Electronic correlations and enhanced spin-orbit coupling in Sr_2RuO_4

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Laser-ARPES
Anna Tamai, Emil Rozbicki, Felix Baumberger

FLATIRON INSTITUTE
Division of Simons Foundation

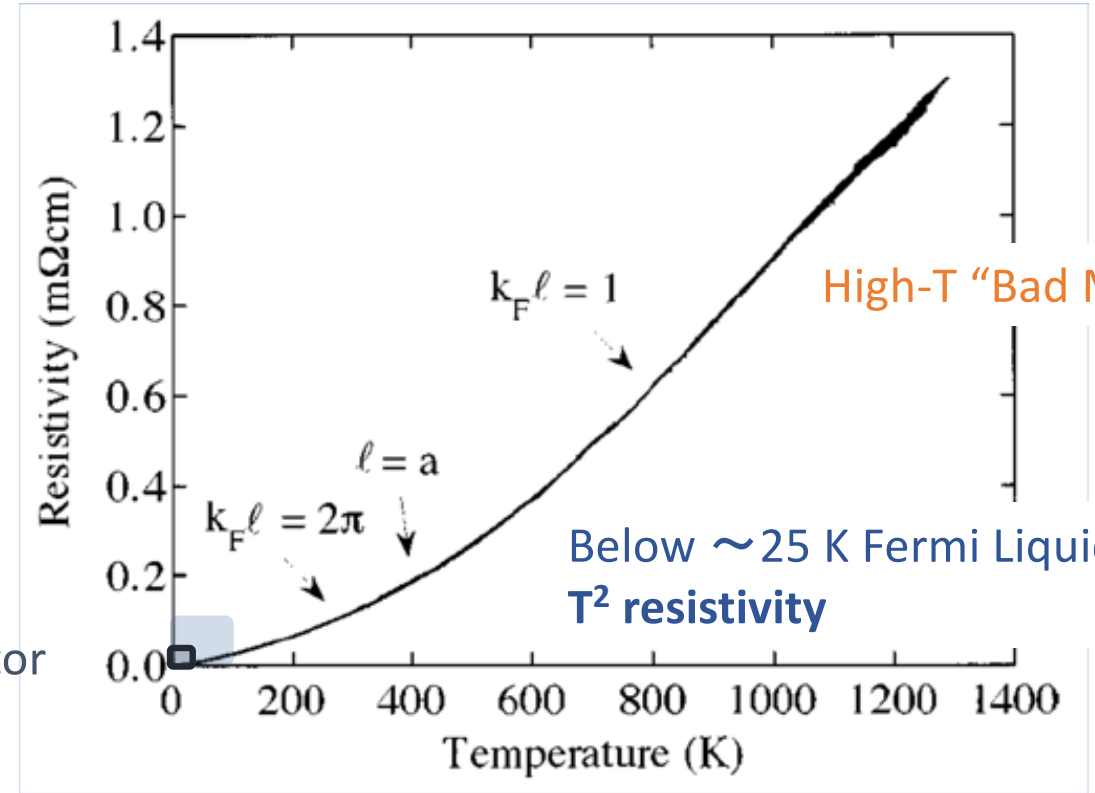
Theory
Manuel Zingl, Minjae Kim, Antoine Georges

COLLÈGE DE FRANCE
1530

University of St Andrews

Samples
Alex Gibbs, Andy Mackenzie

Sr_2RuO_4: Bad metal to low-T superconductors



High-T "Bad Metal"

