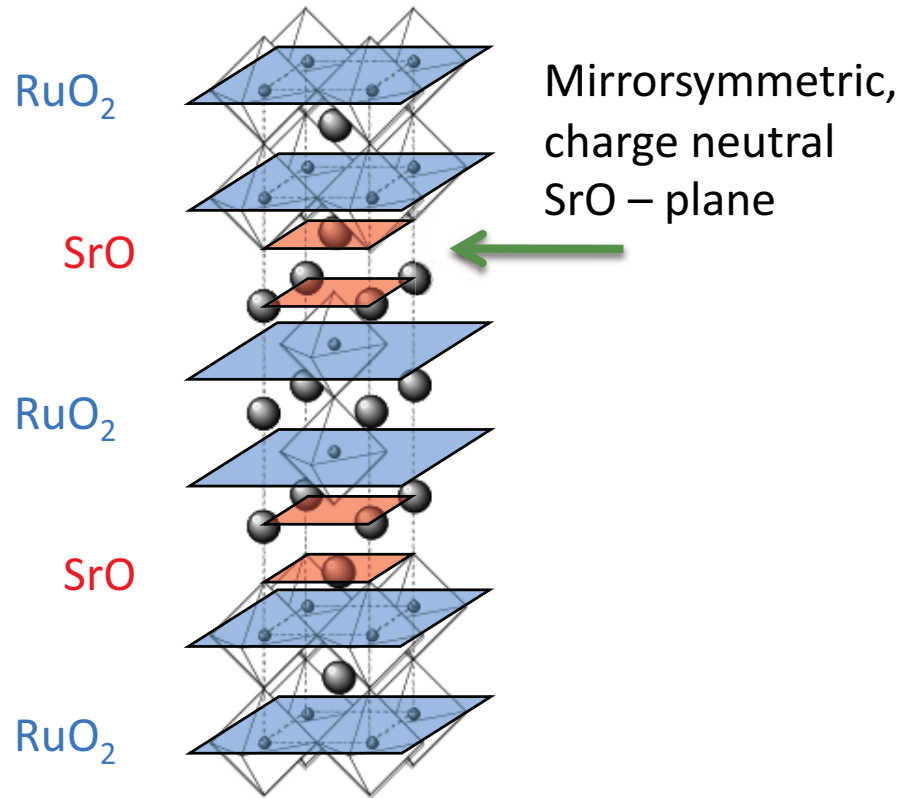
Cleavage plane



1 % Ti doping



Cleavage plane

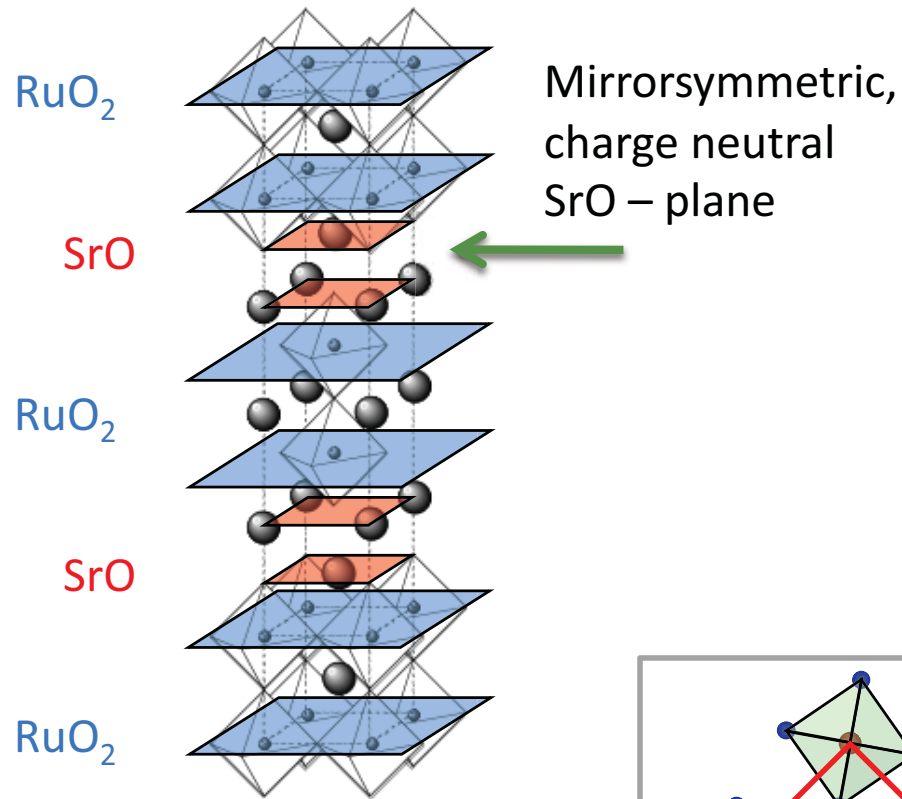


Well defined FL - quasiparticles

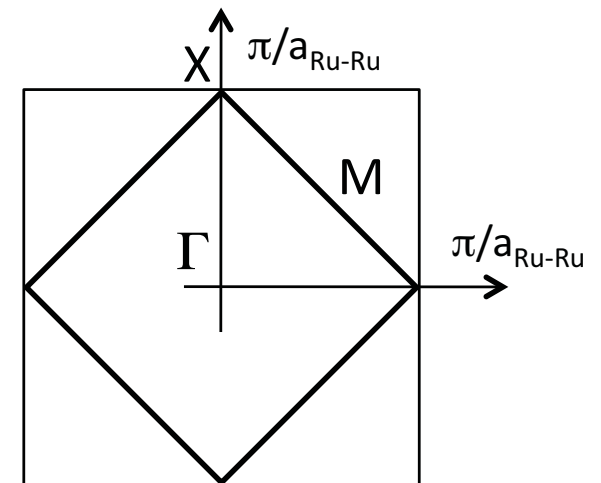
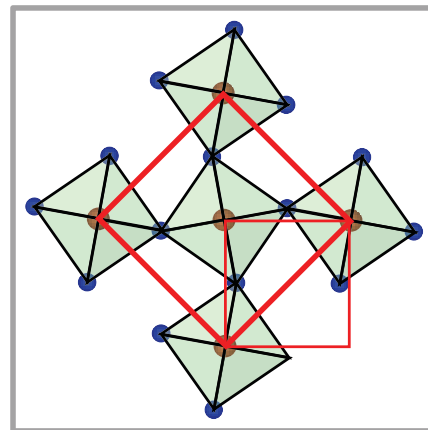
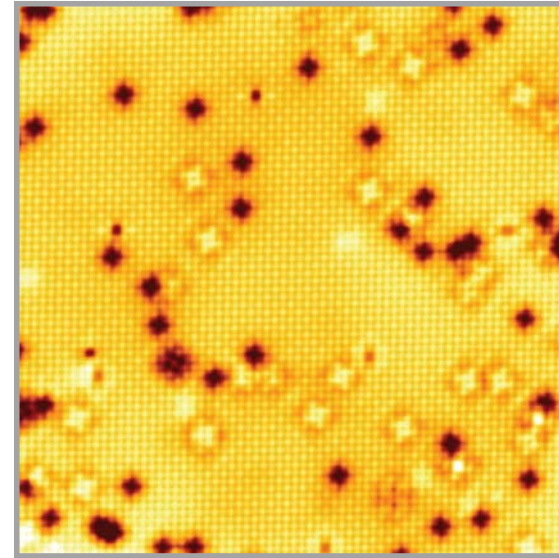
$$\Delta\varepsilon = 1.8 \text{ meV}$$

$$E_i = 4.5 \text{ meV}, \Gamma < 2 \text{ meV}$$

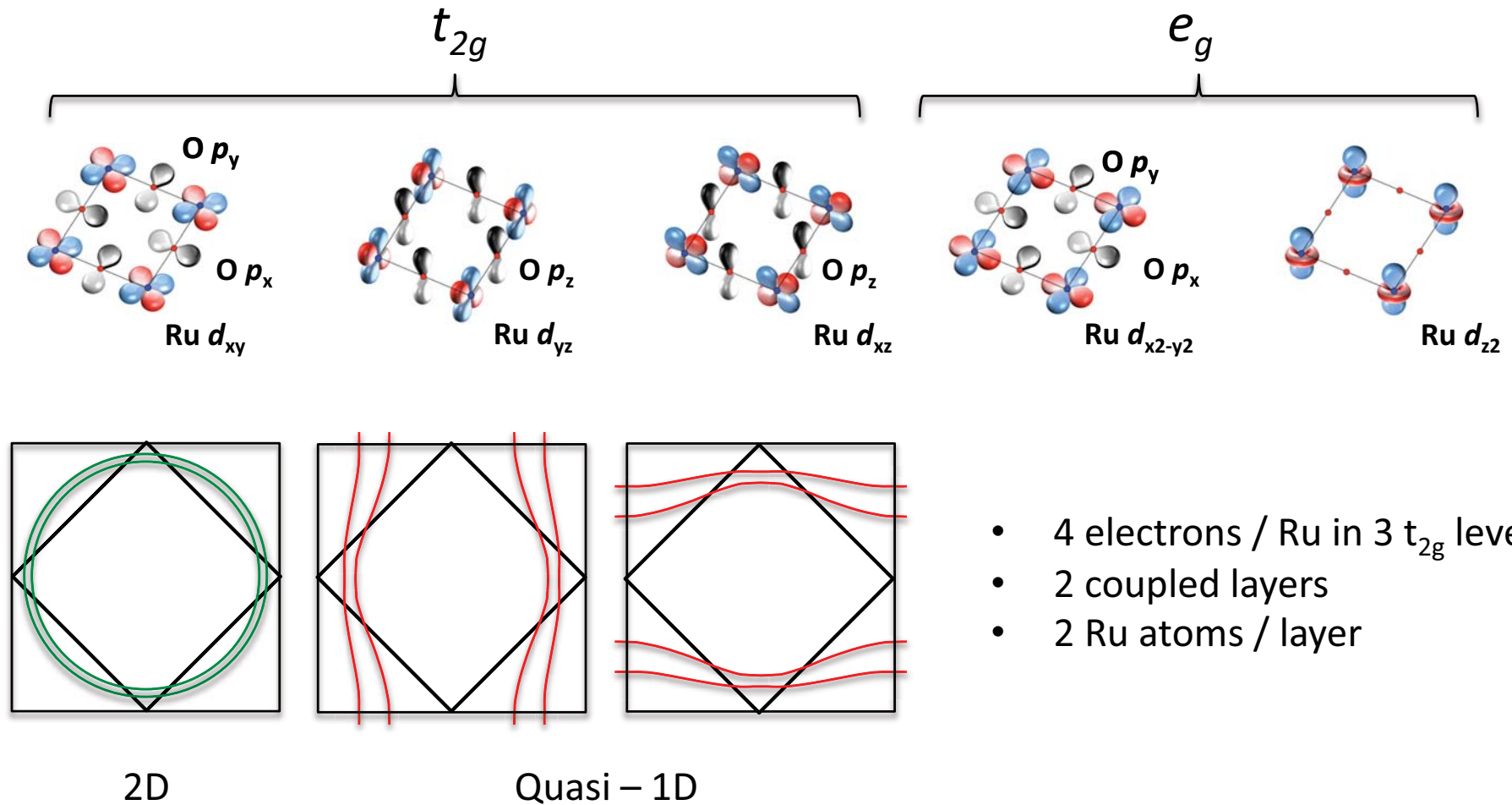
Cleavage plane



1 % Ti doping

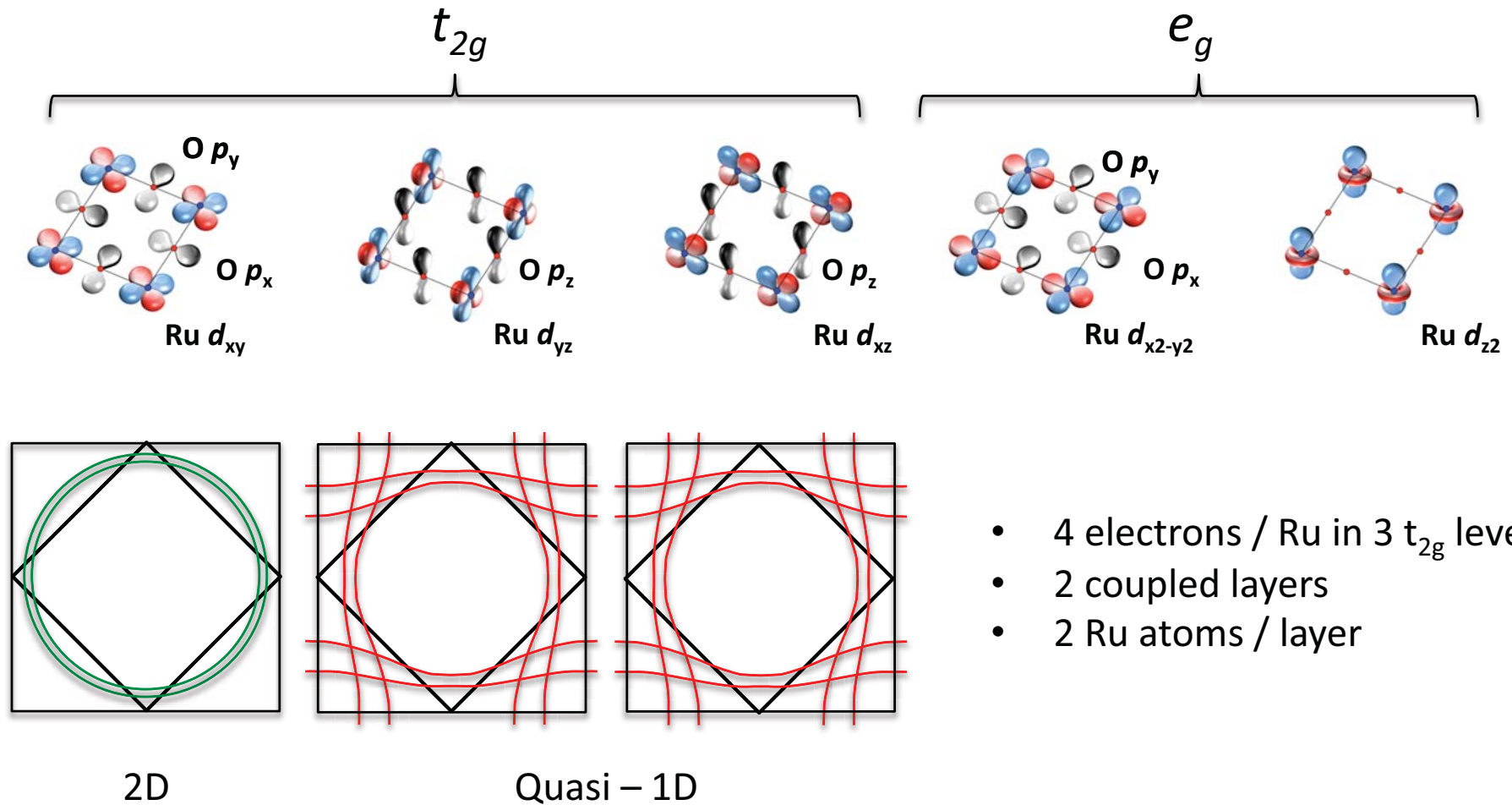


Expected Fermi surface sheets



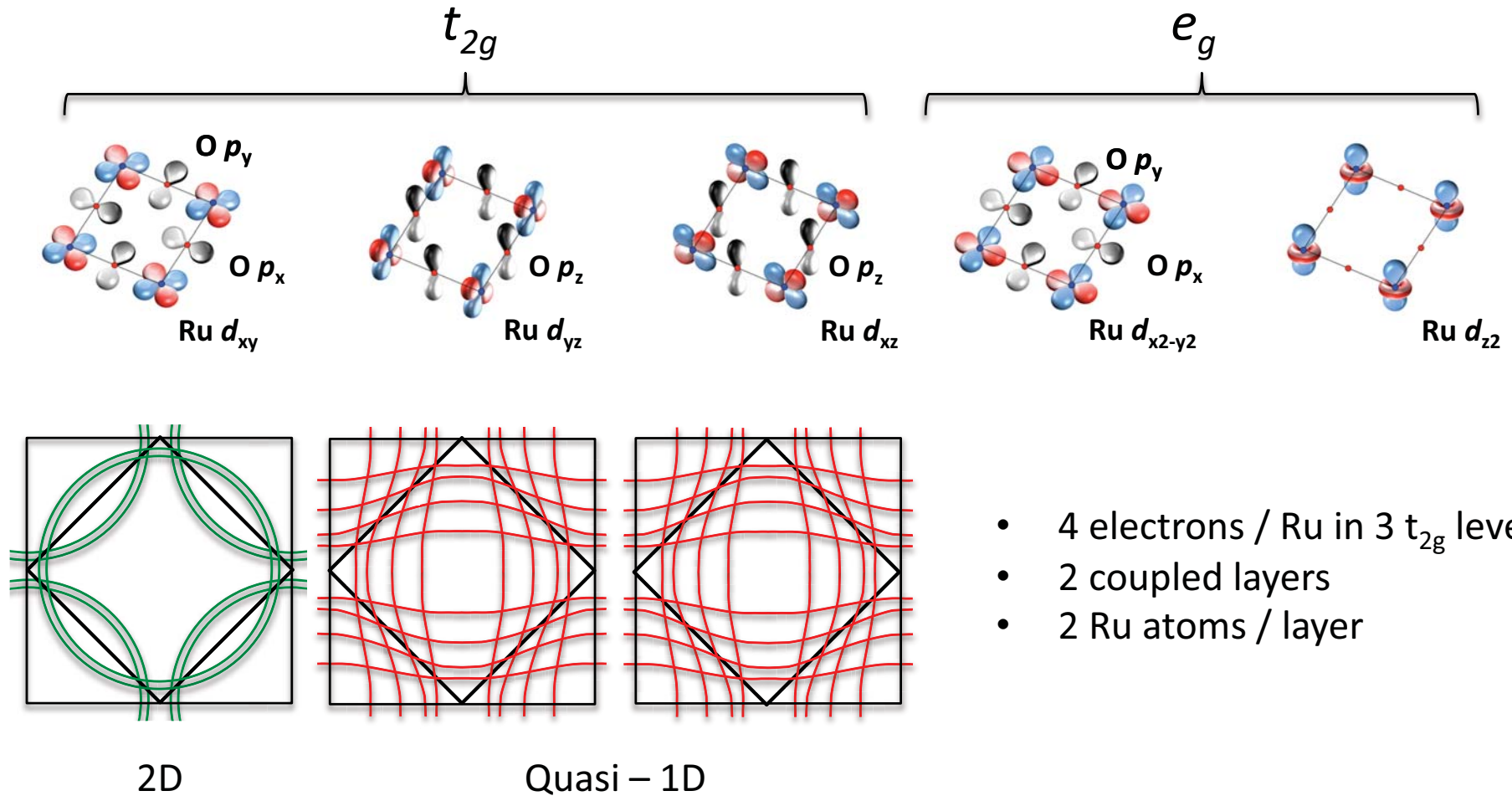
- 4 electrons / Ru in 3 t_{2g} levels
- 2 coupled layers
- 2 Ru atoms / layer

