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1530

Chaire de Physique de la Matière Condensée
Antoine Georges

Cycle 2016-2017
23 mai 2017

Contrôle des fonctionnalités des oxydes

Hétéro-structures, Impulsions Lumineuses

Cours 5

Introduction aux Ruthénates

Sr_2RuO_4: Structure électronique, couplage de Hund et couplage spin-orbite.

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Control of Oxide Functionalities

Heterostructures, Light pulses

Lecture 5

Introduction to Ruthenates.

Sr_2RuO_4: Electronic structure,

Hund's coupling and spin-orbit coupling.

Today's seminar – May 23

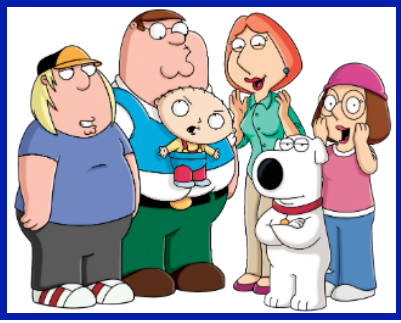
Darrell Schlom

Cornell University

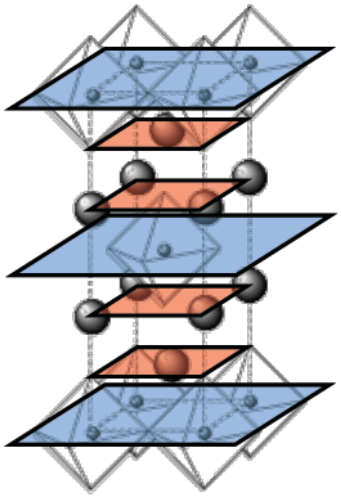
Thin-film alchemy: using epitaxial engineering to unleash the hidden properties of oxides

Image: http://www.mse.cornell.edu/research/resgroups/schlom/group.html

The Ruthenates Family: Overview

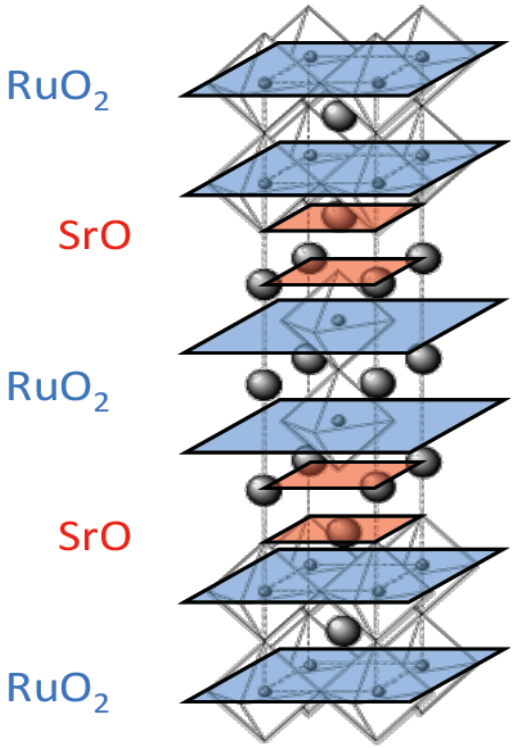


Sr_2RuO_4, n = 1



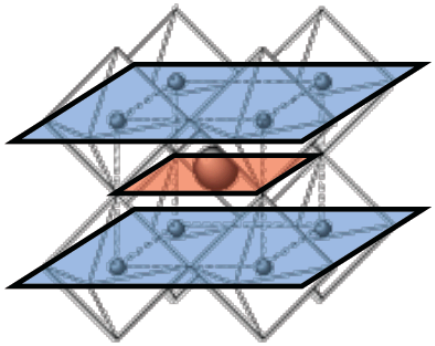
Fermi-Liquid metal
@ low-T
p-wave
superconductor
T_c~1.5K

$Sr_3Ru_2O_7$, n = 2



Strongly enhanced
paramagnet
Metamagnetic

$SrRuO_3$, n = ∞



Itinerant
Ferromagnet
T_{curie} ~ 160K

Controlling dimensionality: the Ruddlesden-Popper series $R_{n+1}M_nO_{3n+1}$ (`layered perovskite')

Unit-cell

n=1

n=2

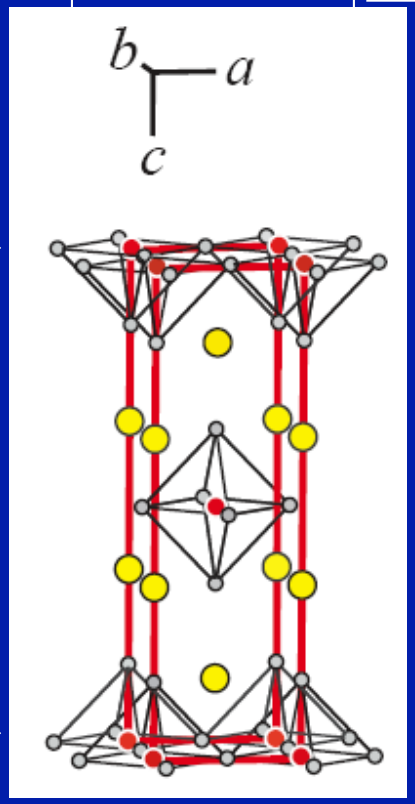
$Sr_3Ru_2O_7$

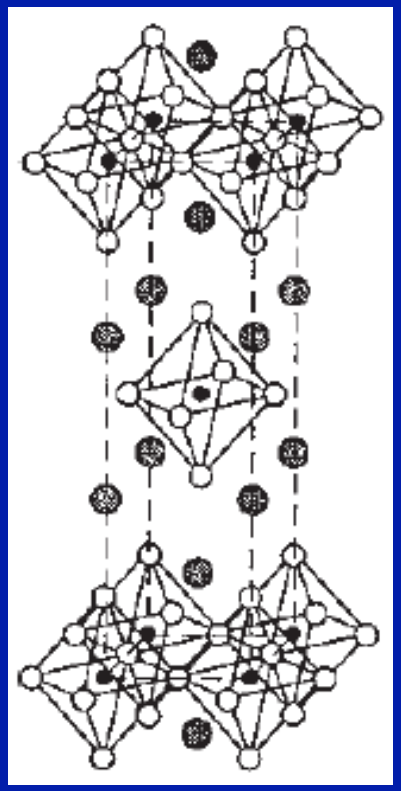
I4/mmm

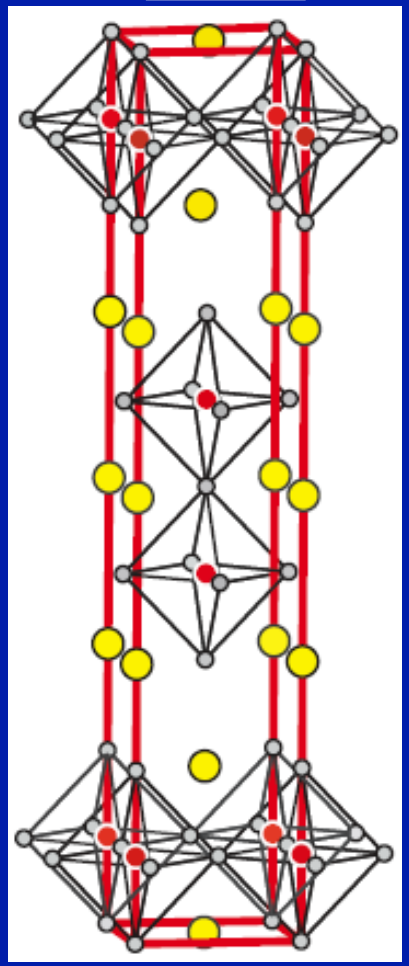
MO_2 layer →

`single-layer ' material

MO_2 layer →







bilayer material

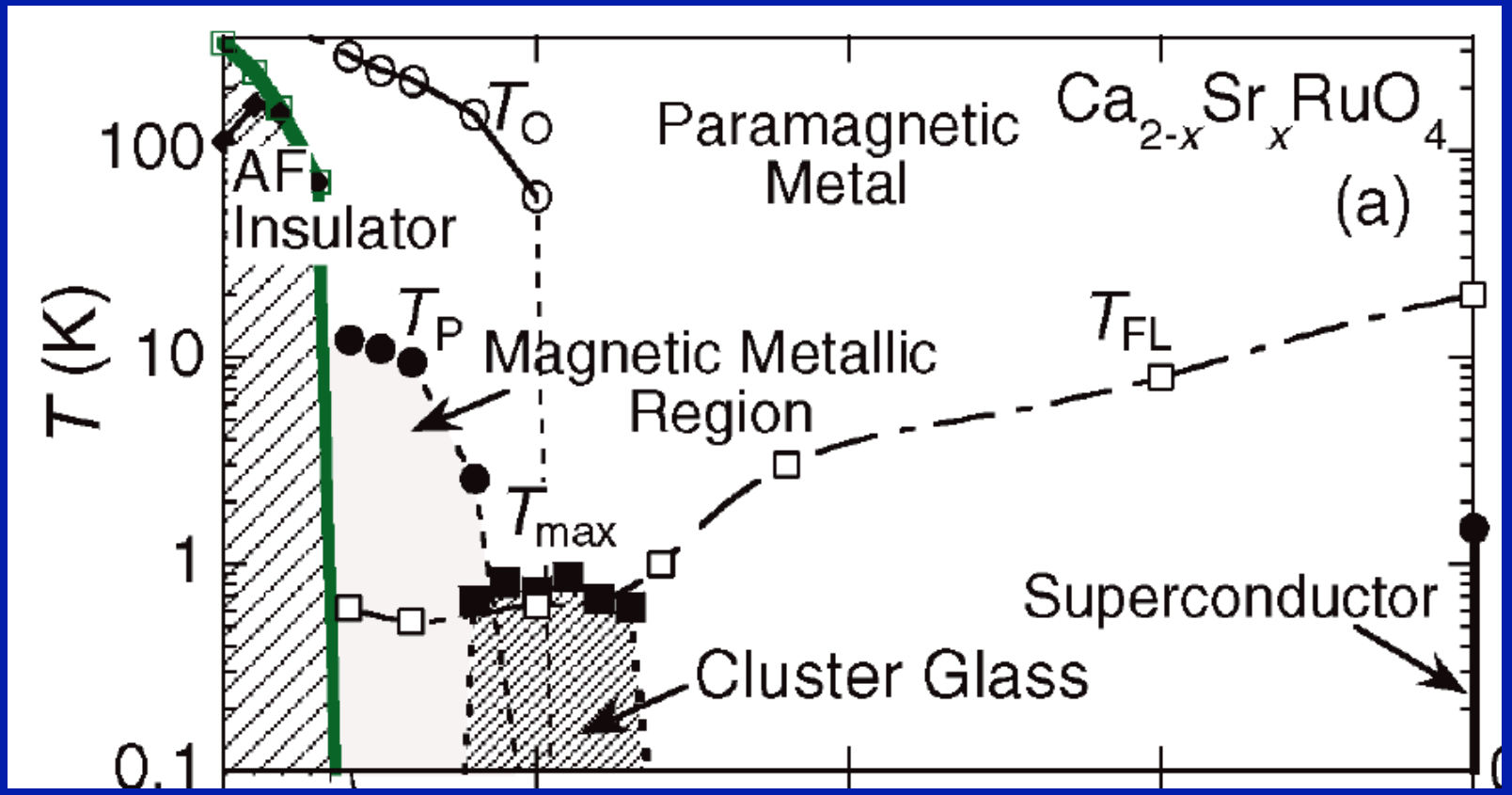
I4/mmm

Sr_2RuO_4

Increasing n : ``from d=2 to d=3"

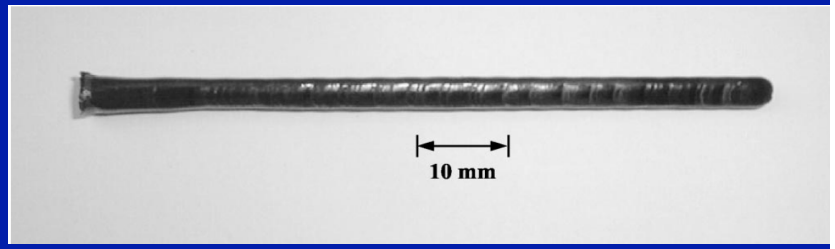
Usual perovskite RMO_3 corresponds to n→infinity

Ca_2RuO_4: The (only) Insulator



Nakatsuji et al. PRL 90, 137202 (2003)

Sr_2RuO_4: the `Helium 3/Drosophila' of transition-metal oxides !

