Understanding orbital physics in correlated materials:

insights from the DFT+DMFT approach

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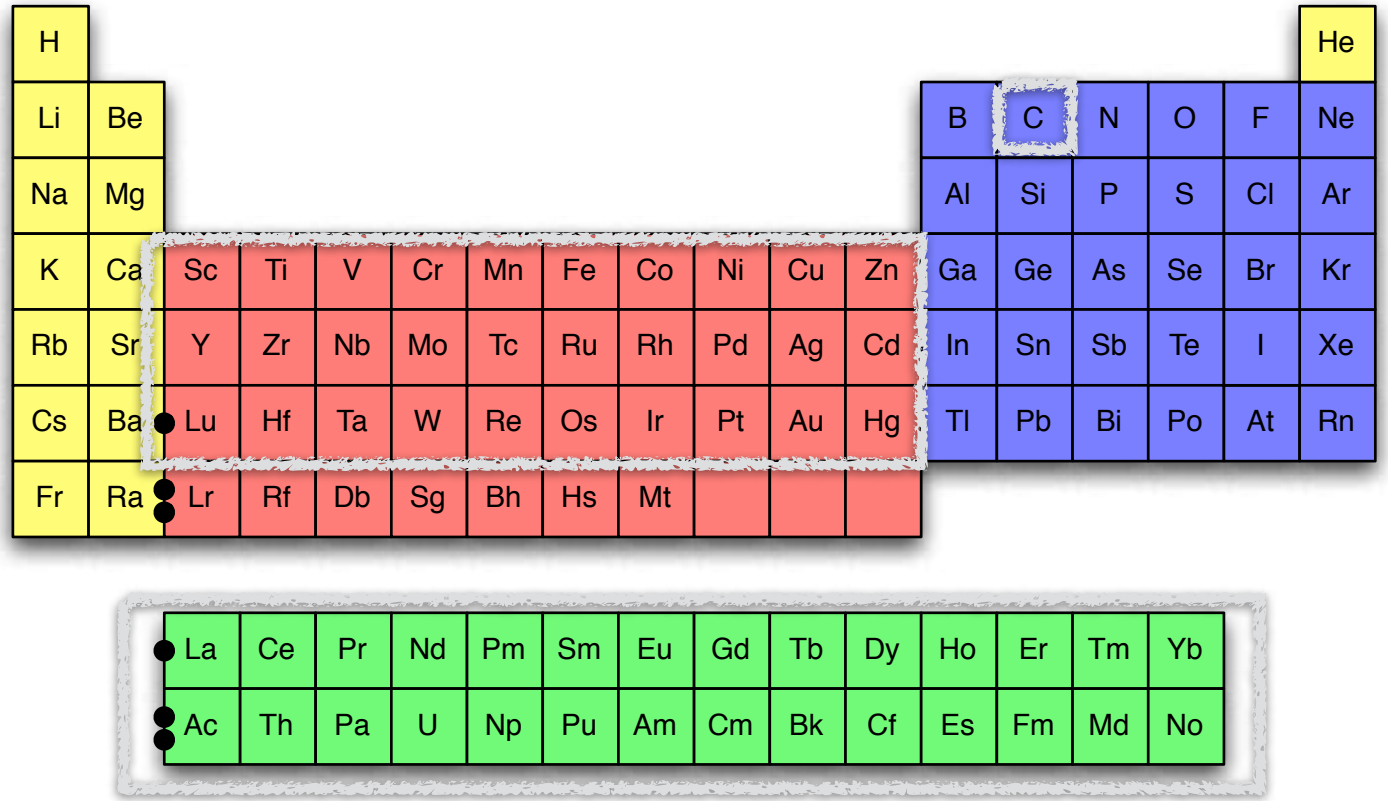
what are correlated materials?

systems for which *single-electron picture* fails *qualitatively*

atomic-like physics survives in the solid



Coulomb-induced metal-insulator transition

heavy-Fermions

unconventional superconductivity

spin-charge separation

.....

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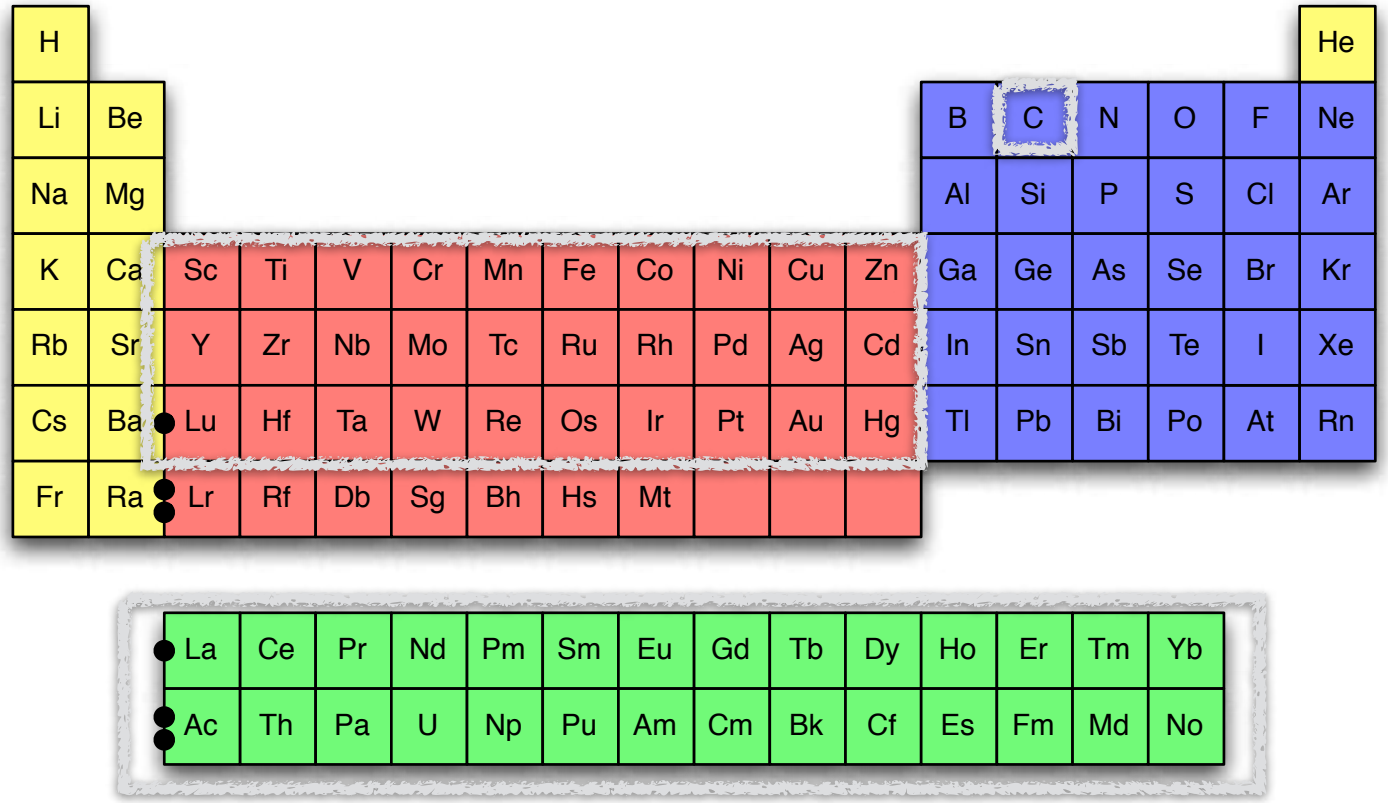

bad news: DFT (Kohn-Sham) band-structure
=single-electron picture

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failure of single-electron picture: ***more is different***

Born-Oppenheimer approximation, non-relativistic

$$\hat{H}_e = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2}\sum_{\alpha\neq\alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}$$

i=electrons

α = nuclei

simple interactions among many particles
can lead to unexpected *emergent* co-operative behavior

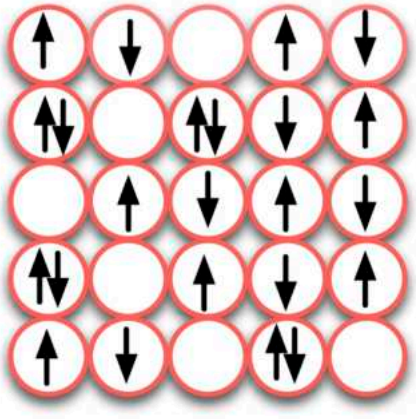
Coulomb-induced metal-insulator transition
heavy-Fermions
unconventional superconductivity
spin-charge separation
.....

Philip Warren Anderson

4 August 1972, Volume 177, Number 4047

SCIENCE

the key phenomenon: Mott transition



Hubbard model

half filling

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

U/W=0:
metal

$m^* \to \infty$

$\Delta E \to U - W$

W/U=0:
insulator

metal with heavy quasiparticles (large masses)

insulator with increasing gap

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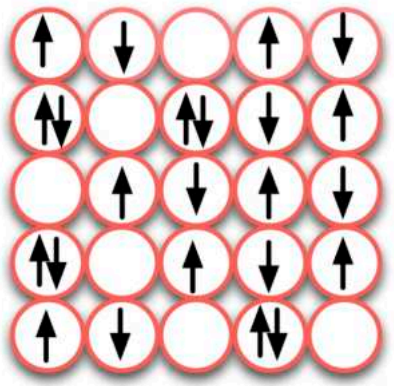
dynamical mean-field theory (DMFT)

$$\hat{H} = \varepsilon_d \sum_i \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

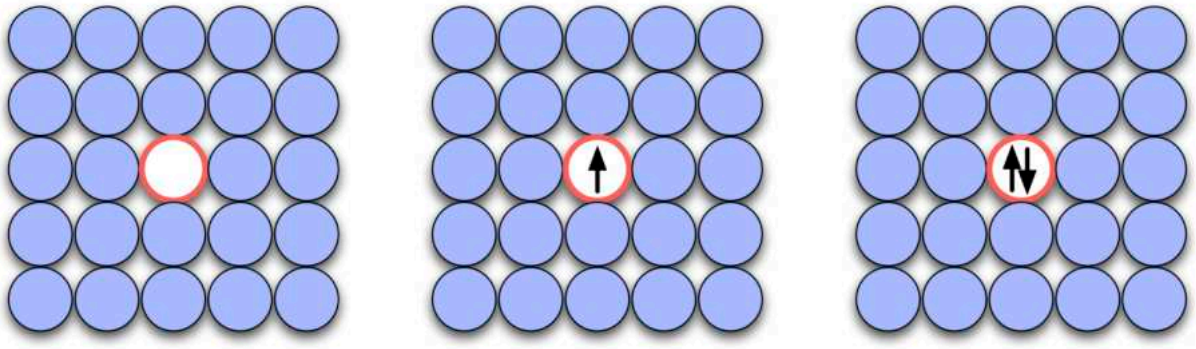


$G^{i,j}$

H^{LDA}

$U^{i,i}$

self-consistent
quantum-impurity model



$$\mathcal{G}^{-1} = G^{-1} + \Sigma$$

$$G = G^{i,i}$$

k-independent self-energy

exact in the infinite coordination number limit

Metzner and Vollhardt, PRL **62**, 324 (1989); Georges and Kotliar, PRB **45**, 6479 (1992).