Expected Fermi surface sheets



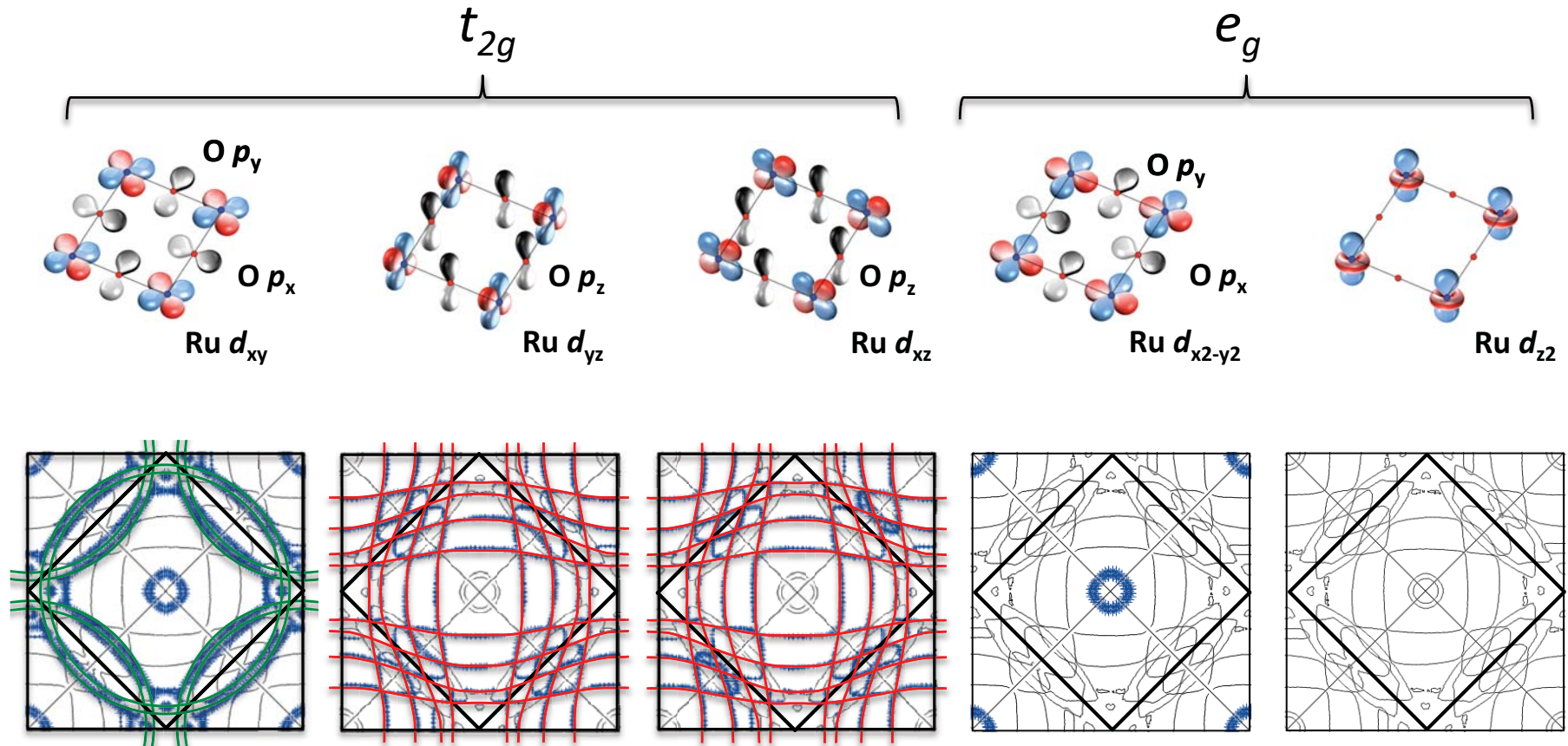
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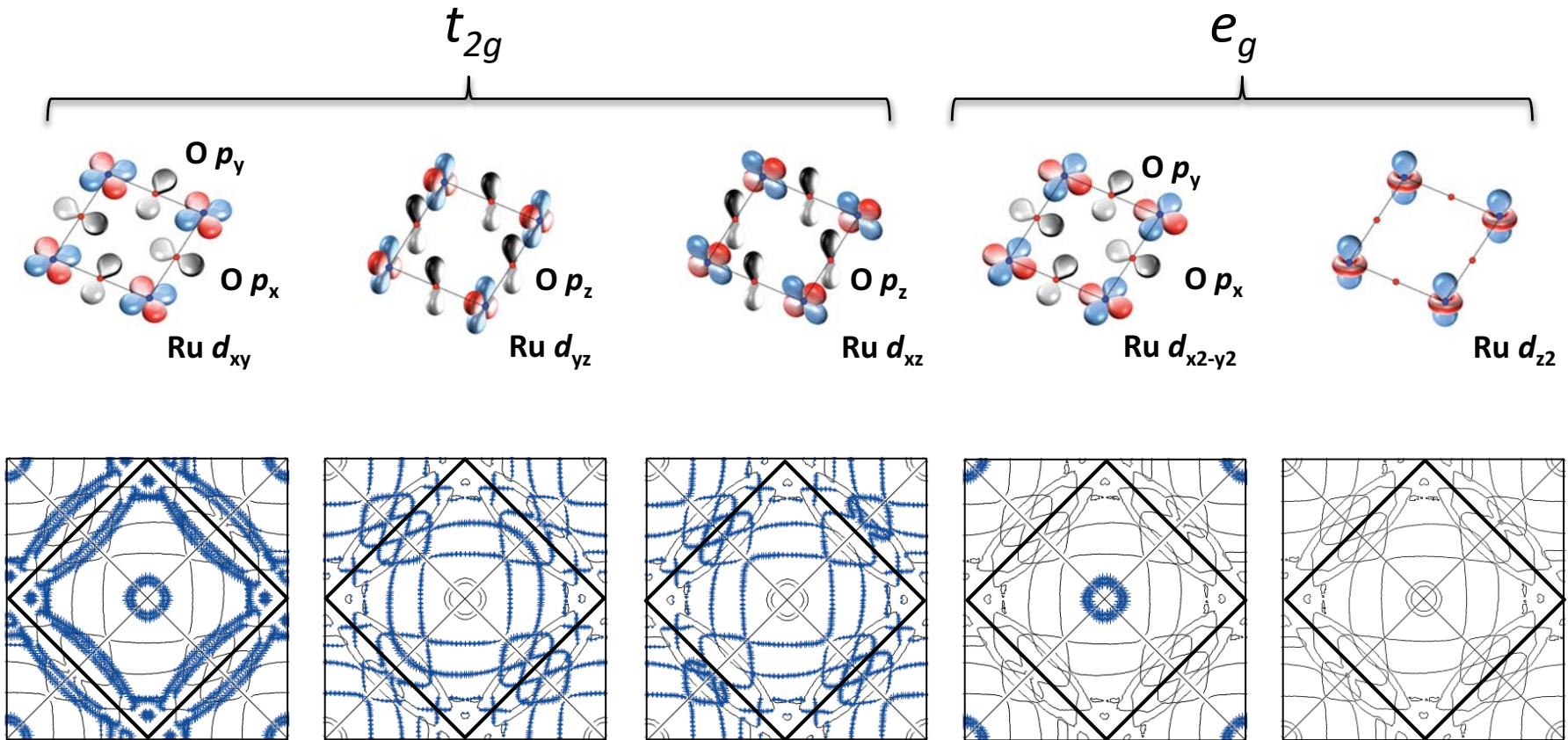


- 4 electrons / Ru in 3 t_{2g} levels
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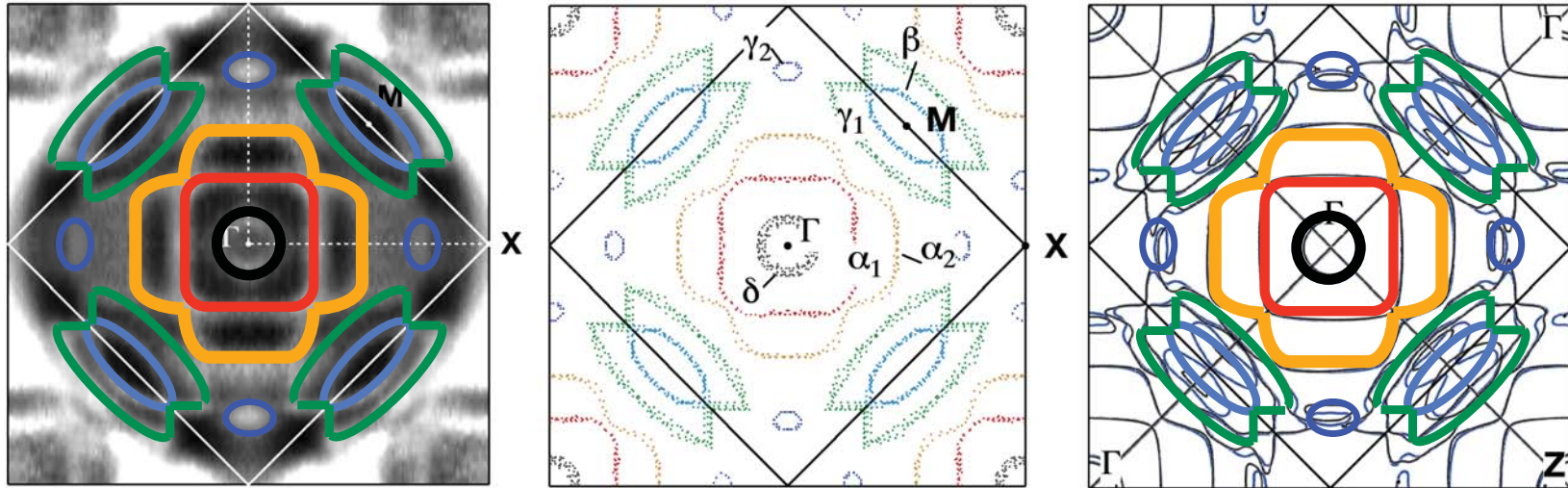
LDA Fermi Surface



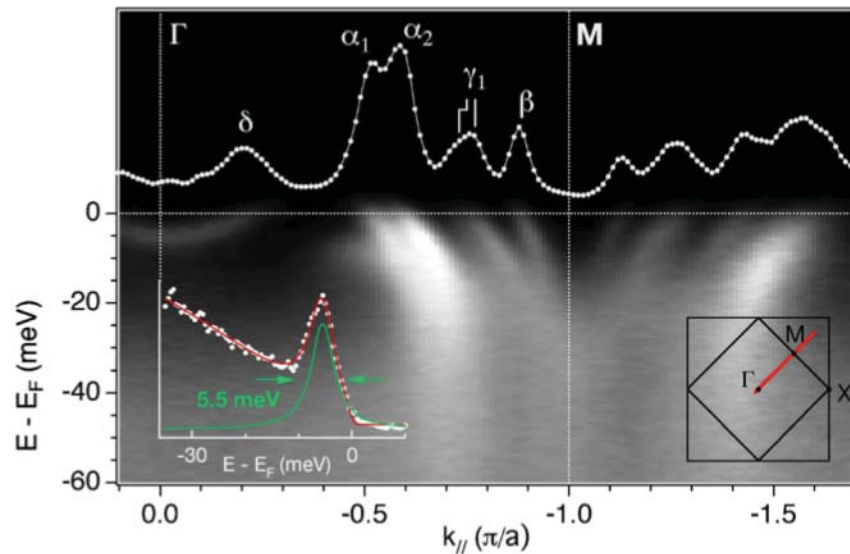
LDA Fermi Surface



Fermi surface & orbital character



LDA+SOC



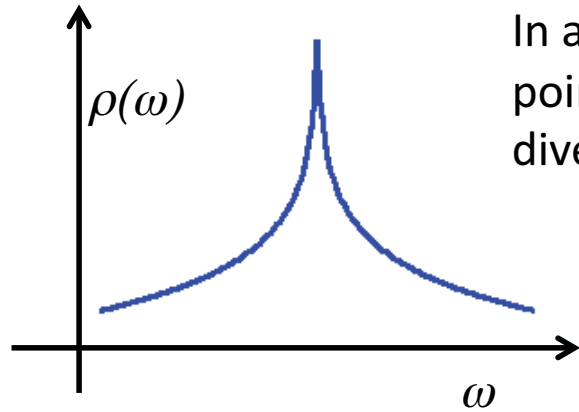
δ e_{2g} $d_{x^2-y^2}$

α_1, α_2 t_{2g} d_{xz}, d_{yz}

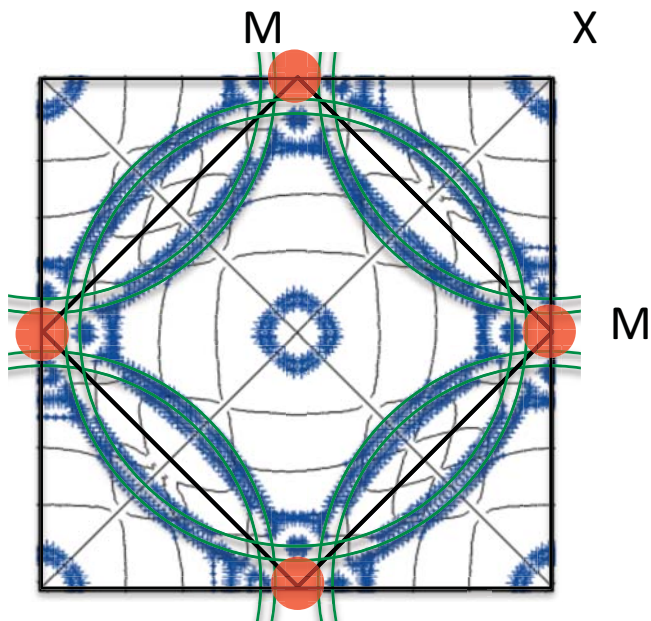
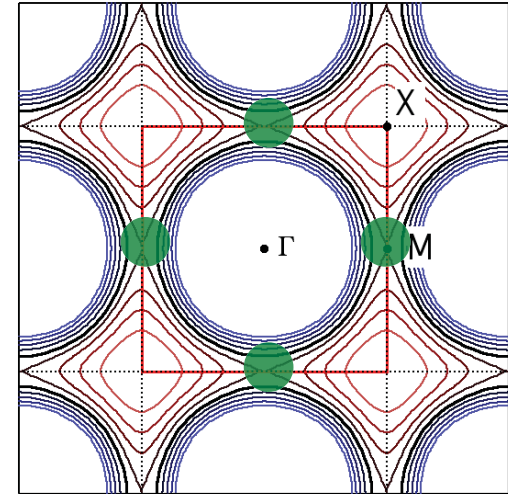
β t_{2g} d_{xz}, d_{yz}

γ_1, γ_2 t_{2g} mainly d_{xy}

Van Hove Singularity



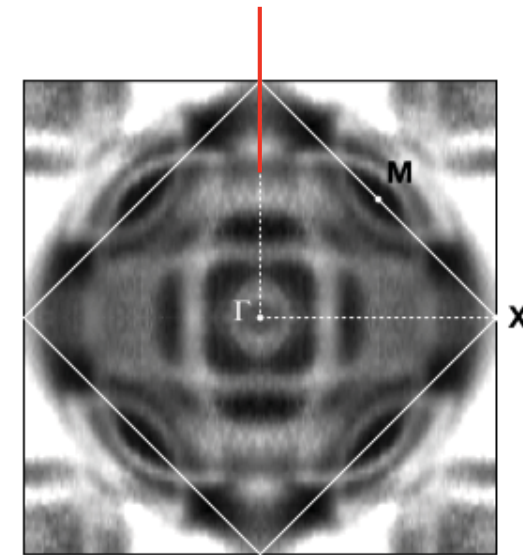
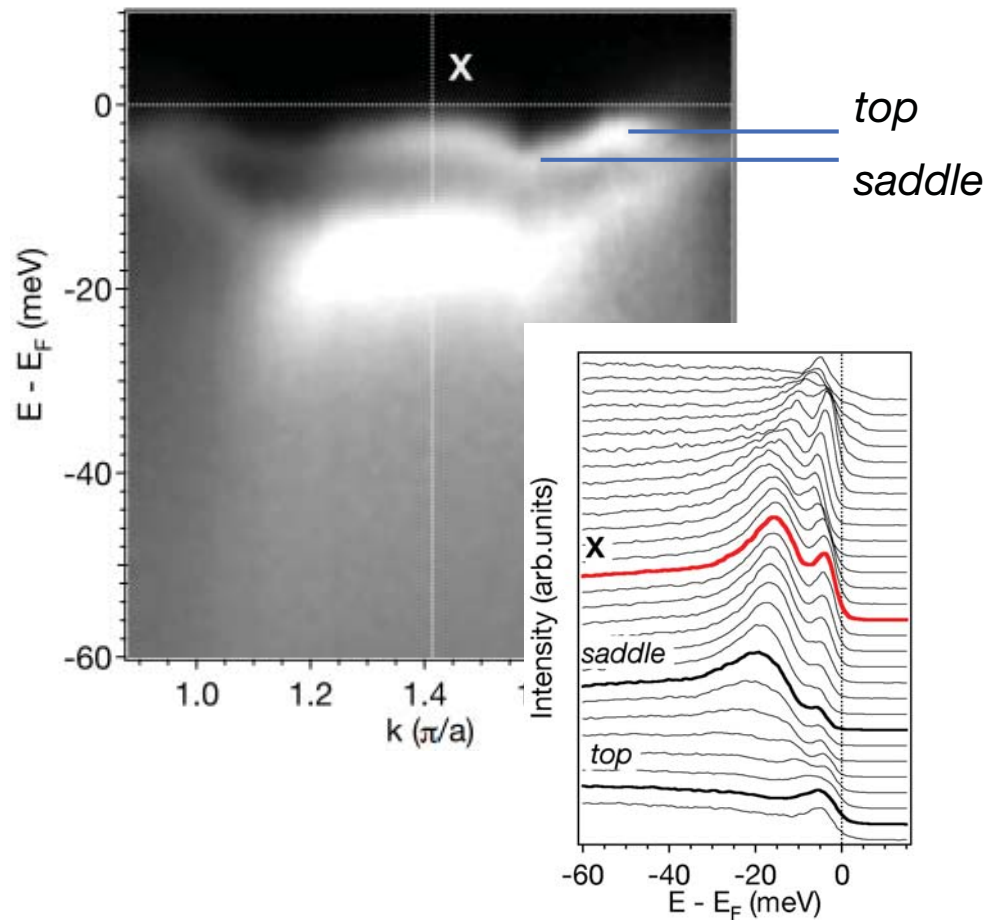
In a 2D band structure a saddle point leads to a logarithmic divergence of $\rho(\omega)$ (vHs) .