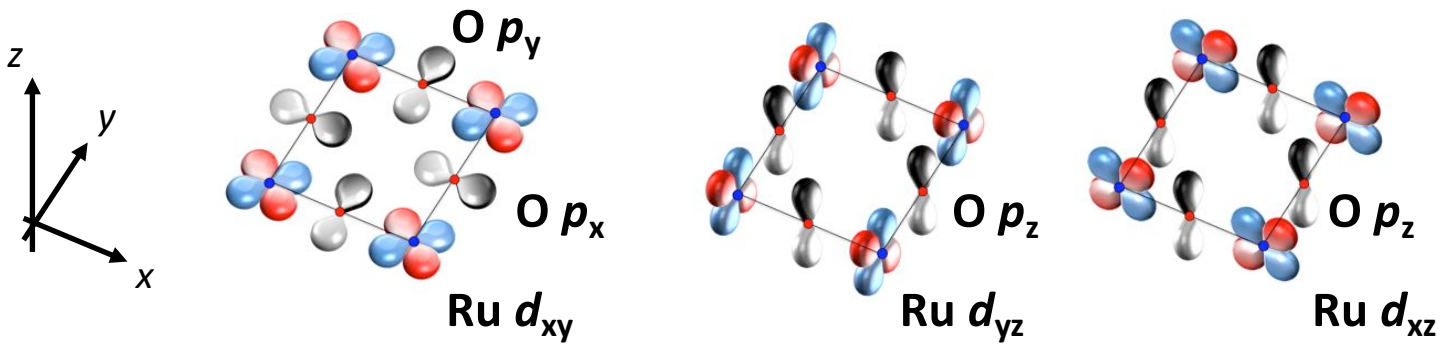
Below ~25 K Fermi Liquid

T^2 resistivity

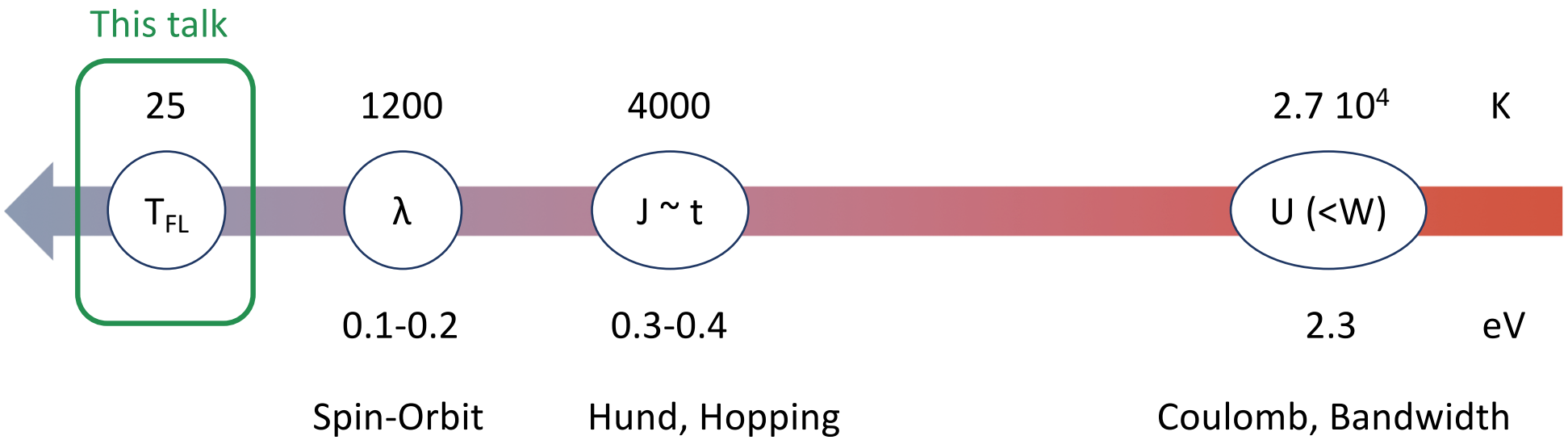
Superconductor

A. W. Tyler et al., PRB 58, R10107 (1998)

Hund's metal

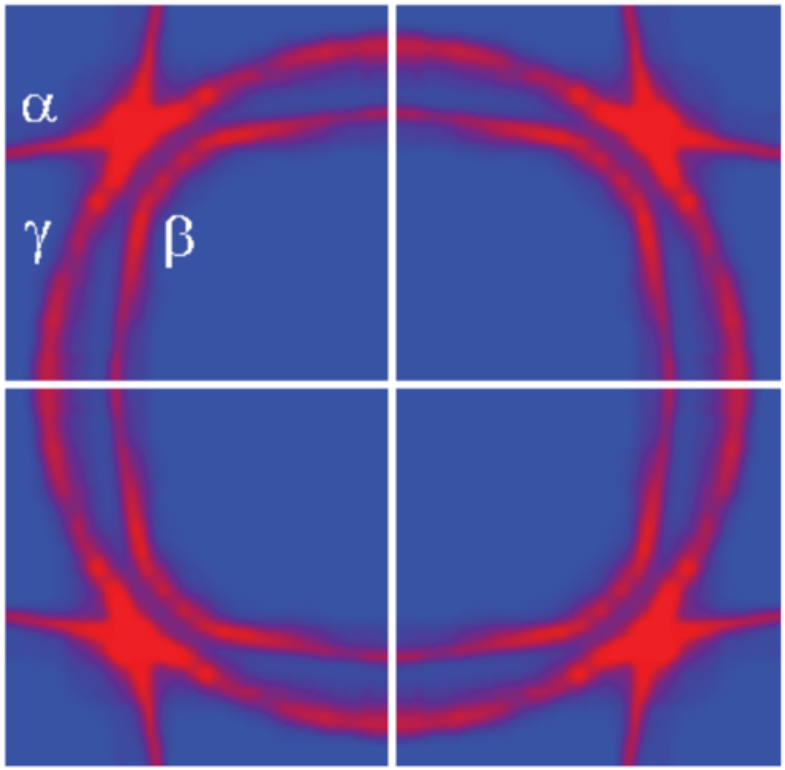


Ru^{4+} :
4 4*d* el./Ru

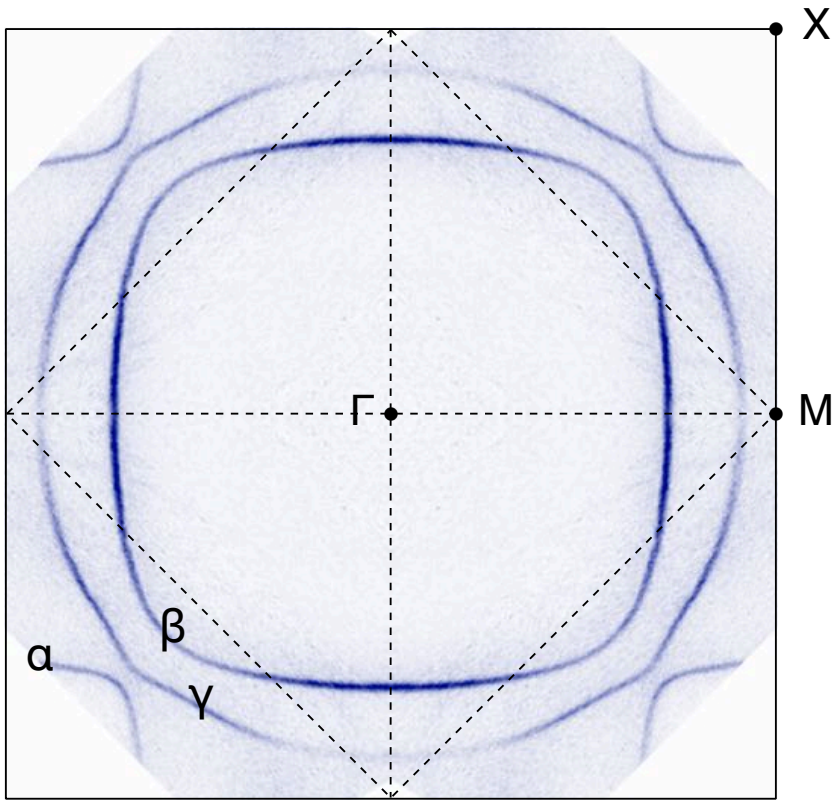


from A. Georges

Laser-ARPES on Sr_2RuO_4

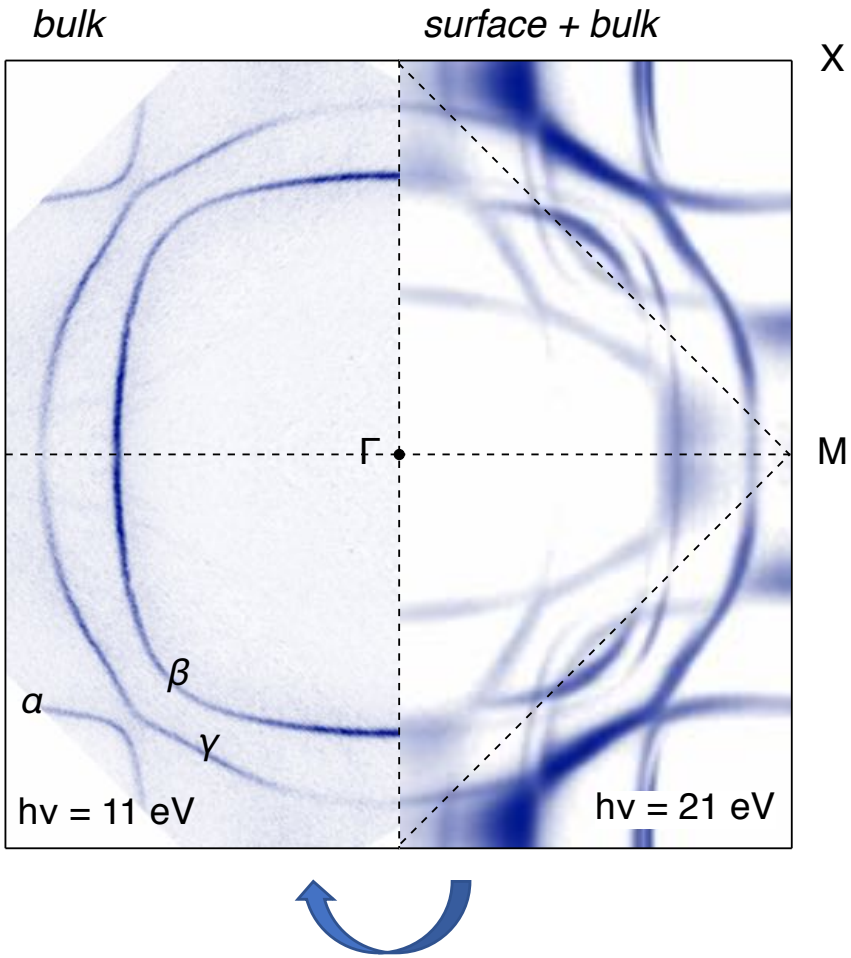


A. Damascelli et al., PRL 85, 5194 (2000)

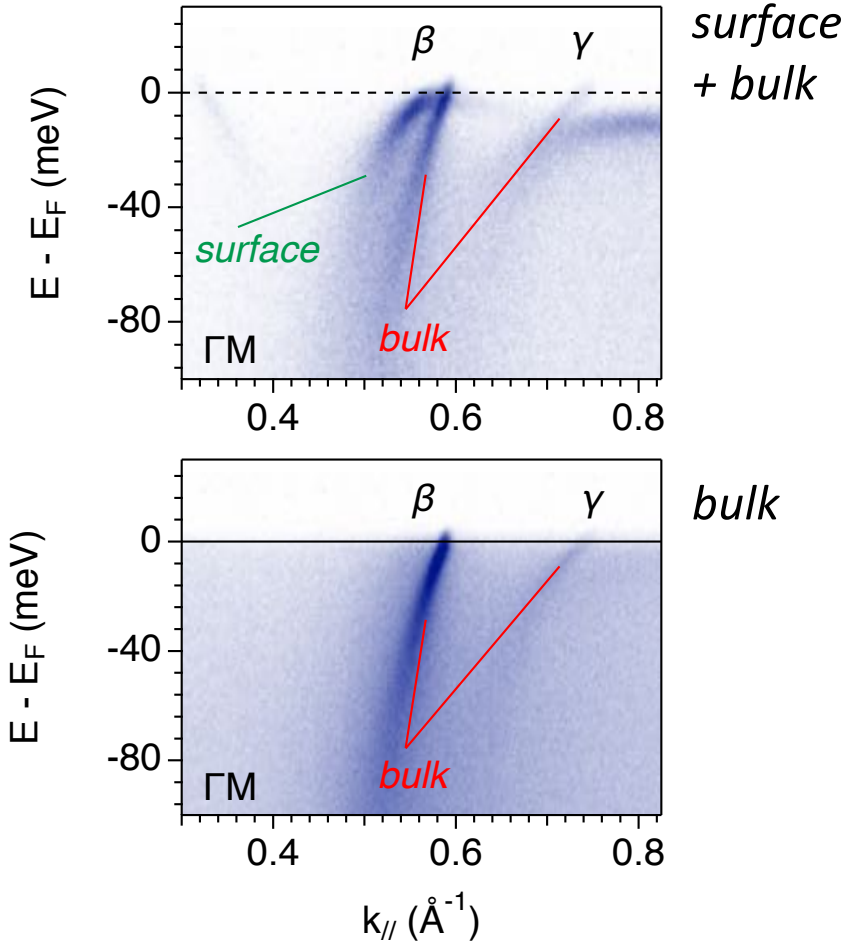