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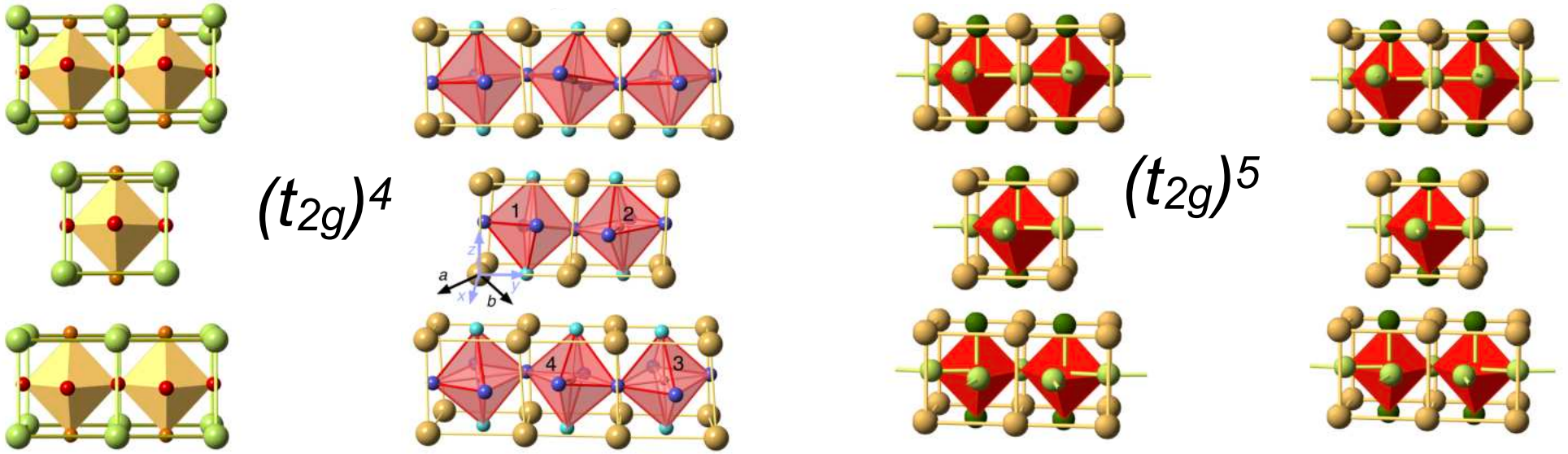
correlated materials: not only W/U

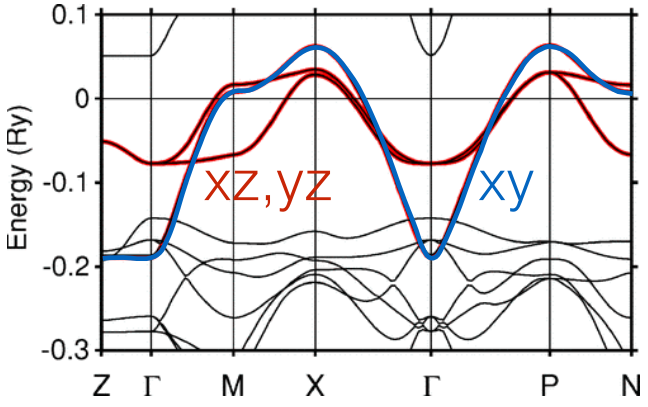
Sr_2RuO_4 Ca_2RuO_4 Sr_2RhO_4 Sr_2IrO_4



$(t_{2g})^4$ $(t_{2g})^5$

metal *insulator* *metal* *insulator*

orbital physics: interplay of spin, orbital, charge, lattice degrees of freedom in the presence of correlations



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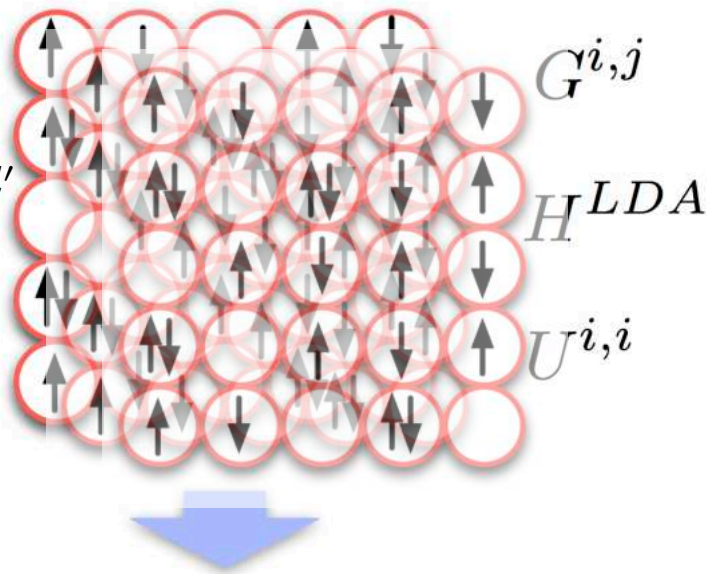
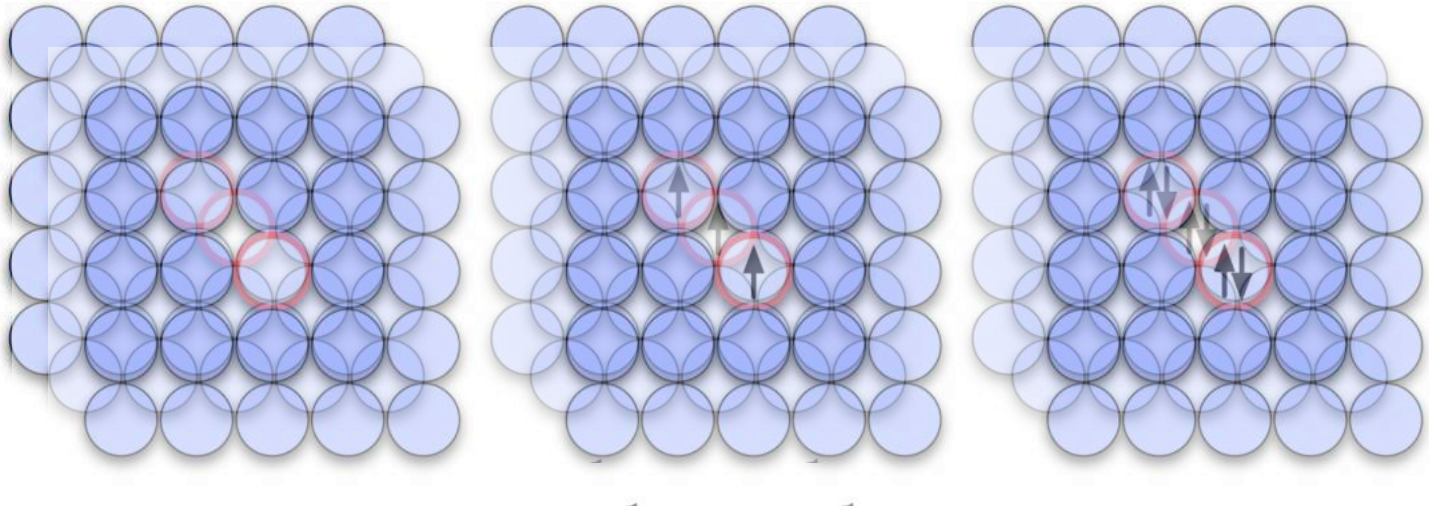
DFT+DMFT: DMFT for Materials

$$\hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cdc'd'} U_{cdd'c'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}$$



realistic
self-consistent
quantum-impurity
(QI) model



we need **minimal** material-specific models
and **flexible and efficient** solvers

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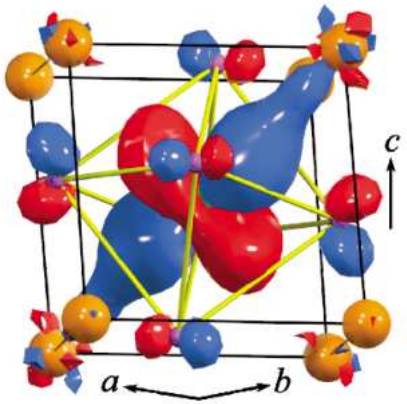
minimal models: DFT-based Wannier functions

VOLUME 92, NUMBER 17 PHYSICAL REVIEW LETTERS week ending 30 APRIL 2004

Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic $3d^1$ Perovskites

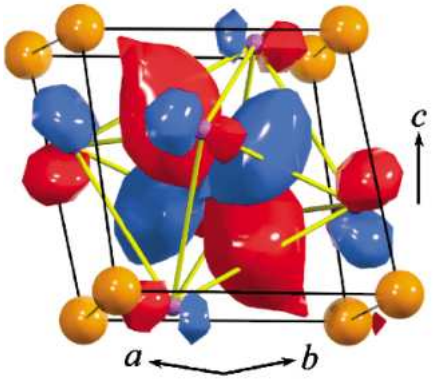
t_{2g}^1

E. Pavarini,[1] S. Biermann,[2] A. Poteryaev,[3] A. I. Lichtenstein,[3] A. Georges,[2] and O. K. Andersen[4]



correlated: DMFT

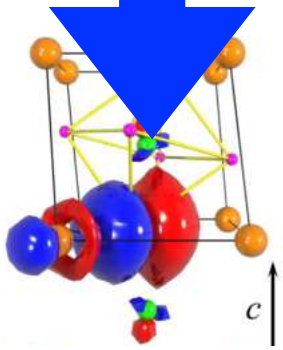
others: Kohn-Sham DFT orbitals



$LaTiO_3$

$YTiO_3$

DFT+DMFT



but screened U,J: cRPA,cLDA

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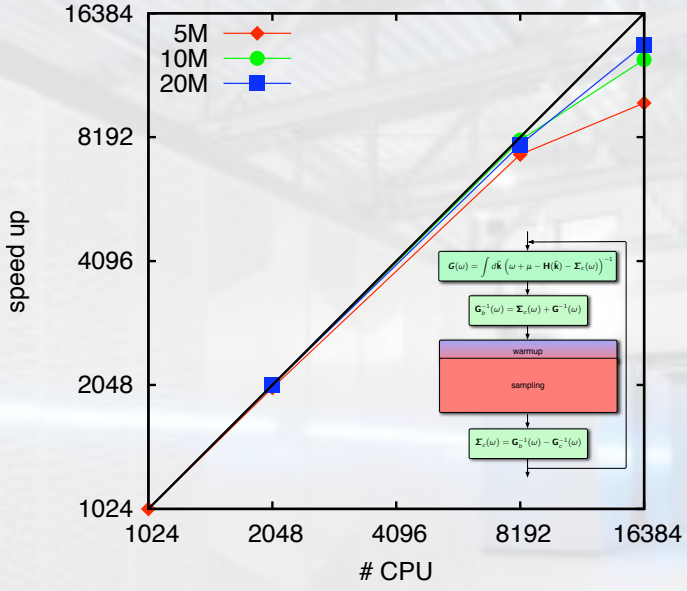
flexible and efficient solvers: our package

$$H = -\sum_{ii'}\sum_{mm'}\sum_{\sigma} t^{ii'}_{mm'} c^{\dagger}_{im\sigma} c_{i'm'\sigma}$$
$$+ U \sum_{im} n_{im\uparrow} n_{im\downarrow}$$
$$+ \frac{1}{2} \sum_{im \neq m' \sigma\sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'}$$
$$- J \sum_{m \neq m'} (c^{\dagger}_{m\uparrow} c^{\dagger}_{m'\downarrow} c_{m'\uparrow} c_{m\downarrow} + c^{\dagger}_{m\uparrow} c^{\dagger}_{m\downarrow} c_{m'\uparrow} c_{m'\downarrow})$$

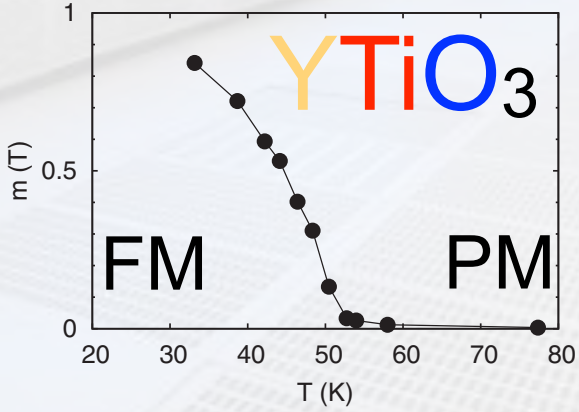
self-energy matrix in spin-orbital space



DMFT and cDMFT

generalized quantum impurity solvers:

general HF QMC
general CT-INT QMC
general CT-HYB QMC



- CT-HYB: A. Flesch, E. Gorelov, E. Koch and E. Pavarini
  Phys. Rev. B **87**, 195141 (2013)
- CT-INT: E. Gorelov et al, PRL 104, 226410 (2010)
- CT-INT+SO: G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini,
  Phys. Rev. Lett. 116, 106402 (2016)

sign problem: smart adapted basis choice

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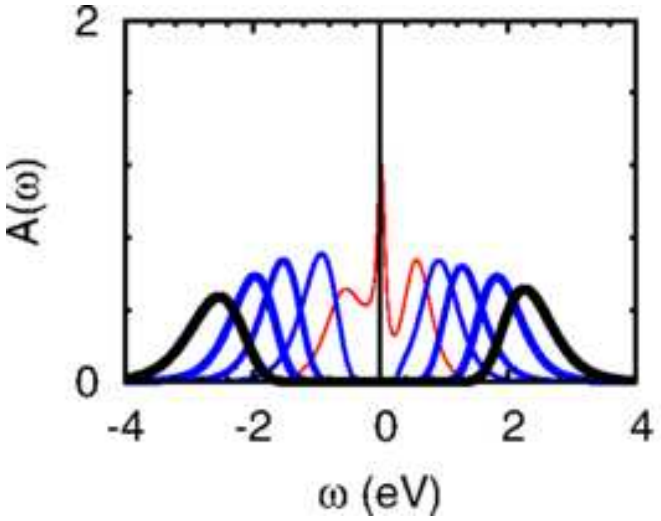
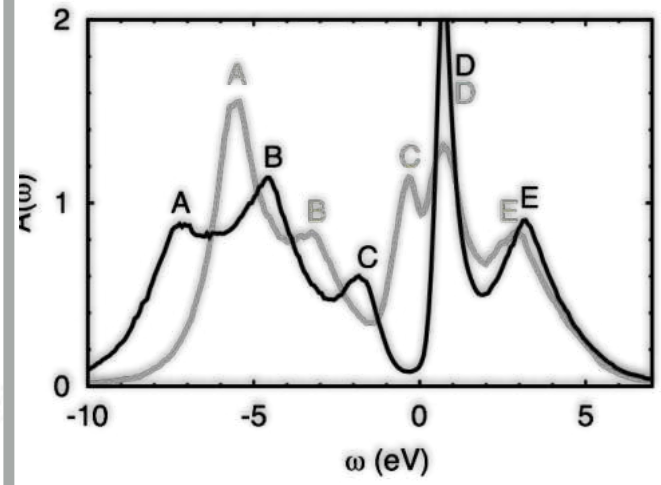
what can we do so far? a lot!