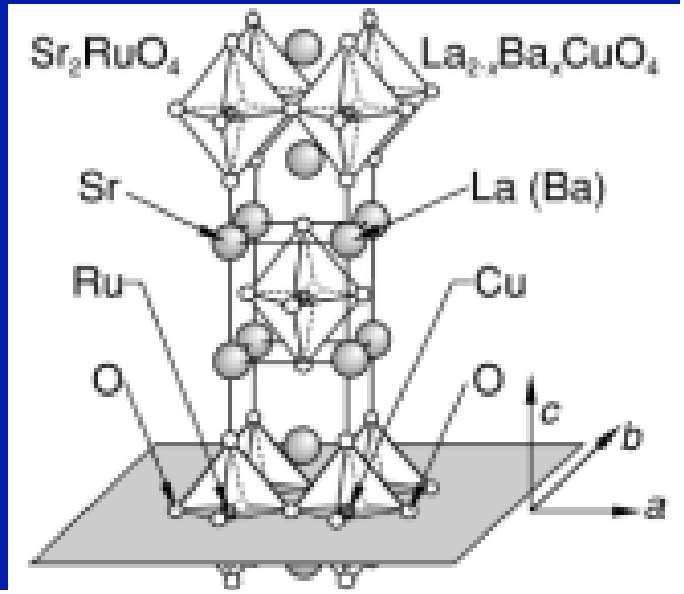


- Huge high-quality crystals !
- Has been investigated with basically all techniques in the experimentalist's toolbox
- 4d-row structural analogue of La_2CuO_4
- Review articles:

- A.Mackenzie and Y.Maeno

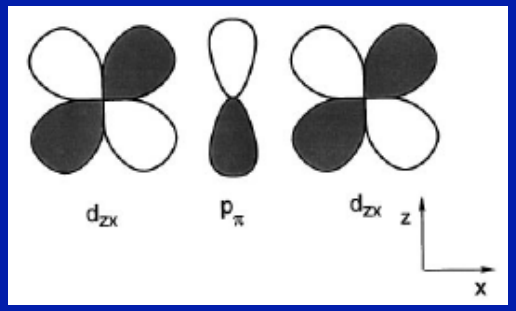
  Rev Mod Phys 75, 657 (2003)
- Bergemann, Adv. Phys. 52, 639 (2003)

  [Focus on dHvA quantum oscillations]

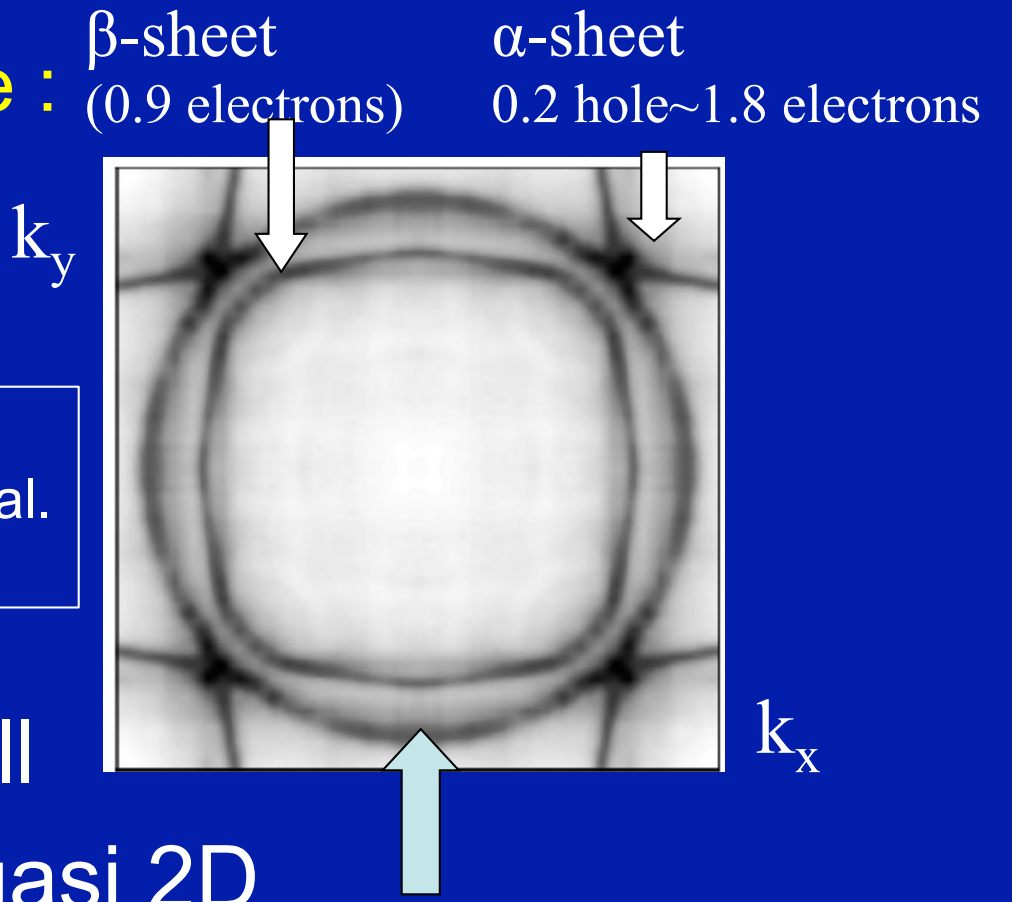


Electronic Structure of Sr_2RuO_4

Basic electronic structure :



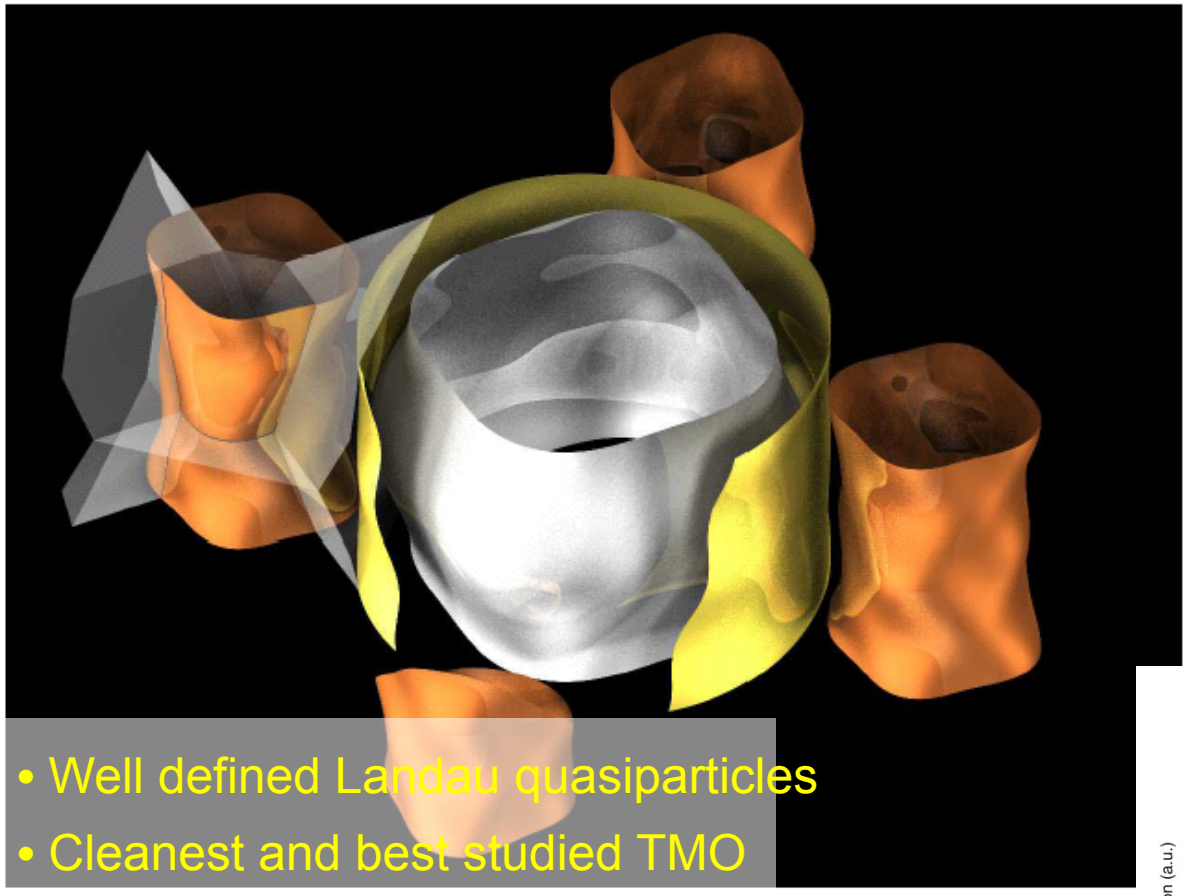
ARPES:
Damascelli et al.
PRL 2000



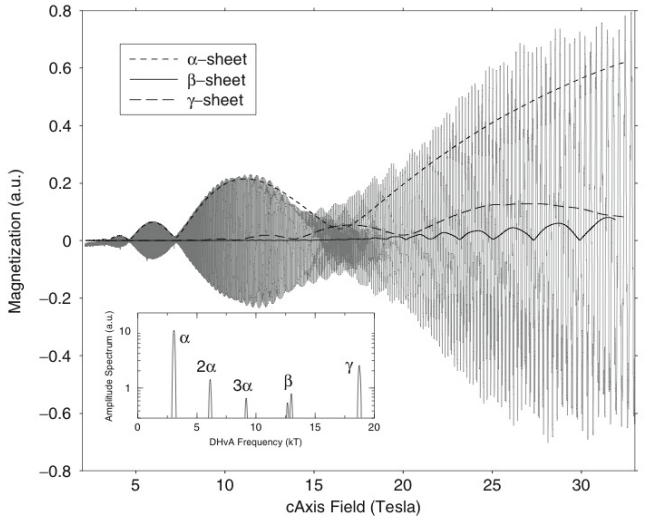
- 4 electrons in t_{2g} shell
- d_{xy} orbital yields a quasi 2D band → γ-sheet of FS

- d_{xz}, (resp. d_{yz}) → bands with directional hopping along x (resp. y) → α,β sheets