A. Tamai et al., PRX 9, 021048 (2019)

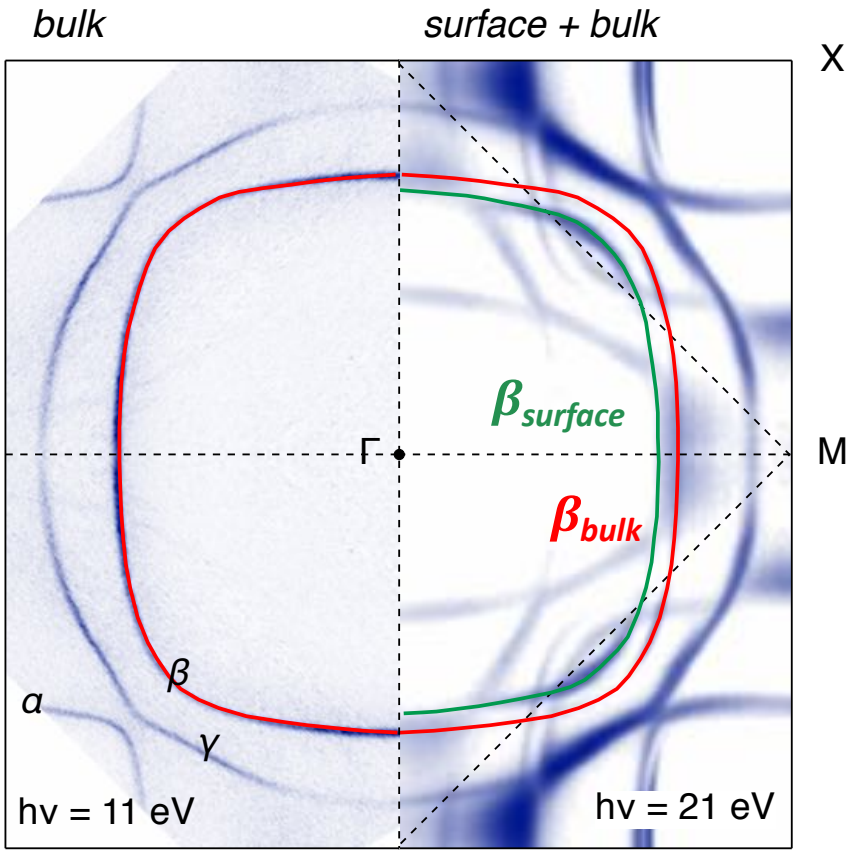
Sr_2RuO_4 - surface vs bulk

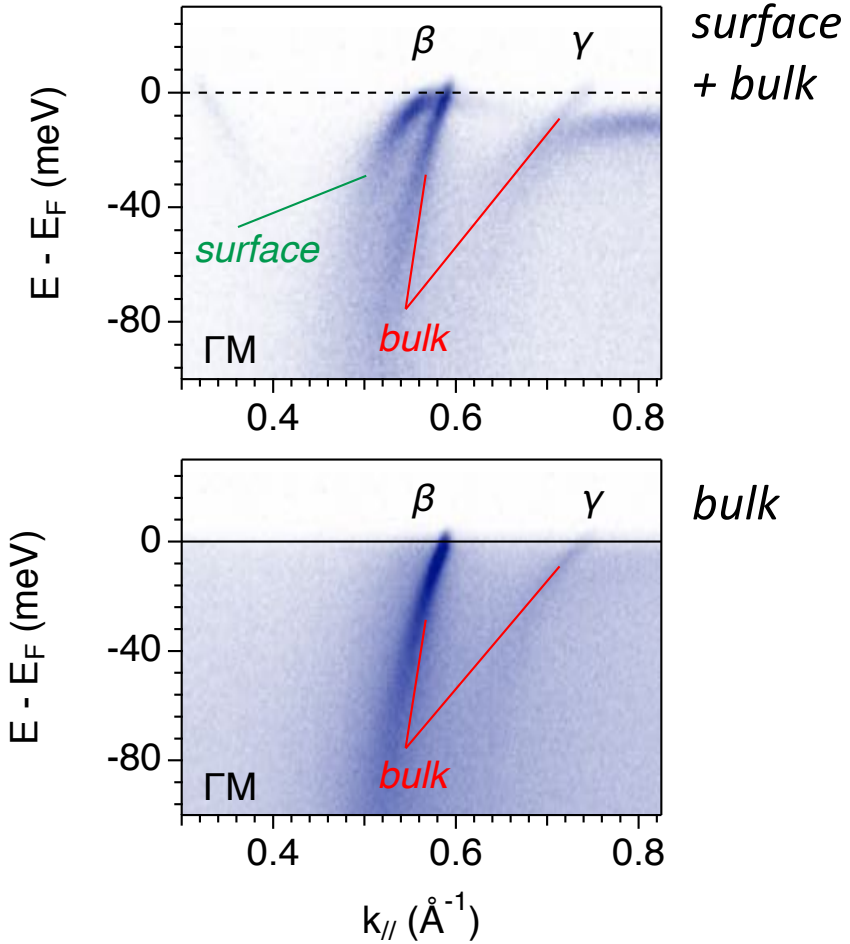


0.5 Langmuir CO at 120 K

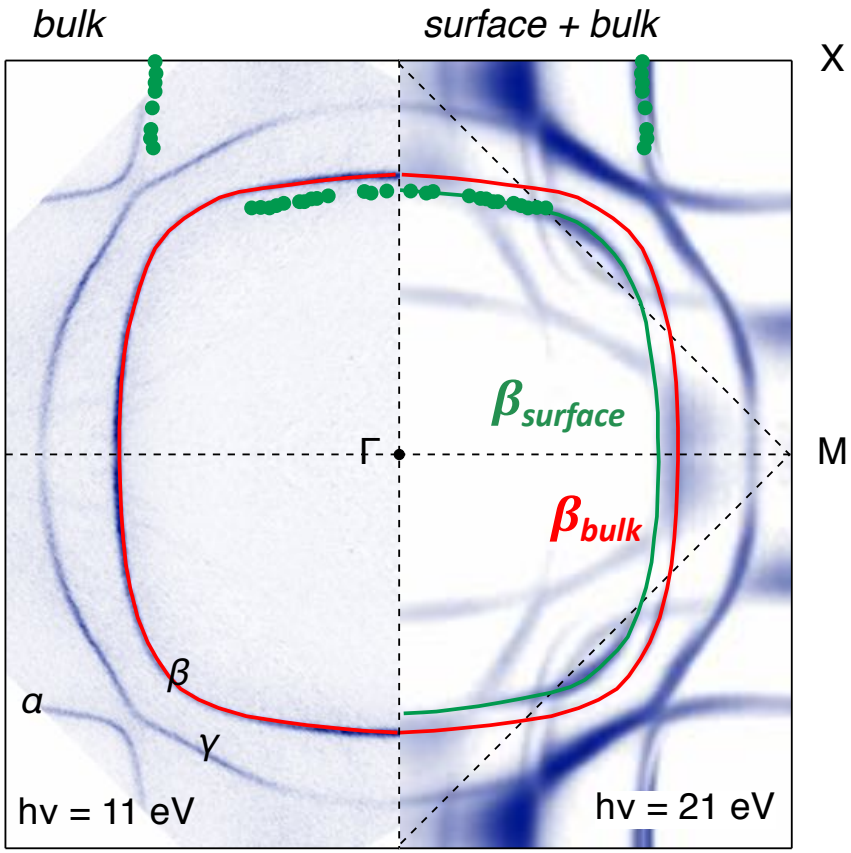


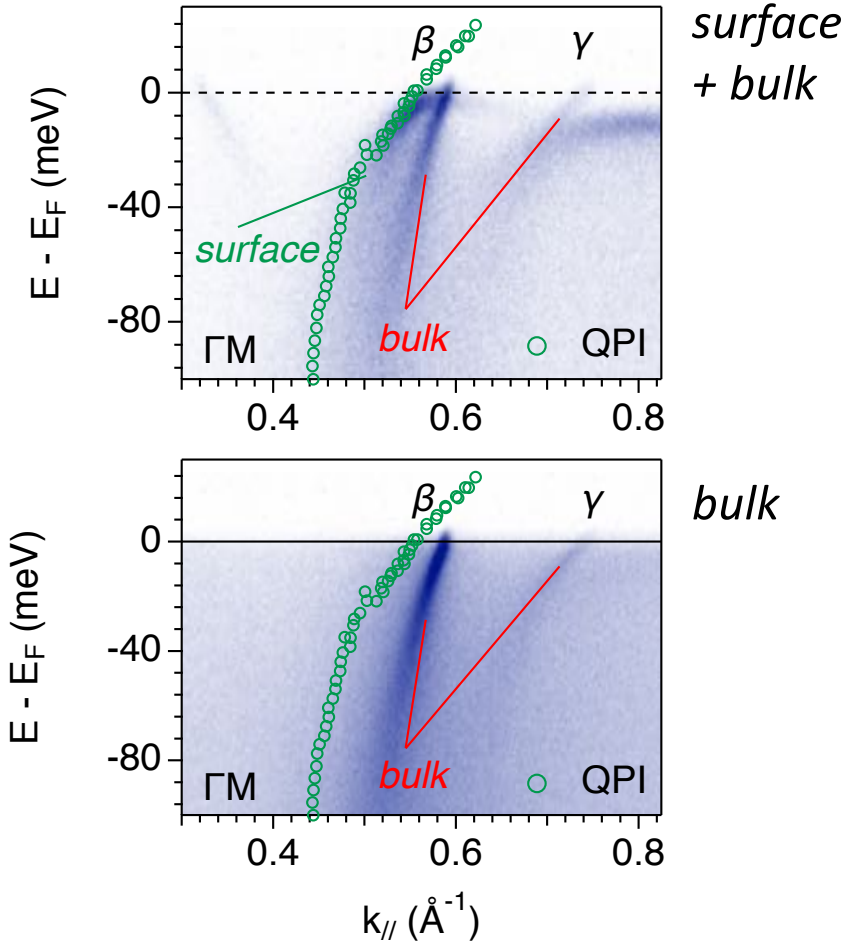
Sr_2RuO_4 - surface vs bulk





Sr_2RuO_4 - surface vs bulk



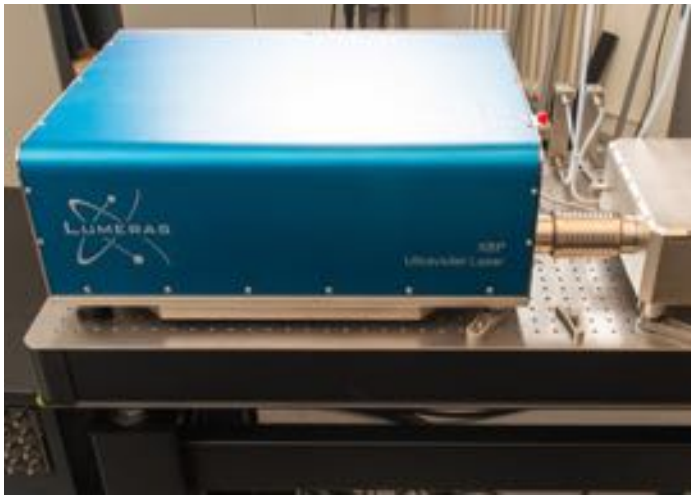


R. Sharma, PNAS 201916463 (2020)

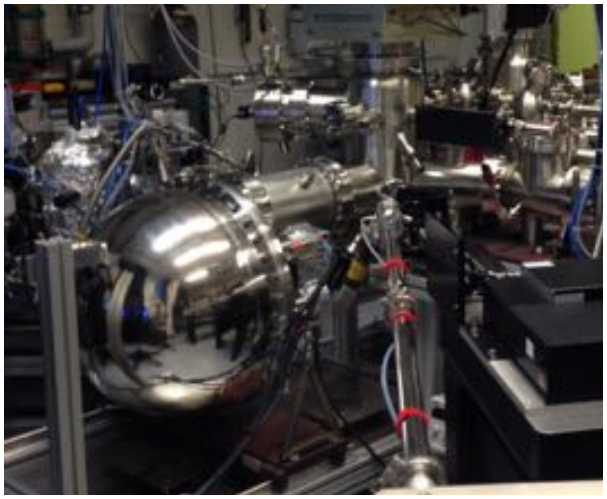
Z. Wang, Nat. Phys. **13**, 799 (2017)