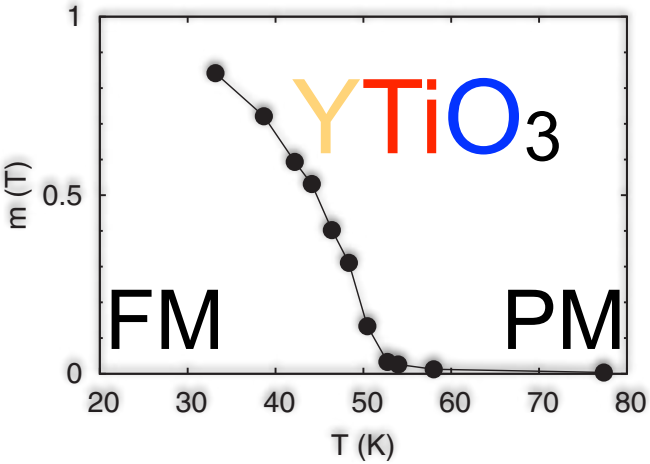
spectral functions



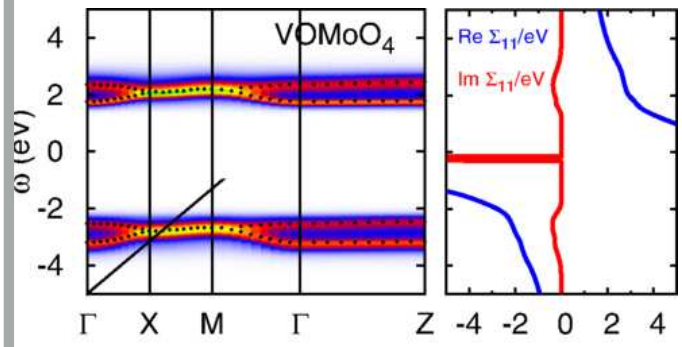
many orbitals



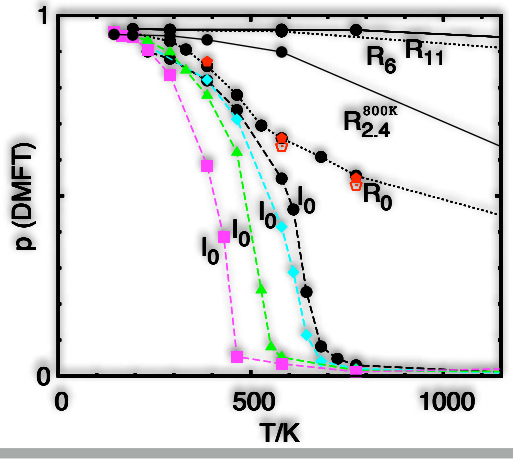
low T



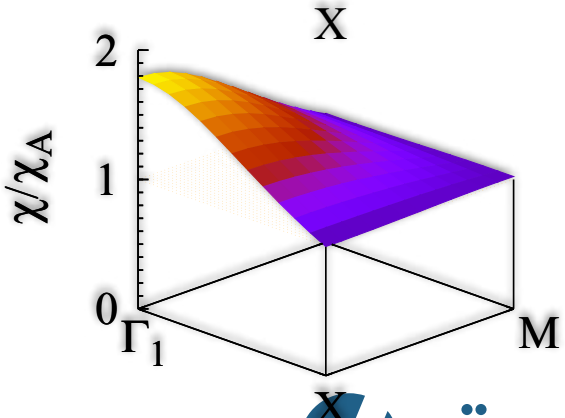
correlated bands



phase transitions



susceptibilities



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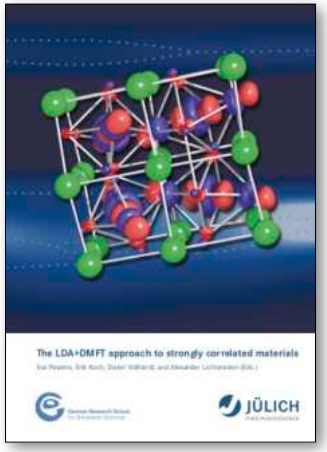
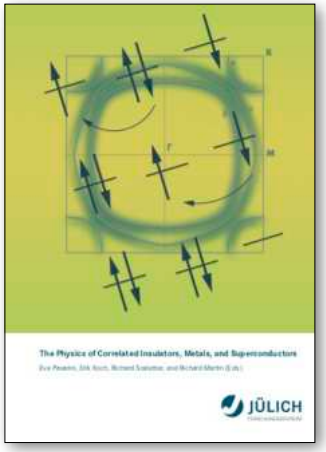
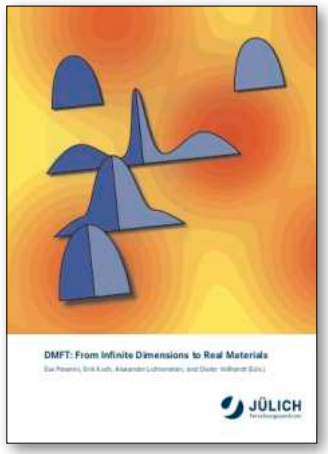
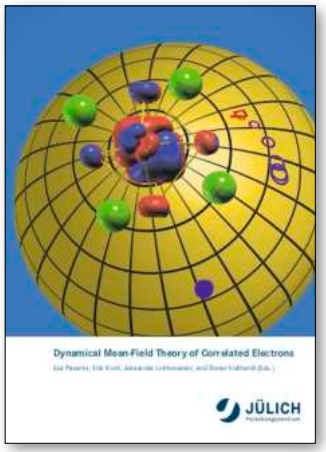
want to know more?

Autumn School on Correlated Electrons









La Rivista del Nuovo Cimento (2021) 44:597–640
https://doi.org/10.1007/s40766-021-00025-8

REVIEW PAPER

Check for updates

Solving the strong-correlation problem in materials

Eva Pavarini[1]

Received: 24 March 2021 / Accepted: 11 June 2021 / Published online: 14 July 2021

www.cond-mat.de/events/correl.html

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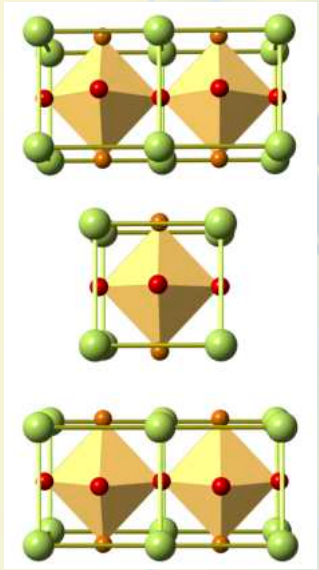
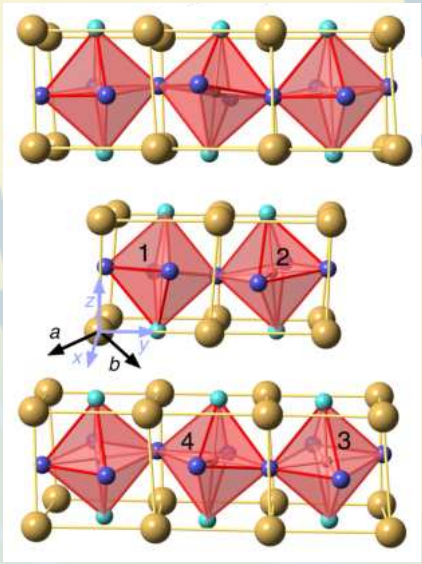
Sr_2RuO_4 and its family

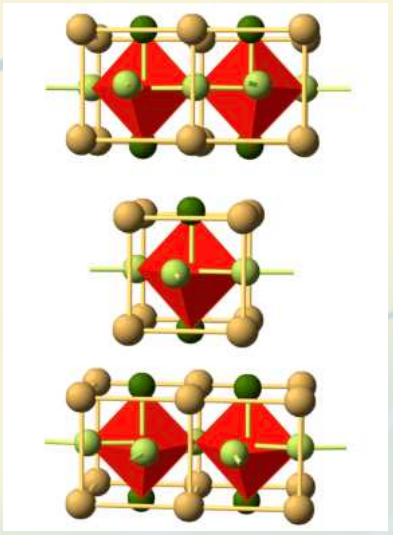
disentangling complexity

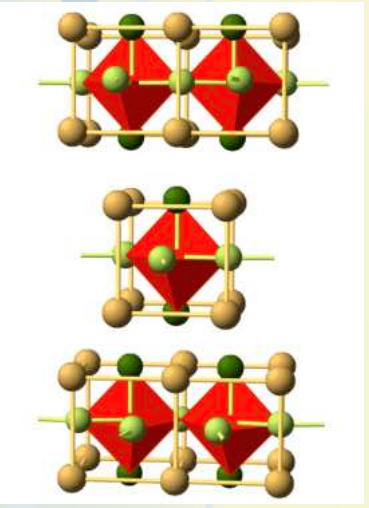
building a unifying picture

Sr_2RuO_4 Ca_2RuO_4 Sr_2RhO_4 Sr_2IrO_4









$(t_{2g})^4$ $(t_{2g})^5$

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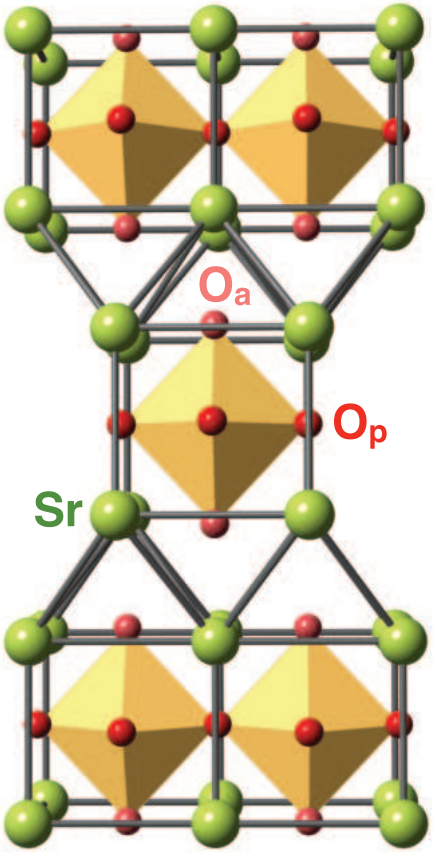
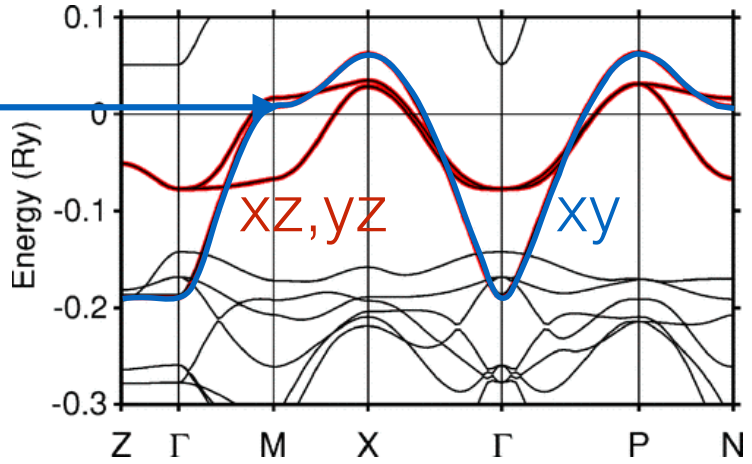
Sr_2RuO_4: a paradigmatic system



xy vHS



$$H = -\sum_{ii'}\sum_{mm'}\sum_{\sigma\sigma'} t^{i,i'}_{m\sigma,m'\sigma'} c^{\dagger}_{im\sigma} c_{i'm'\sigma'}$$

$$+\frac{1}{2}\sum_{i}\sum_{mm'pp'}\sum_{\sigma\sigma'} U_{mm'pp'} c^{\dagger}_{im\sigma} c^{\dagger}_{im'\sigma'} c_{ip'\sigma'} c_{ip\sigma}$$