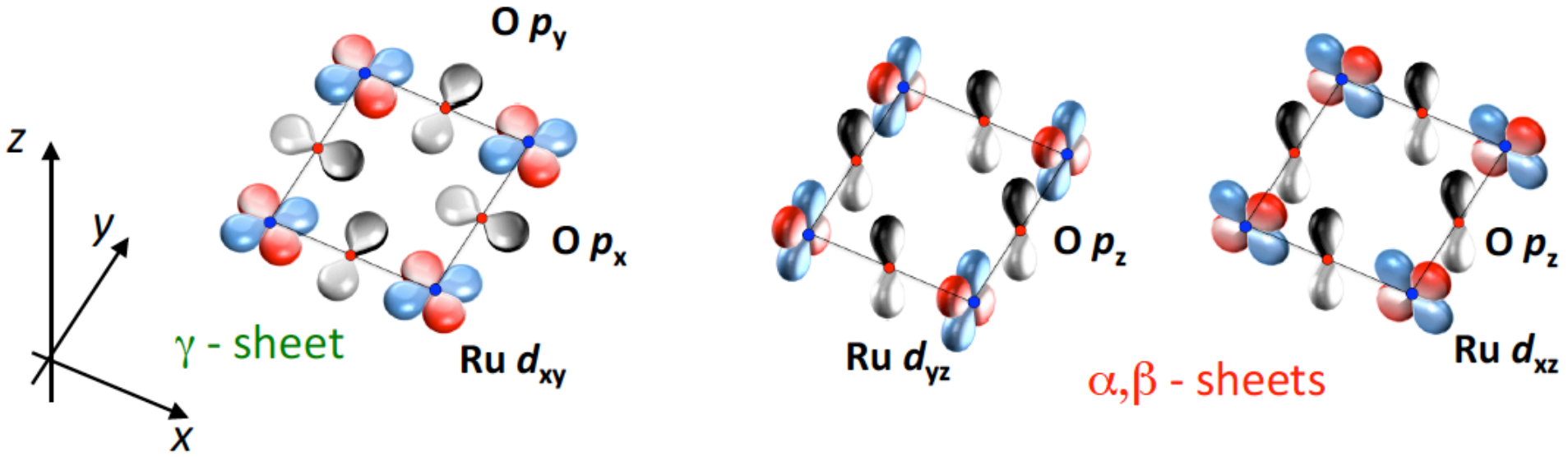
Sr_2RuO_4 - Low-T normal state: a model Fermi liquid

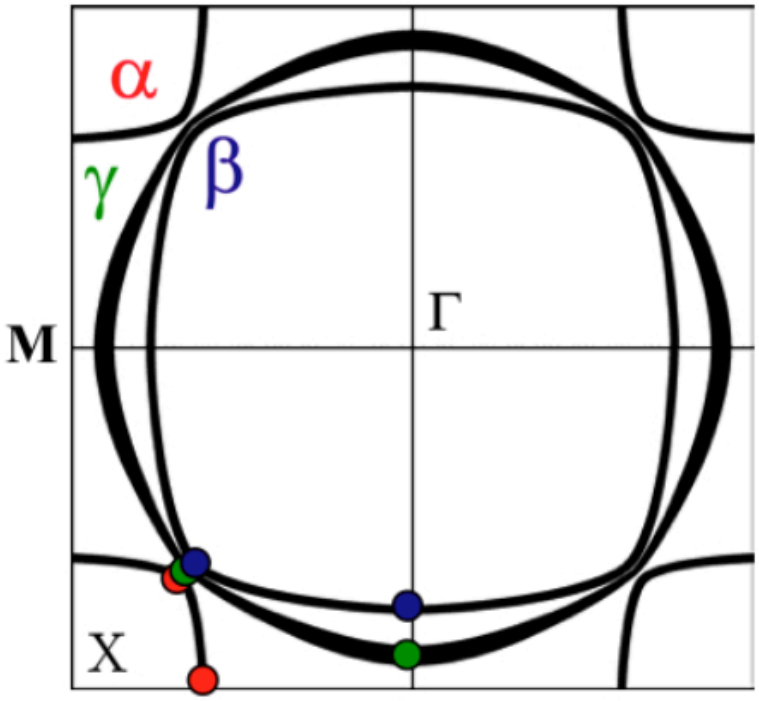


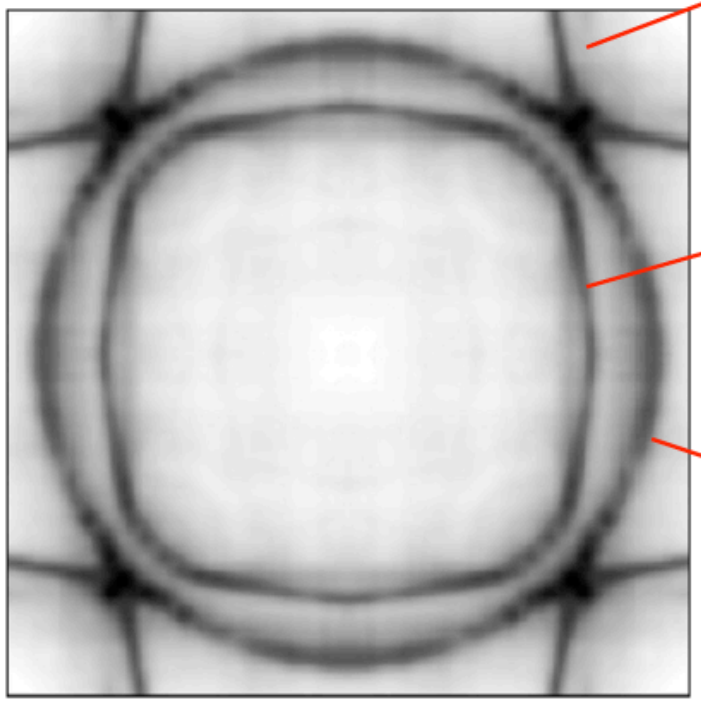
- Well defined Landau quasiparticles
- Cleanest and best studied TMO

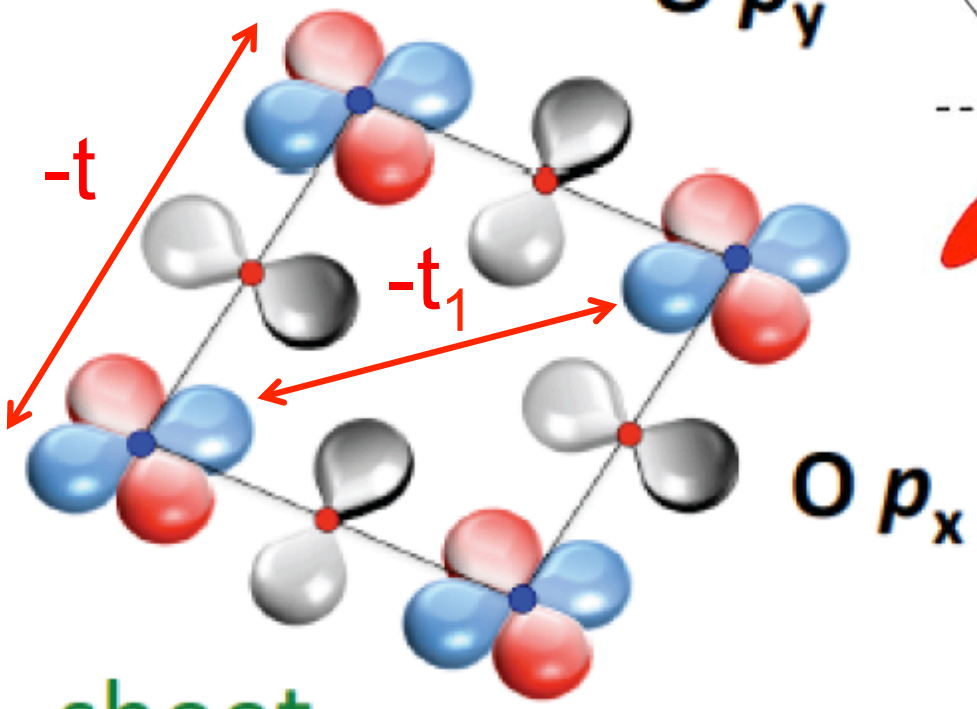


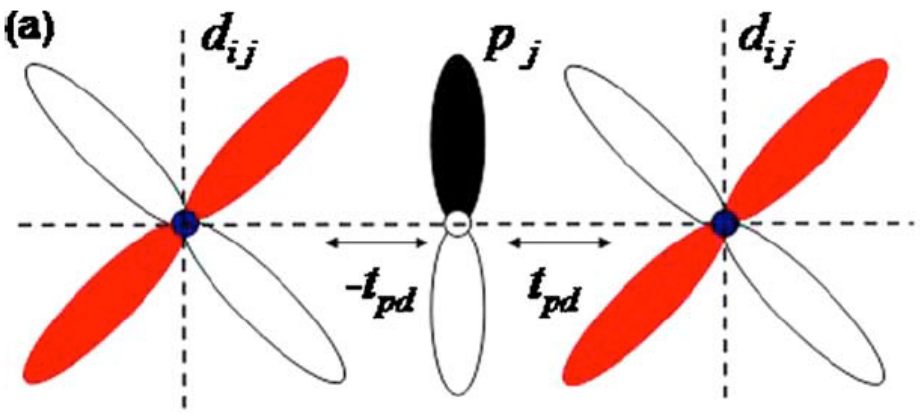
Mackenzie *et al.* PRL **76**, 3786
Bergemann *et al.* PRL **84**, 2662
Bergemann *et al.* Adv. Phys. **52**, 639


z
y
x
O p_y
O p_x
Ru d_{xy}
γ - sheet
O p_z
Ru d_{yz}
O p_z
Ru d_{xz}
α,β - sheets


α
γ
β
M
Γ
X


α (d_{xz})
β (d_{yz})
γ (d_{xy})