Single 2D band in a square lattice
→ Saddle points at the M point

d_{xy} - band topography

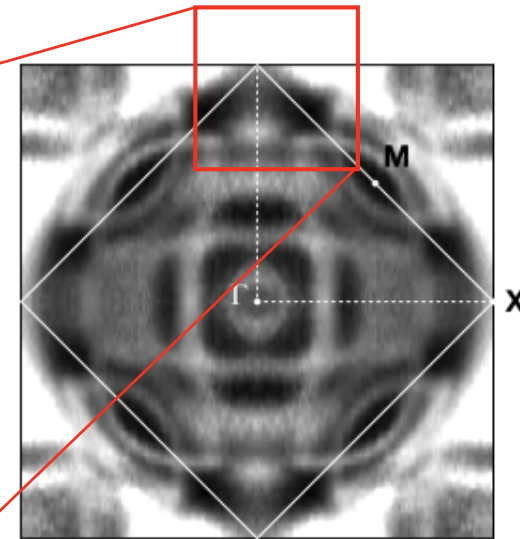
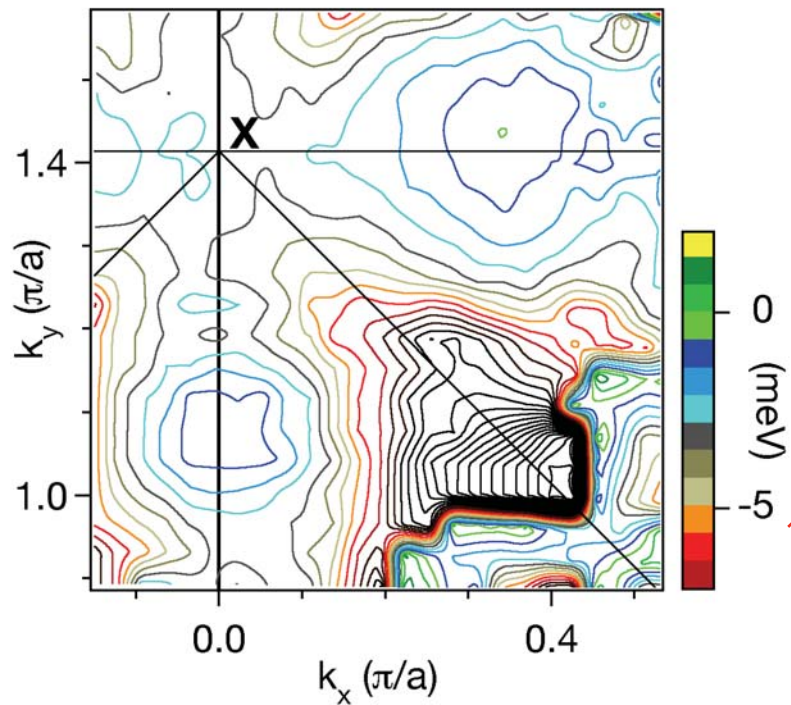
d_{xy} - band topography



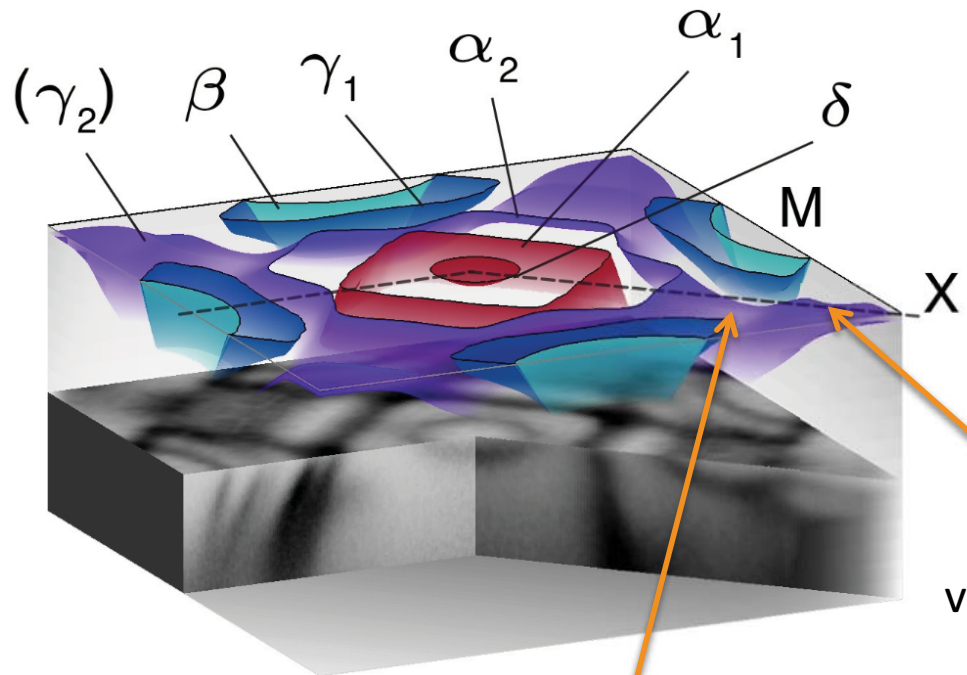
≈ 3 meV dispersion
over 30% of BZ

d_{xy} - band topography

d_{xy} - band topography

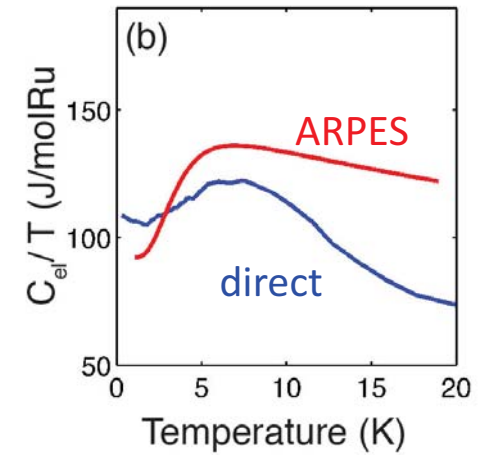
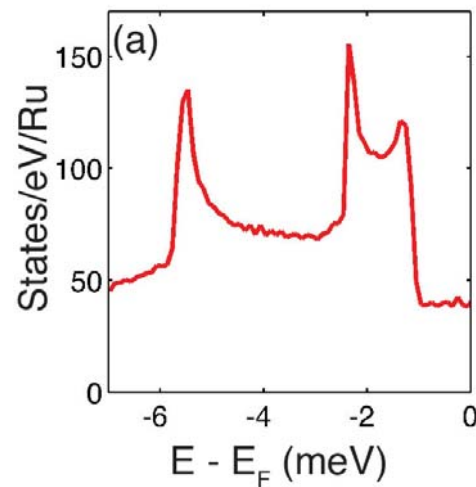


Full low-energy electronic structure



vHs at -6 meV

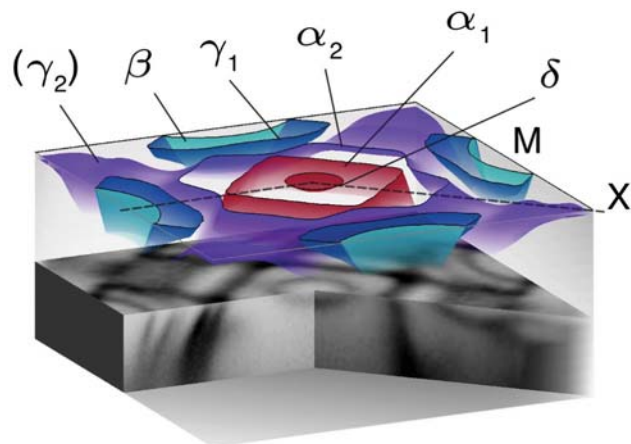
vHs at -2.5 meV



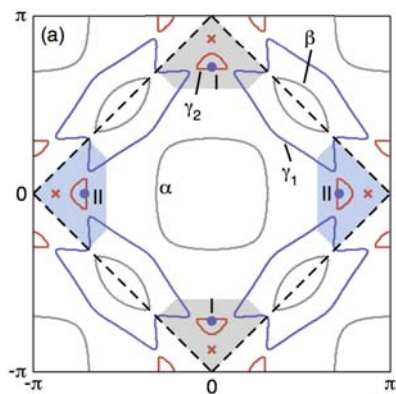
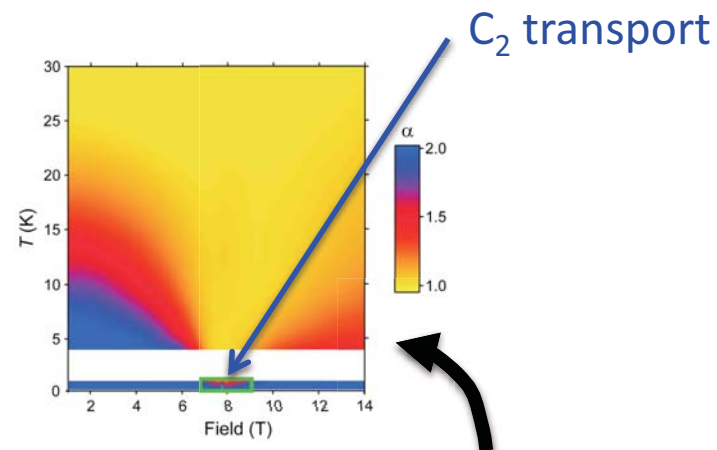
$$C_{el} = \frac{\partial}{\partial T} \int d\varepsilon \varepsilon g(\varepsilon) f(\varepsilon, T)$$



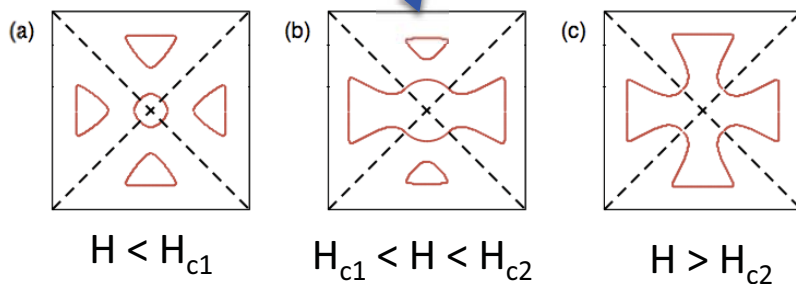
Sr₃Ru₂O₇: microscopic model based on ARPES



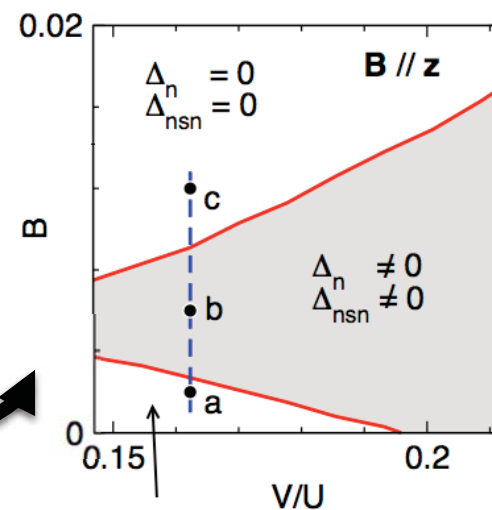
Iamai et al. PRL 101, 026407



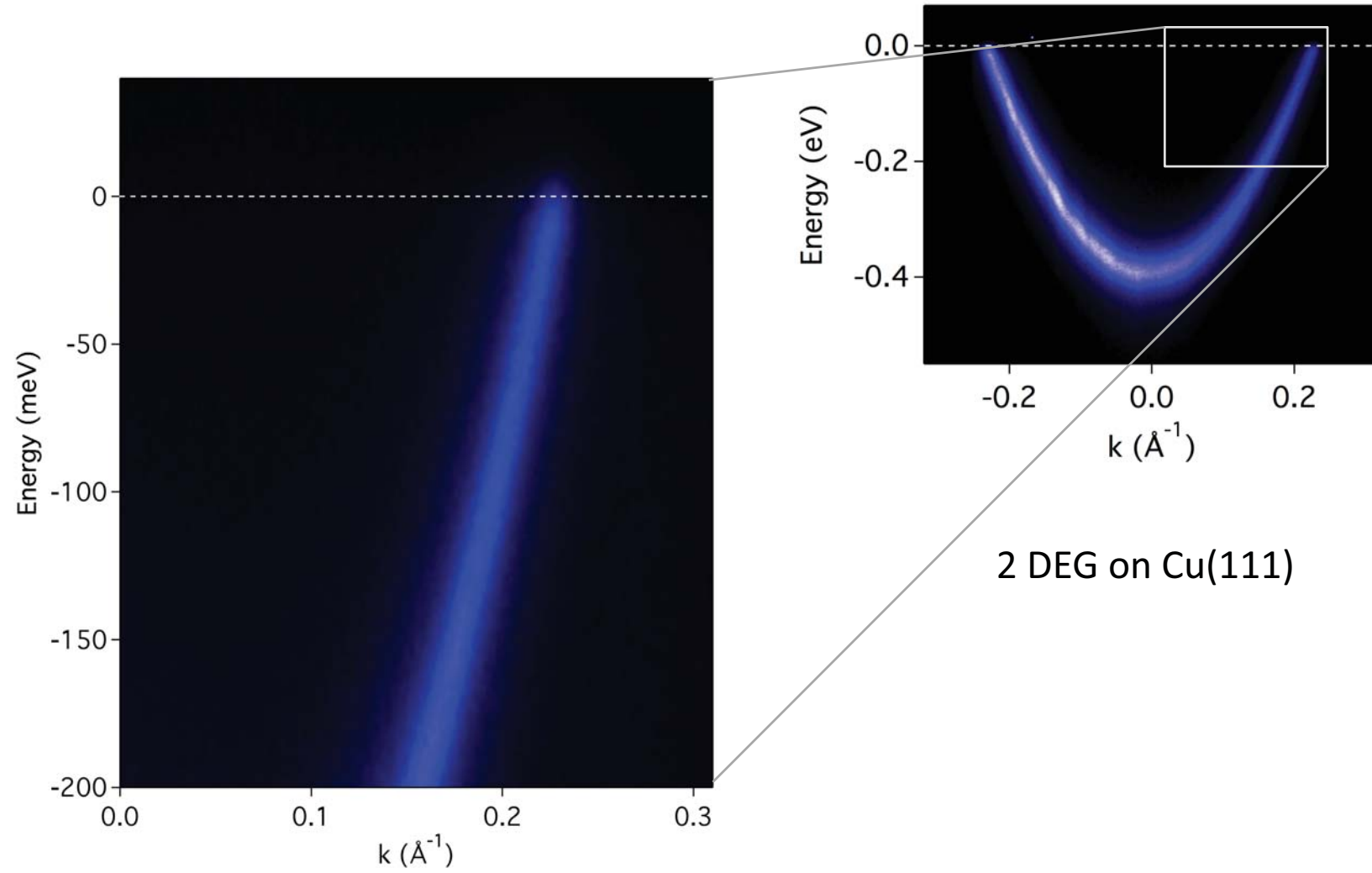
Nematic γ_2 band



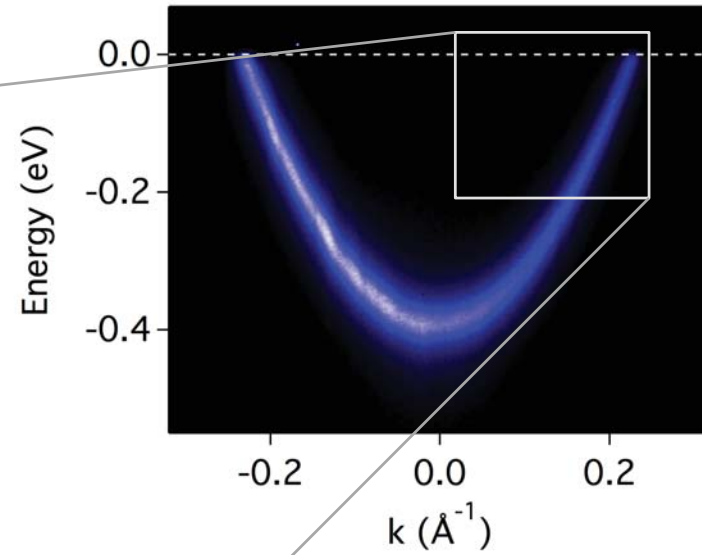
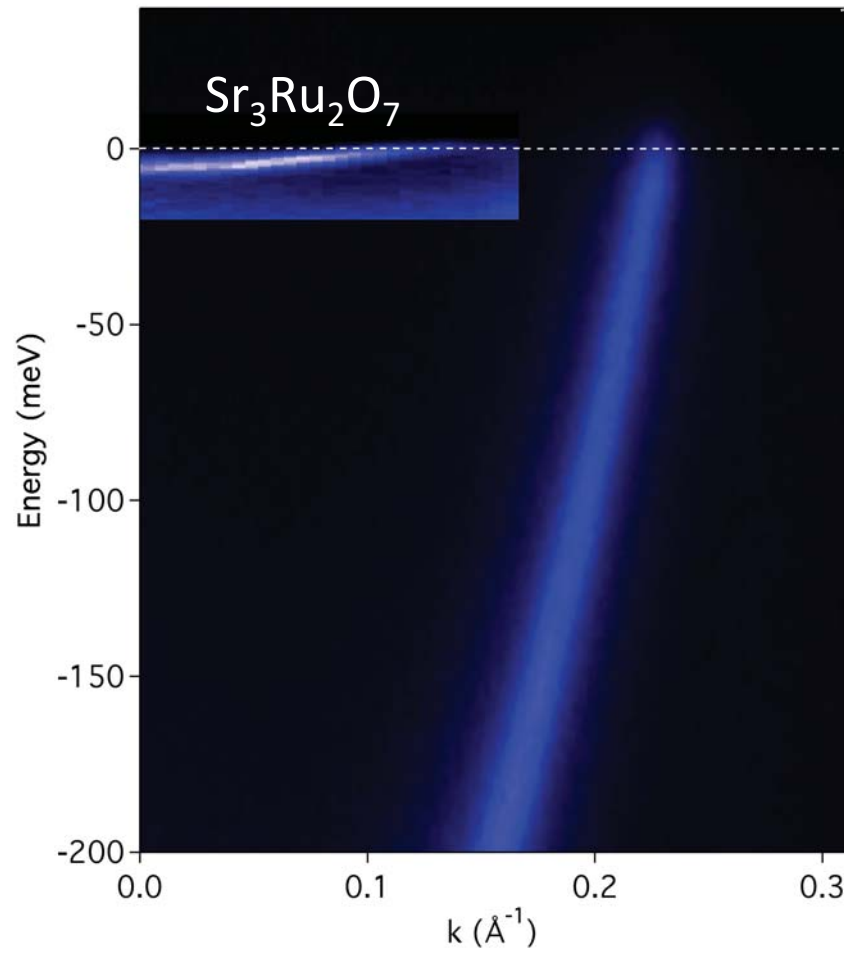
Mean field phase diagram