Geneva laser-ARPES lab

sub – 4 K 6 axis goniometer

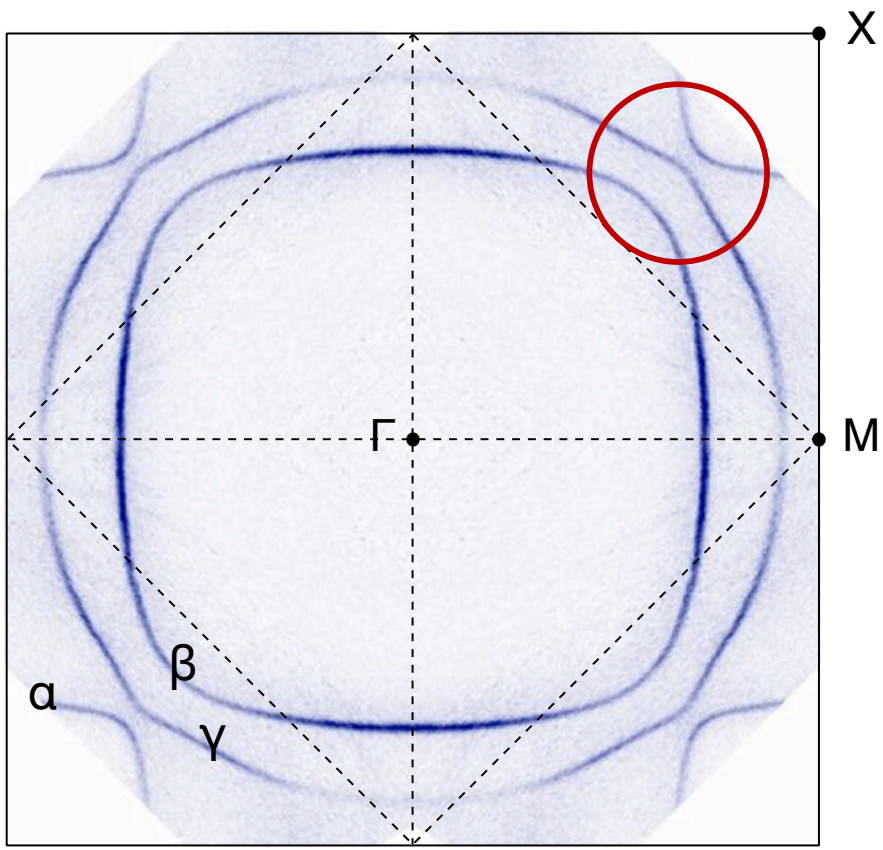


11eV laser – Lumeras
50 MHz / 30 ps, 10^{12} γ/s



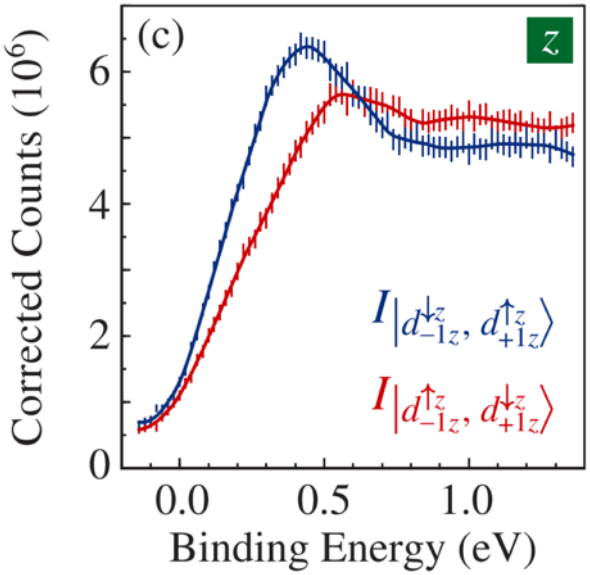
MBS electron spectrometer
$\Delta\varepsilon \approx 0.7$ meV

Spin-orbit coupling



- DFT : λ_{LDA}= 100 meV
- Exp: band bottom of α, β : λ = 130 ± 30 meV

Veenstra, PRL **112**, 127002 (2013)

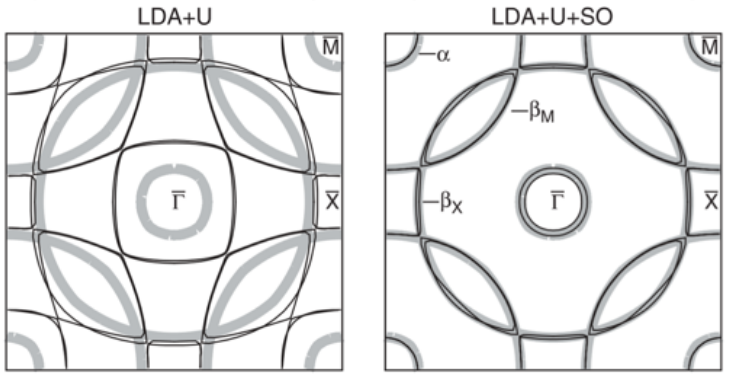


See also Haverkort, PRL **101**, 26406 (2008)

Theoretical work

- *Coulomb-Enhanced Spin-Orbit Splitting: The Missing Piece in the Sr_2RhO_4 Puzzle*

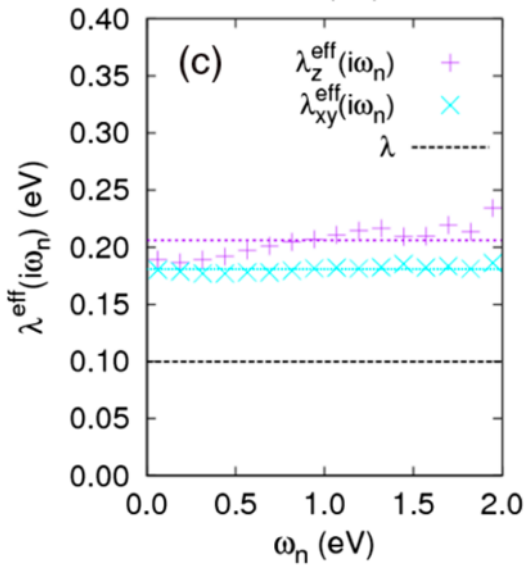
  Liu, Andersen et al., Phys. Rev. Lett. **101**, 026408 (2008)



- DMFT: off diagonal contributions in self-energy

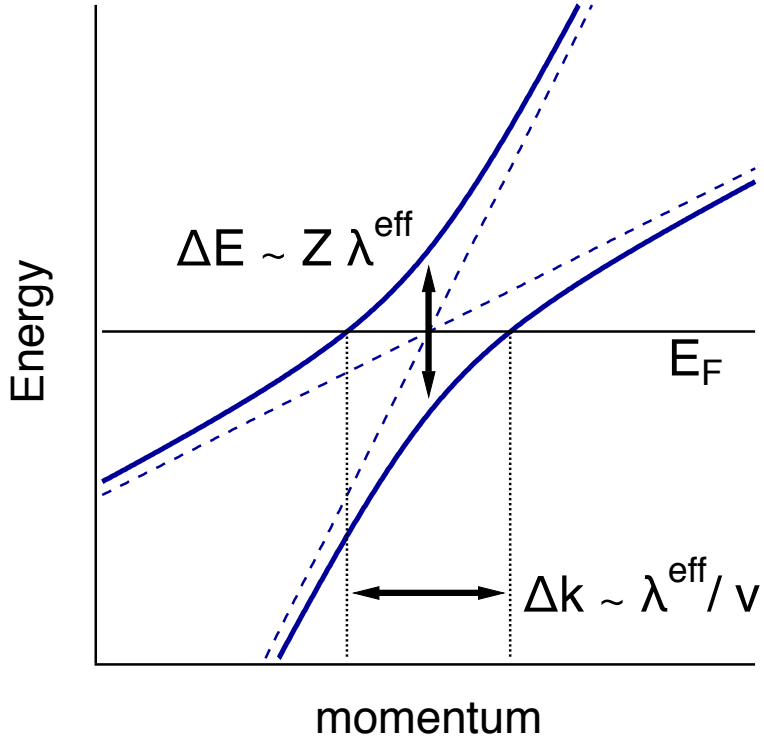
  Zhang, Pavarini et al., Phys. Rev. Lett. 116, 106402 (2016)
  Kim, Georges et al., Phys. Rev. Lett. 120, 126401 (2018)

$\lambda_{eff} \approx 2\ \lambda_{LDA}$ for Sr_2RuO_4



Spin-orbit gaps

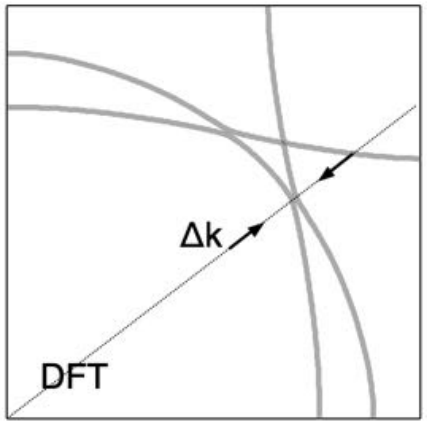
$Z = (Z_1 Z_2)^{½}$



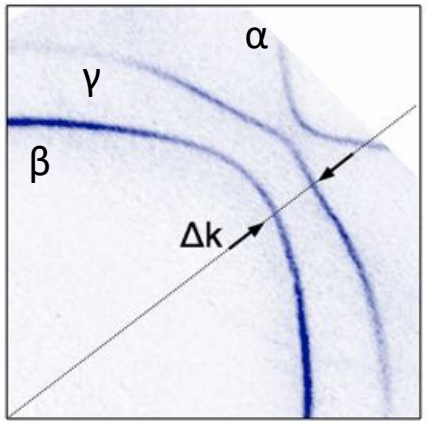
$v = (v_1^{bare} v_2^{bare})^{½}$

Kim, Georges et al., Phys. Rev. Lett. 120, 126401 (2018).