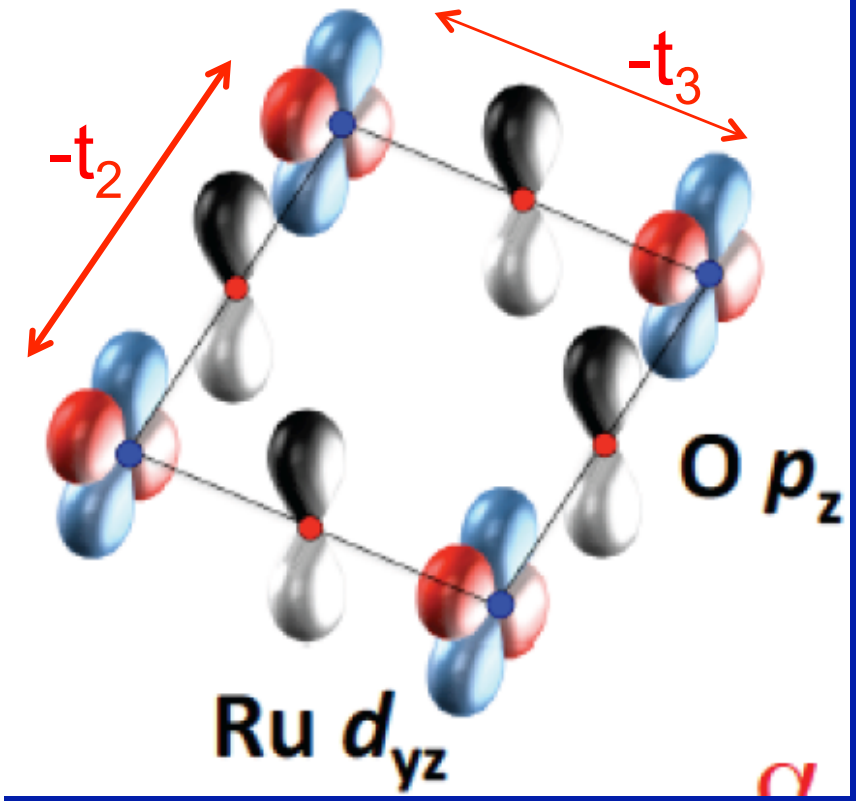


$$-t = t_{pd}\frac{1}{\varepsilon_d - \varepsilon_p}(-t_{pd})$$

$$\Rightarrow t > 0$$

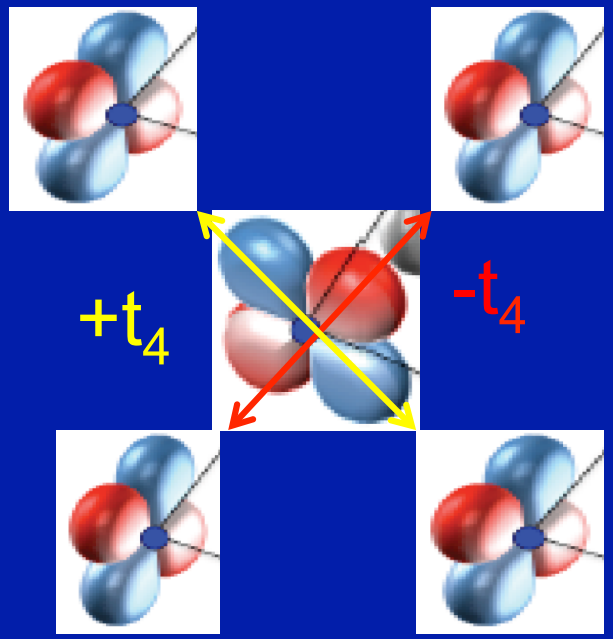
$$\varepsilon^{xy}(k) = \varepsilon_0^{xy} - 2t(\cos k_x + \cos k_y) - 4t_1 \cos k_x \cos k_y$$

$t \simeq 0.42\text{eV}$, $t_1 \simeq 0.17\text{eV}$ fits LDA dispersion



t_2 ~ 0.30 eV >> t_3 ~ 0.03 eV

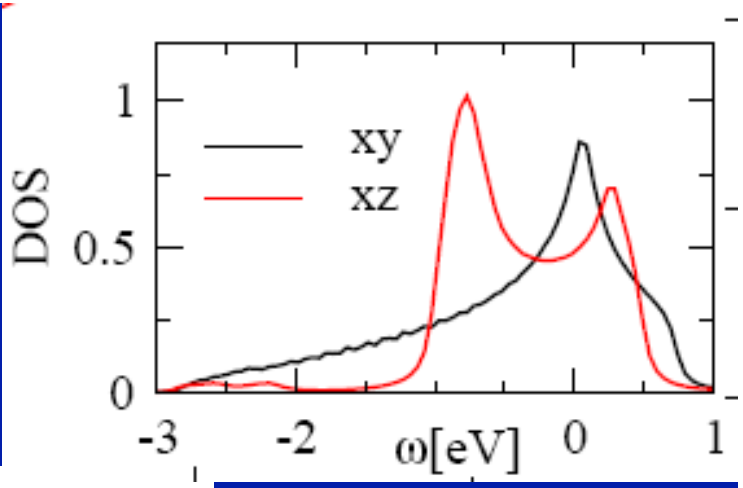
Inter-orbital hopping (very small, along diagonals t_4~0.04 eV):



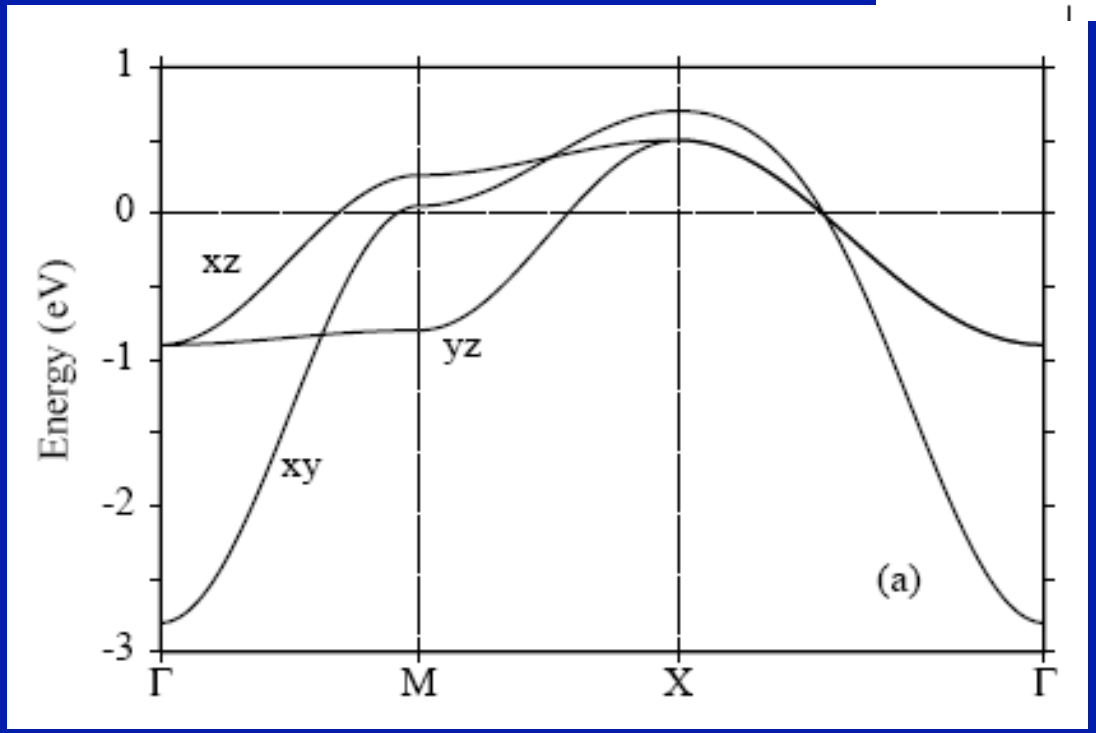
$$-2t_4\left[\cos(k_x-k_y)-\cos(k_x+k_y)\right]=-4t_4\sin k_x\sin k_y$$

$$\begin{pmatrix} -2t_2\cos k_x-2t_3\cos k_y & -4t_4\sin k_x\sin k_y \\ -4t_4\sin k_x\sin k_y & -2t_2\cos k_y-2t_3\cos k_x \end{pmatrix}$$

Bands (LDA, no SO)



~ 1.5 eV
(xz,yz)



~ 3.6 eV
(xy band)

But kinetic energies of all bands comparable

Note: van Hove singularity close to Fermi level for xy-orbital

A PUZZLE :

Why are transition-metal oxides of the 4d series strongly correlated metals, while not being close to a Mott insulating state ?

Sr_2RuO_4 has t_{2g} bandwidth ~ 4eV,
and estimated U for t_{2g} shell about 2.5 eV at most.
Nevertheless effective mass enhancement (over LDA)
of xy-band is ~ 5 (~3 for xz, yz) !!

Outstanding puzzles about this compound…

- A 4d material, bandwidth ~ 3.6 eV
  Not very large U (< 3eV)
- Yet, strongly correlated : effective mass enhancement (vs. band/LDA value) as large as ~ 5
- Strong orbital dependence: largest m*/m for broader band (xy) !

- T^2 law obeyed only below ~ 30K
- → Low Fermi Liquid energy/temperature scale
- Complex crossover in resistivity, from FL at low-T all the way to `bad metal' (above Mott Ioffe Regel) at hi-T

Effective masses

TABLE II. Summary of quasiparticle parameters of Sr_2RuO_4.

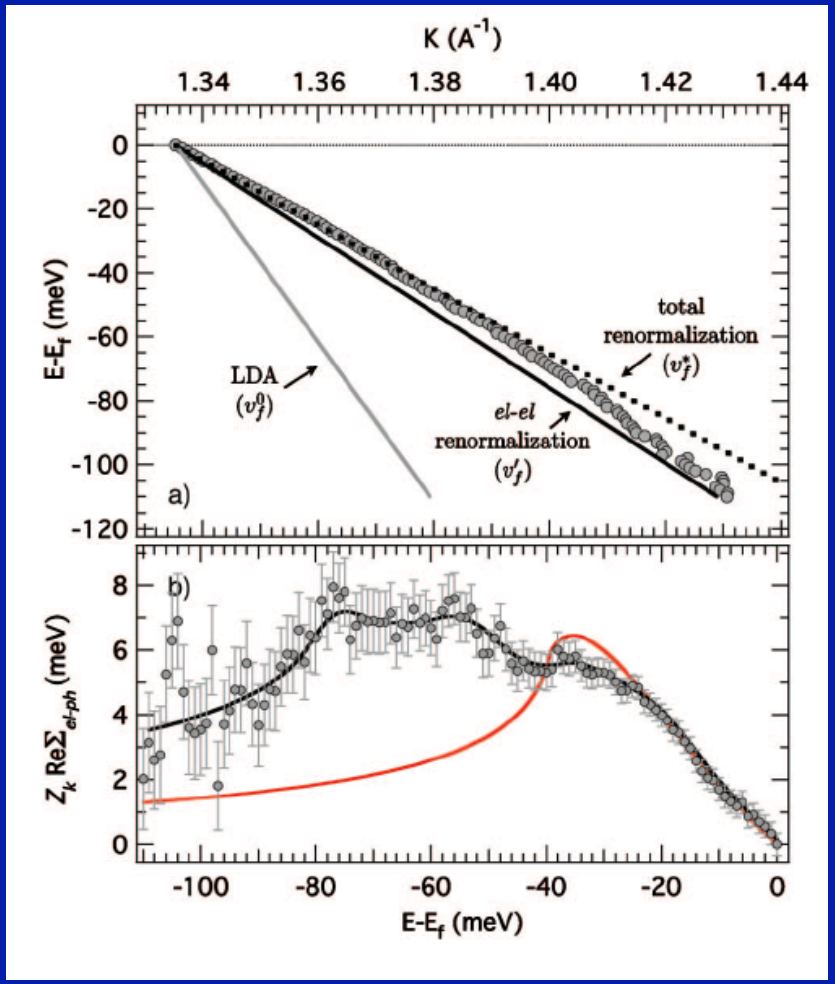
Fermi-surface sheet	α	β	γ
Character	Holelike	Electronlike	Electronlike
k_F (Å^{-1})[a]	0.304	0.622	0.753
m^* (m_e)[b]	3.3	7.0	16.0
m^*/m_{band}[c]	3.0	3.5	5.5
v_F (ms^{-1})[d]	1.0×10^5	1.0×10^5	5.5×10^4
$\langle v_\perp^2 \rangle$ (m^2 s^{-2})[e]	7.4×10^5	3.1×10^6	1.0×10^5
$t_\perp$ (K)[f]	7.3	15.0	2.7

-Rather large !

- Strongly orbital dependent.