Renormalization



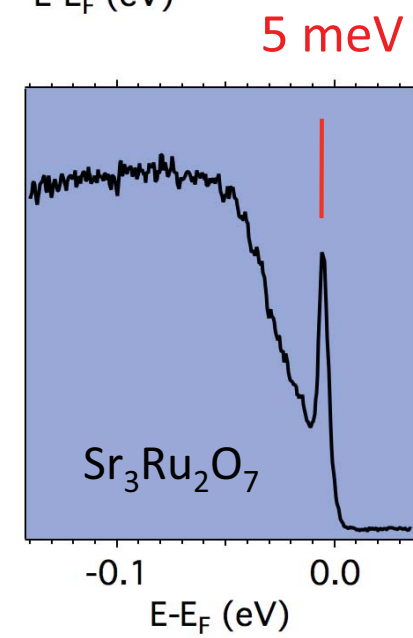
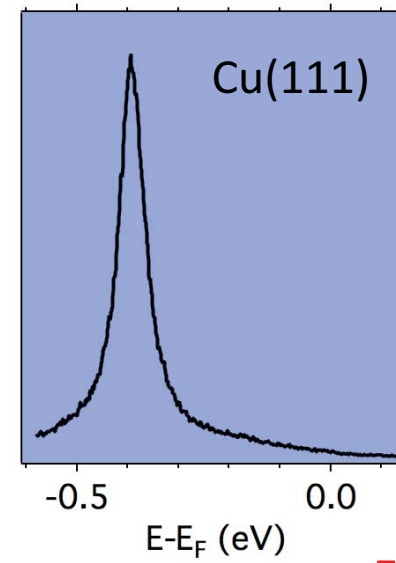
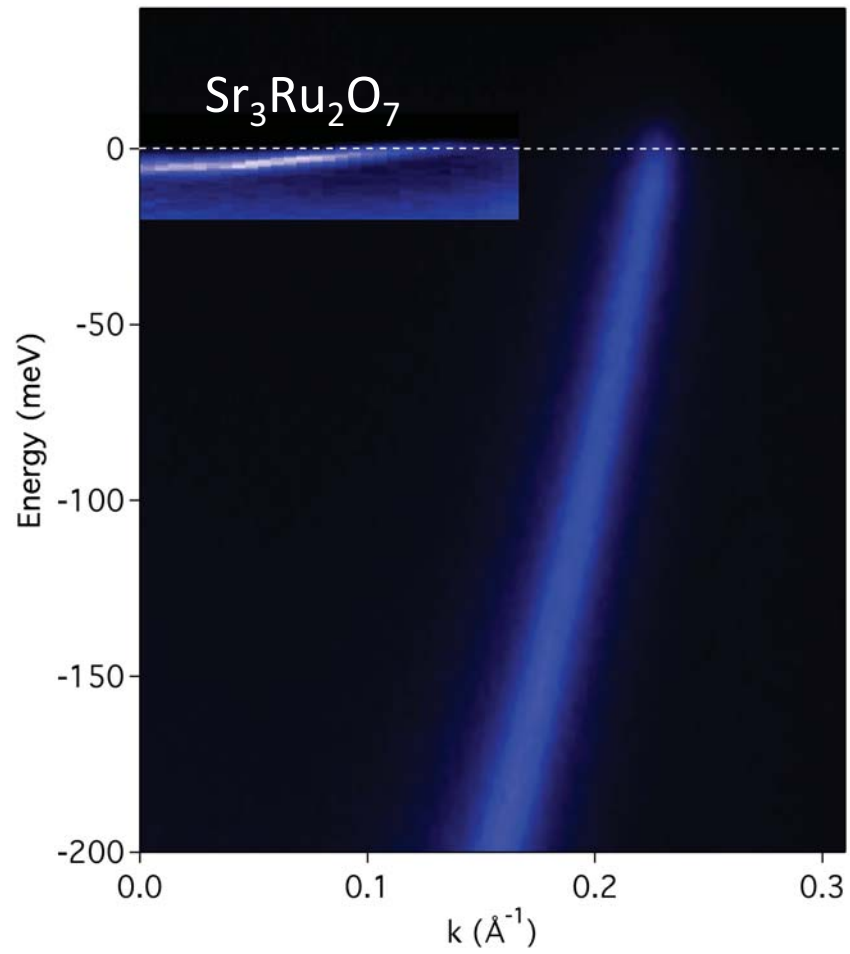
Renormalization



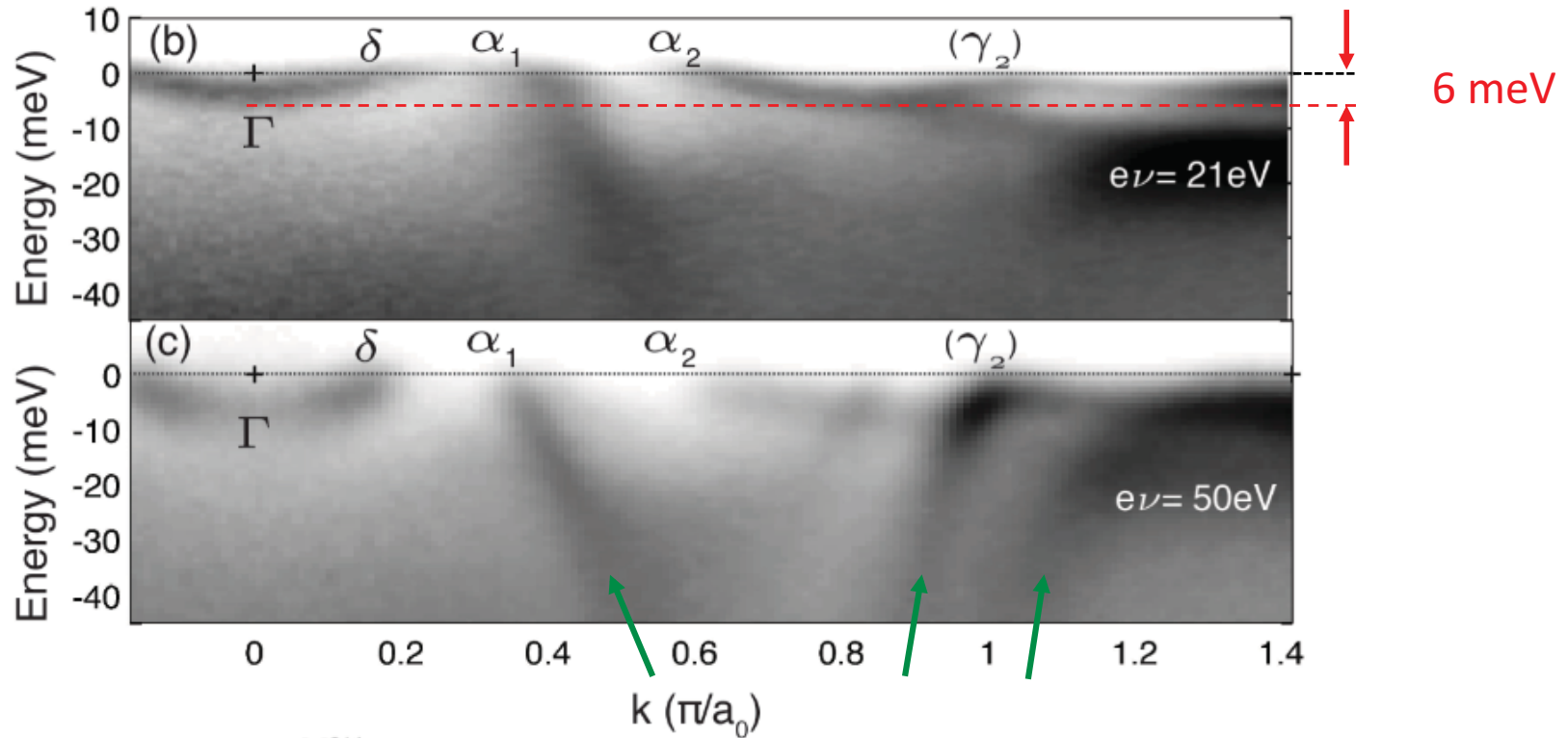
2 DEG on Cu(111) :
 $m^*/m_{\text{LDA}} \approx 1$

$\text{Sr}_3\text{Ru}_2\text{O}_7$:
 $m^*/m_{\text{LDA}} \approx 25$

Renormalization

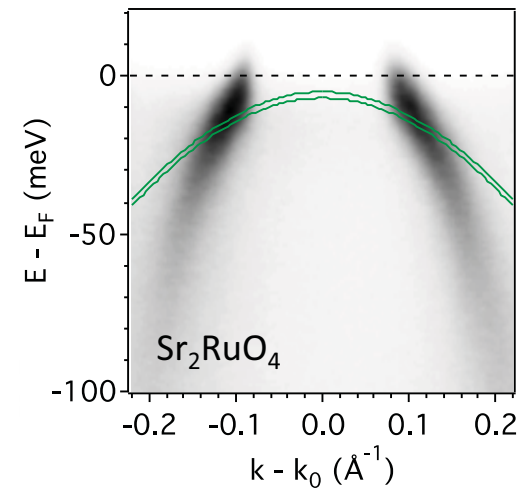
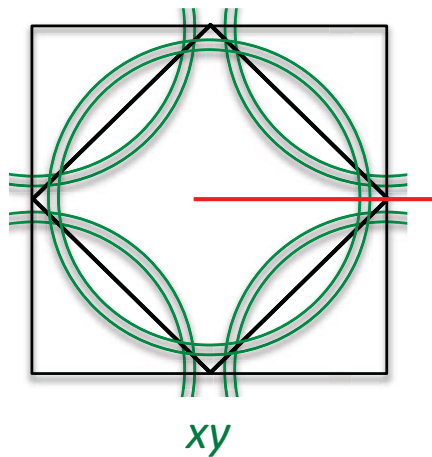
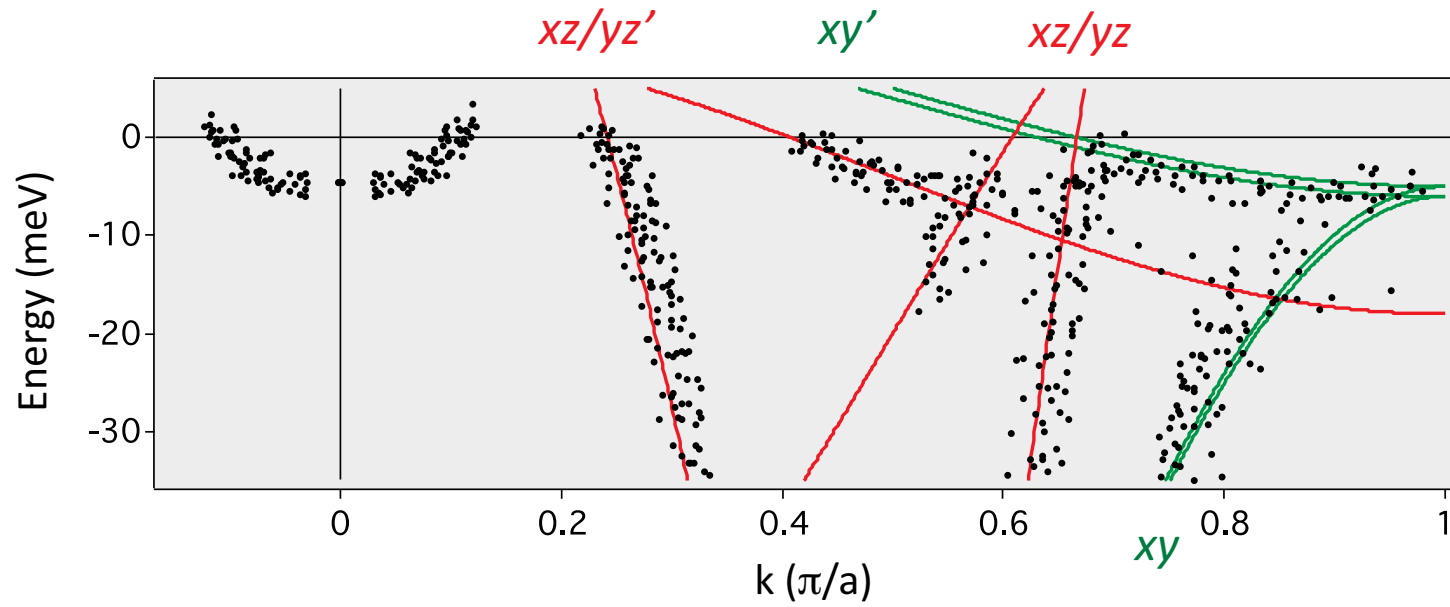


Quasiparticle dispersion

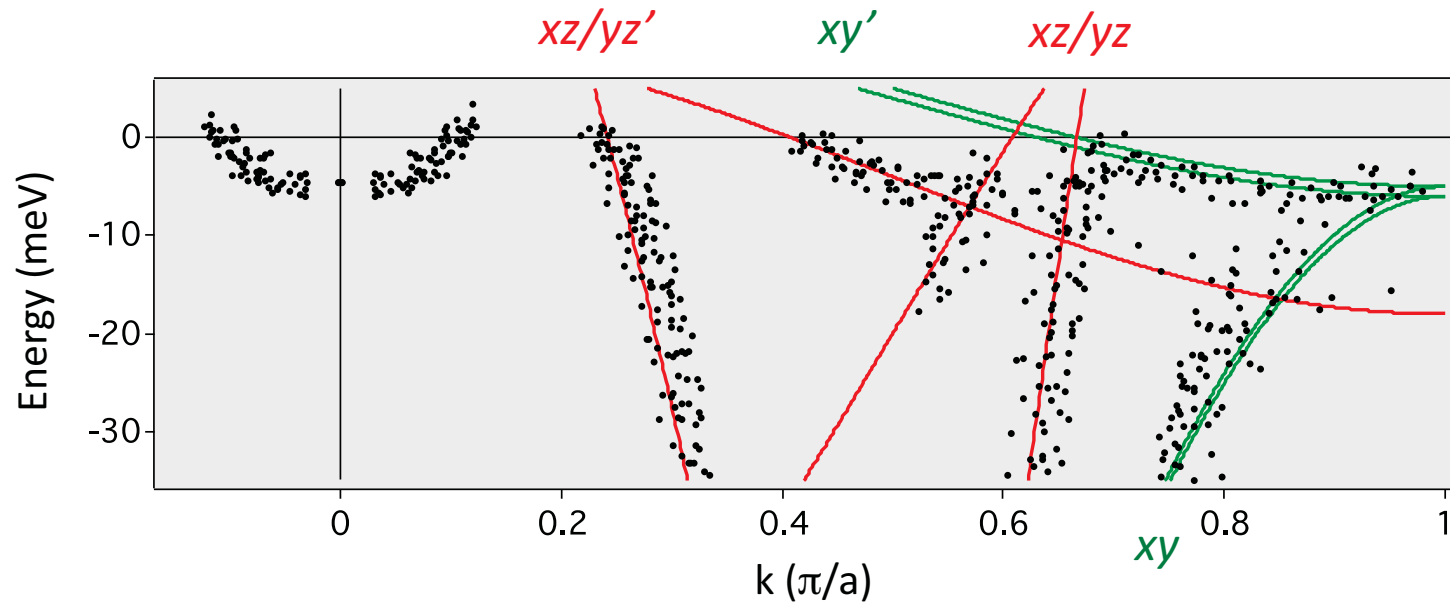


1. Energy scale of 3 – 6 meV across multiple bands
2. Coexistence of flat and dispersive bands

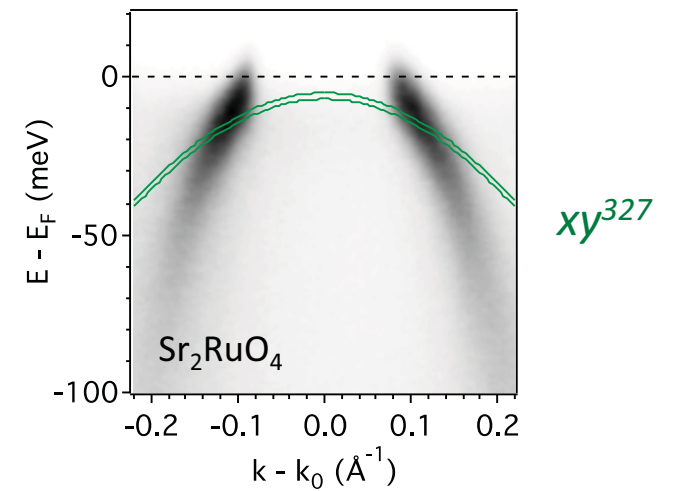
Quasiparticle dispersion



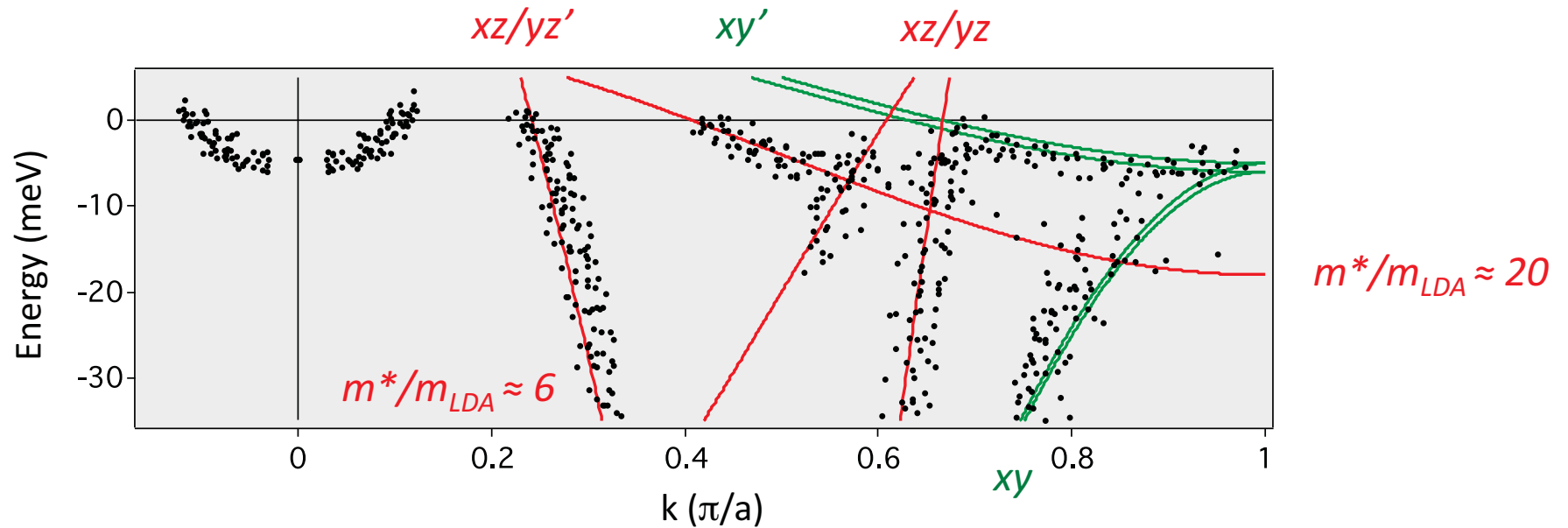
Quasiparticle dispersion



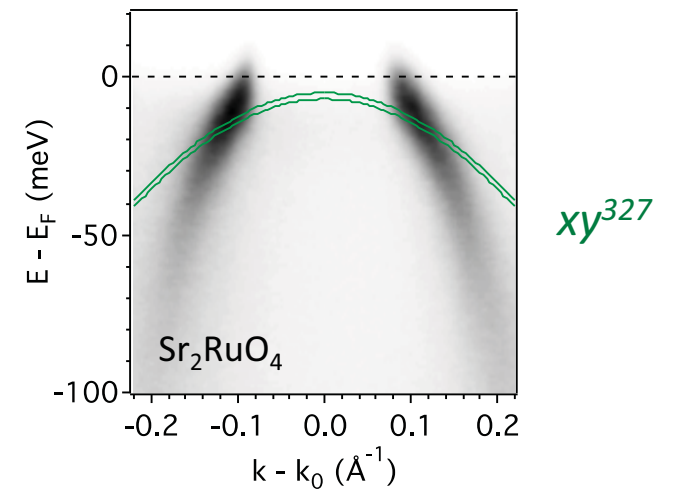
- backfolding
- 'light' bands are similar to Sr_2RuO_4