Ru t_{2g}^4

xy-band 2-dimensional

xz/yz-bands 1-dimensional

$W_{xy} \sim 2W_{xz/yz}$

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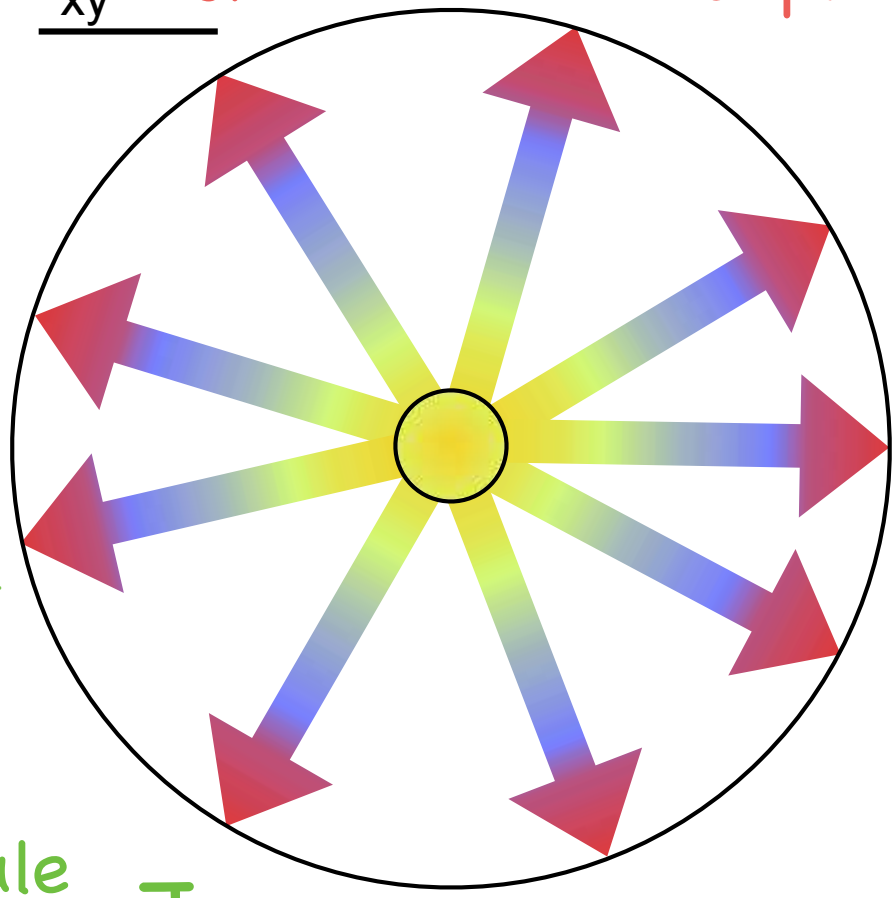
many energy scales are similar



crystal-field splitting

xz/yz

xy

ε_{CF}

spin-orbit coupling

λ

screened Coulomb repulsion

U

$dU=U_{xy}-U_{xz/yz}$

n filling

t_{2g}^n

$W_{xz/yz}$

$W_{xy}\sim 2W_{xz/yz}$

Hund's rule coupling

J

xy vH singularity ?

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minimal Hubbard model: t_{2g} bands

$$H = -\sum_{ii'}\sum_{mm'}\sum_{\sigma\sigma'} t^{i,i'}_{m\sigma,m'\sigma'} c^{\dagger}_{im\sigma} c_{i'm'\sigma'}$$

$$+ \frac{1}{2}\sum_{i}\sum_{mm'pp'}\sum_{\sigma\sigma'} U_{mm'pp'} c^{\dagger}_{im\sigma} c^{\dagger}_{im'\sigma'} c_{ip'\sigma'} c_{ip\sigma}$$

$$H_{\mathrm{SO}} = \sum_{i\mu} H^{i\mu}_{\mathrm{SO}} = \sum_{i\mu}\sum_{m\sigma m'\sigma'} \lambda^{i}_{\mu} \xi^{i\mu}_{m\sigma m'\sigma'} c^{\dagger}_{im\sigma} c_{im'\sigma'}$$

local spin-orbit interaction

example: Hund's rule coupling J & van-Hove singularity

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]
[1]*Centre de Physique Théorique, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France*
[2]*Jožef Stefan Institute, Jamova 39, Ljubljana, Slovenia*
[3]*Institute of Theoretical and Computational Physics, TU Graz, Petersgasse 16, Graz, Austria*
[4]*Nanosystem Research Institute, AIST, Tsukuba 305-8568, Japan*
[5]*Japan Science and Technology Agency, CREST, Kawaguchi 332-0012, Japan*
[6]*Physics Department and Center for Materials Theory, Rutgers University, Piscataway New Jersey 08854, USA*
[7]*Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France*
(Received 27 October 2010; published 2 March 2011)

We calculate the electronic structure of Sr_2RuO_4, treating correlations within dynamical mean-field theory. The approach successfully reproduces several experimental results and explains the key properties of this material: the anisotropic mass renormalization of quasiparticles and the crossover into an incoherent regime above a low temperature scale. While the orbital differentiation originates from the proximity of the van Hove singularity, strong correlations are caused by the Hund's coupling. The generality of this mechanism for other correlated materials is pointed out.

Hund's metal

xy vH singularity

and mass inversions

$W_{xy} > W_{xz}$

but $m^*_{xy} > m^*_{xz}$

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.

J [eV]	$m^*/m_{\mathrm{LDA}}\|_{xy}$	$m^*/m_{\mathrm{LDA}}\|_{xz}$	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

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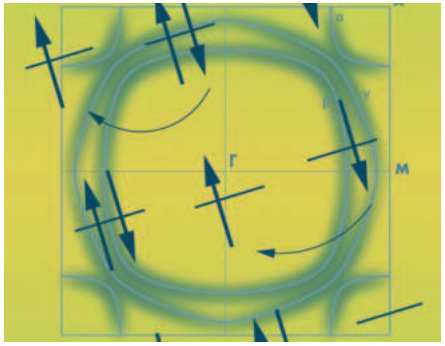
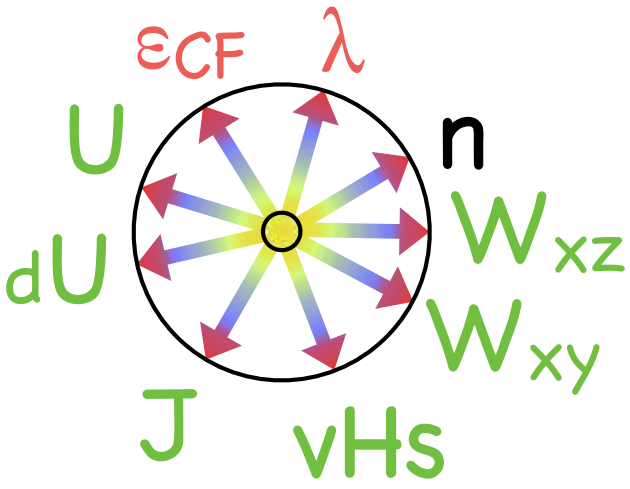
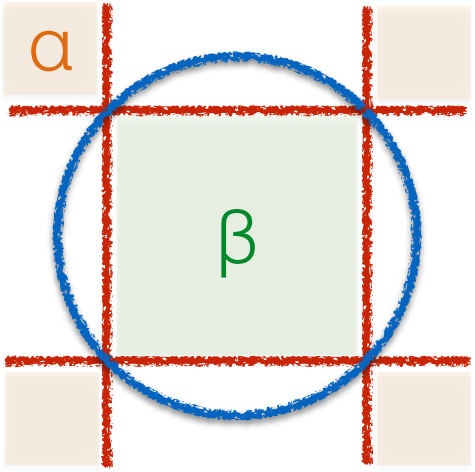
example: the Fermi surface puzzle

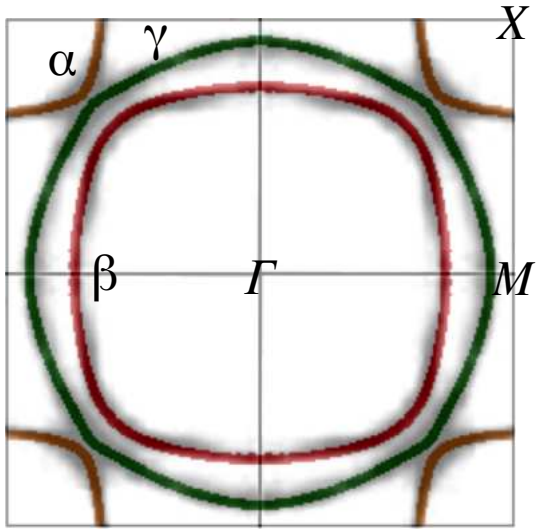


$$\varepsilon_{CF} + \Delta\varepsilon_{CF}(U) - \Delta'\varepsilon_{CF}(dU) \sim \varepsilon_{CF}$$

$$\lambda + \Delta\lambda \sim 2\lambda$$







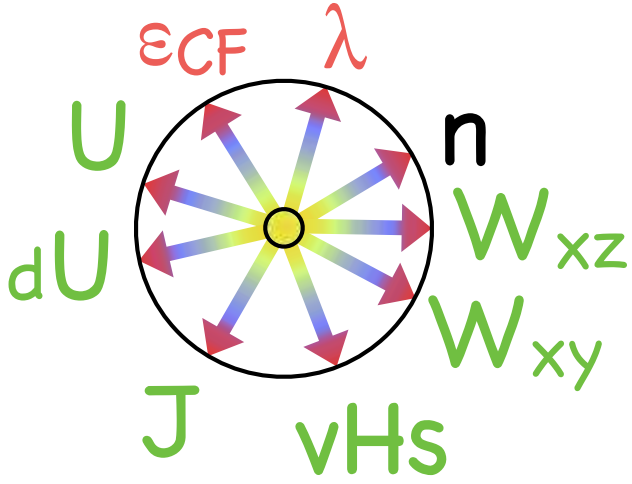
theory:

G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)

experiments:

A. Damascelli, D. H. Lu, K. M. Shen, N. P. Armitage, F. Ronning, D. L. Feng, C. Kim, Z.-X. Shen, T. Kimura, Y. Tokura, Z. Q. Mao, and Y. Maeno, Phys. Rev. Lett. **85,** 5194 (2000)

the Sr_2RuO_4 family: exploit complexity



H
Li Be B
Na Mg Al
K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga
Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In
Cs Ba Lu Hf Ta W Re Os Ir Pt Au Hg Tl
Fr Ra Lr Rf Db Sg Bh H