Enhanced SOC at the Fermi surface

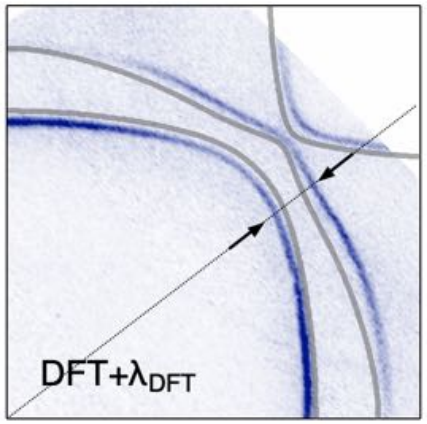


$\Delta k = 0$



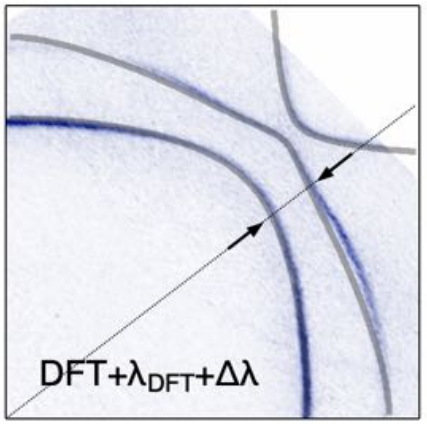
$\Delta k_{QP} = 0.094(9)$ Å^{-1}

LDA + SOC



$\Delta k = 0.046$ Å^{-1}

Enhanced SOC



$\Delta k = 0.093$ Å^{-1}

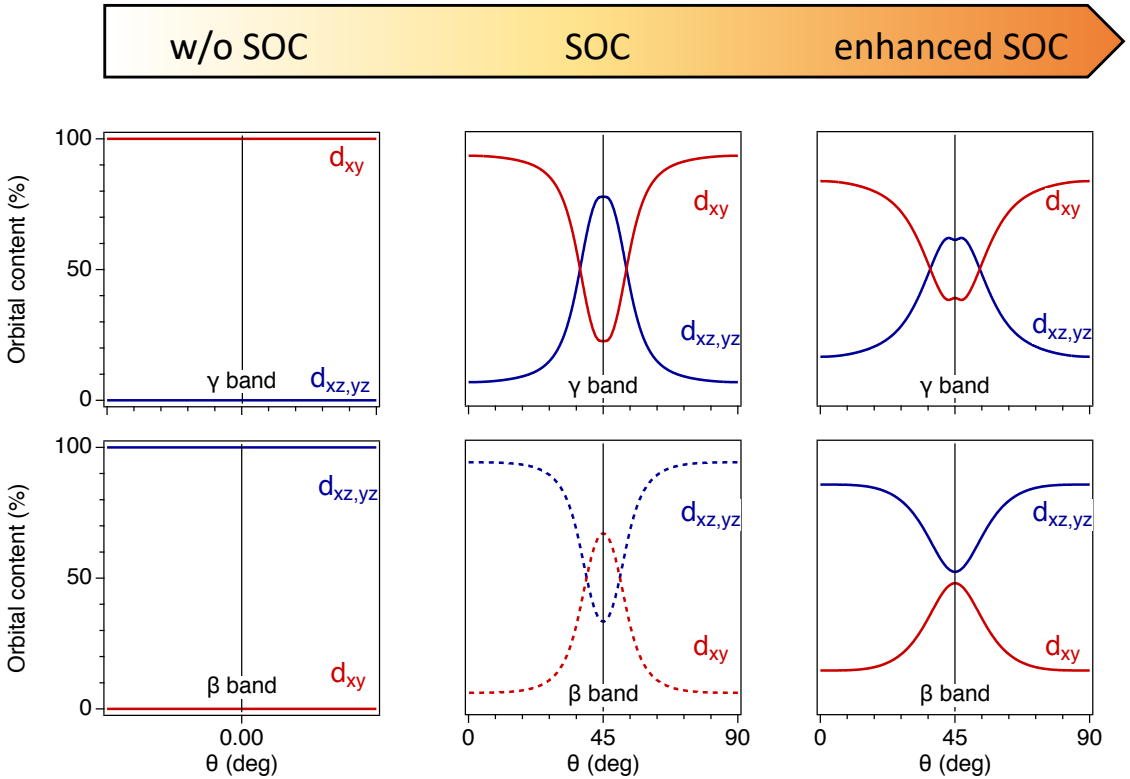
ARPES : $\lambda_{eff} = \lambda_{bare} (\Delta k_{QP} / \Delta k_{LDA+SOC}) \approx 200$ meV