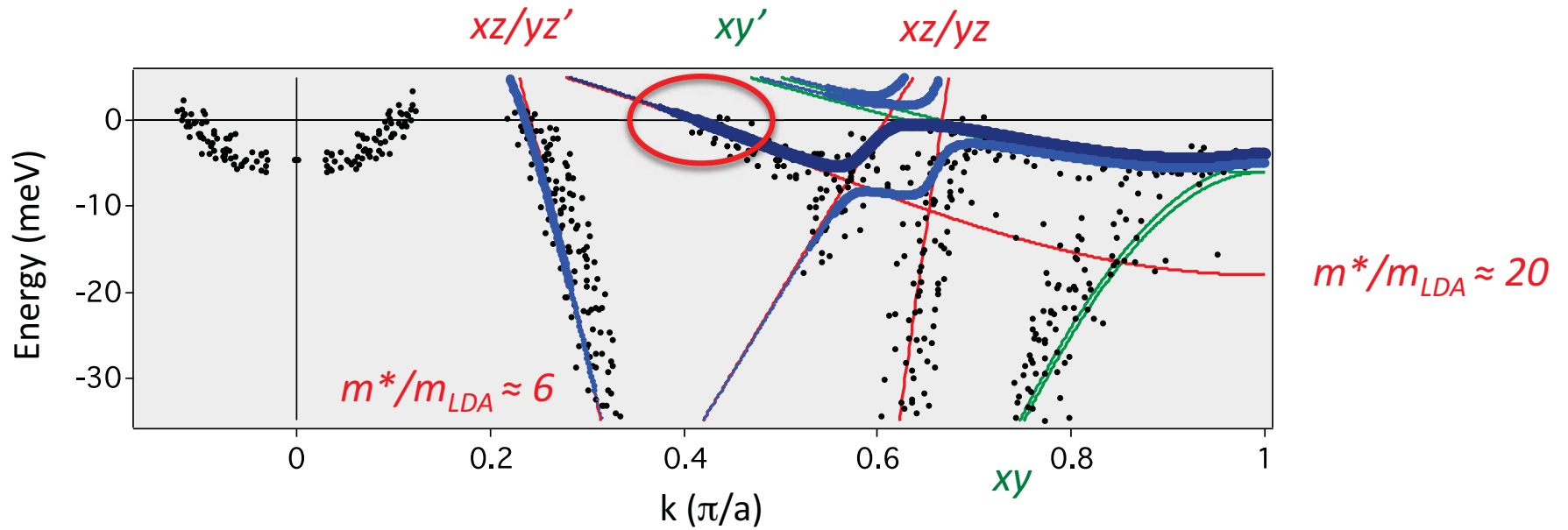
Quasiparticle dispersion



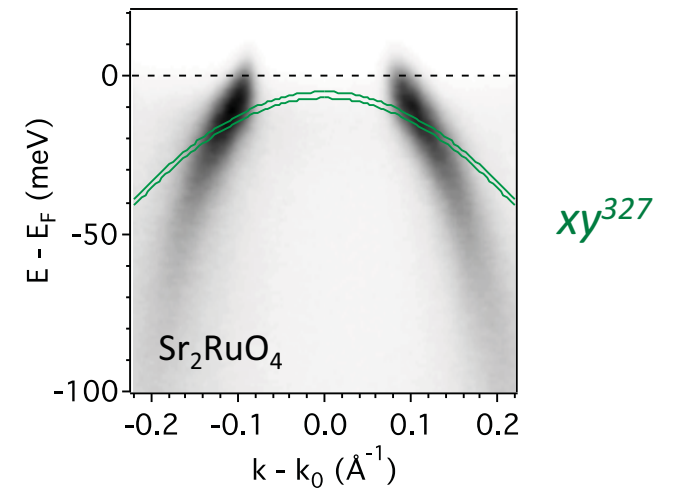
- backfolding
- 'light' bands are similar to Sr_2RuO_4
- **Bilayer split xz/yz bands have different renormalization**



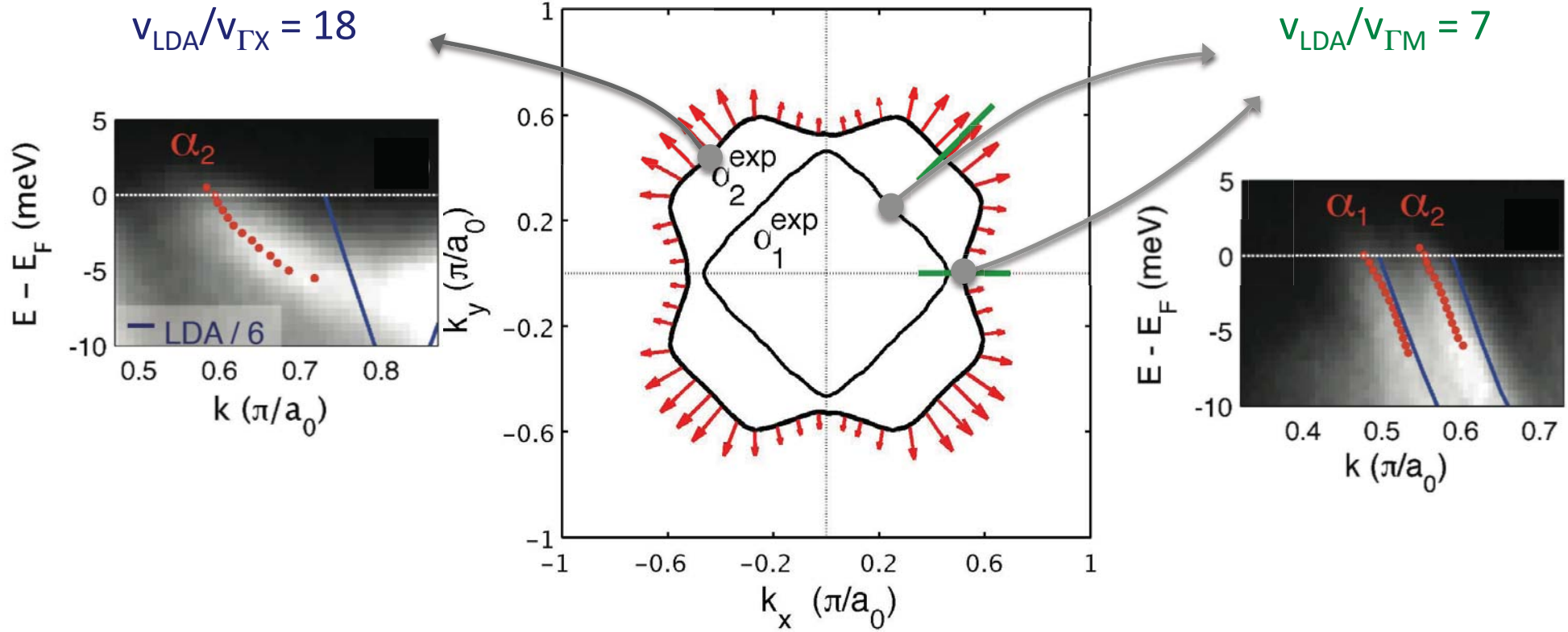
Quasiparticle dispersion



- backfolding
- 'light' bands are similar to Sr_2RuO_4
- Bilinear split xz/yz bands have different renormalization
- hybridization

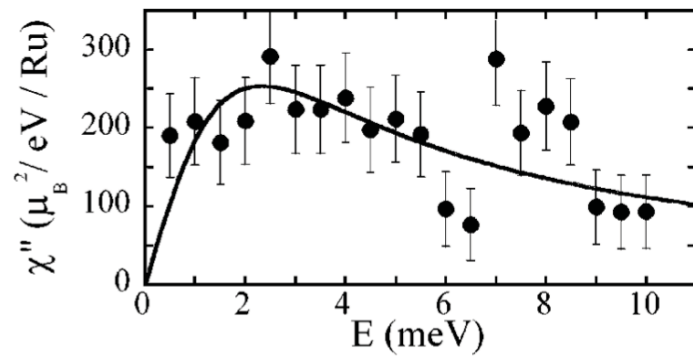
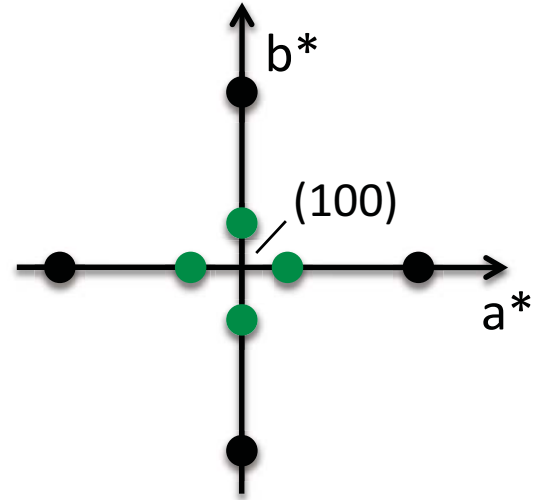
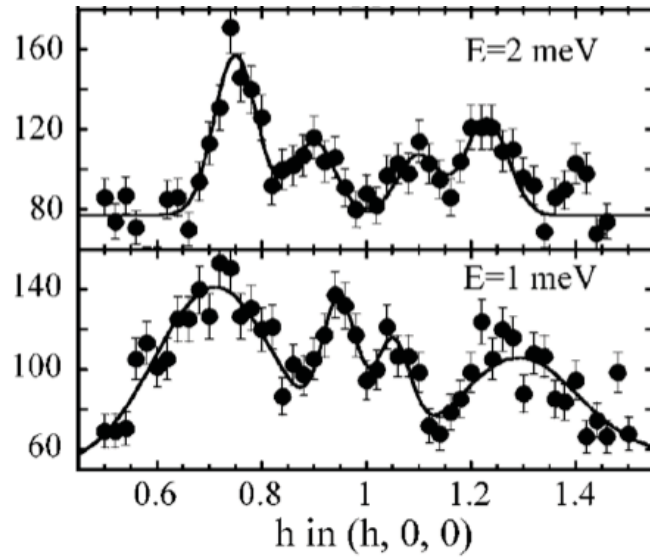


$d_{xz/yz}$ sheets



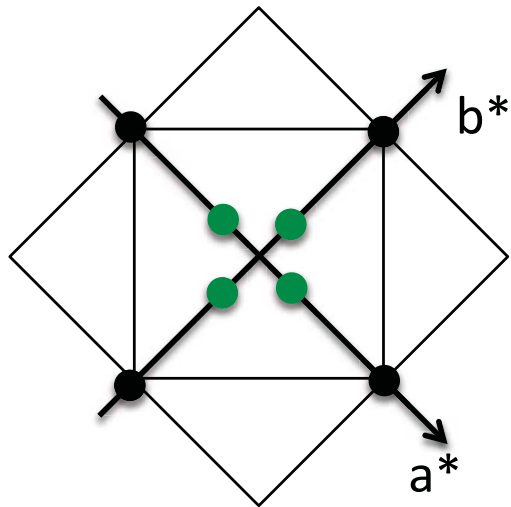
Mass enhancement is strongly anisotropic
 → Bosonic modes ?

Neutron Scattering

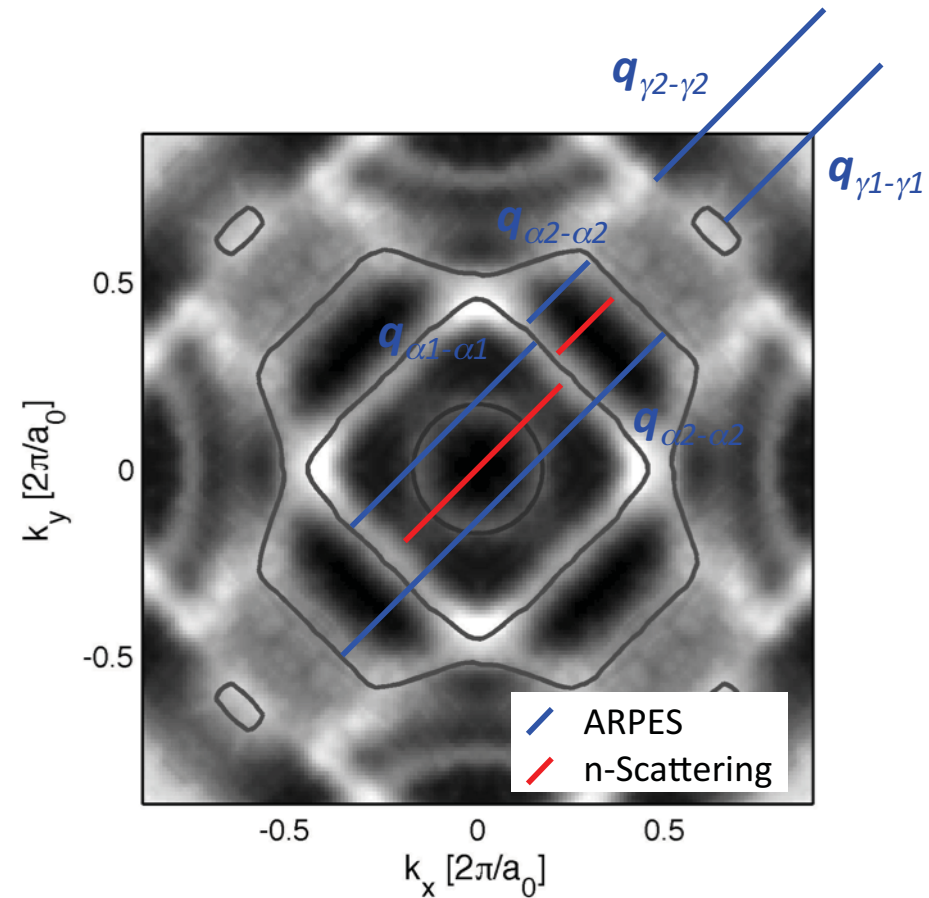


Strong incommensurate AF fluctuations
2 distinct \mathbf{q} - vectors
Peak around 3 meV

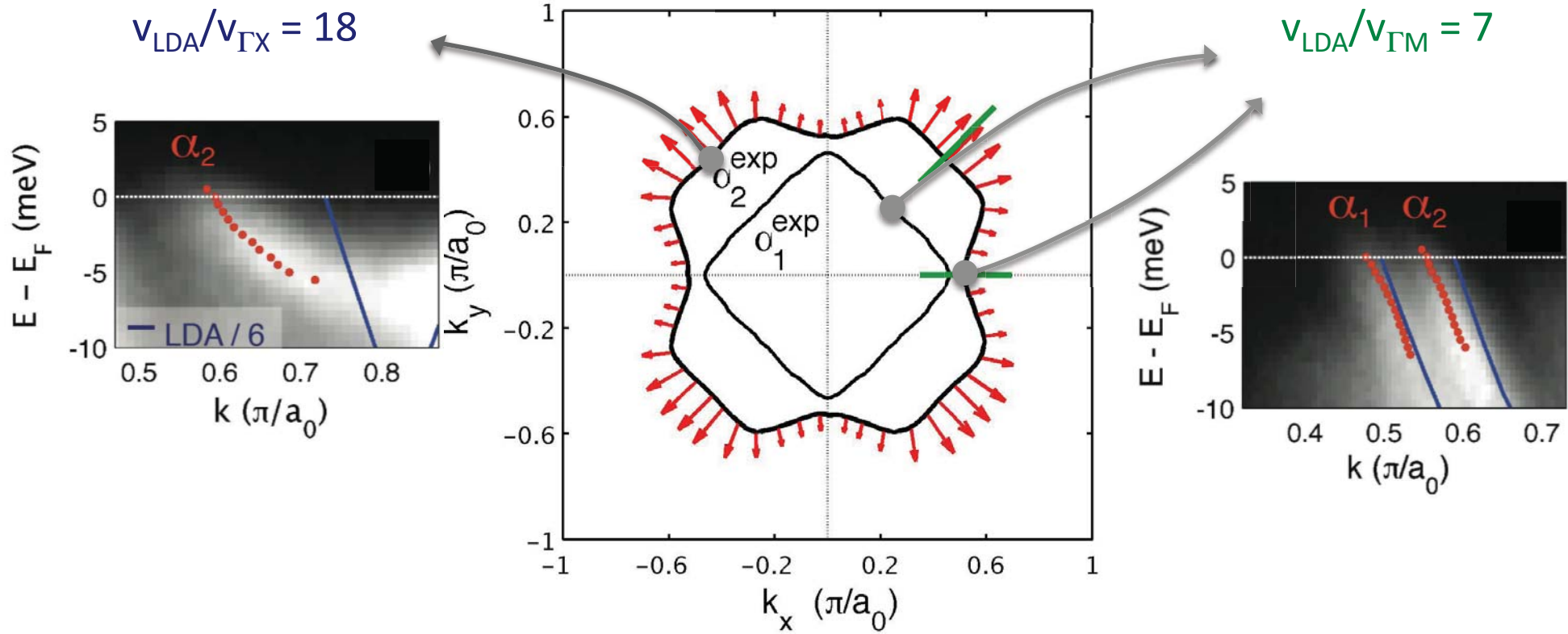
Nesting vectors



- Neutron \mathbf{q} -vectors connect large parts of the FS
- NMR: AF fluctuations dominate even at QCP (Kitagawa, PRL 2005)



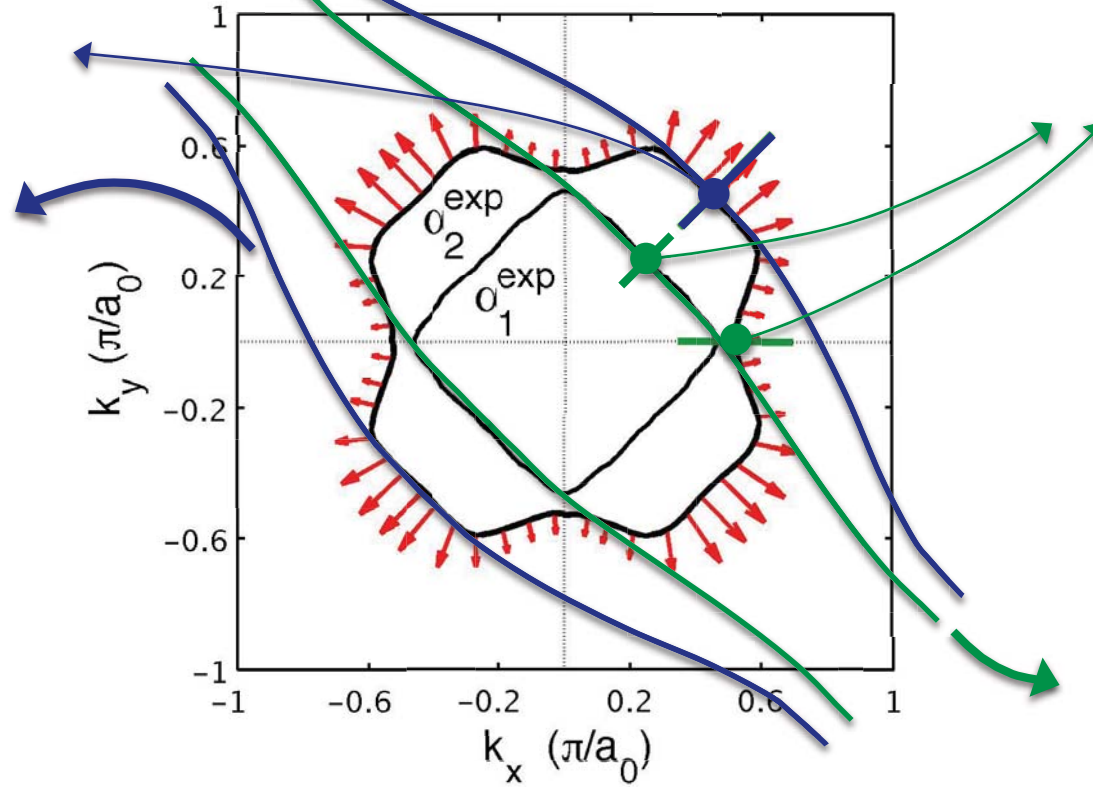
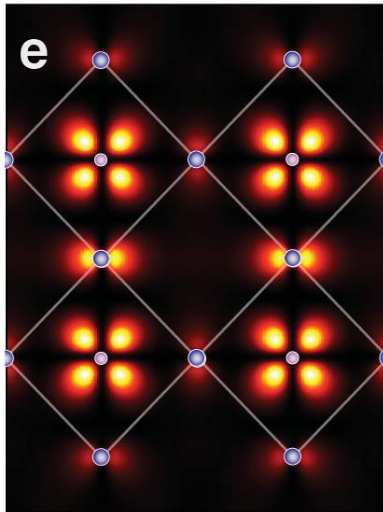
$d_{xz/yz}$ sheets