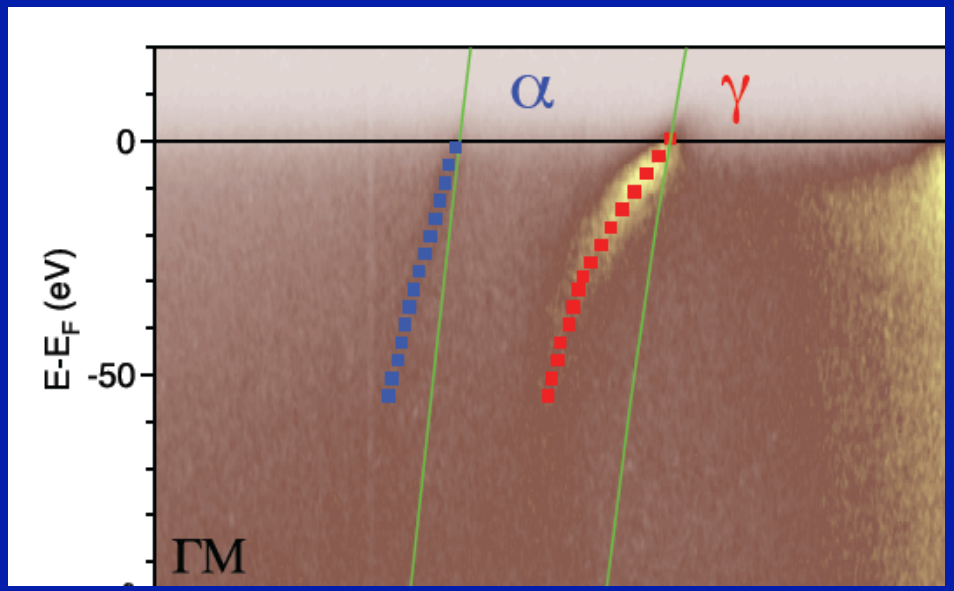
- The widest band has the largest eff. mass enhancement !

Mass renormalisation from ARPES



Ingle et al.
PRB 72, 205114 (2005)

F.Baumberger et al.
From 2012 seminar
@College de France
See website



Crossovers as a function of temperature (or energy-scale):

- At low $T<T_{FL}$ ~ 25K, Sr_2RuO_4 is a Fermi-liquid: quasiparticles with m*/m ~ 3-5, T^2 resistivity, FL optical scattering rate, etc…
- As T is increased, quasiparticles 'undress' BUT SURVIVE until the Ioffe-Regel-Mott criterion is reached (above 600 K) → `resilient quasiparticles'
- In this regime, fluctuating spin degrees of freedom, but orbital degrees don't
- Above T_{MIR}: incoherent bad metal.

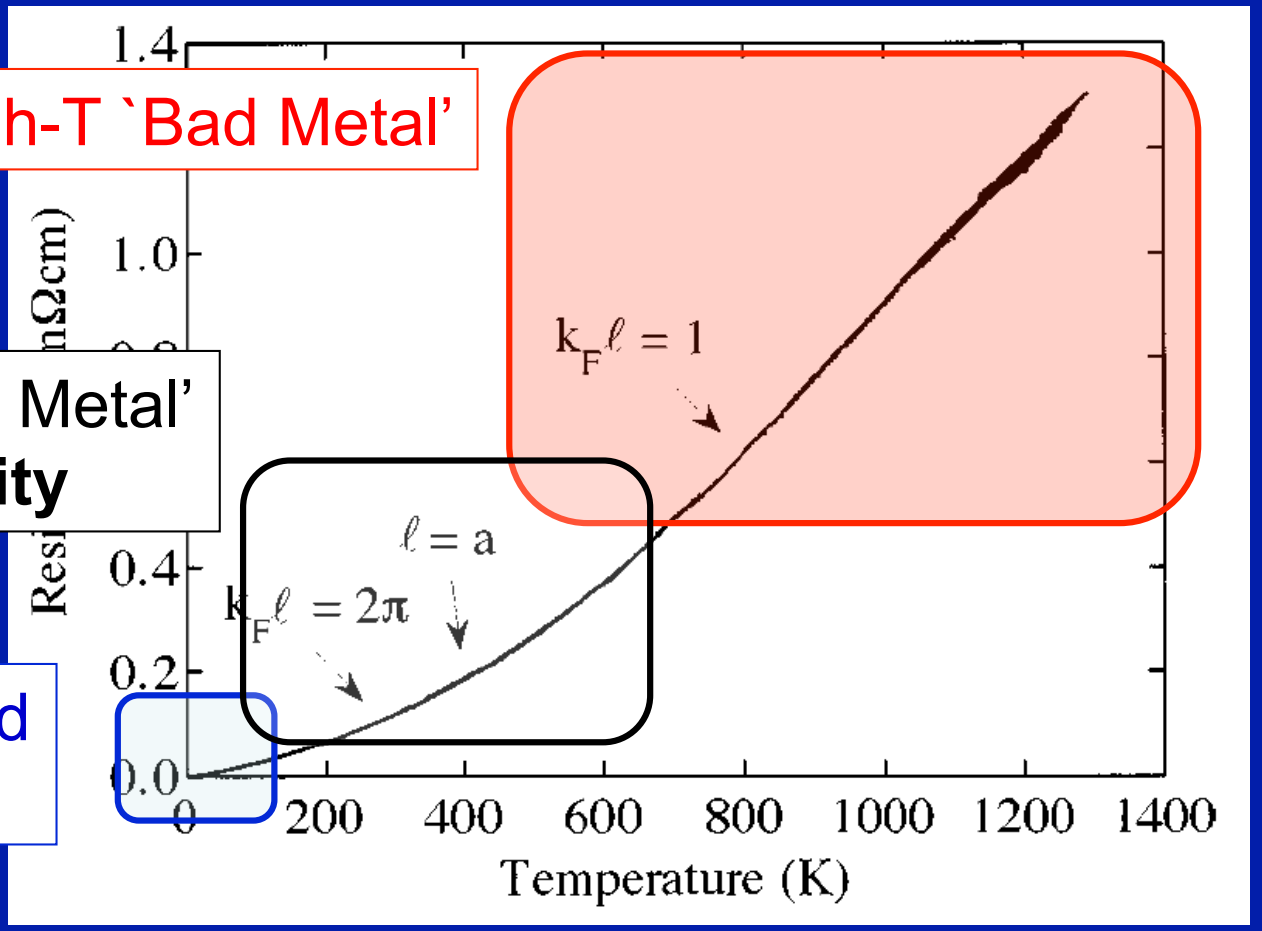
Theoretical studies of crossovers from FL to bad metals, see:
Deng et al. PRL 110, 086401 (2013); Xu et al PRL 111, 036401 (2013)

The three regimes of transport:

High-T `Bad Metal'

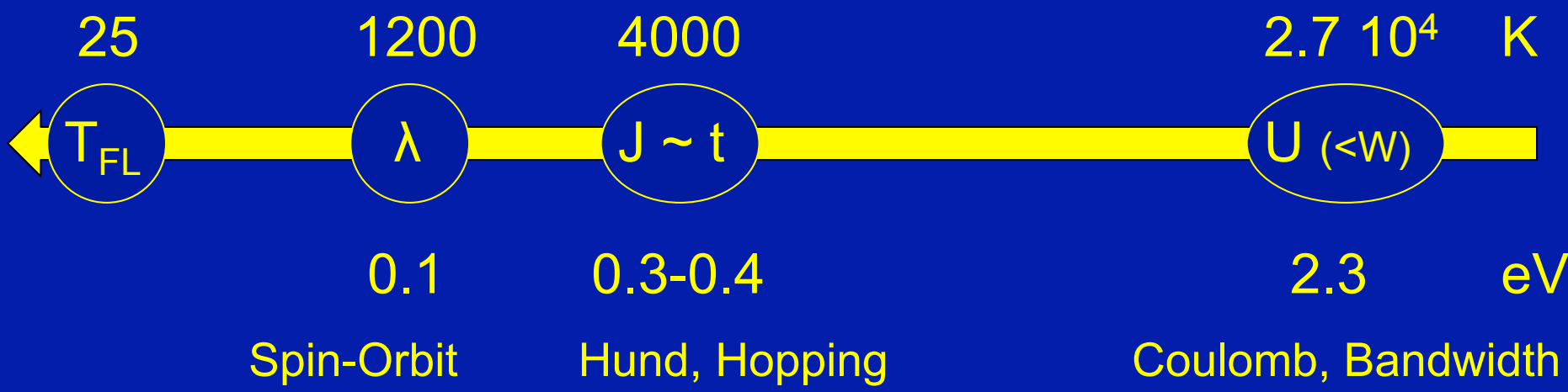
Intermediate-T `OK Metal'
but not T^2 resistivity

Low-T Fermi Liquid
Good metal



Crossovers are crucial in strongly correlated materials !

Hierarchy of energy scales and coupling constants



Fundamental question and program:

High energy: atomic multiplets

of a t_{2g} shell with d^4 configuration

→ Fluctuating spin and orbital degrees of freedom

Low energy: Formation of quasiparticles, Fermi Liquid

How does this process occur

as we flow down in energy scale ? → DMFT

Take-Home Message - 1

- Treat first largest energy scales: U,J,t
- Because U (<,~ W) not so large, Hund's coupling is playing a key role
- Ruthenates can be characterized as `Hund's metals': they are strongly correlated metals mostly because of the action of J
- Note: the van-Hove singularity also plays an important role for the xy-orbital

PRL 106, 096401 (2011) PHYSICAL REVIEW LETTERS week ending 4 MARCH 2011

Coherence-Incoherence Crossover and the Mass-Renormalization Puzzles in Sr_2RuO_4

Jernej Mravlje,[1,2] Markus Aichhorn,[3,1] Takashi Miyake,[4,5] Kristjan Haule,[6] Gabriel Kotliar,[6] and Antoine Georges[1,7,5]

General Relevance

A large class of materials

including: transition-metal oxides of the 4d series (this talk)

and also iron pnictides/chalcogenides

→ cf. Rutgers group (Kotliar, Haule et al) + R.Valenti's talk here

→ are best characterized as

`Hund's metals'

They are not close to a Mott transition

but still display strong correlations

because of the Hund's rule coupling

Some articles of the `Hund's metals' saga…

- Haule and Kotliar New J. Phys. 11, 025021 (2009) [Fe-superconductors]
- Werner, Gull Troyer and Millis, PRL 101, 166405 (2008)
- Mravlje et al. PRL 106, 096401 (2011) [Sr2RuO4]
- Mravlje et al. PRL 108, 197202 (2012) [SrTcO3]
- de'Medici et al. PRL 107, 256401 (2011)
- … And many more

Recent review article:
AG, de'Medici and Mravlje
Annual Reviews Cond. Mat. Phys Vol 4 (2013)
arXiv:1207.3033

Two key players & collaborators:

Luca de' Medici
(ESPCI-LPEM)

Jernej Mravlje
Joszef Stefan Institute
Ljubljana, Slovenia
Formerly at Collège de France,
& École Polytechnique

→ *Review article*
(Annual Reviews, Vol.4, 2013)
arXiv:1207.3033

The Hund's coupling is the suspect !
(together with van-Hove physics for xy-band)
Effective masses enhancements from DMFT:

J [eV]	$m^*_{xy}/m_{\rm LDA}$	$m^*_{xz}/m_{\rm LDA}$	T^*_{xy}[K]	T^*_{xz}[K]	$T_>$[K]
0.0, 0.1	1.7	1.7	> 1000	> 1000	> 1000
0.2	2.3	2.0	300	800	> 1000
0.3	3.2	2.4	100	300	500
0.4	4.5	3.3	60	150	350

Table I. Mass enhancement of the xy and xz orbitals, as a function of Hund's coupling, for $U = 2.3$ eV. Other columns: coherence temperatures as defined in the text.