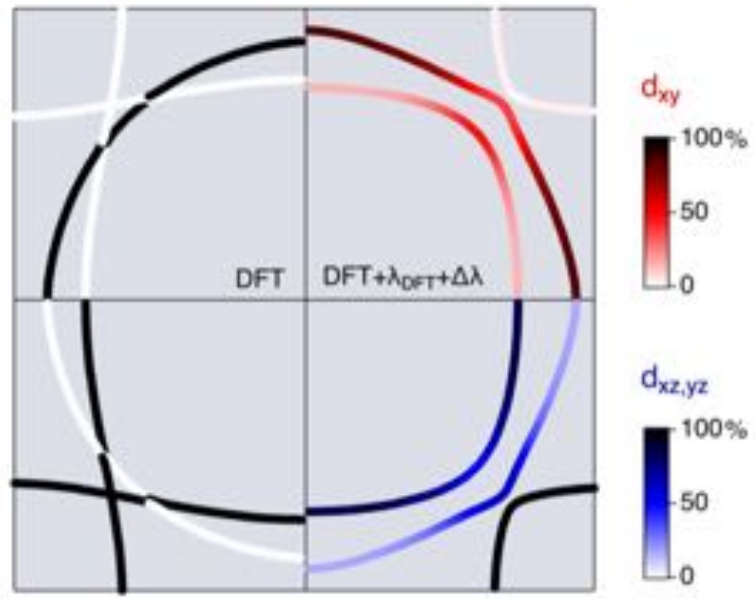
LDA : $\lambda_{bare} \approx 100$ meV

DMFT : $\lambda_{eff} \approx 200$ meV

A. Tamai et al. PRX 9, 021048 (2019)
M. Kim, A. Georges et al. PRL 120, 126401 (2018)

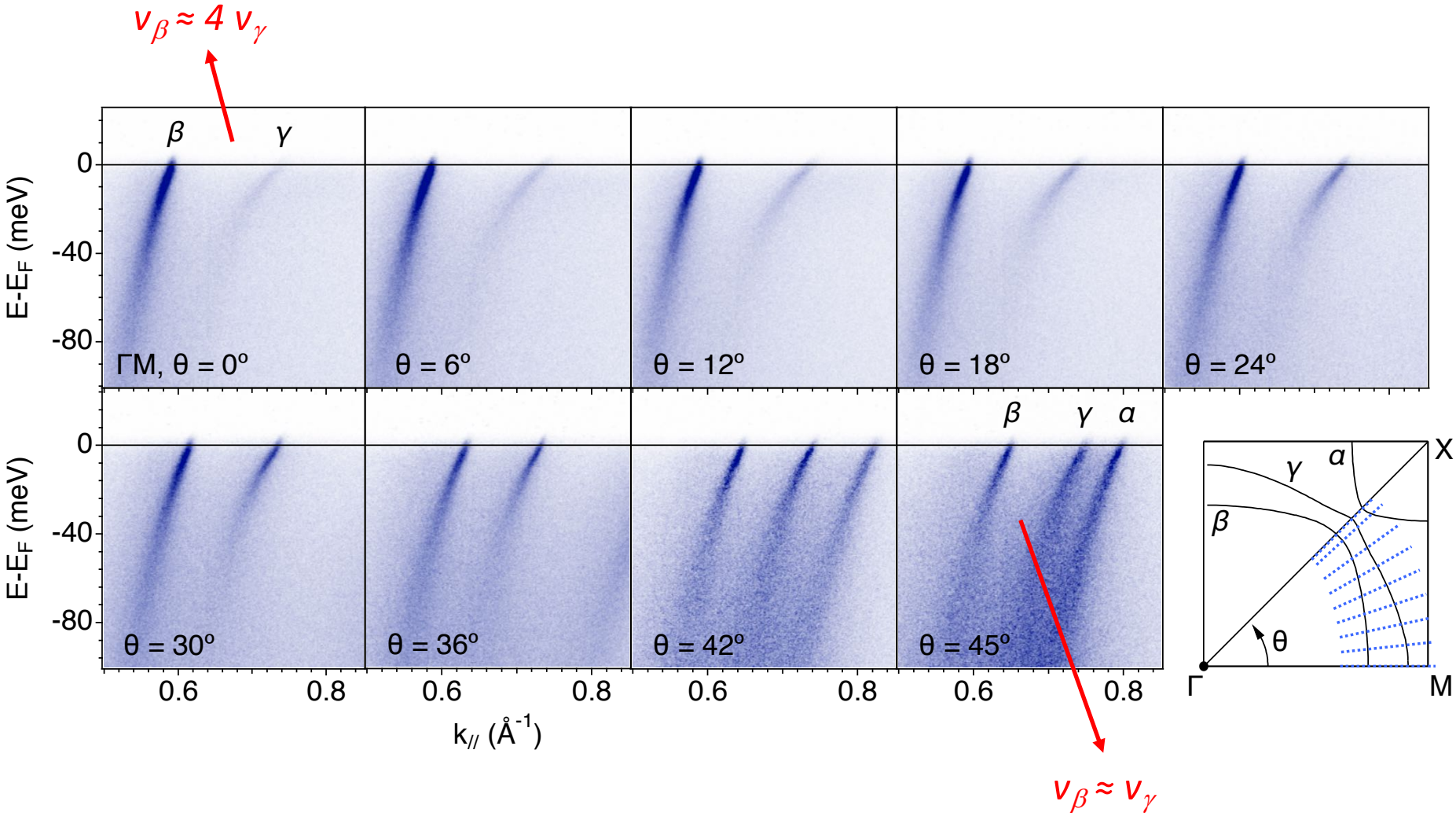
Orbital character at the FS



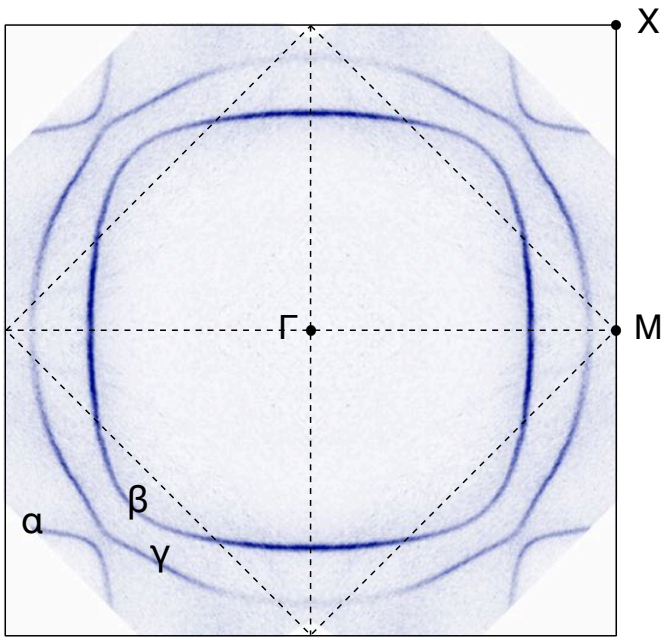


Orbital content of quasiparticle states is strongly angular dependent due to SOC

Quasiparticle dispersion



Sr_2RuO_4 – effective masses



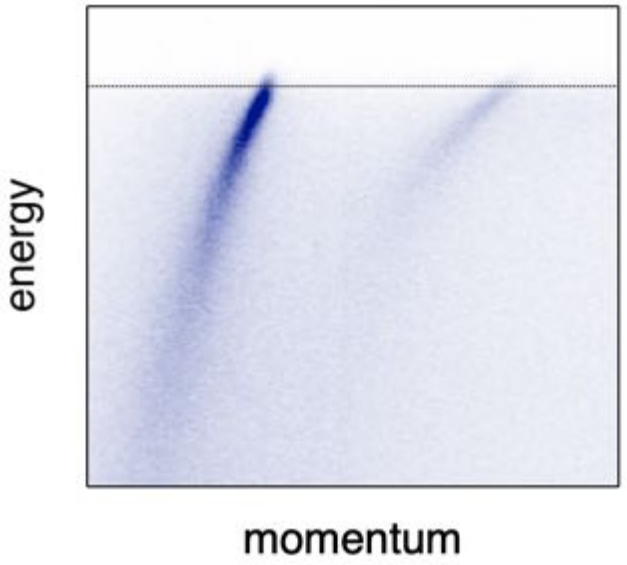
Cyclotron masses

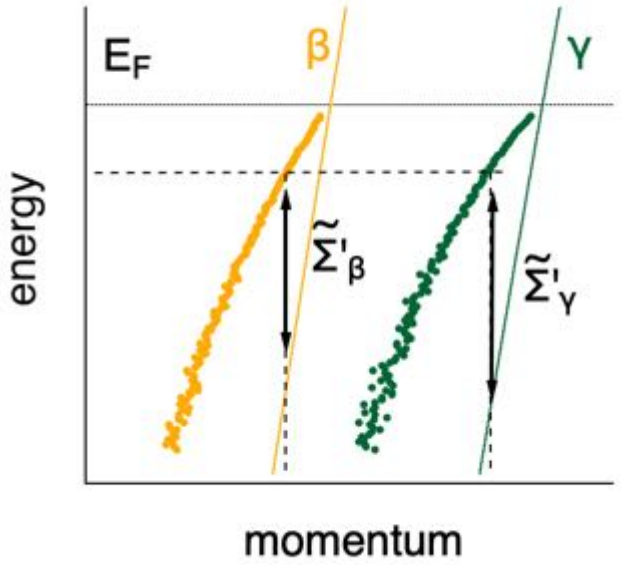
$$m^* = \frac{\hbar^2}{2\pi}\frac{\partial A_{FS}}{\partial \epsilon} = \frac{\hbar^2}{2\pi}\int_0^{2\pi}\frac{k_F(\theta)}{\partial\epsilon/\partial k(\theta)}d\theta$$

	ARPES	dHvA
γ	17.3(2) m_e	16 m_e
β	6.1(1) m_e	7 m_e

A. Tamai et al., PRX 9, 021048 (2019)
Bergemann et al., Adv. Phys. 52, 639 (2003)
Mackenzie et al., Phys. Rev. Lett. 76, 3786 (1996)
Mackenzie et al., J. Phys. Soc. Japan 67, 385 (1998)

Extracting self-energies



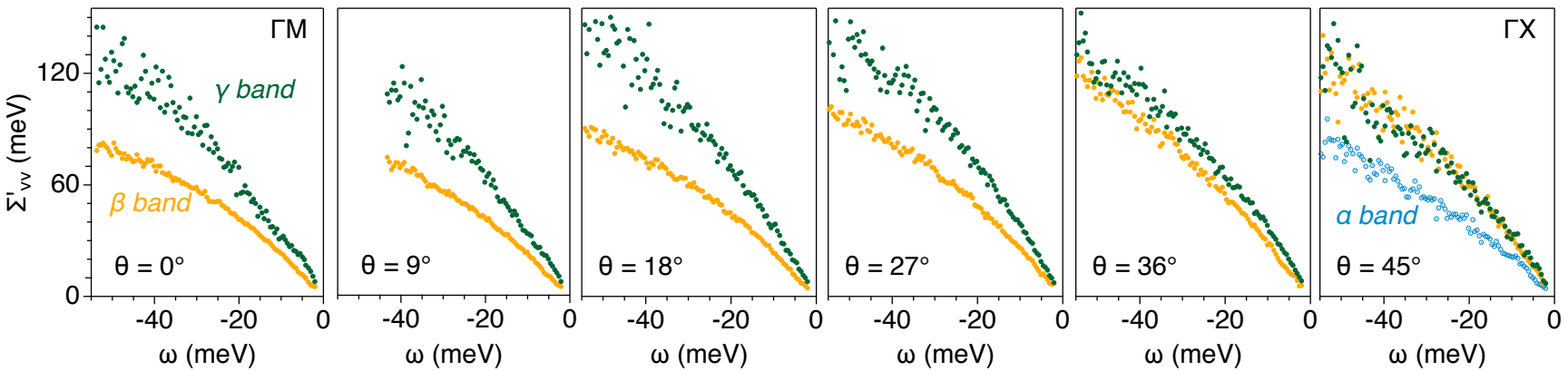


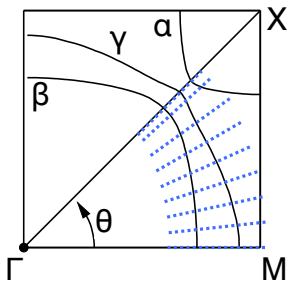
Bare Hamiltonian :

DFT + λ + Δλ

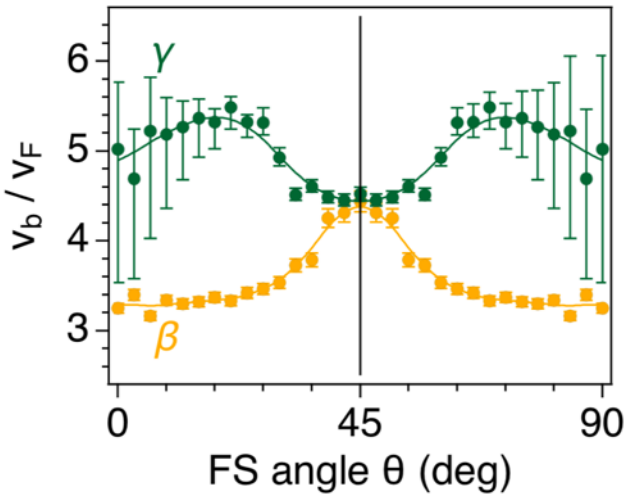
Correlation effect
(but frequency independent)

Self-energy of bulk bands



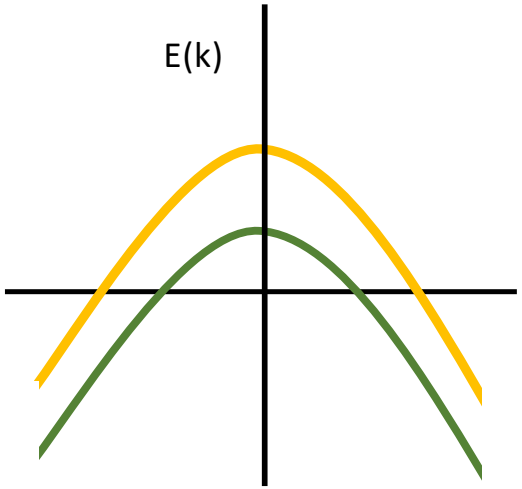


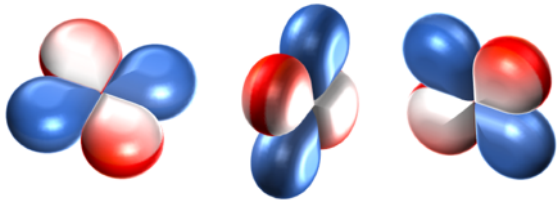
Fermi surface



- Anisotropic Coulomb interactions ?
- Long wavelength spin fluctuations ?
- Electron – phonon coupling?

Self-energy: band basis vs orbital basis





$\nu, \nu' = \alpha, \beta, \gamma$

$m, m' = d_{xy}, d_{yz}, d_{xz}$

$|\chi_m(\mathbf{R})\rangle$: *Wannier functions*

$U_{m\nu}(\boldsymbol{k}) = \langle \chi_m(\boldsymbol{k}) | \psi_\nu(\boldsymbol{k}) \rangle$

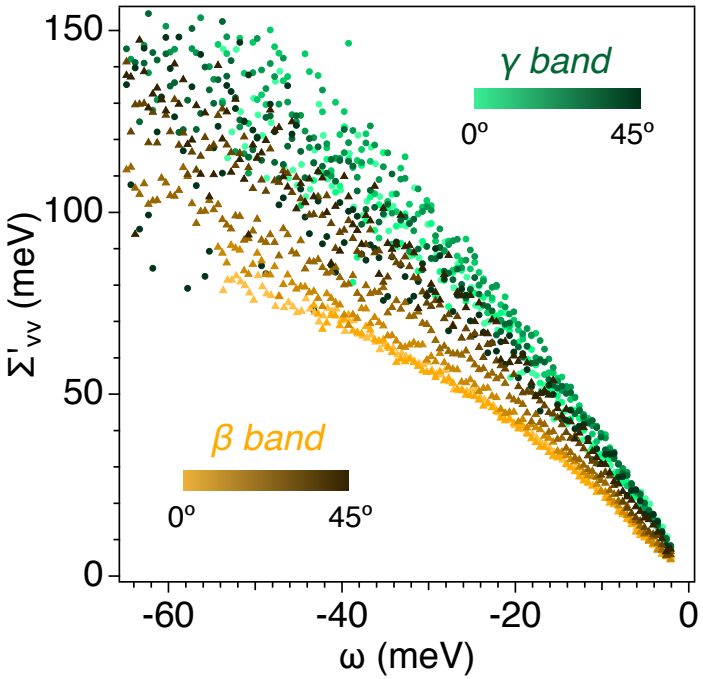
$|U_{m\nu}(\boldsymbol{k})|^2$: *Orbital* character of each band

$$\hat{H}^0_{mm'}(\boldsymbol{k}) = \sum_\nu U_{m\nu}(\boldsymbol{k})\, \varepsilon_\nu(\boldsymbol{k})\, U^*_{m'\nu}(\boldsymbol{k})$$