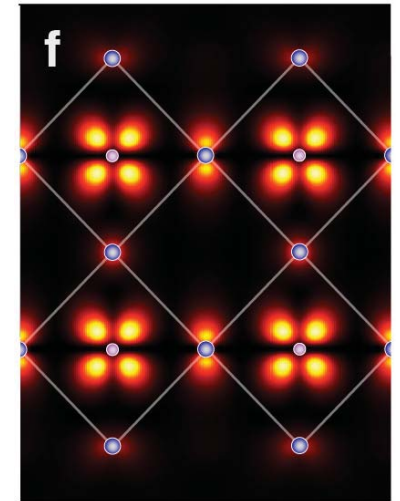
$Sr_2RuO_4 - d_{xz/yz} : m^*/m_{band} \approx 3$

$d_{xz/yz}$ sheets

$$v_{\text{LDA}}/v_{\Gamma X} = 18$$

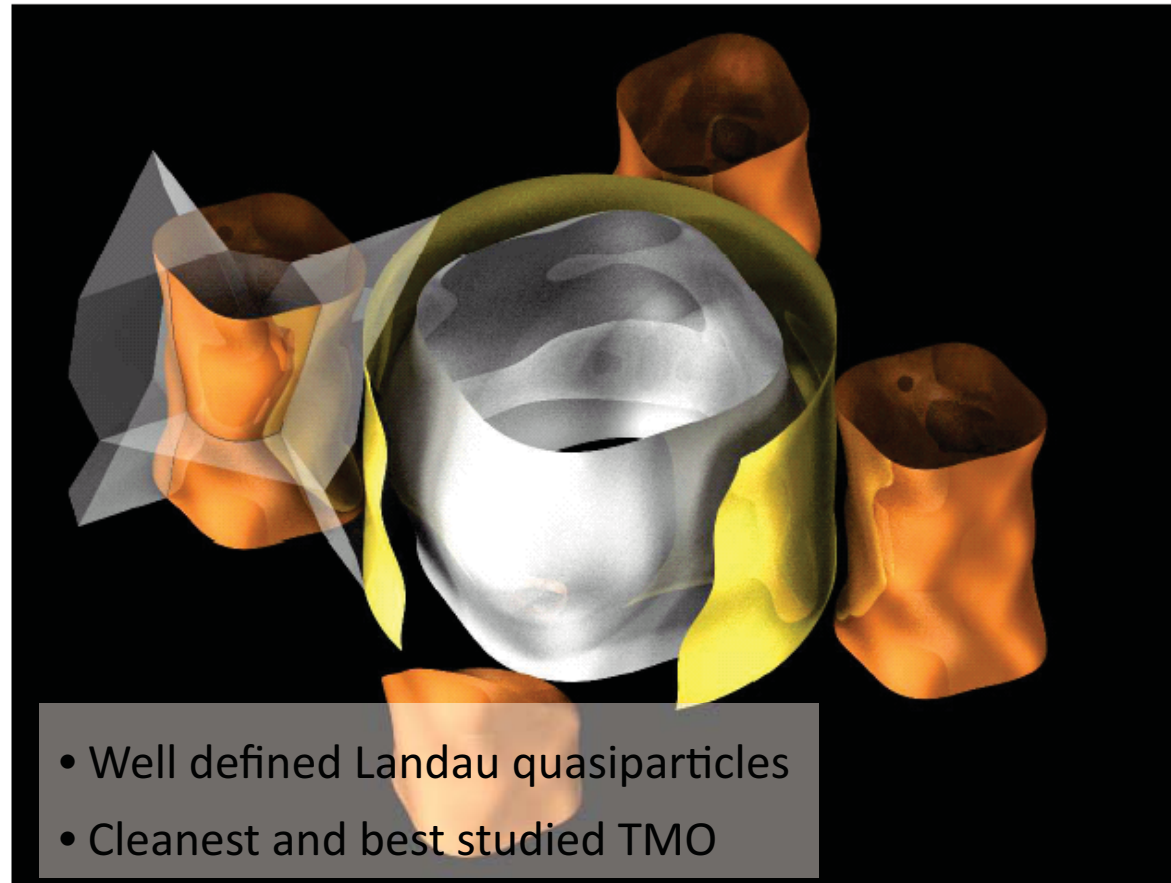


$$v_{\text{LDA}}/v_{\Gamma M} = 7$$



Renormalization strength correlates with $p - d$ hybridization

Sr_2RuO_4 - normal state: a model Fermi liquid

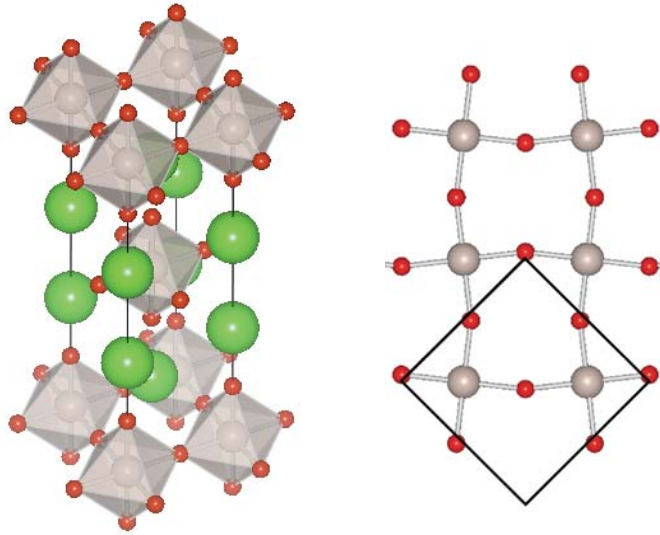


Mackenzie *et al.* PRL **76**, 3786

Bergemann *et al.* PRL **84**, 2662

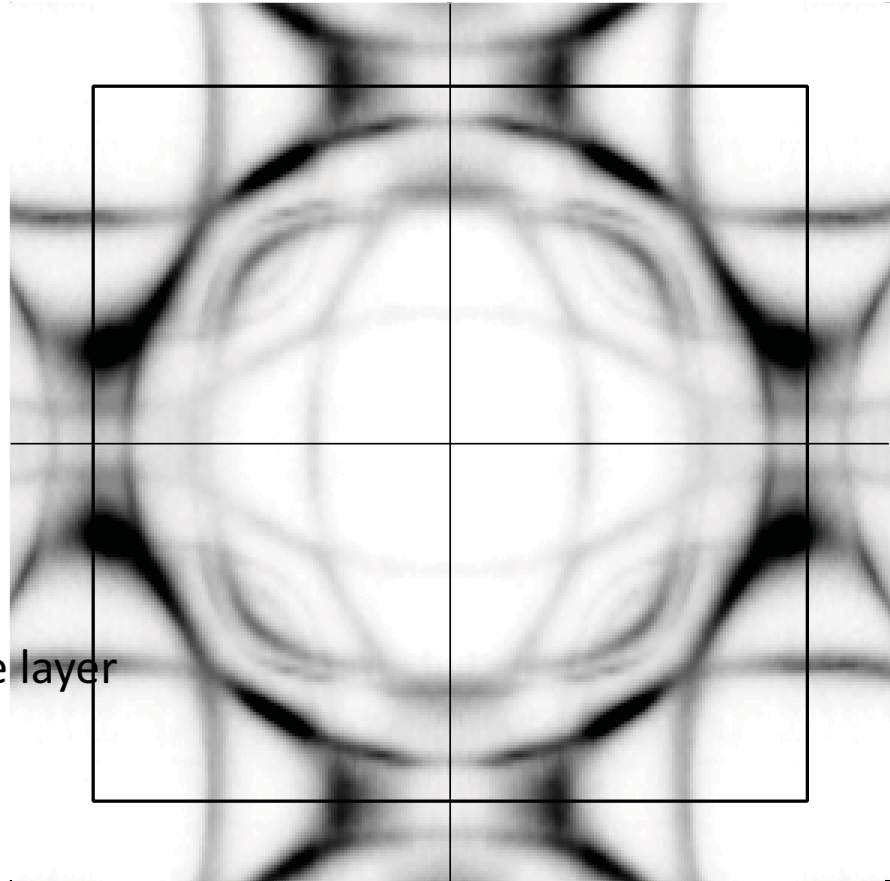
Bergemann *et al.* Adv. Phys. **52**, 639

Surface reconstruction



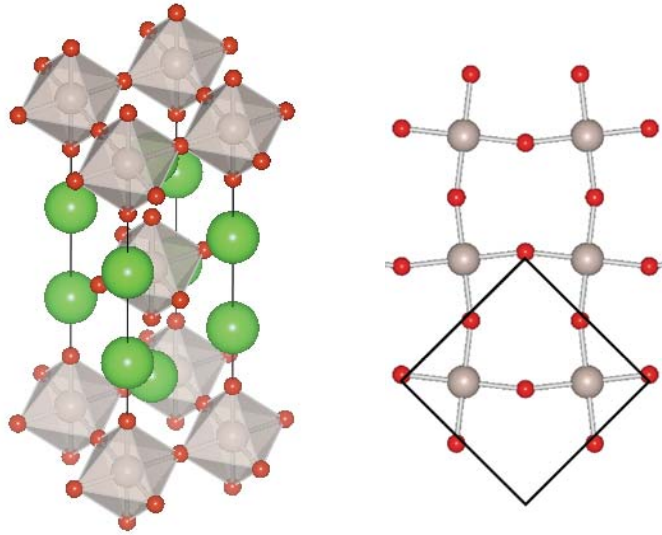
$\sqrt{2} \times \sqrt{2}$ $R45^\circ$ reconstruction of surface layer

$\approx 6^\circ$ rotation around c -axis



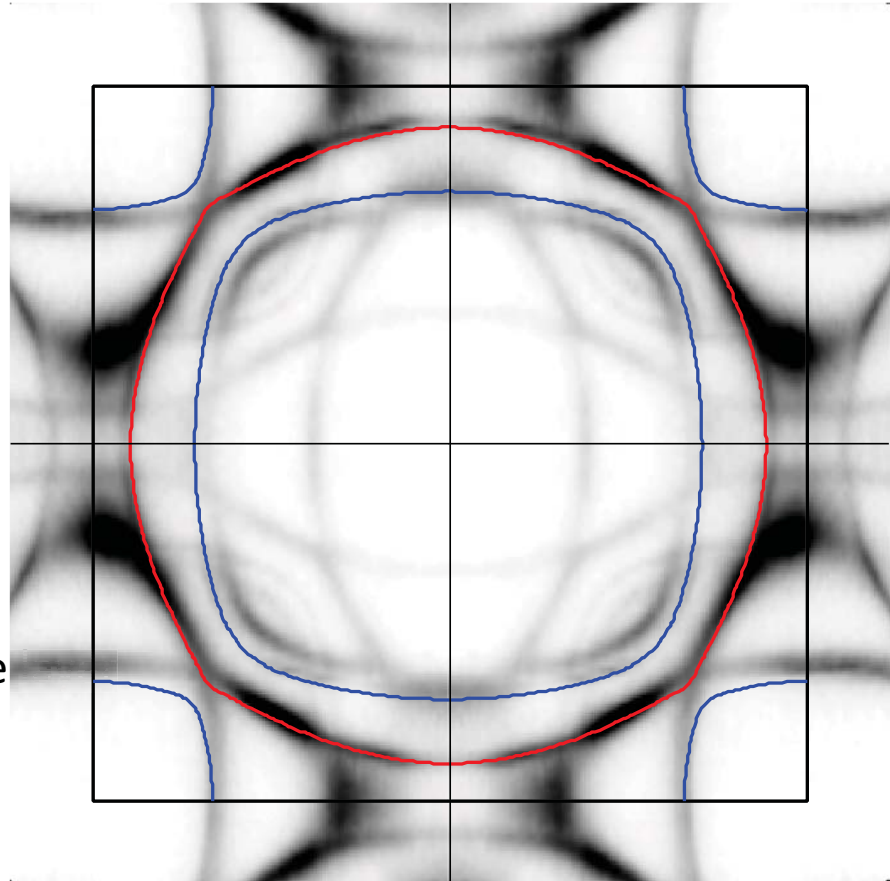
see also A. Damascelli et al. PRL **85**, 5194 (2000),
K.M. Shen et al, PRB **64**, 180502R (2001)

Surface reconstruction



$\sqrt{2} \times \sqrt{2}$ $R45^\circ$ reconstruction of surface

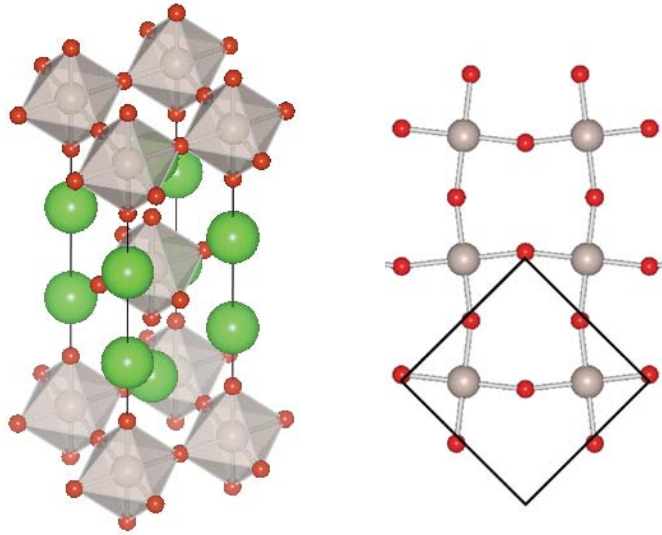
$\approx 6^\circ$ rotation around c -axis



bulk bands

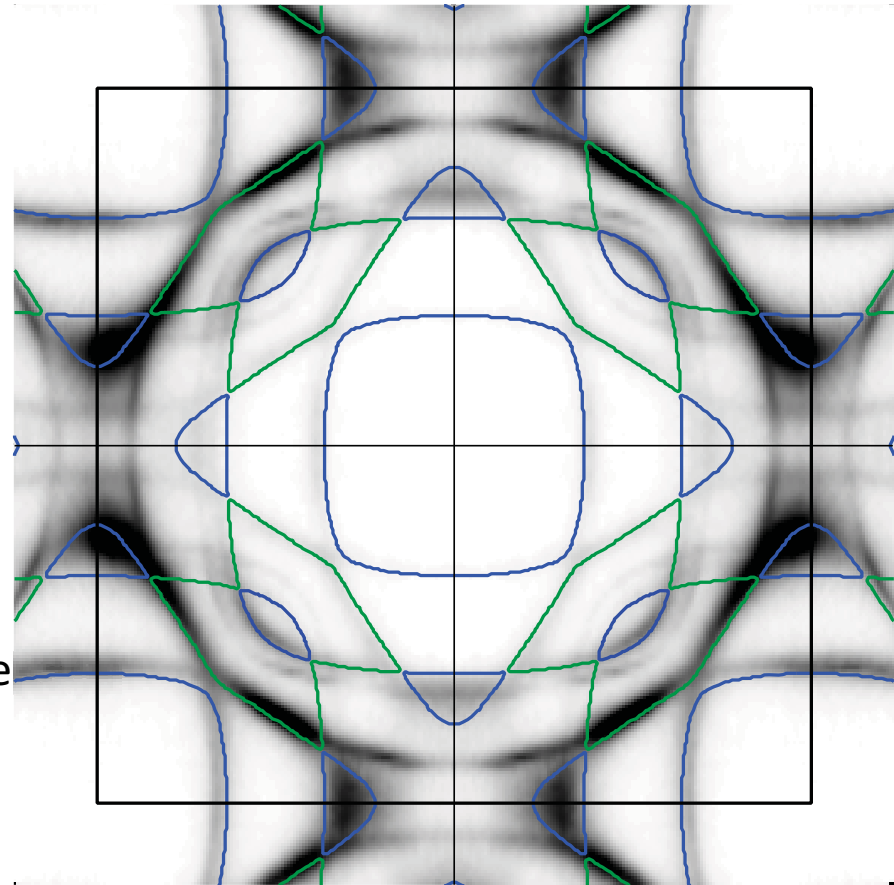
see also A. Damascelli et al. PRL **85**, 5194 (2000),
K.M. Shen et al, PRB **64**, 180502R (2001)

Surface reconstruction



$\sqrt{2} \times \sqrt{2}$ $R45^\circ$ reconstruction of surface

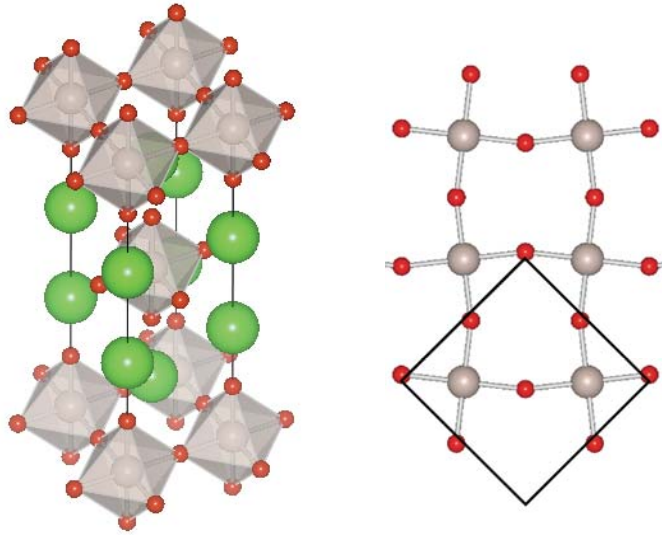
$\approx 6^\circ$ rotation around c -axis



hybridized surface layer bands

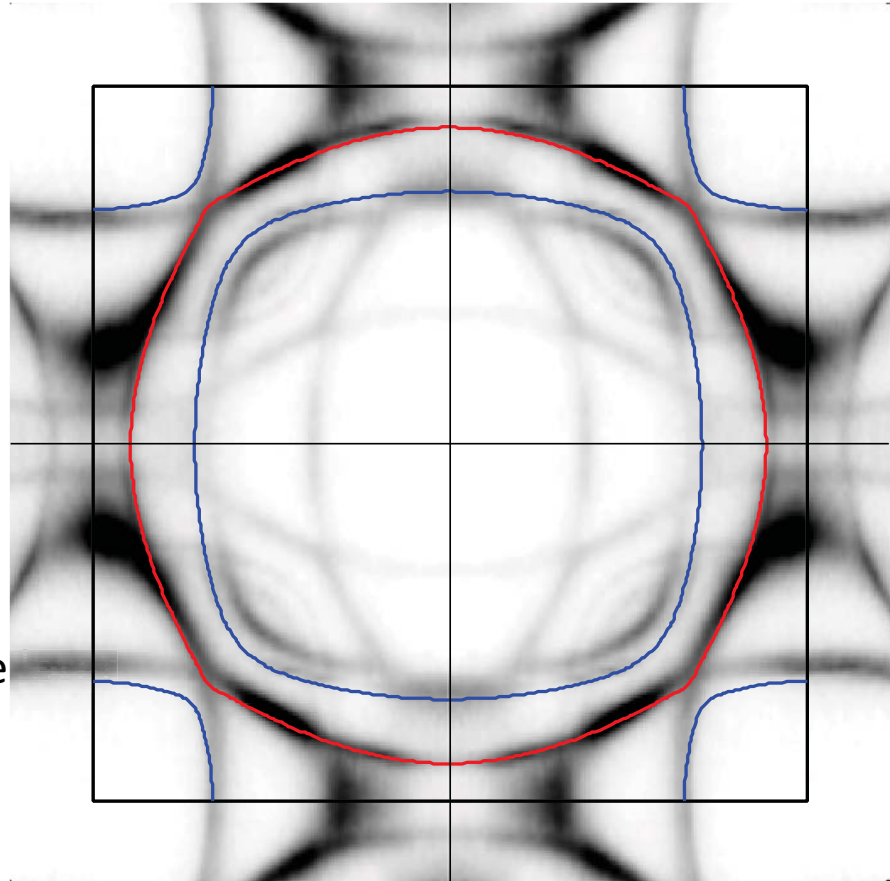
see also A. Damascelli et al. PRL **85**, 5194 (2000),
K.M. Shen et al, PRB **64**, 180502R (2001)