U=2.3 eV

- Increase of effective mass as J is increased
- Orbital differentiation: xy heavier (due to van Hove singularity)
- Comparable mass enhancement would require U=5eV at J=0 !

Interactions: Kanamori hamiltonian:

[J.Kanamori, Prog. Theor. Phys. 30 (1963) 275]

$$H_{\mathrm{K}} = U \sum_{m} \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U' \sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J) \sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} +$$
$$-J \sum_{m\neq m'} d^{+}_{m\uparrow} d_{m\downarrow}\, d^{+}_{m'\downarrow} d_{m'\uparrow} + J \sum_{m\neq m'} d^{+}_{m\uparrow} d^{+}_{m\downarrow}\, d_{m'\downarrow} d_{m'\uparrow}$$

EXACT for a t_{2g} shell

Useful reference: Sugano, Tanabe & Kamimura,
Multiplets of transition-metal ions in crystals
Academic Press, 1970

Assuming furthermore ~ spherical symmetry of the screened interaction V_c , one can show that: U' = U-2J

In this case, the hamiltonian can be written:

$$H_{t_{2g}} = (U - 3J)\,\frac{\hat{N}(\hat{N}-1)}{2} - 2J\,\vec{S}^2 - \frac{J}{2}\vec{L}^2 + \frac{5}{2}J\,\hat{N}$$

$$\hat{N} = \sum_{m\sigma} \hat{n}_{m\sigma} \;,\; \vec{S} = \frac{1}{2}\sum_{m}\sum_{\sigma\sigma'} d^{\dagger}_{m\sigma}\vec{\tau}_{\sigma\sigma'}d_{m\sigma'} \;,\; L_m = i\sum_{m'm''}\sum_{\sigma}\epsilon_{mm'm''}d^{\dagger}_{m'\sigma}d_{m''\sigma},$$

Total charge, spin and orbital iso-spin operators

$U(1)_c \otimes SU(2)_s \otimes SO(3)_o$ symmetry

Spectrum of atomic t_{2g} hamiltonian with U'=U-2J

N	S	L	Degeneracy $= (2S+1)(2L+1)$	Energy
0,[6]	0	0	$\boxed{1}$	0
1,[5]	1/2	1	$\boxed{6}$	$-5J/2,[10\mathcal{U}-5J/2]$
2,[4]	1	1	$\boxed{9}$	$\mathcal{U}-5J,[6\mathcal{U}-5J]$
2,[4]	0	2	5	$\mathcal{U}-3J,[6\mathcal{U}-3J]$
2,[4]	0	0	1	$\mathcal{U},[6\mathcal{U}]$
3	3/2	0	$\boxed{4}$	$3\mathcal{U}-15J/2$
3	1/2	2	10	$3\mathcal{U}-9J/2$
3	1/2	1	6	$3\mathcal{U}-5J/2$

Table 1: Eigenstates and eigenvalues of the t_{2g} Hamiltonian $\mathcal{U}\hat{N}(\hat{N}-1)/2 - 2J\vec{S}^2 - J\vec{T}^2/2$ in the atomic limit ($\mathcal{U} \equiv U - 3J$). The boxed numbers identifies the ground-state multiplet and its degeneracy, for $J > 0$.

- Hund's rule ground-state in each particle-number sector
- Symmetry broken by J from SU(6) to U(1)c×SU(2)s×SO(3)o
- → Degeneracies lifted by J

In Lecture 3, we have seen one face of the Hund's coupling:

- Drives materials with a ½ filled (sub)shell closer to the Mott insulating state
- Drives all other cases further away from the Mott insulating state

But this is NOT the whole story …

cf. van der Marel&Sawatzky PRB 37 (1988) 10674 ;
L. de' Medici PRB 83 (2011) 205112

So, what is U_{eff} ? N electrons in M orbitals (0≤N≤2M)

1) If M<N (or M>N) non half-filled shell: only the interaction between parallel spins matters U'-J=U-3J

$$U_{\text{eff}} = (U' - J)\left[\frac{(N+1)N}{2} + \frac{(N-1)(N-2)}{2} - 2\frac{N(N-1)}{2}\right] = U - 3J$$

U_{eff} = U' = U-3J

The Hund's coupling reduces U_{eff}

2) If N=M (half-filled shell)

$|\uparrow\downarrow,\uparrow,\uparrow\rangle$

$$E_0(N+1) = (U' - J)\frac{N(N-1)}{2} + U + U'(N-1)$$

$$U_{\text{eff}} = (U' - J)\left[\frac{N(N-1)}{2} + \frac{(N-1)(N-2)}{2} - 2\frac{N(N-1)}{2}\right] + U + U'(N-1)$$

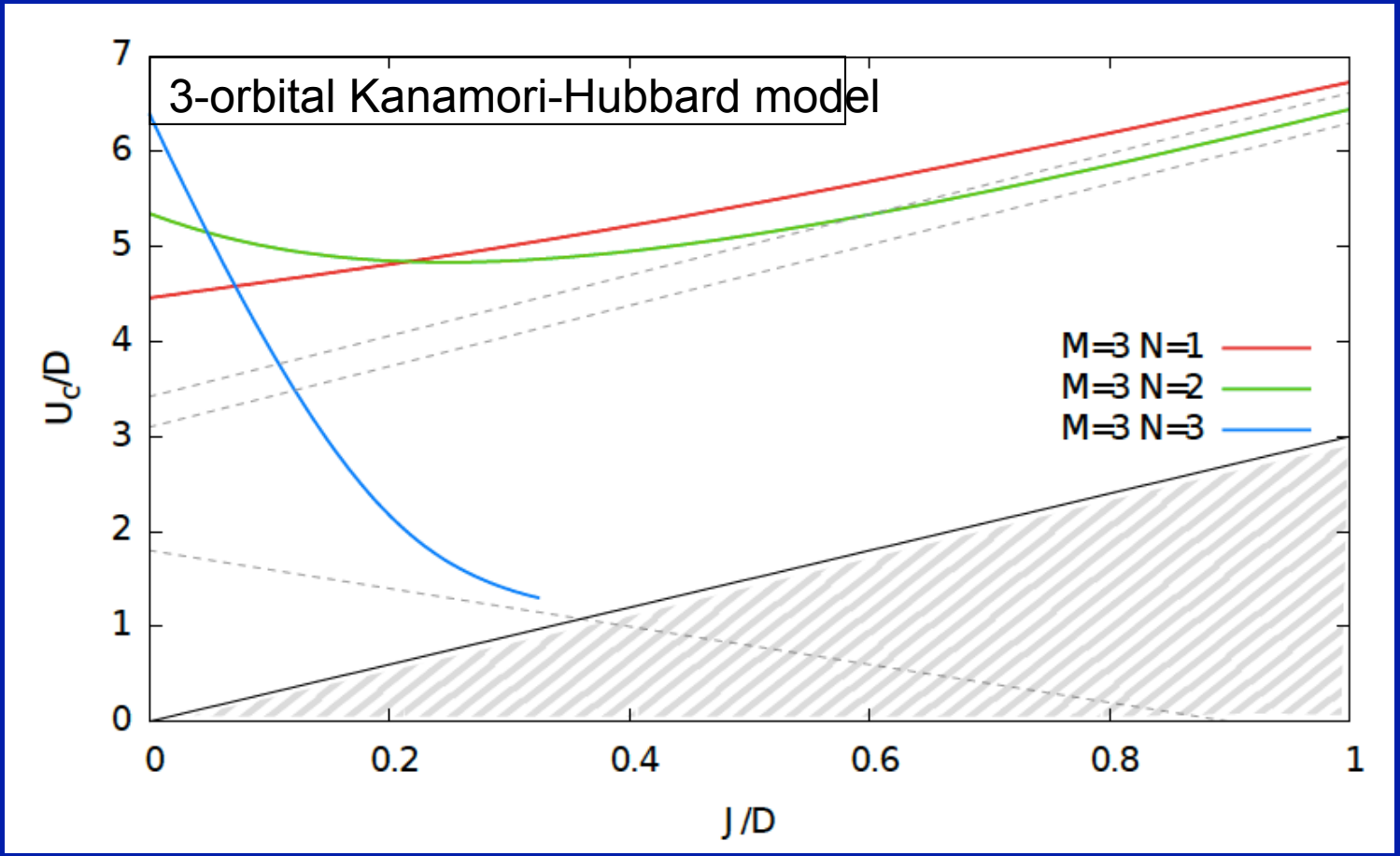
$$= U + (N-1)J$$

U_{eff} = U+(N-1)J

The Hund's coupling increases U_{eff}

→ Half-filled (sub)shells are usually robust Mott insulators

Condition for Mott state: key difference between ½-filled (sub)shell and other cases 3-orbitals with ½-bandwidth D - DMFT

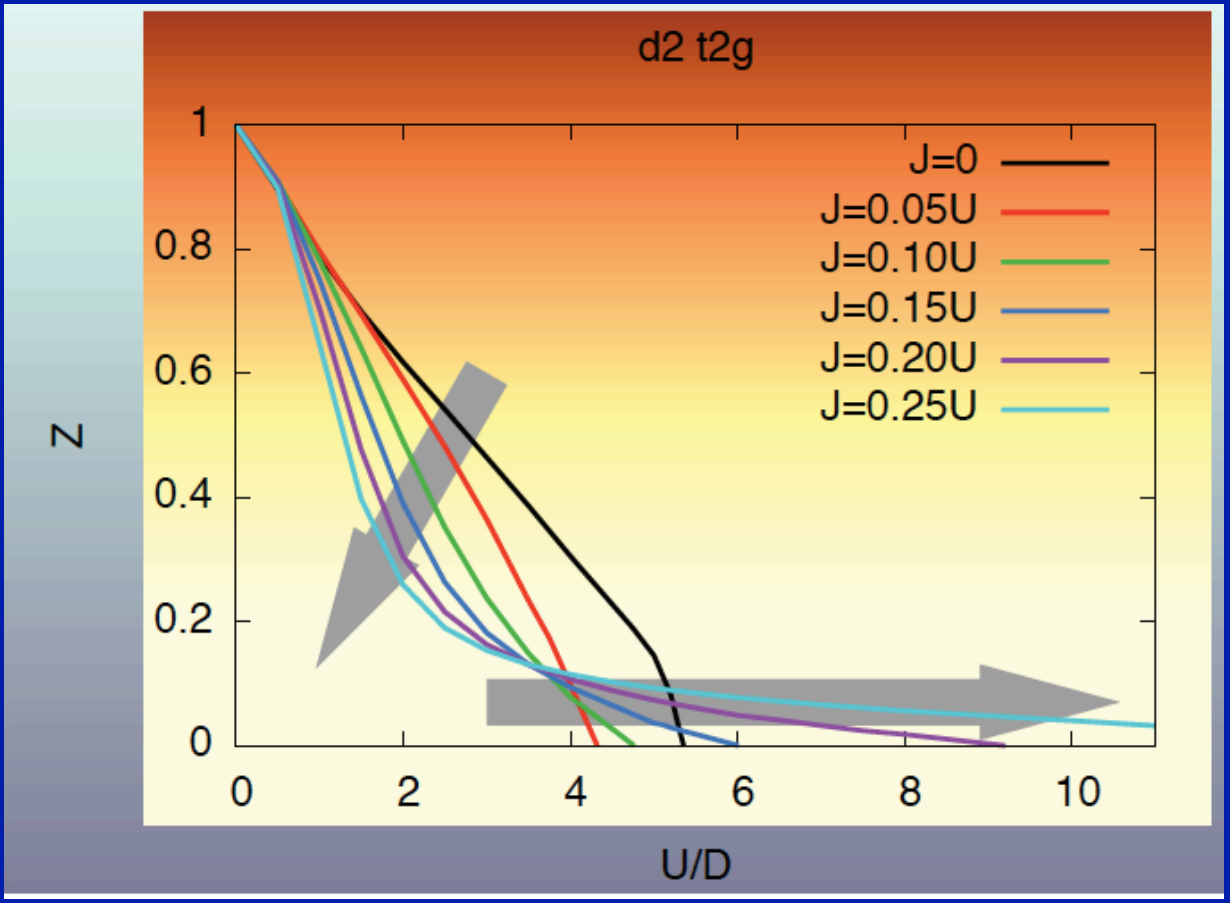


Cf. L. de' Medici, PRB 83, 205112 (2011)

cf. early work on V_5S_8
Fujimori et al. PRB (1991)