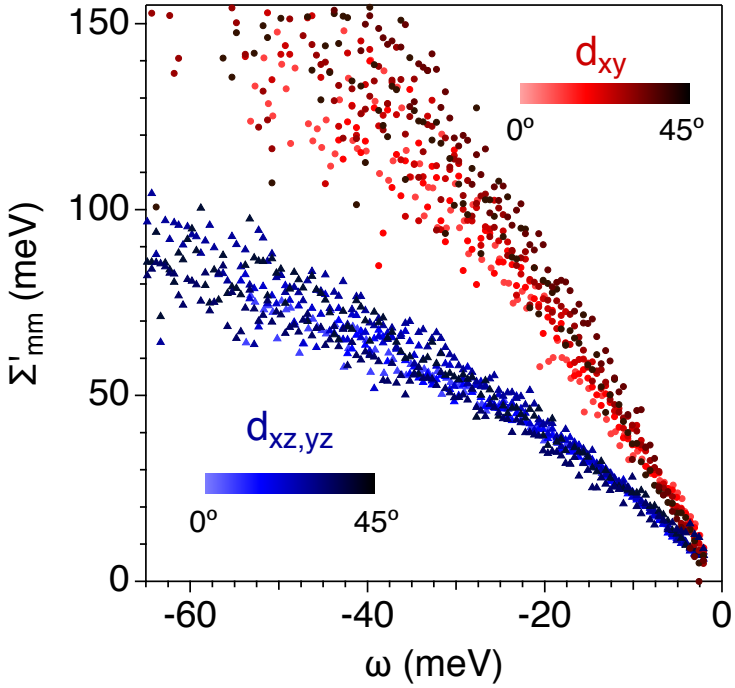
$$\Sigma_{mm'}(\omega, \boldsymbol{k}) = \sum_{\nu\nu'} U_{m\nu}(\boldsymbol{k})\, \Sigma_{\nu\nu'}(\omega, \boldsymbol{k})\, U^*_{m'\nu'}(\boldsymbol{k})$$

Self-energy: Band basis vs Orbital basis

$\nu, \nu' = \alpha, \beta, \gamma$

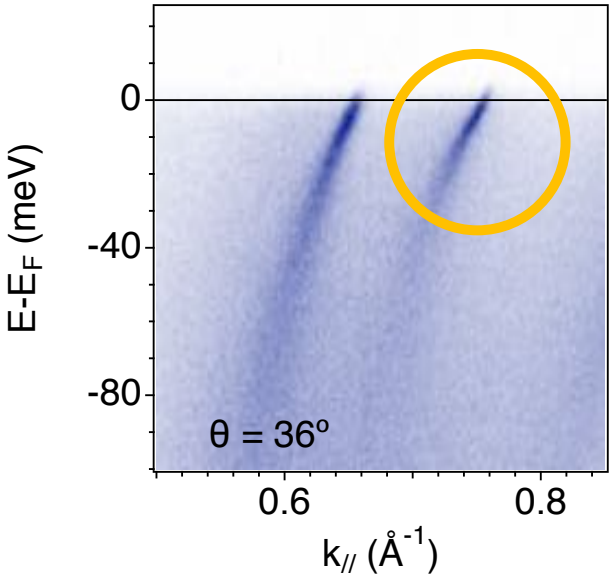


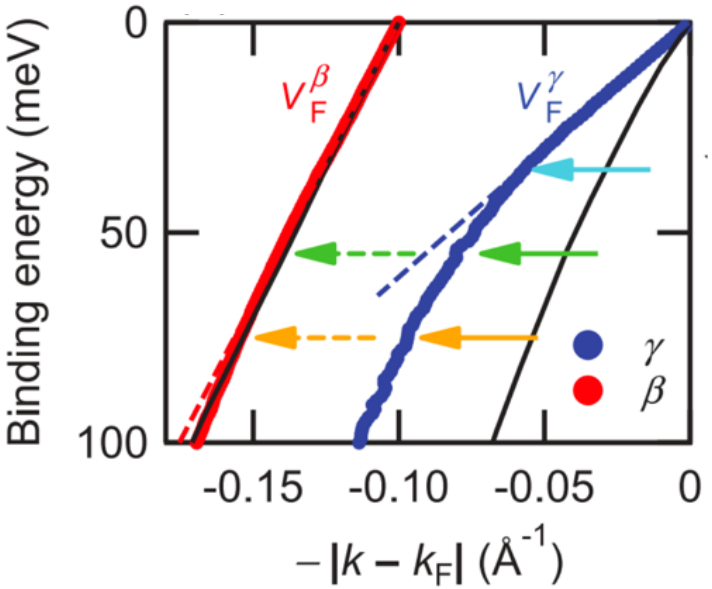
$m, m' = d_{xy}, d_{yz}, d_{xz}$



collapse of the angular dependence

Self energy and ‘kinks’



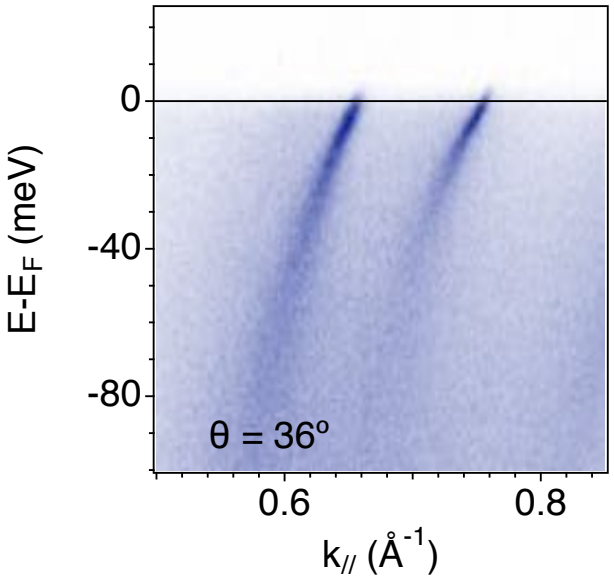


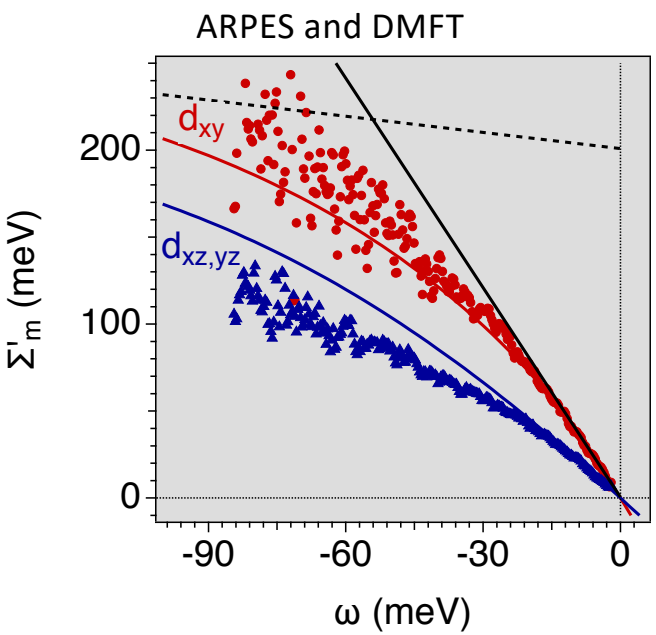
Iwasawa, PRL (2010)

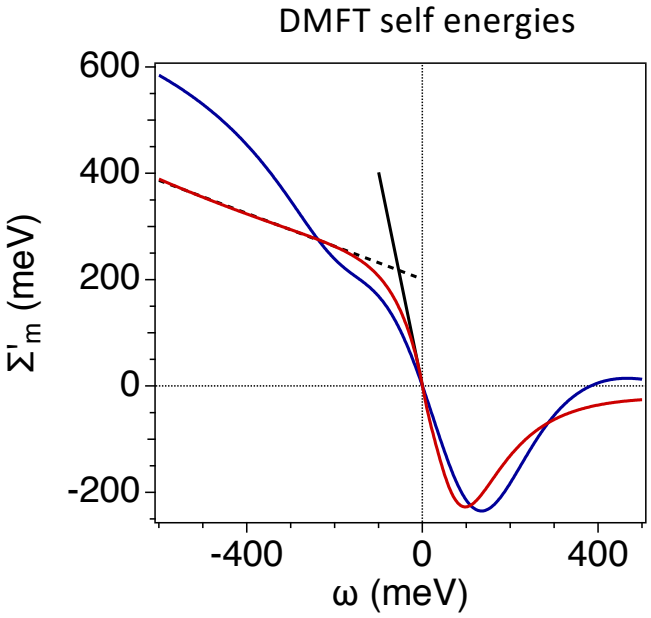
Electron-phonon kinks :

Iwasawa, Phys. Rev. B **72**, 104514 (2005), Ingle, Phys. Rev. B **72**, 205114 (2005), Iwasawa, Phys. Rev. Lett. **105**, 226406 (2010), Kim, Journal of Physics and Chemistry of Solids 72, 556 (2011), Iwasawa, Sci. Rep. **3**, 1930 (2013), Wang, Nat. Phys. **13**, 799 (2017)

Self energy and ‘kinks’