Surface reconstruction



$\sqrt{2} \times \sqrt{2}$ $R45^\circ$ reconstruction of surface

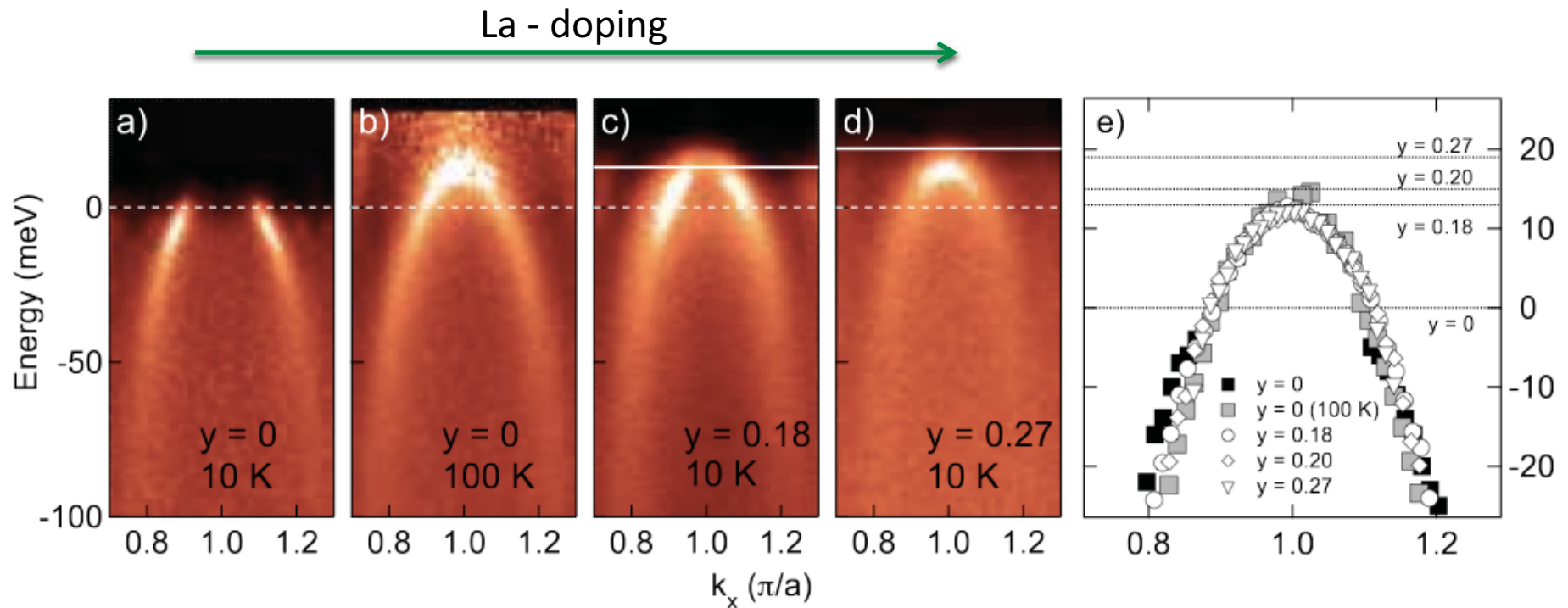
$\approx 6^\circ$ rotation around c -axis



bulk bands

see also A. Damascelli et al. PRL **85**, 5194 (2000),
K.M. Shen et al, PRB **64**, 180502R (2001)

Mass enhancement in Sr_2RuO_4



Weak coupling to modes, little influence of vHs energy

γ - band : $m^*/m = 6.1$

α - band : $m^*/m = 2.8$

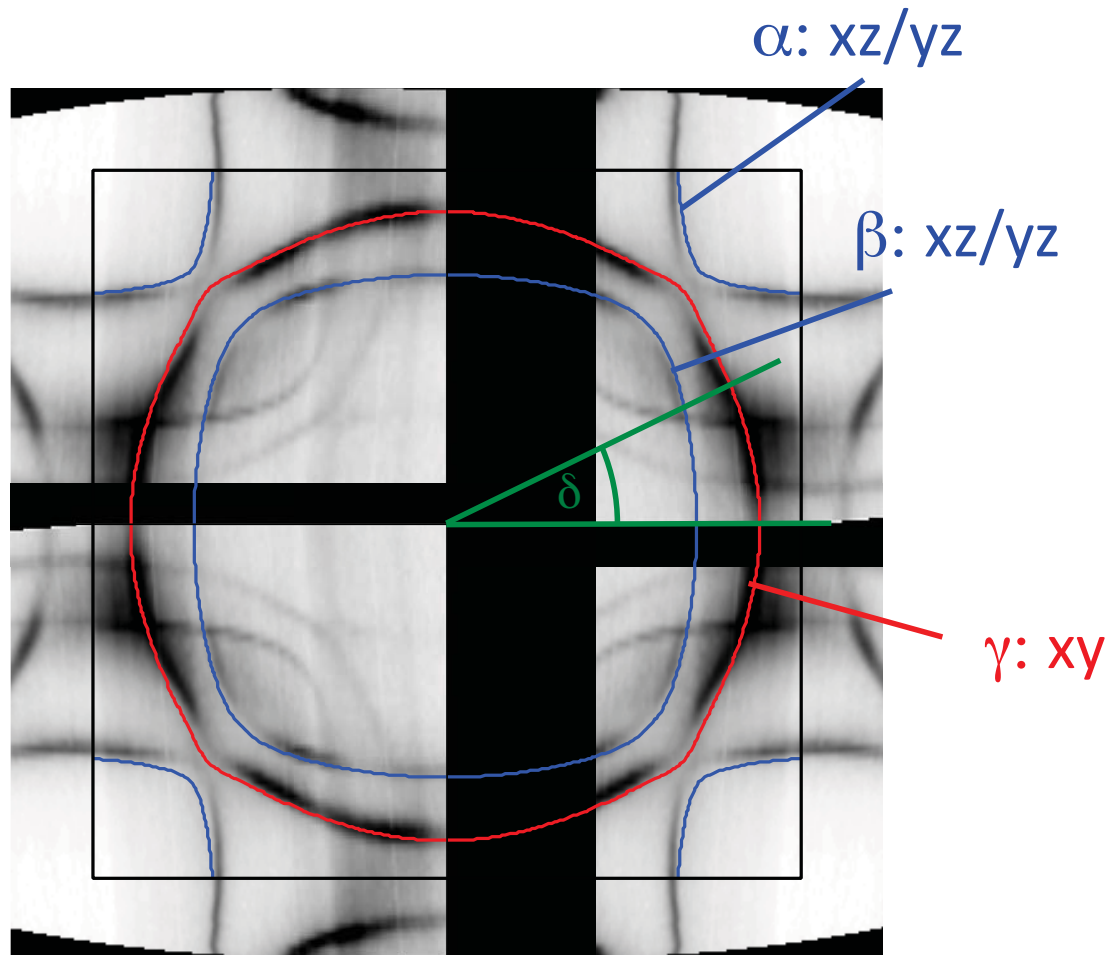
β - band : $m^*/m = 2.6$

DMFT:

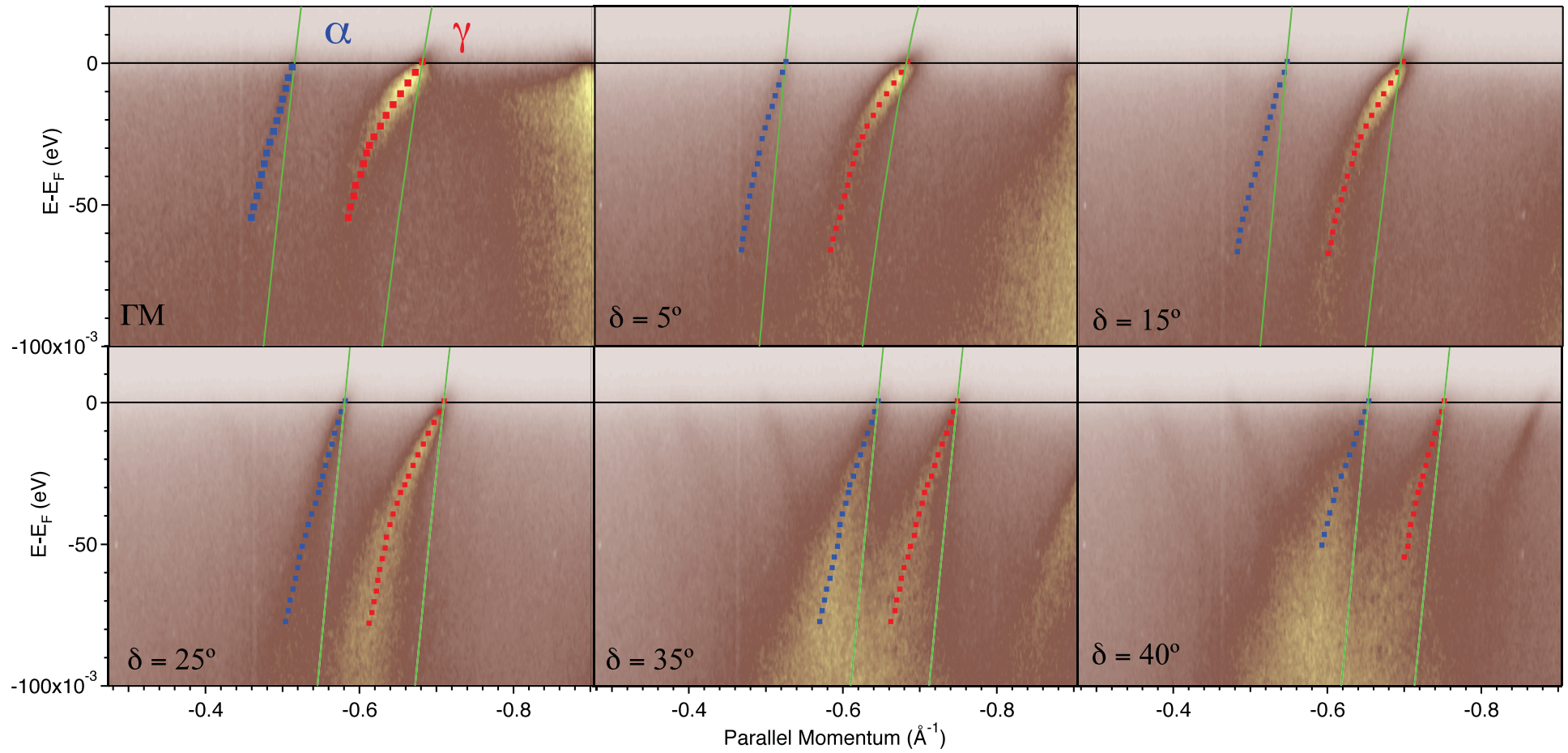
1. Hund's rule coupling

2. vHs in xy - sheet

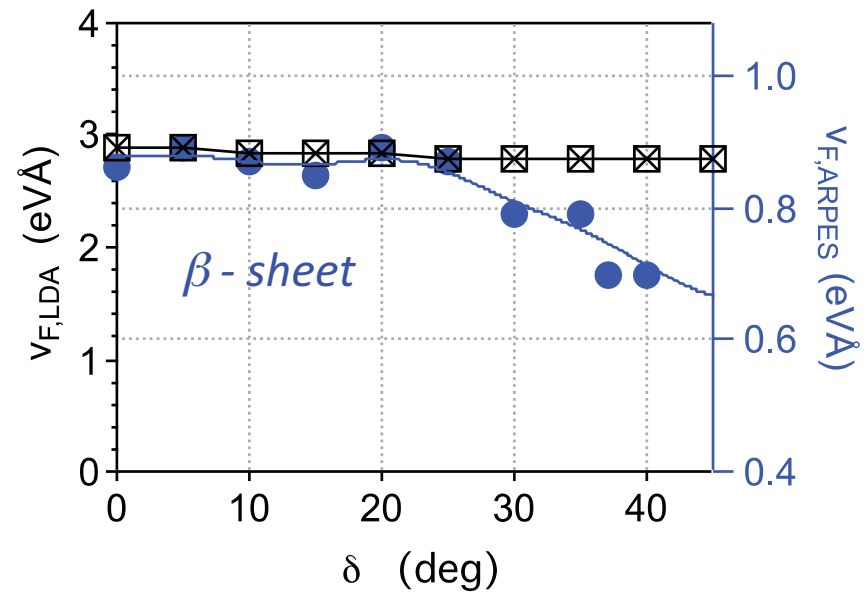
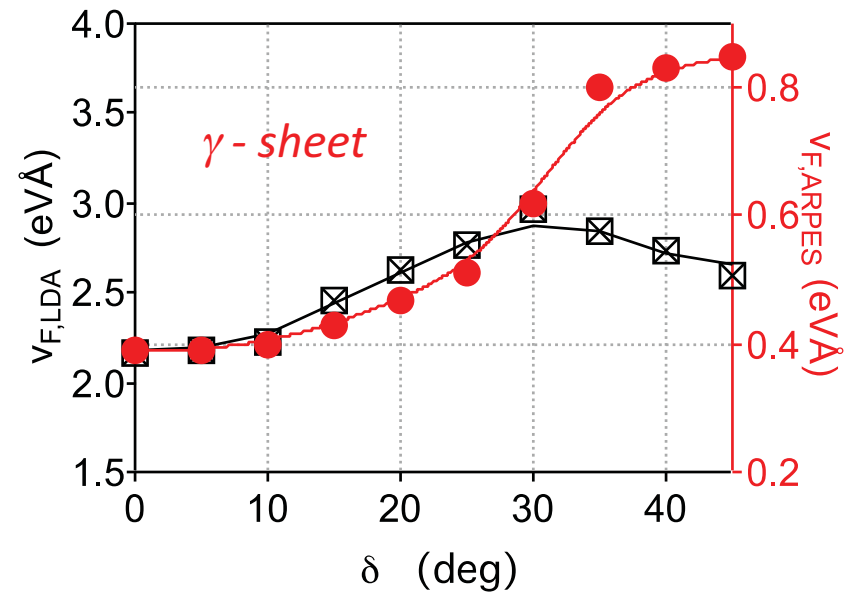
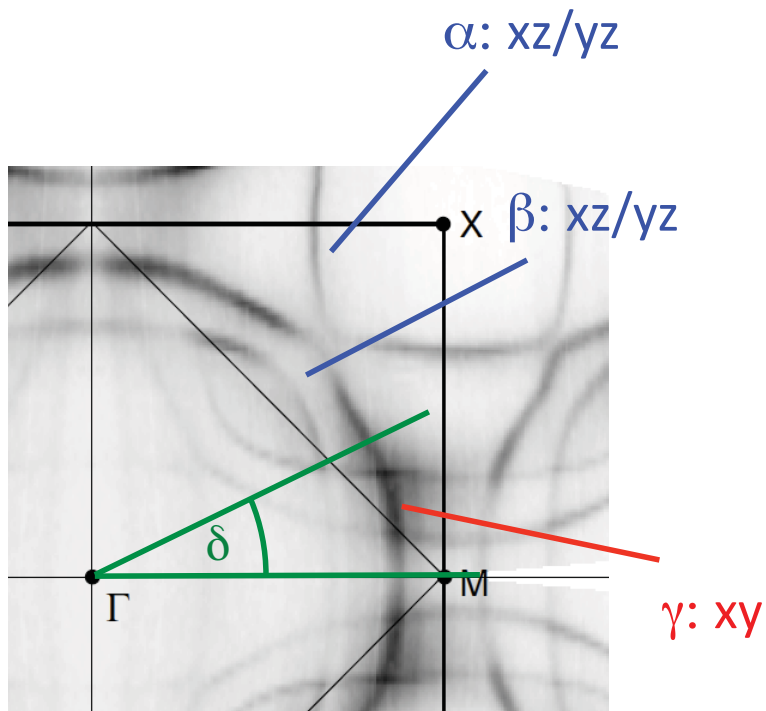
Renormalization along full Fermi surface



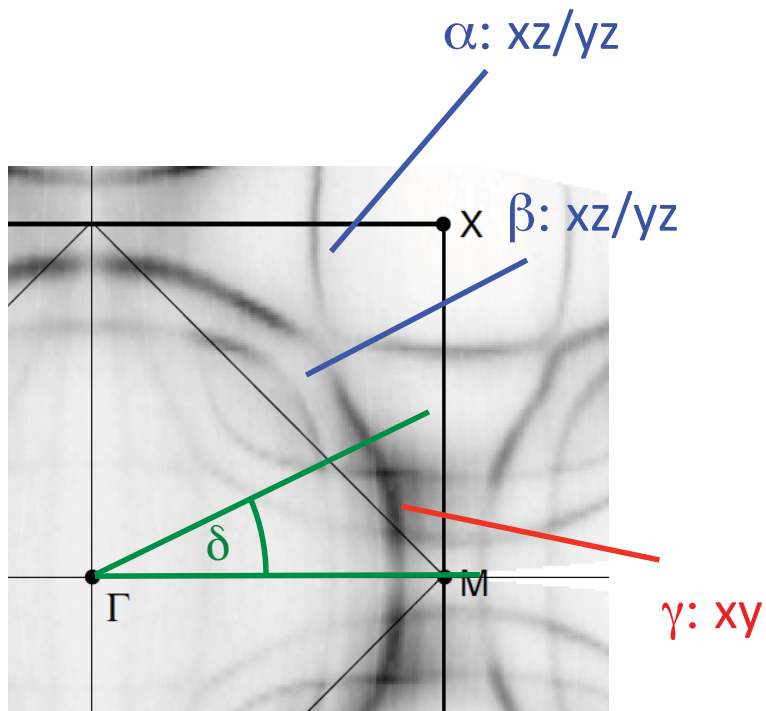
Renormalization along full Fermi surface