For all filling except ½-filling and a single electron and hole:
Hund's coupling suppresses coherence scale →
Reduces quasiparticle coherence scale, smaller Z, larger m*/m

Explanation requires Kondo-logy: see Adv. Cont. Mat Phys review



But also increases U_c → Enhances range of metallic state

For ‘generic’ filling (i.e. not ½ filled and not just a single electron or hole) …

… J is « Janus-faced » : it has two ANTAGONISTIC effects

Janus is the latin god of beginnings/ transitions. He is often associated with doors and entrances and has two faces.

First promoted to being a physicist by P.G. de Gennes

PRL 107, 256401 (2011) PHYSICAL REVIEW LETTERS week ending 16 DECEMBER 2011

Janus-Faced Influence of Hund’s Rule Coupling in Strongly Correlated Materials

Luca de’ Medici,[1] Jernej Mravlje,[2,3,4] and Antoine Georges[2,4,5,6]

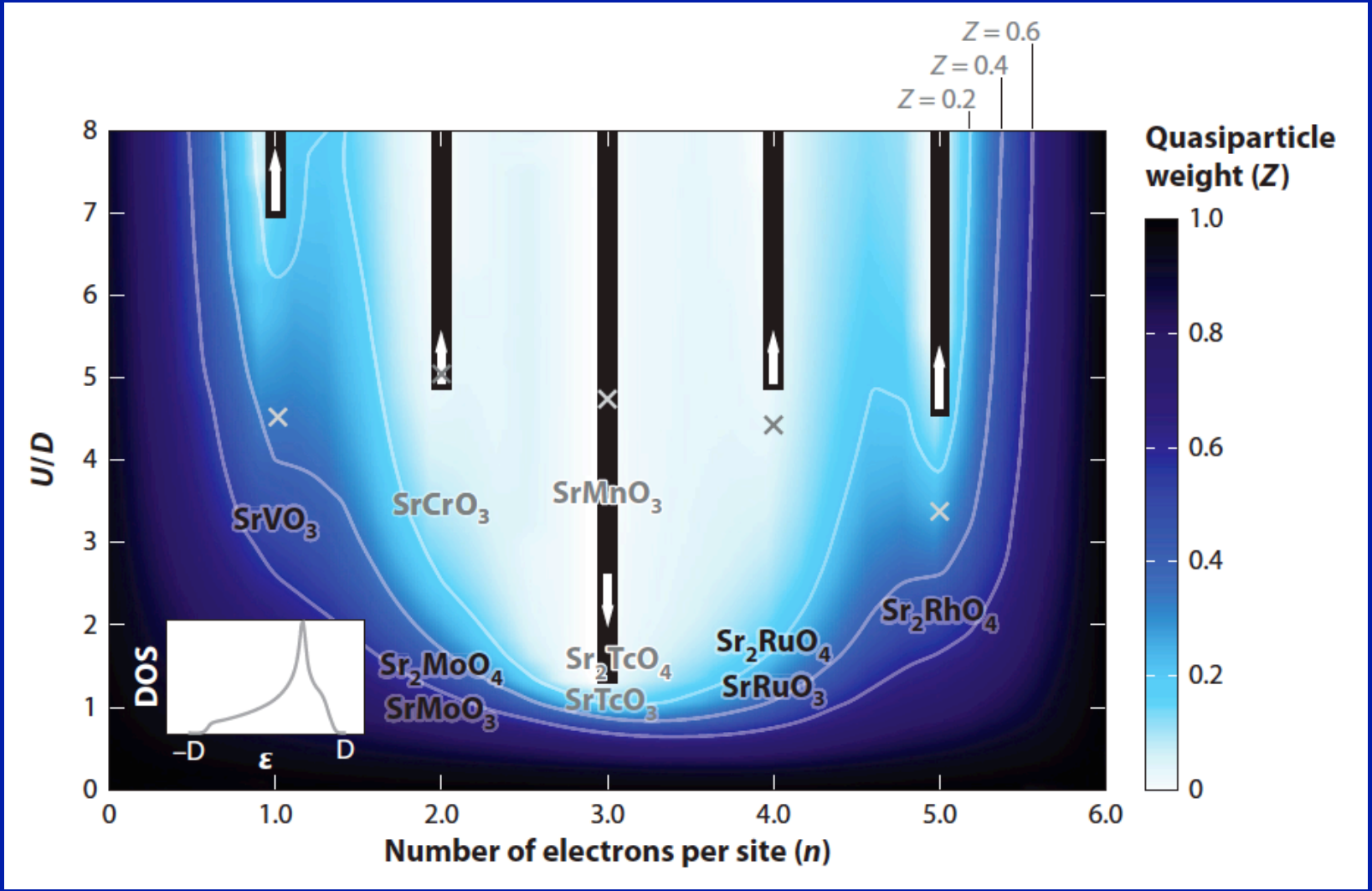
Putting together the two effects, the Hund's coupling:

- Drives the system
away from the Mott state
- But at the same time lowers the
quasiparticle coherence scale
(below which the local atomic multiplet is quenched)
i.e makes the metal more correlated

This applies to all cases, except occupancies N=1,2M-1,M

Drawing a map of early transition-metal oxides (both 3d and 4d) with Hund's rule coupling as guidance

Correlation effects in 4d oxides due to J, not to Mott physics (except when strong splitting between orbitals)



3d oxides: U/D ~ 4
4d oxides: U/D ~ 2

Hund's metals: distinct crossover scales for orbital and spin degrees of freedom

~ 1000K

Fermi Liquid

Metal with fluctuating spins
No orbital fluctuations

PRL 117, 036401 (2016) PHYSICAL REVIEW LETTERS week ending 15 JULY 2016

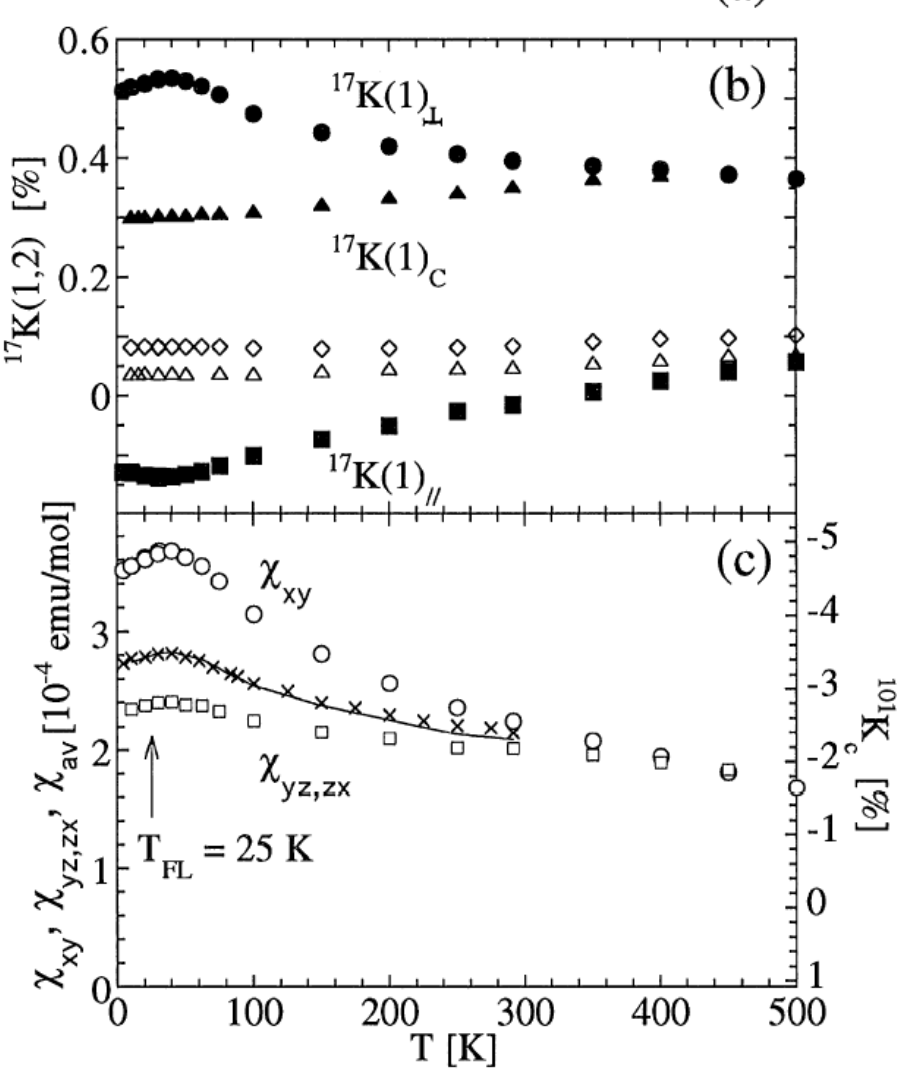
Thermopower and Entropy: Lessons from Sr_2RuO_4

Jernej Mravlje[1] and Antoine Georges[2,3,4]

Nature of intermediate-T regime: experimental evidence

- Curie-Weiss susceptibility (not Pauli)
- Seebeck coefficient
- → entropy of fluctuating degrees of freedom.