Ca_2RuO_4

W,εCF

Sr_2RuO_4 Sr_2RhO_4

n

λ, W/U

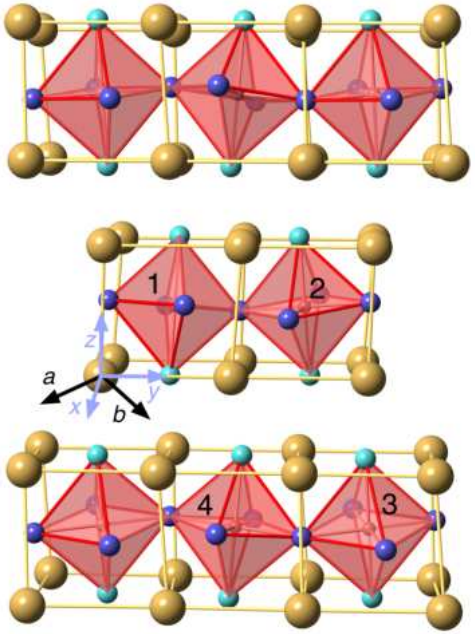
Sr_2IrO_4

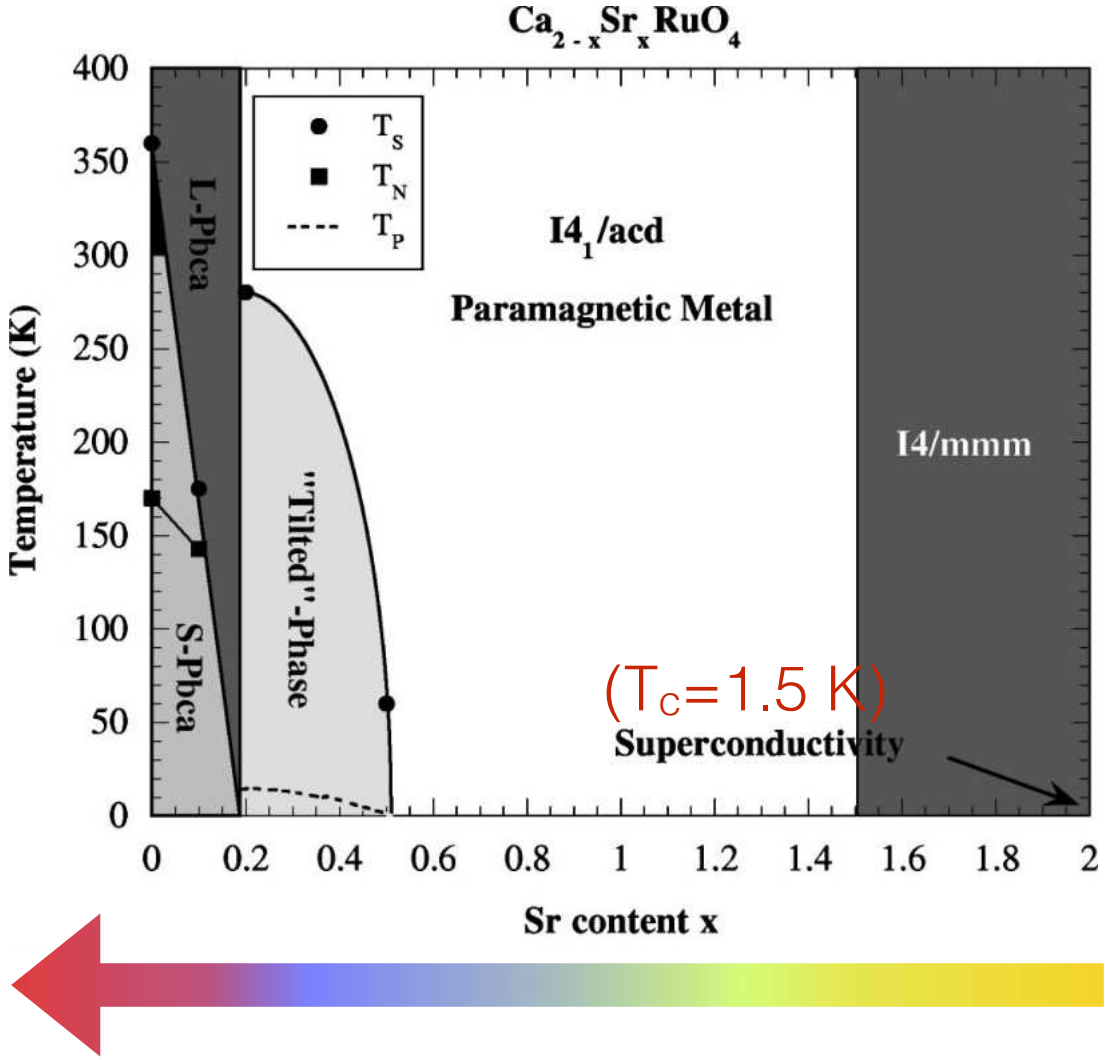
some known facts..

replacing Sr with Ca: metal-insulator transition

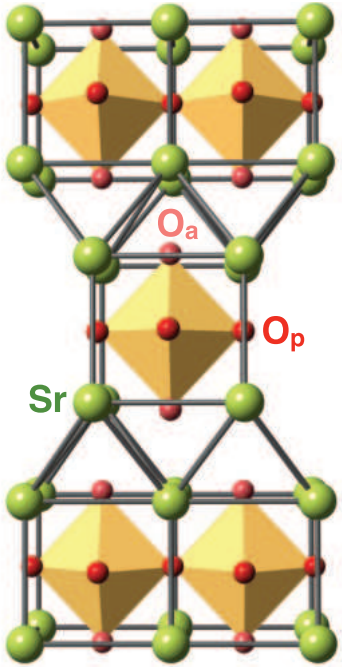
Ru 4d t_{2g}^4

Ca_2RuO_4





Sr_2RuO_4



O. Friedt *et al.*, PRB **63**, 174432 (2001)

Nature of Mott transition

PRL **104,** 226401 (2010) PHYSICAL REVIEW LETTERS week ending 4 JUNE 2010

Nature of the Mott Transition in Ca_2RuO_4

E. Gorelov,[1] M. Karolak,[2] T. O. Wehling,[2] F. Lechermann,[2] A. I. Lichtenstein,[2] and E. Pavarini[1]

[1]*Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany*
[2]*I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany*

(Received 12 January 2010; published 1 June 2010)

We study the origin of the temperature-induced Mott transition in Ca_2RuO_4. As a method we use the local-density approximation + dynamical mean-field theory. We show the following. (i) The Mott transition is driven by the change in structure from long to short **c**-axis layered perovskite (*L-Pbca* → *S-Pbca*); it occurs together with orbital order, which follows, rather than produces, the structural transition. (ii) In the metallic *L-Pbca* phase the orbital polarization is ∼0. (iii) In the insulating *S-Pbca* phase the lower energy orbital, ∼*xy*, is full. (iv) The spin-flip and pair-hopping Coulomb terms reduce the effective masses in the metallic phase. Our results indicate that a similar scenario applies to $Ca_{2-x}Sr_xRuO_4$ ($x \leq 0.2$). In the metallic $x \leq 0.5$ structures electrons are progressively transferred to the xz/yz bands with increasing x; however, we find no orbital-selective Mott transition down to ∼300 K.

$\varepsilon_{CF} + \Delta\varepsilon_{CF}$ $xy^2xz^1yz^1$

λ (spin-orbit coupling) **not** essential for MIT, but key to magnetism

Phys. Rev. B **95**, 075145 (2017); Phys. Rev. B **101**, 205128 (2020)

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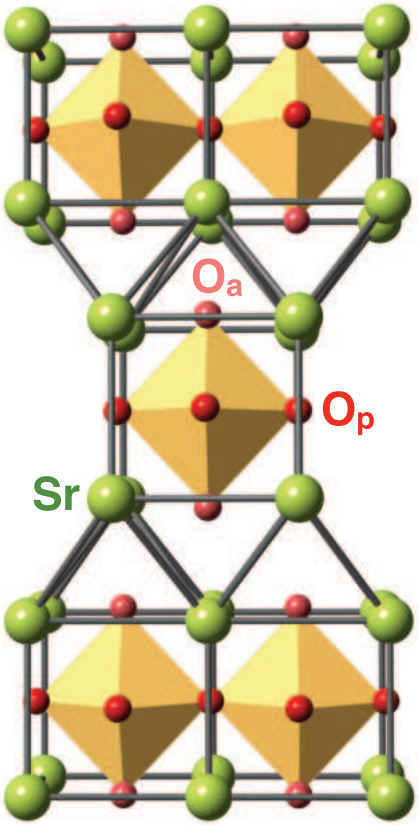
replacing Ru with Rh

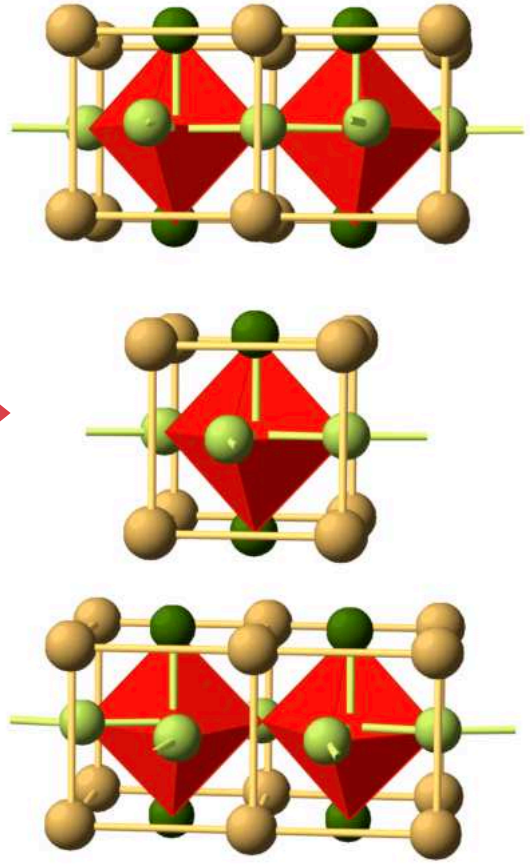
Sr_2RuO_4



t_{2g}^4

4d

Sr_2RhO_4



t_{2g}^5

4d

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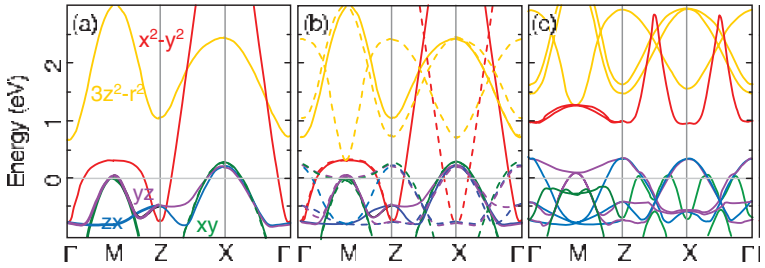
rotations: xy-band FS missing

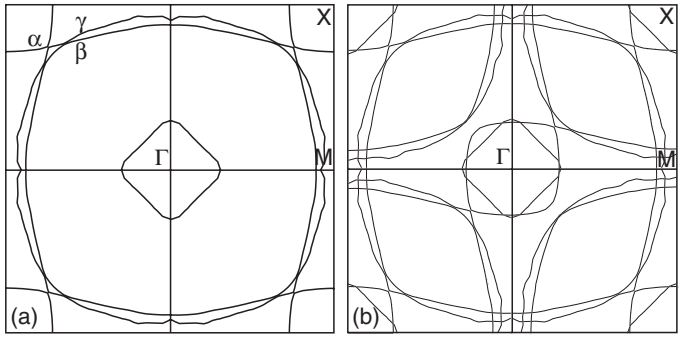
PRL **97,** 106401 (2006) PHYSICAL REVIEW LETTERS week ending 8 SEPTEMBER 2006

Missing *xy*-Band Fermi Surface in 4*d* Transition-Metal Oxide Sr_2RhO_4: Effect of the Octahedra Rotation on the Electronic Structure

B. J. Kim,[1] Jaejun Yu,[1] H. Koh,[2] I. Nagai,[3] S. I. Ikeda,[3] S.-J. Oh,[1] and C. Kim[4]

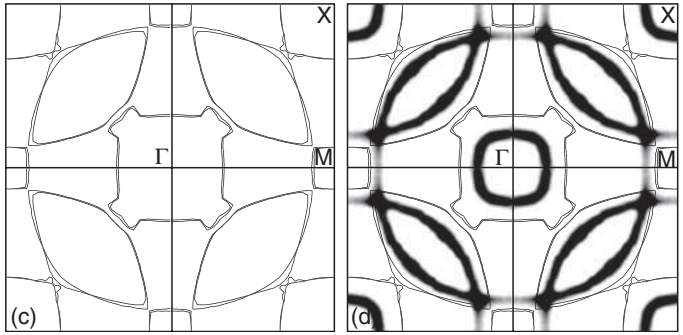


undistorted



undistorted+folded

distorted



distorted
vs experiments

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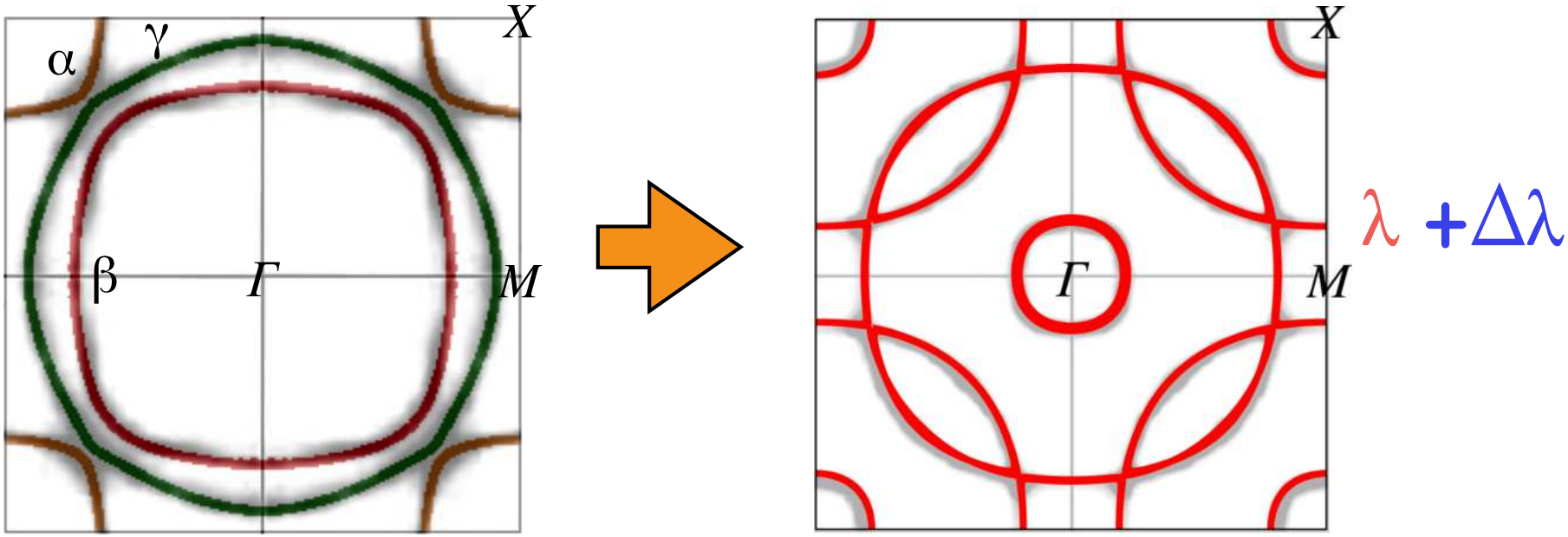
Ru → Rh: moderate masses, xy band full

t_{2g}^4 t_{2g}^5

Sr_2RuO_4: Sr_2RhO_4:



theory:

G. Zhang, E. Gorelov, E. Sarvestani, and E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)
G. Zhang and E. Pavarini, Phys. Rev. B **99**, 125102 (2019)

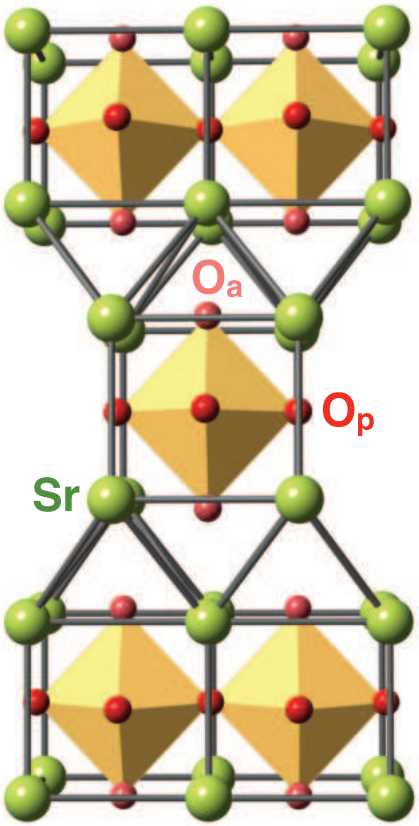
experiments:

A. Damascelli, D. H. Lu, K. M. Shen, N. P. Armitage, F. Ronning, D. L. Feng, C. Kim, Z.-X. Shen, T. Kimura, Y. Tokura, Z. Q. Mao, and Y. Maeno, Phys. Rev. Lett. **85,** 5194 (2000)

B. J. Kim, J. Yu, H. Koh, I. Nagai, S. I. Ikeda, S.-J. Oh, and C. Kim, Phys. Rev. Lett. **97,** 106401 (2006)

replacing Ru with Ir

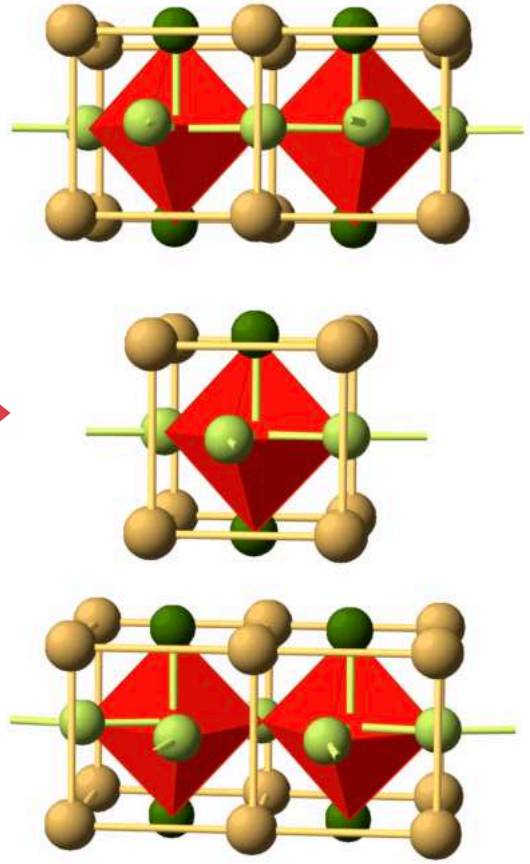
Sr_2RuO_4



t_{2g}^4

4d

$Sr_2(Rh/Ir)O_4$



t_{2g}^5

4d/5d

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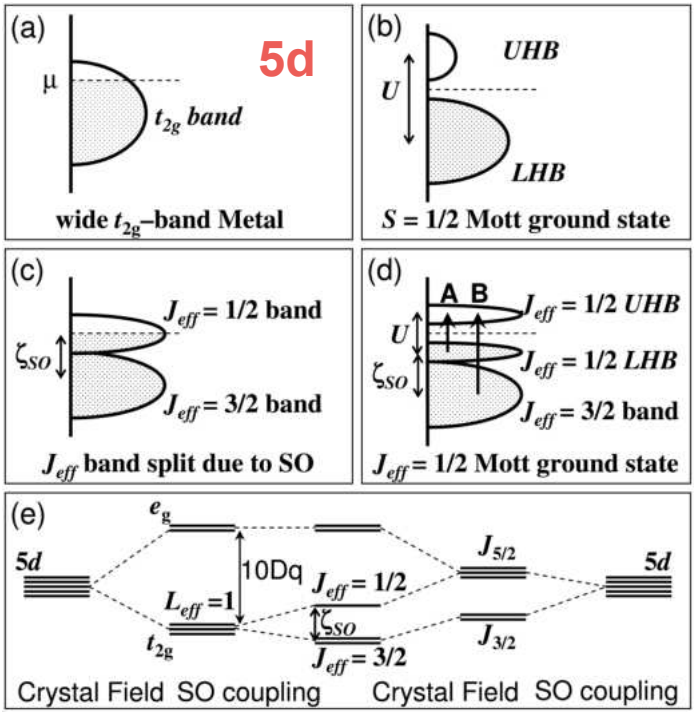
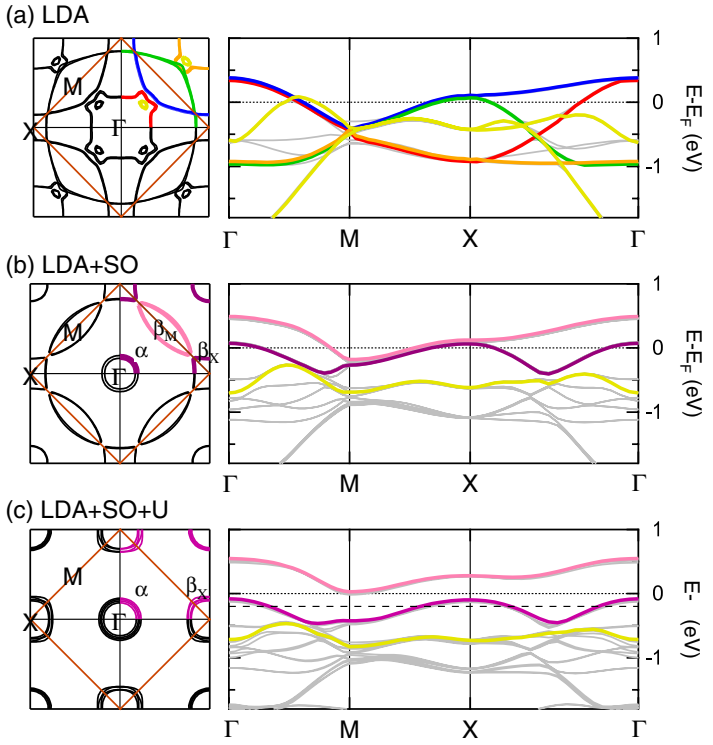
Sr_2IrO_4: t_{2g} analogous of HTSCs?

PRL **101,** 076402 (2008) PHYSICAL REVIEW LETTERS week ending 15 AUGUST 2008

Novel $J_{eff} = 1/2$ Mott State Induced by Relativistic Spin-Orbit Coupling in Sr_2IrO_4

B. J. Kim,[1] Hosub Jin,[1] S. J. Moon,[2] J.-Y. Kim,[3] B.-G. Park,[4] C. S. Leem,[5] Jaejun Yu,[1] T. W. Noh,[2] C. Kim,[5] S.-J. Oh,[1] J.-H. Park,[3,4,*] V. Durairaj,[6] G. Cao,[6] and E. Rotenberg[7]





angle-resolved photoemission, optical conductivity,

x-ray absorption measurements

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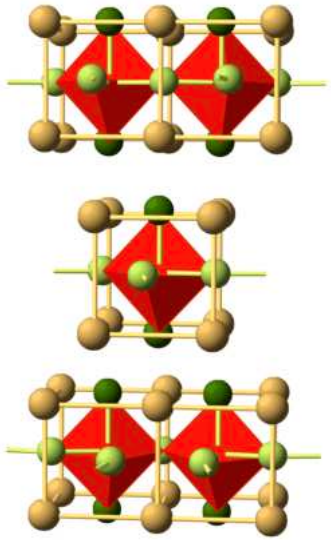
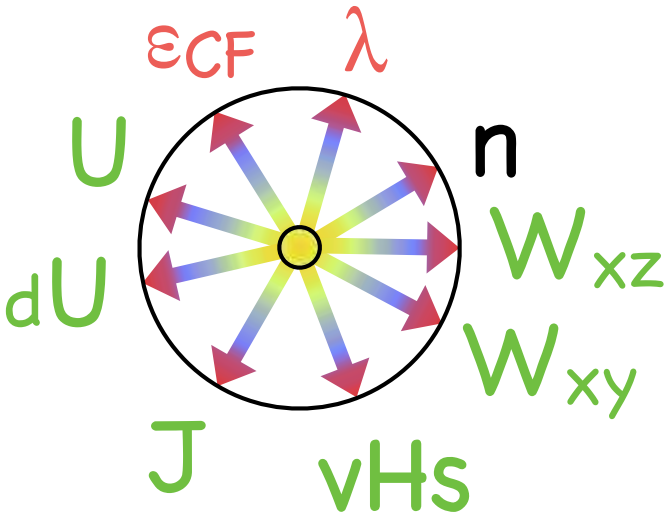
no, rather j_{eff}=1/2 spin-orbital order

spin-orbit large but non sufficiently for 1-band picture

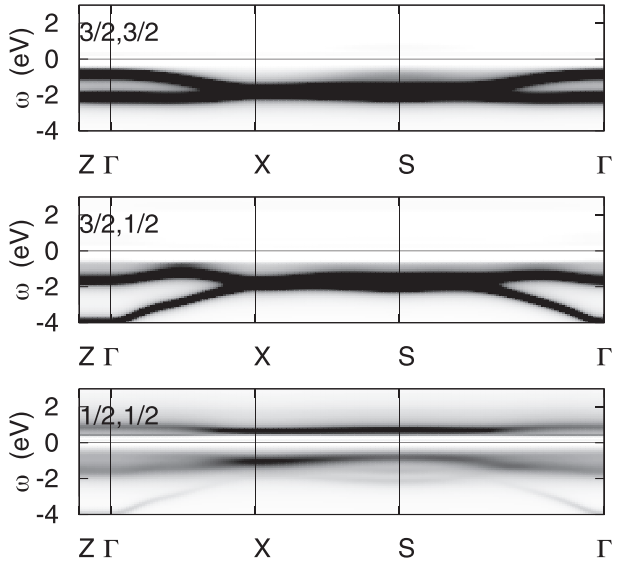


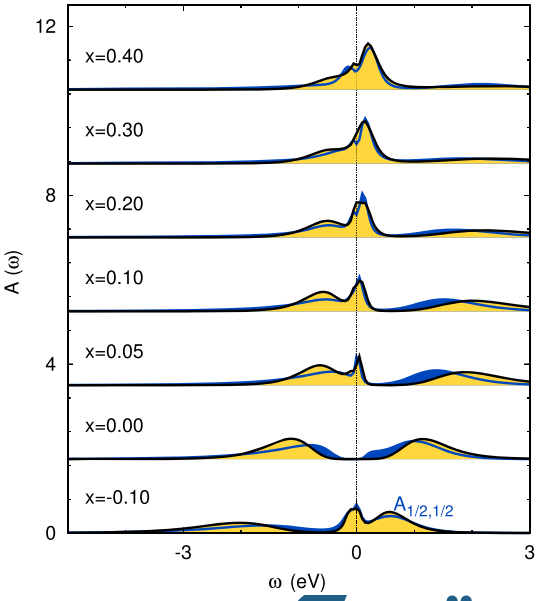


PHYSICAL REVIEW LETTERS **131,** 036504 (2023)