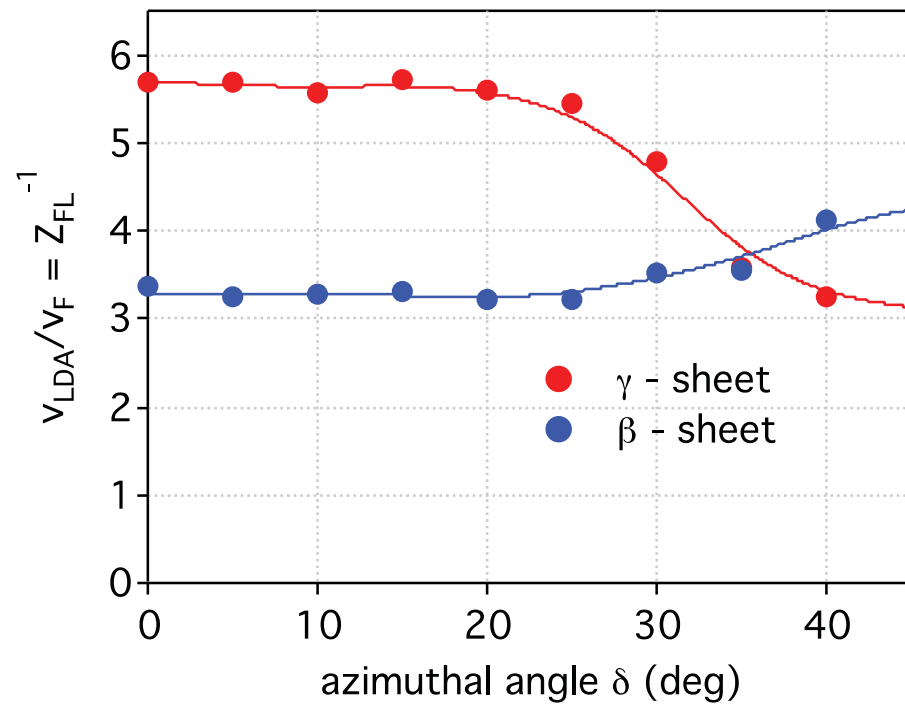
Fermi velocities



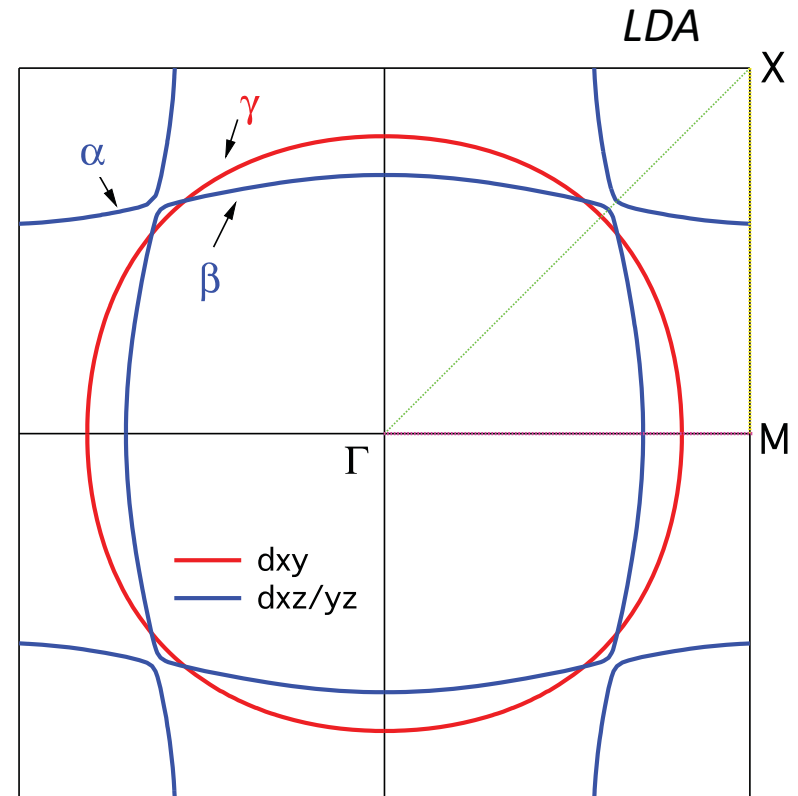
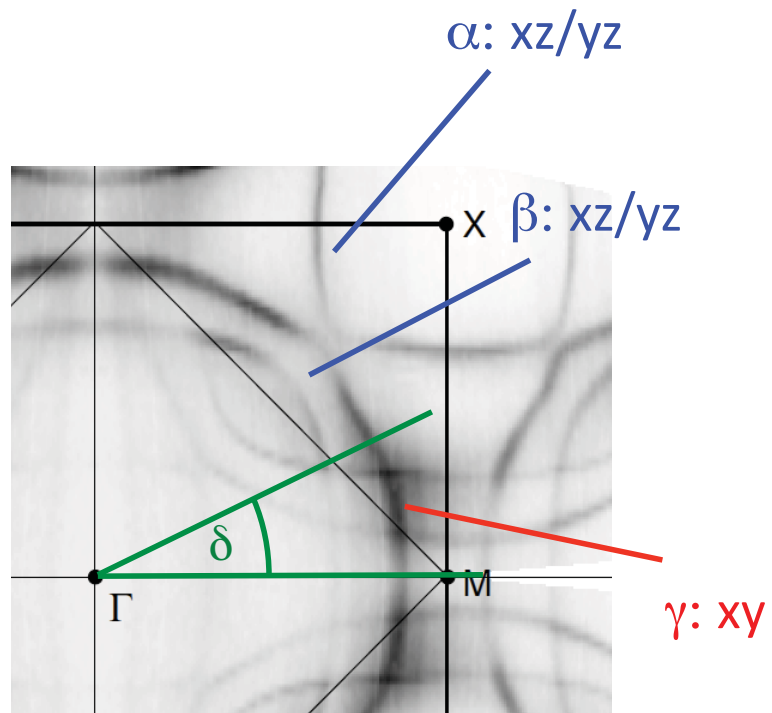
Mass enhancement



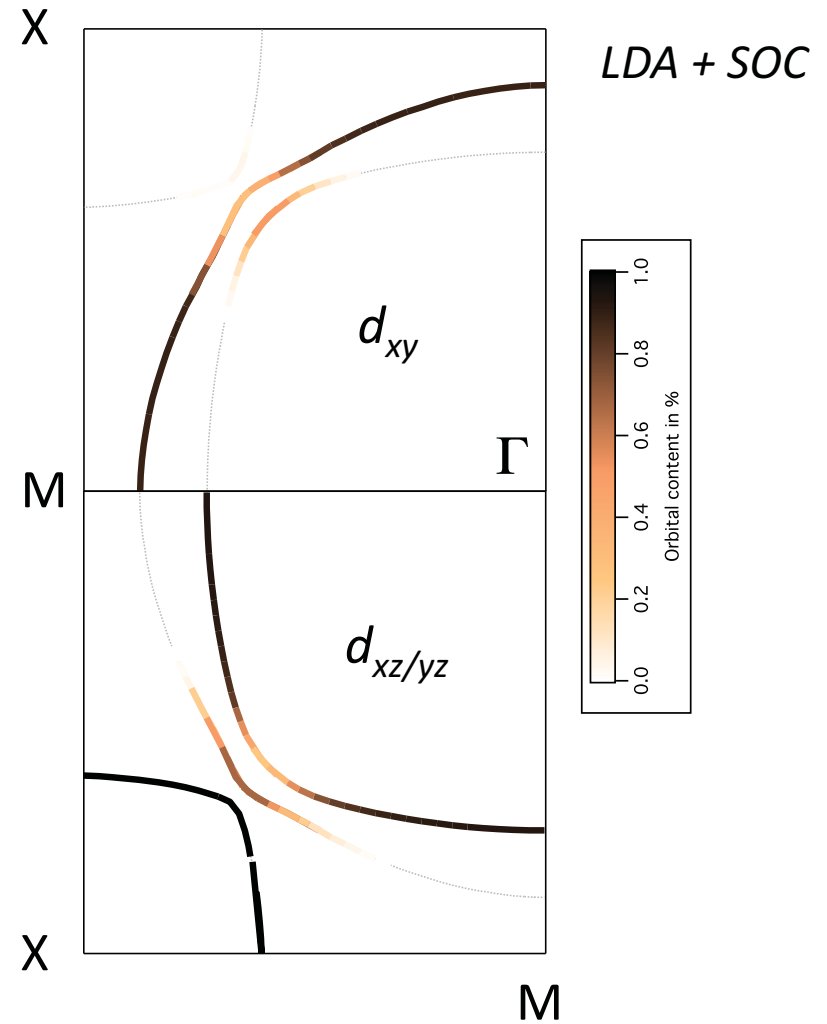
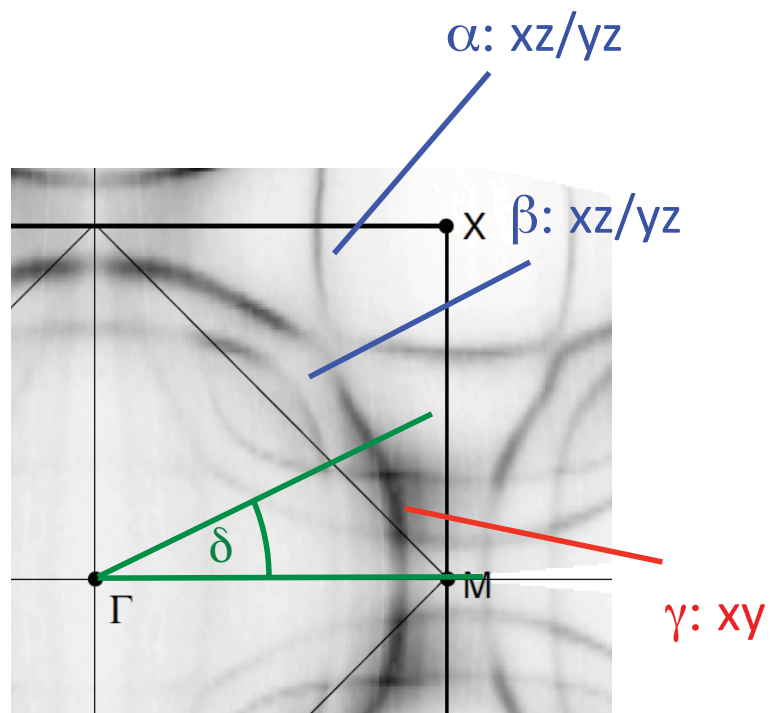
$$Z_{FL}^{-1} = 1 - \left. \frac{\partial \text{Re} \Sigma(\omega)}{\partial \omega} \right|_{\omega=0} = \frac{m^*}{m} = \frac{v_{LDA}}{v_F}$$



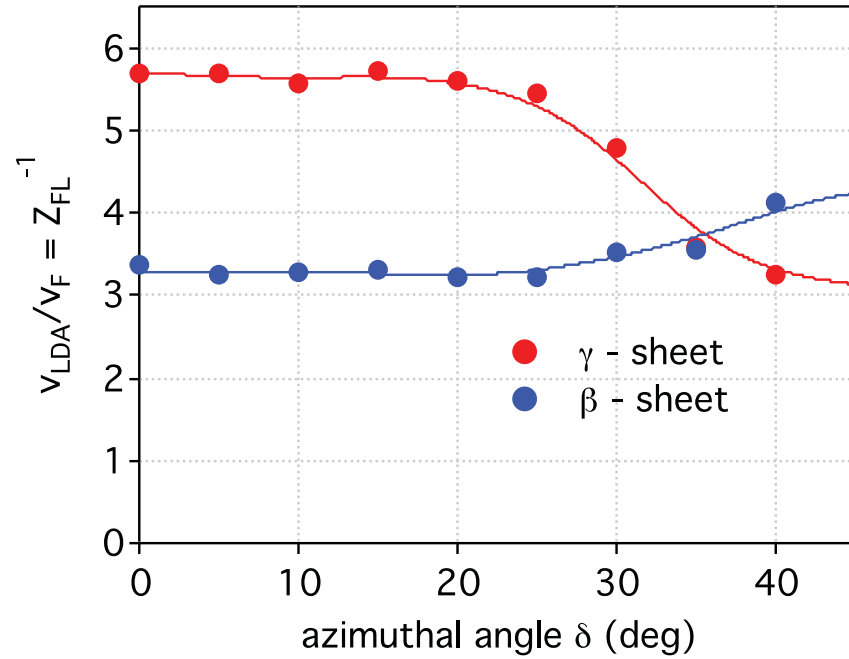
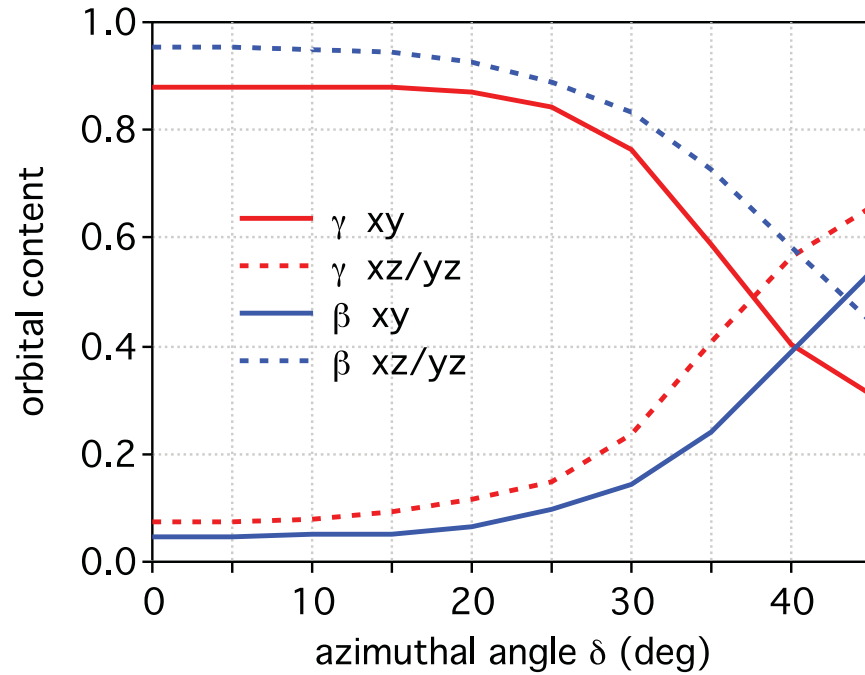
Sr_2RuO_4 – spin-orbit coupling



Sr_2RuO_4 – spin-orbit coupling



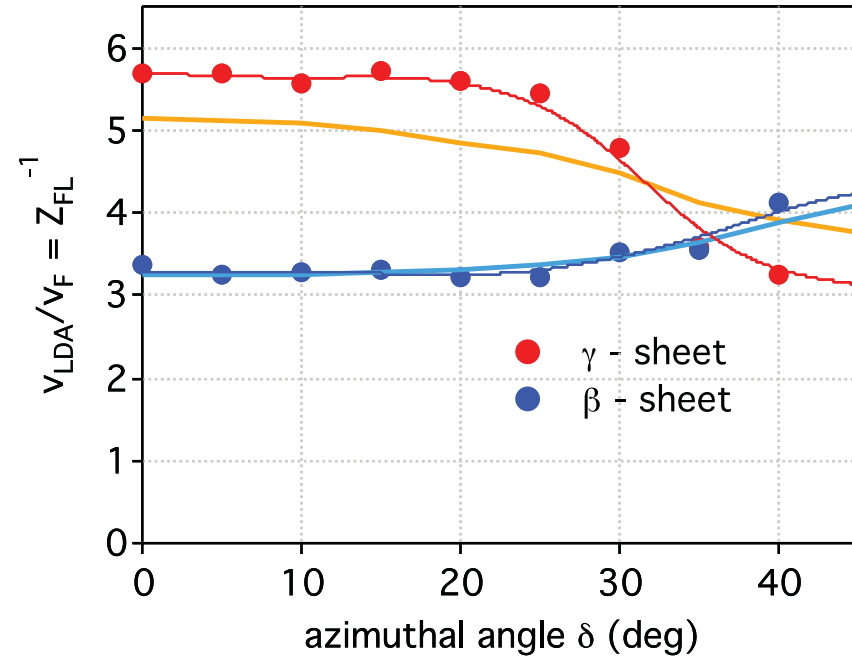
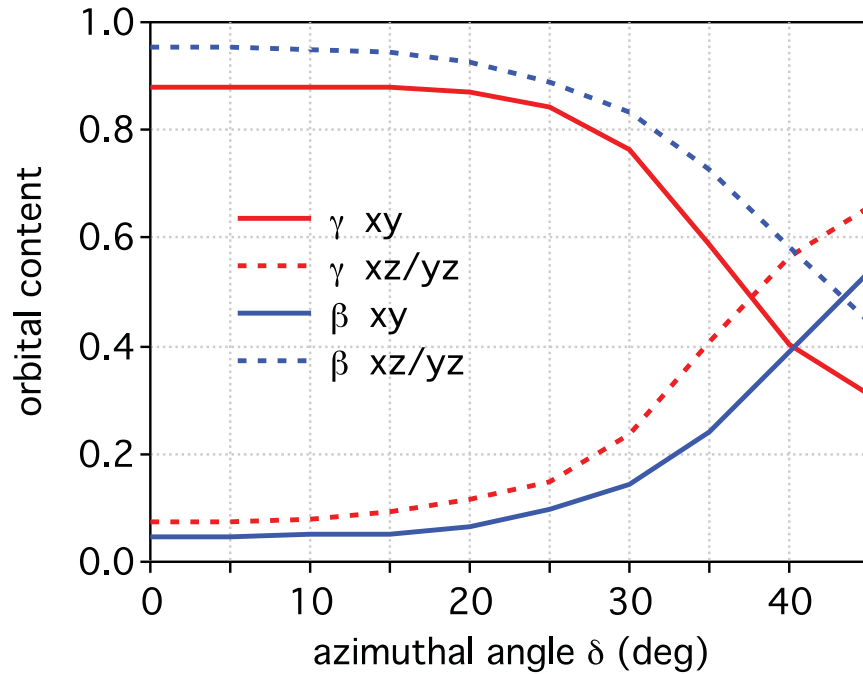
DMFT



$$Z^{xy} = 5.1^{-1}$$

$$Z^{xz/yz} = 3.2^{-1}$$

DMFT



$$Z^{xy} = 5.1^{-1}$$

$$Z^{xz/yz} = 3.2^{-1}$$

$$Z_{\gamma}^{-1} = c_{\gamma}^{xy} / Z^{xy} + c_{\gamma}^{xz/yz} / Z^{xz/yz}$$

$$Z_{\beta}^{-1} = c_{\beta}^{xy} / Z^{xy} + c_{\beta}^{xz/yz} / Z^{xz/yz}$$

summary

1. Quantum criticality in $\text{Sr}_3\text{Ru}_2\text{O}_7$ is related to low-lying van Hove singularities.
2. Key features of the electronic structure consistent with assumptions in mean-field models of nematic state.
 - I. Large mass enhancement with $m^*/m_{\text{LDA}} > 20$
 - II. vHs of the d_{xy} sheet at -3 meV
3. Hybridization is essential to understand the mass renormalization puzzle in ruthenates.

Thank you