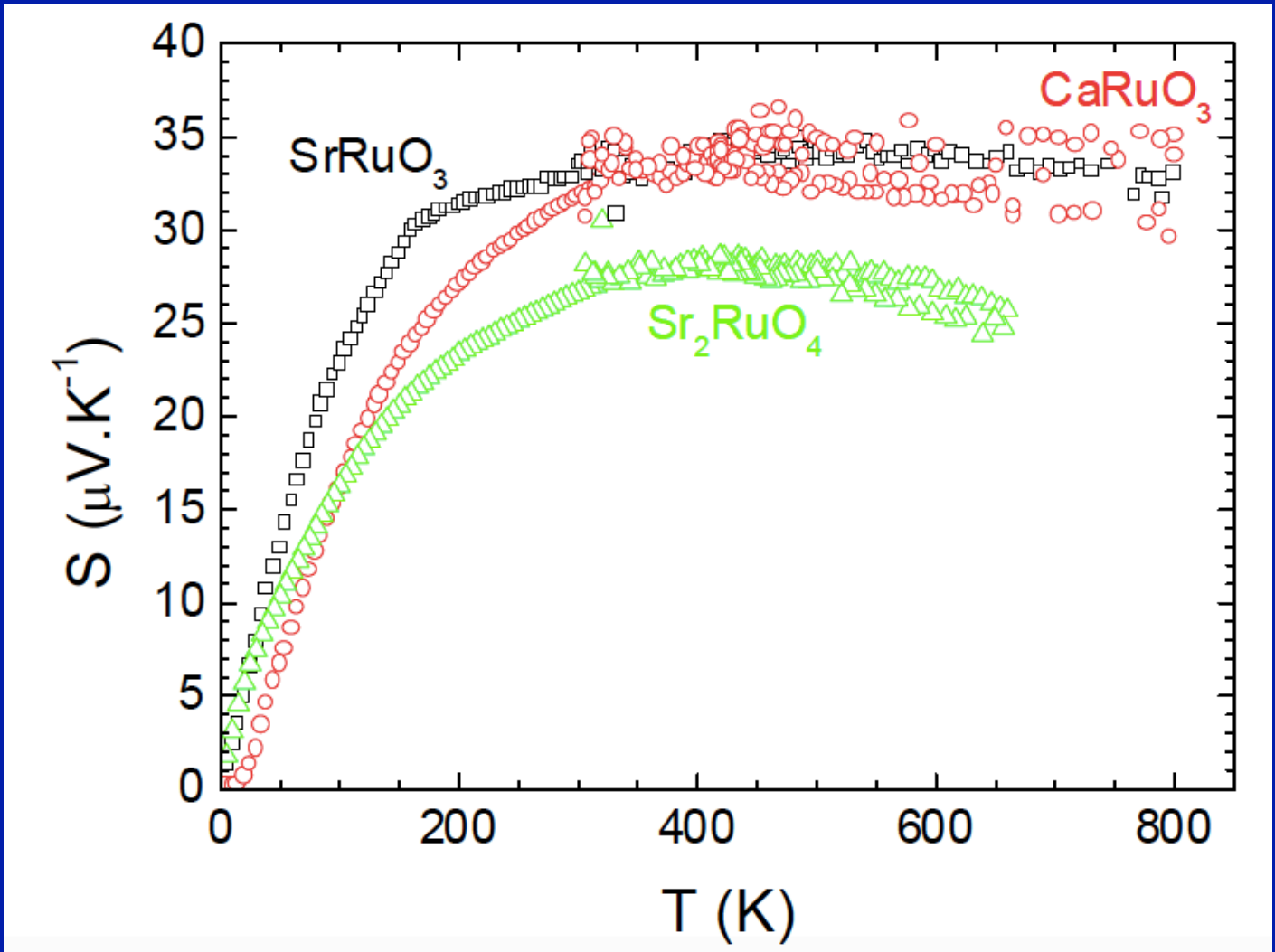
FIG. 1. (a) Top view (left panel) and side view (right panel) of the local geometry of the RuO_2 plane (Ru $4d$ and O $2p\pi$ orbitals). (b) ^{17}O NMR shift $^{17}K(1,2)$ at the planar O(1) and apical O(2) sites. $^{17}K(1)_c$ [▲], $^{17}K(1)_{\parallel}$ [■], $^{17}K(1)_{\perp}$ [●], $^{17}K(2)_c$ [△], and $^{17}K(2)_{ab}$ [◇]. (c) The uniform spin susceptibility χ_{xy} of $4d_{xy}$ orbital [○] and $\chi_{yz,zx}$ of $4d_{yz,zx}$ orbital [□], deduced from $^{17}K(1)$ based on Eqs. (1a)–(1c) with $C = D = 34$ kOe/μ_B. Also plotted are the average $\chi_{av} \equiv (\chi_{xy} + 2\chi_{yz,zx})/3$ [solid line], and ^{101}Ru Knight shift $^{101}K_c$ [×]. Notice that we invert the scale of $^{101}K_c$ to account for the negative hyperfine coupling, and offset the origin by 1.08% [9] to account for $^{101}K_{orb}$.



Imai et al PRL 81 3006 (1998)

Ruthenates: Seebeck

Yoshino et al. JPSJ 1996, Fu et al. PRL 2008, Keawprak Mat Trans 2008, Klein et al. PRB 2006; Present graph from Klein PhD thesis, Caen, 2006



Conspicuous plateau at ~ 25-35μV/K around room temperature

	Ru^{3+}	Ru^{4+}	Ru^{5+}
Configuration électronique			
Dégénérescence de spin ($\Gamma^{\sigma}=2S+1$) SPIN	2	3	4
Dégénérescence orbitalaire (Γ) ORBITAL	3	3	1
Dégénérescence totale ($\beta = \Gamma.\Gamma^{\sigma}$) TOTAL	6	9	4

Spin and Orbital degeneracies for Ru t2g shell (Klein, PhD)

Spin + orbital leads to, for a Ru^{4+} shell

$$\alpha_H = \frac{k_B}{2e} \ln \frac{4}{6} \simeq -17.66\,\mu V/K < 0\,!$$

SPIN-ONLY (as suggested by Klein, Hebert Maignan et al) leads to, according to this revisited Heikes analysis:

$$\alpha_H = \frac{k_B}{2e} \ln \frac{4}{2} \simeq 30\,\mu V/K$$

- For an atomic shell with INTEGER occupancy N (such as Ru^{4+} with N= 4electrons in Ru-3d shell)

$$N = \langle n \rangle = \frac{d_{N-1}(N-1)e^{-\beta(E_{N-1}-\mu(N-1))} + d_N N e^{-\beta(E_N-\mu N)} + (N+1)d_{N+1}e^{-\beta(E_{N+1}-\mu(N+1))}}{d_{N-1}e^{-\beta(E_{N-1}-\mu(N-1))} + d_N e^{-\beta(E_N-\mu N)} + d_{N+1}e^{-\beta(E_{N+1}-\mu(N+1))}}.$$

The configurational entropy term is then ABSENT and one simply gets (note also factor of 1/2 in front):

$$\alpha_H = \frac{k_B}{2e} \log \frac{d_{N-1}}{d_{N+1}}.$$

Can this expression explain the ~ universal value observed in ruthenates ?

But what about spin-orbit coupling ?

- Experimental evidence that SO coupling is important for Fermiology: several papers. e.g. Veenstra et al. PRL 112, 127002 (2014) spin-resolved ARPES
- Theoretical studies e.g. Zhang et al. PRL 116, 106402 (2016)
- Paper in preparation:

  Kim, Mravlje and AG

SO hamiltonian for a t_{2g} shell

Angular momentum in cubic harmonic basis set:

- **Orbital matrices (l=1)** $\{|z\rangle, |x\rangle, |y\rangle\}$

$$L_x^p = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \qquad L_y^p = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad L_z^p = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

- **Orbital matrices (l=2)** $\{|xy\rangle, |yz\rangle, |zx\rangle, |3z^2 - r^2\rangle, |x^2 - y^2\rangle\}$

$$L_x^d = \begin{pmatrix} 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{3}i & -i \\ i & 0 & 0 & 0 & 0 \\ 0 & \sqrt{3}i & 0 & 0 & 0 \\ 0 & i & 0 & 0 & 0 \end{pmatrix} \qquad L_y^d = \begin{pmatrix} 0 & i & 0 & 0 & 0 \\ -i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3}i & -i \\ 0 & 0 & -\sqrt{3}i & 0 & 0 \\ 0 & 0 & i & 0 & 0 \end{pmatrix} \qquad L_z^d = \begin{pmatrix} 0 & 0 & 0 & 0 & 2i \\ 0 & 0 & i & 0 & 0 \\ 0 & -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -2i & 0 & 0 & 0 & 0 \end{pmatrix}$$

When restricted to t_{2g}, acts like MINUS the L=1 generators of SO(3)

$$\lambda \vec{\ell}_d \cdot \vec{s} \to -\lambda \vec{\ell}_p \cdot \vec{s}$$

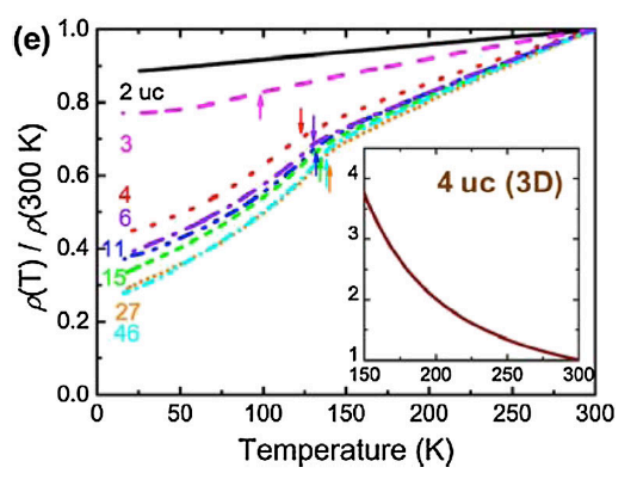
$$\to \sum_{mm'\sigma\sigma'} d^{\dagger}_{m\sigma} \frac{1}{2} \vec{\sigma}_{\sigma\sigma'} \cdot \vec{L}^{p}_{mm'} d_{m'\sigma'}$$

$$[xy\uparrow, yz\uparrow, xz\uparrow; xy\downarrow, yz\downarrow, xz\downarrow]$$

$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon_{xy} & 0 & 0 & 0 & \frac{\lambda_{xy}}{2} & \frac{i\lambda_{xy}}{2} \\ 0 & \varepsilon_{yz} & -\frac{i\lambda_z}{2} & -\frac{\lambda_{xy}}{2} & 0 & 0 \\ 0 & \frac{i\lambda_z}{2} & \varepsilon_{xz} & -\frac{i\lambda_{xy}}{2} & 0 & 0 \\ 0 & -\frac{\lambda_{xy}}{2} & \frac{i\lambda_{xy}}{2} & \varepsilon_{xy} & 0 & 0 \\ \frac{\lambda_{xy}}{2} & 0 & 0 & 0 & \varepsilon_{yz} & \frac{i\lambda_z}{2} \\ -\frac{i\lambda_{xy}}{2} & 0 & 0 & 0 & -\frac{i\lambda_z}{2} & \varepsilon_{xz} \end{pmatrix}.$$

What I have NOT talked about

- Thin-film and Heterostructures of Ruthenates
- → Darrell Schlom's seminar
- Ex: Ferromagnetism of $SrRuO_3$



PRL **103,** 057201 (2009) PHYSICAL REVIEW LETTERS week ending 31 JULY 2009

Fundamental Thickness Limit of Itinerant Ferromagnetic $SrRuO_3$ Thin Films

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We report on a fundamental thickness limit of the itinerant ferromagnetic oxide $SrRuO_3$ that might arise from the orbital-selective quantum confinement effects. Experimentally, $SrRuO_3$ films remain metallic even for a thickness of 2 unit cells (uc), but the Curie temperature T_C starts to decrease at 4 uc and becomes zero at 2 uc. Using the Stoner model, we attributed the T_C decrease to a decrease in the density of states (N_o). Namely, in the thin film geometry, the hybridized Ru $d_{yz,zx}$ orbitals are terminated by top and bottom interfaces, resulting in quantum confinement and reduction of N_o.