Multiorbital Nature of Doped Sr_2IrO_4

Guoren Zhang[1,2] and Eva Pavarini[3,4]
[1]*School of Sciences, Nantong University, Nantong, 226019, People's Republic of China*
[2]*Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, People's Republic of China*
[3]*Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany*
[4]*JARA High-Performance Computing, Forschungszentrum Jülich, 52425 Jülich, Germany*





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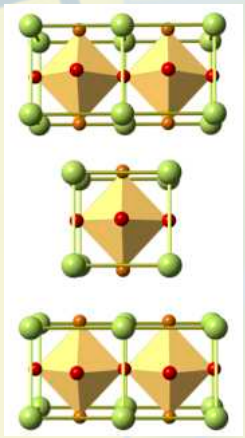
$(t_{2g})^n$

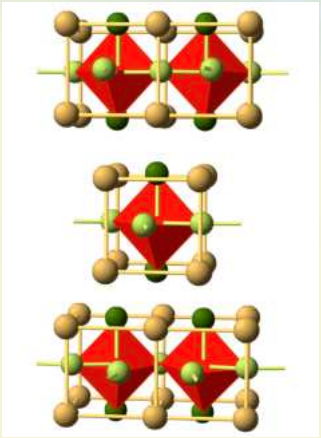
Sr_2RuO_4



correlated metal

$m_{xy} > m_{xz/yz}$

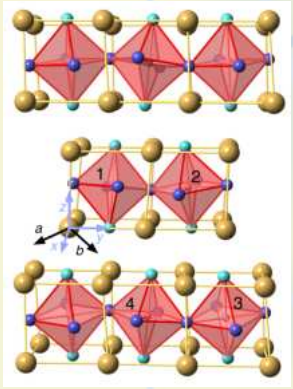
Sr_2RhO_4



weakly correlated metal

only 2-bands
xz/yz at Fermi surface

Ca_2RuO_4



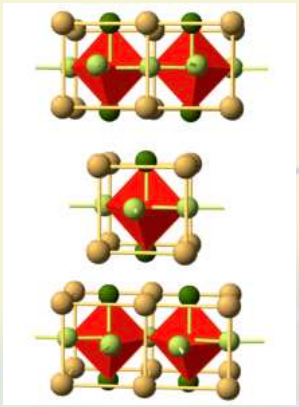
small gap insulator

xy-orbital order

spin-orbit important
only for magnetism

$(t_{2g})^4$

Sr_2IrO_4



spin-orbit Mott insulator
small gap

j=1/2 orbital order
only 1-band half-fillled

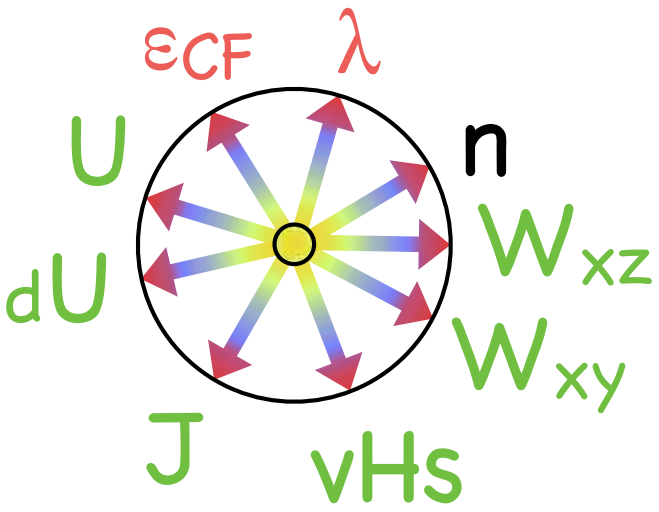
$(t_{2g})^5$

can we build a unifying picture?

yes!

ε_{CF} changes natural occupations

build map of CF (ε_{CF}) effects!



PHYSICAL REVIEW LETTERS **132,** 236505 (2024)

Map of Crystal-Field Effects in Correlated Layered t_{2g}^n Perovskites

Neda Samani,[1] Guoren Zhang,[1,2,3] and Eva Pavarini[1,4]
[1]*Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany*
[2]*School of Physics and Technology, Nantong University, Nantong 226019, People's Republic of China*
[3]*Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, People's Republic of China*
[4]*JARA High-Performance Computing, Forschungszentrum Jülich, Germany*

(natural orbitals=eigenvalues of occupation matrix)

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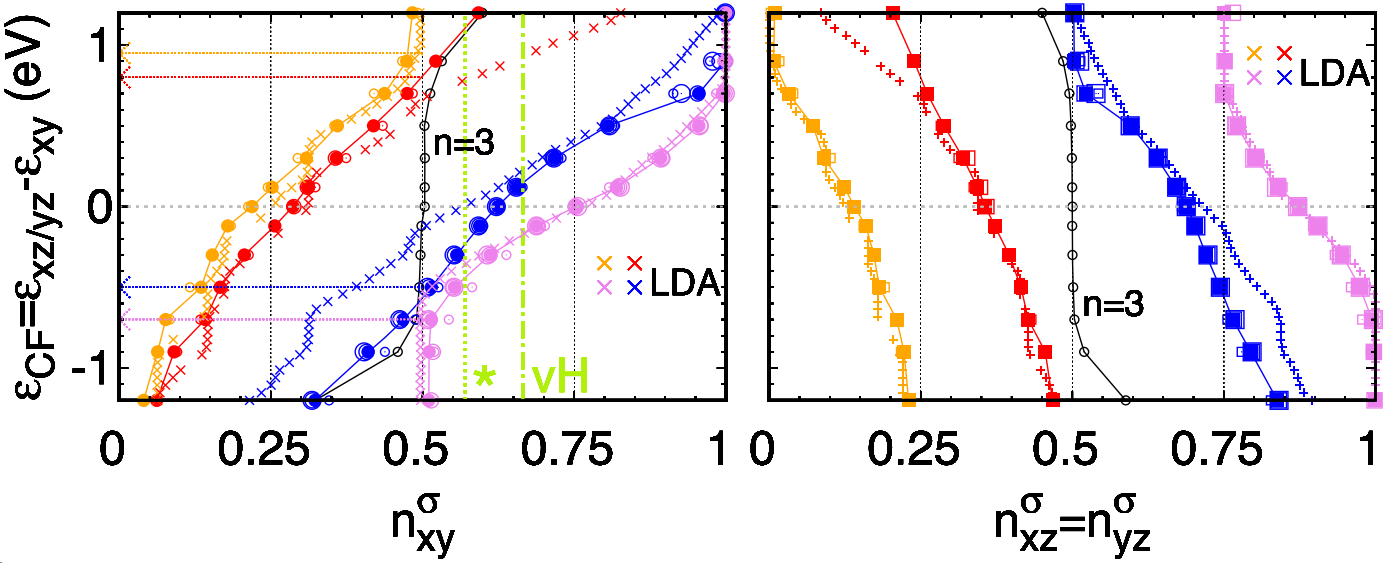
ε_{CF} changes natural occupations

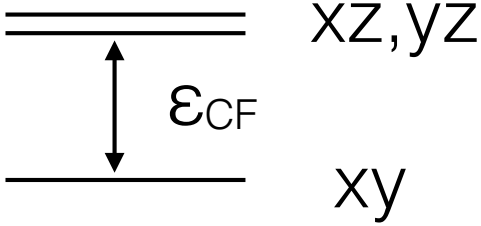
$\lambda = 0$ natural orbitals=xy,xz/yz

t_{2g}^{n}



n=1
n=2
n=4
n=5

CF splitting



$n=n_{xy}+2n_{xz/yz}$

crosses: U=0

closed symbols: finite U

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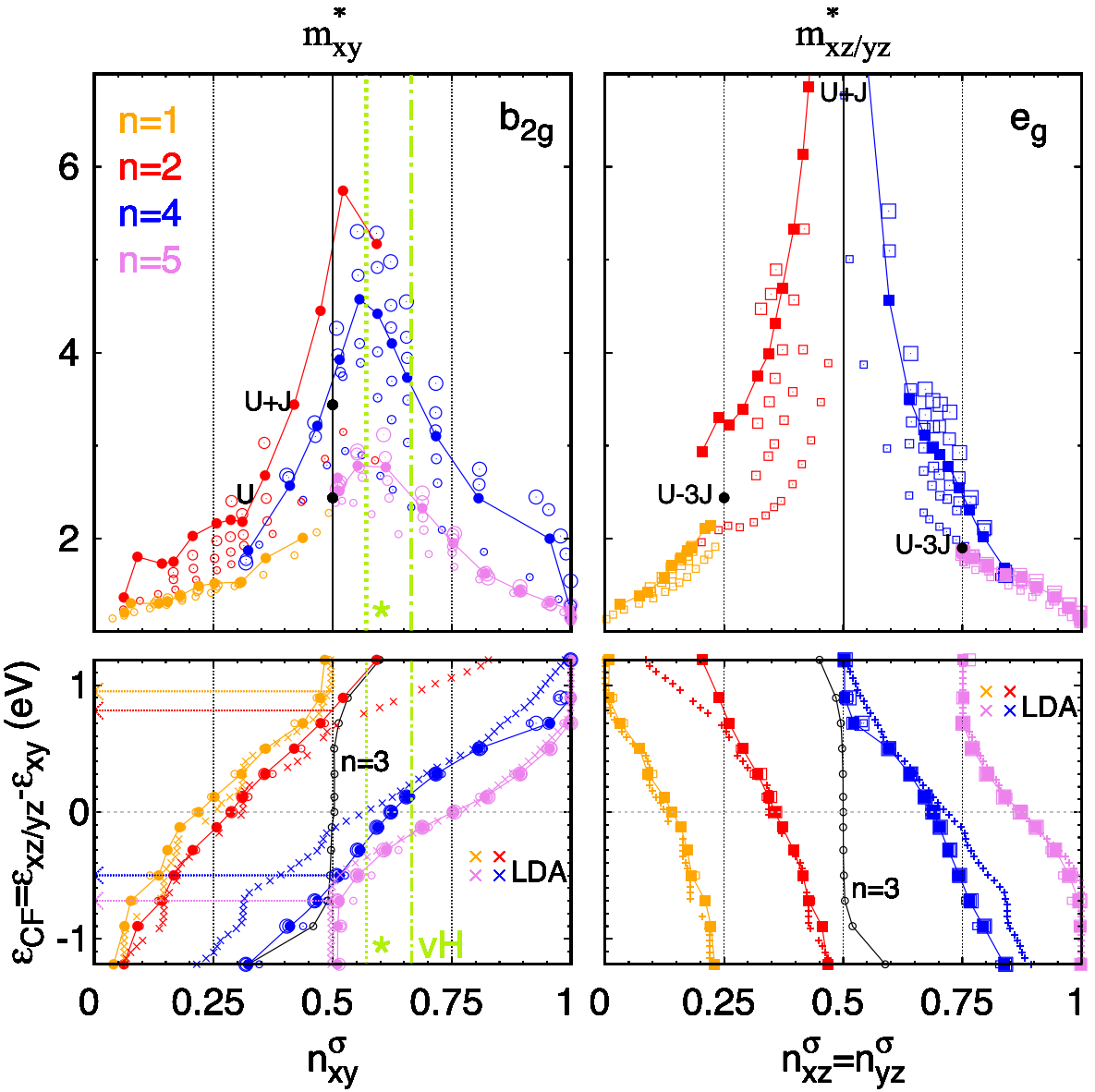
map of crystal-field splitting: effective masses