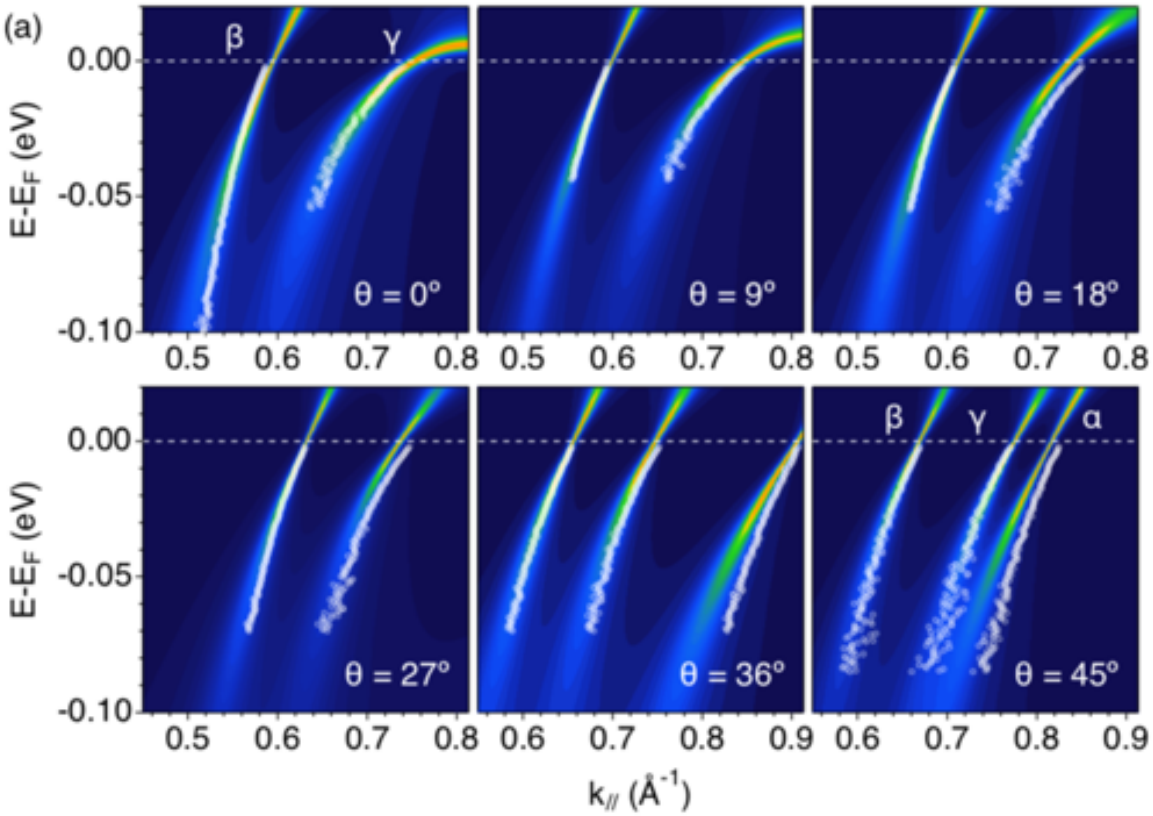


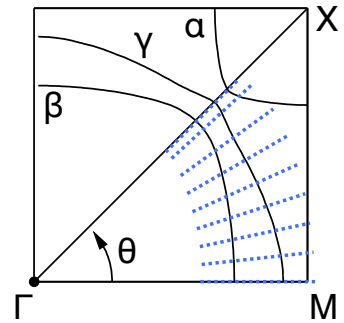


- ‘kink’ well described by DMFT
- deviations from linearity for $\omega > 20$ meV (FL Crossover temperature T_{FL}~ 25 K)

Single-site DMFT vs ARPES

QP dispersion

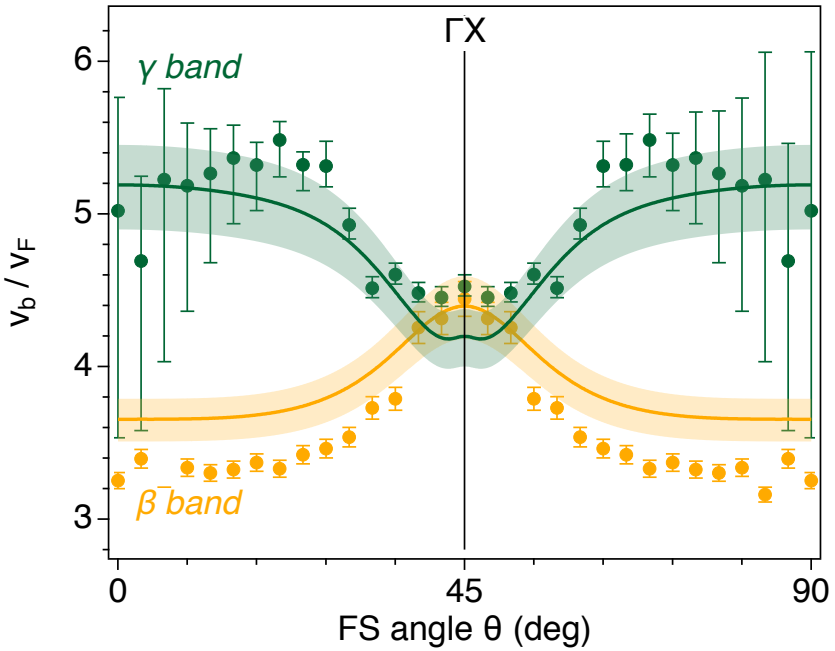




Dots: ARPES ϵ(k)
Colors: DMFT spectral function

Single-site DMFT vs ARPES

mass enhancement



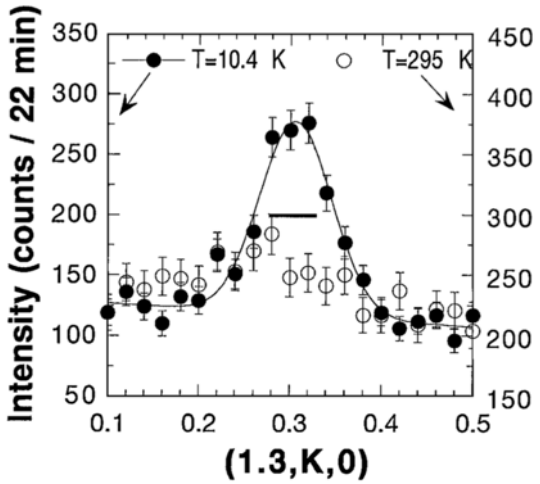
A. Tamai, PRX 9, 021048 (2019)

$$\frac{v_b}{v_F^{\nu}(\theta)} = \sum_m \frac{1}{Z_m} |U_{m\nu}(\theta)|^2$$

DMFT: Z_{xy}= 0.18, $Z_{xz/yz}$= 0.3

J. Mravlje, PRL 106 096401 (2011)
F. Kugler, PRL 124 016401 (2020)

Where is the signature of spin fluctuations ?

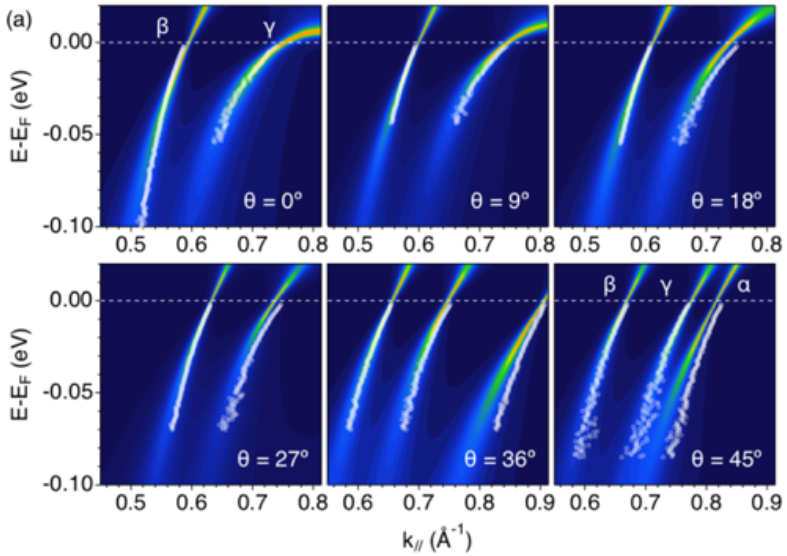


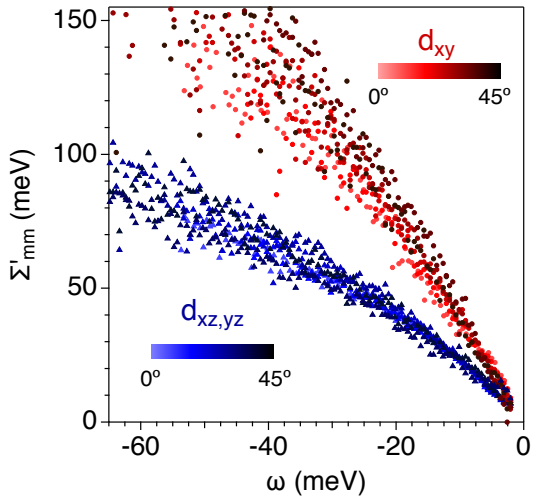
- Incommensurate AF at Q=(2π/3,2π/3)

  Y. Sidis et al., PRL 83, 3320 (1999)

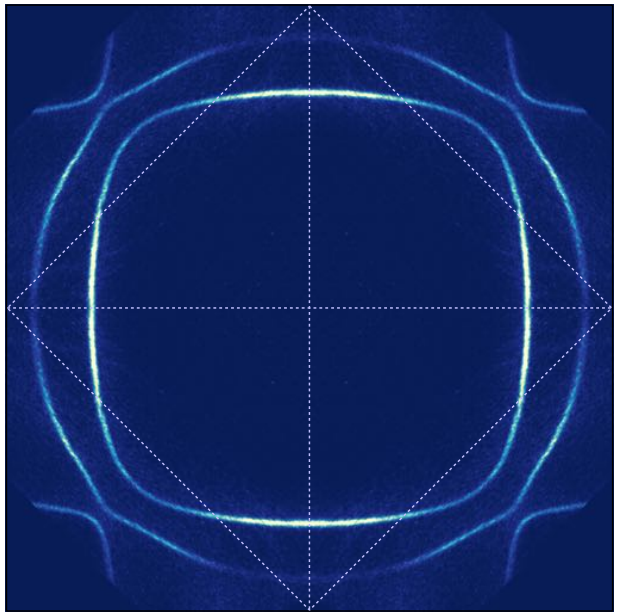
- FM near (π,π) and (0,0)

  P. Steffens et al., PRL 122, 047004 (2019)





Sr_2RuO_4 - Conclusions



Sr_2RuO_4 *laser-ARPES*

- Correlation induced enhancement of SOC (λ_{eff} = 200 meV)
- The momentum anisotropy of self energy can be attributed to SOC-driven orbital mixing
- Electronic origin of ‘kinks’

Dominant role of local-interactions

A. Tamai, PRX 9, 021048 (2019)