t_{2g}^n

$\lambda = 0$



m diverges: insulator*

m=1: not correlated*

moderate (realistic) U,J, fixed U/W

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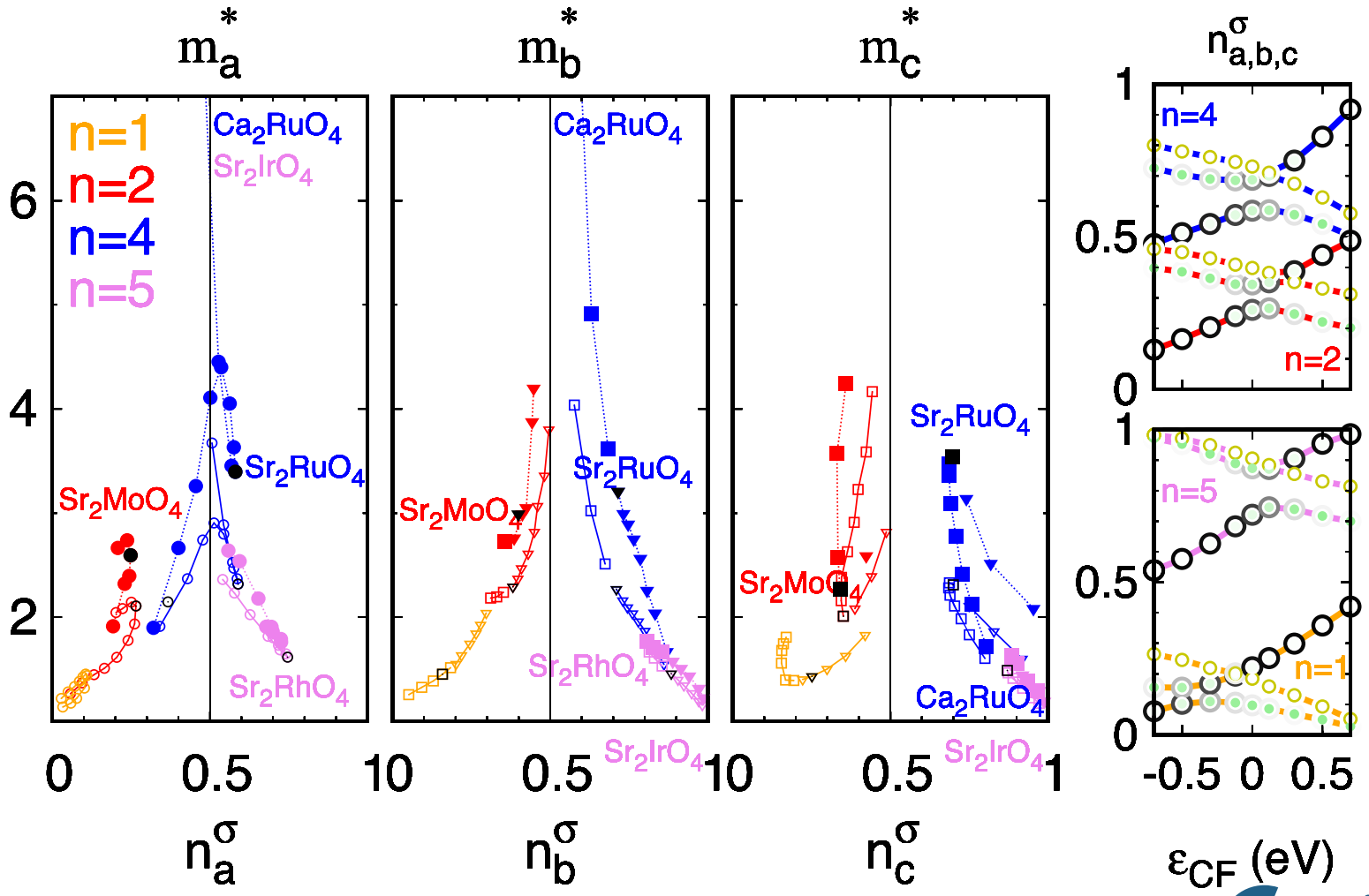
switch on moderate spin-orbit coupling

λ as in Sr_2RuO_4 (4d)



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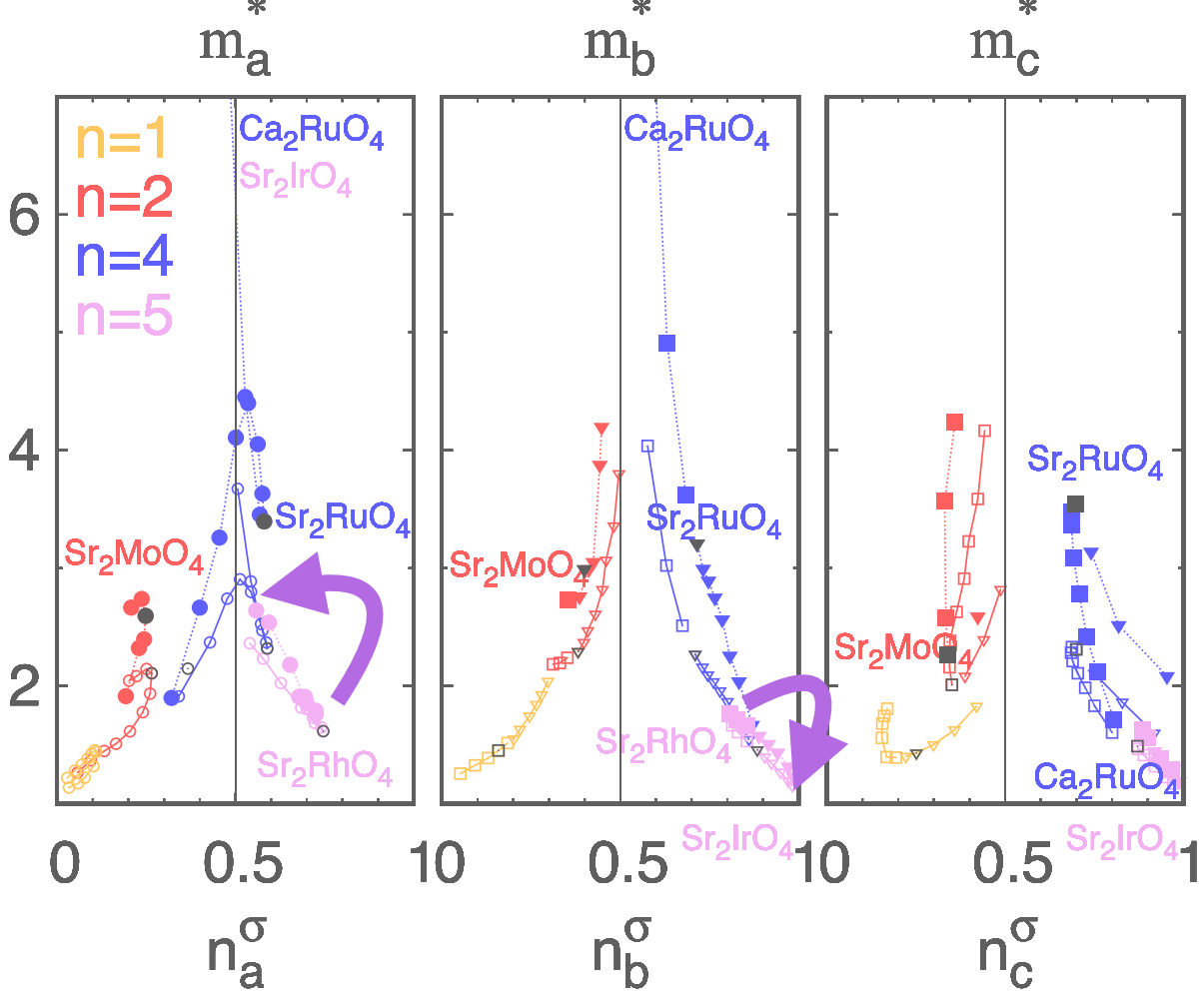
putting the map to a test: Sr_2IrO_4

λ as in Sr_2RuO_4 (4d)

change of configuration effect:

mass-matrix trace invariant: $m_a^* \sim 1+3(m_{av}-1)$



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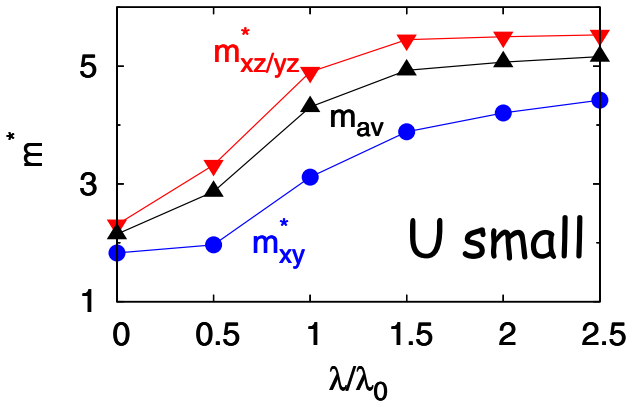
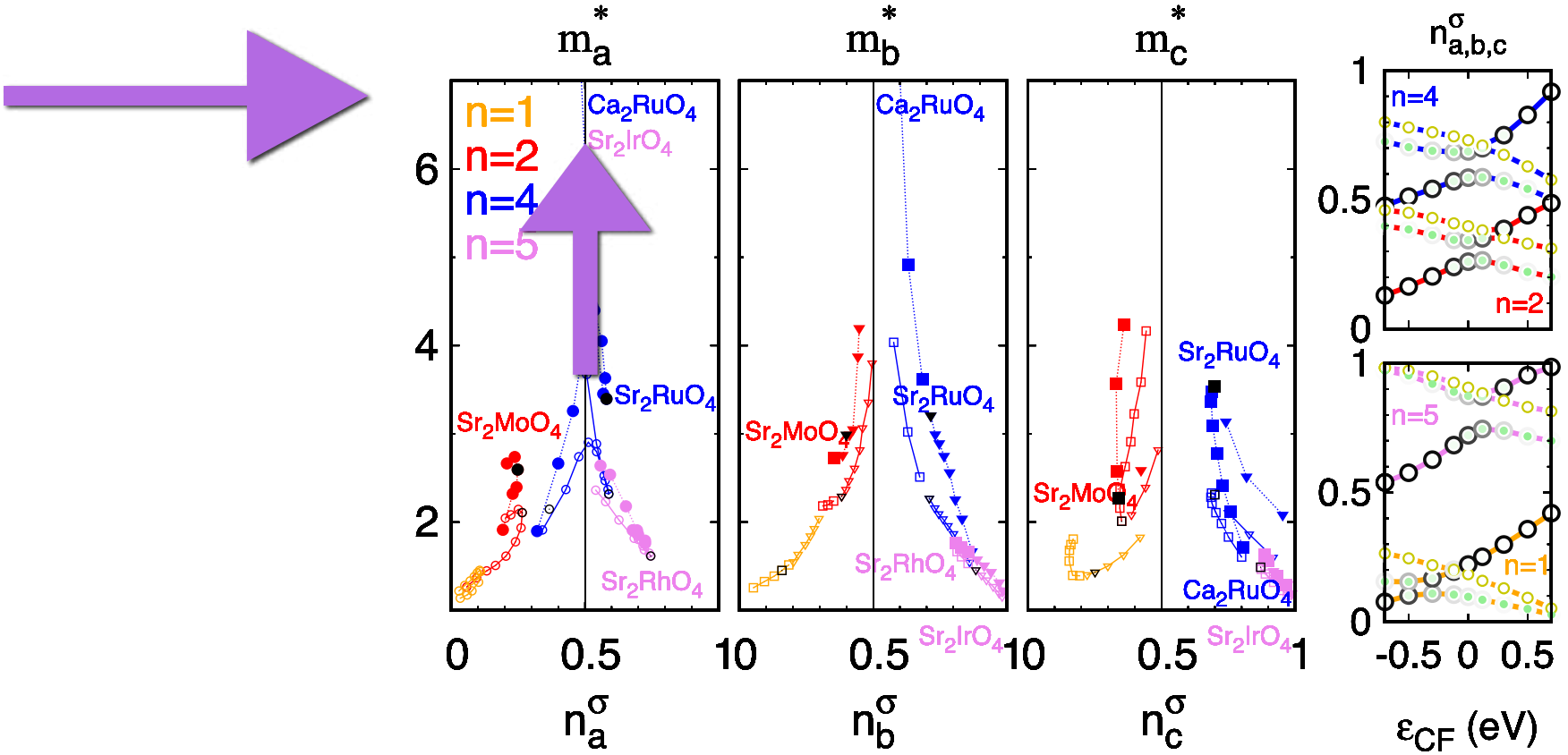
putting the map to a test: Sr_2IrO_4



λ two times larger (5d)

suppression of spin-orbital fluctuations



putting the map to a test: pressure effects

Sr_2IrO_4: persistence of insulating state state under very high pressure

(tetragonal till 40 GPa)

IOP Publishing

Journal of Physics: Condensed Matter

J. Phys.: Condens. Matter **26** (2014) 255603 (5pp)

doi:10.1088/0953-8984/26/25/255603

Persistent non-metallic behavior in Sr_2IrO_4 and $Sr_3Ir_2O_7$ at high pressures

D A Zocco[1,6], J J Hamlin[1,7], B D White[1], B J Kim[2,3], J R Jeffries[4], S T Weir[4], Y K Vohra[5], J W Allen[3], and M B Maple[1]

PHYSICAL REVIEW B **101**, 144102 (2020)

Persistent insulating state at megabar pressures in strongly spin-orbit coupled Sr_2IrO_4

Chunhua Chen,[1,2] Yonghui Zhou,[1,*] Xuliang Chen,[1] Tao Han,[3] Chao An,[3] Ying Zhou,[3] Yifang Yuan,[1,2] Bowen Zhang,[1,2] Shuyang Wang,[1,2] Ranran Zhang,[1] Lili Zhang,[4] Changjin Zhang,[1,3,5] Zhaorong Yang,[1,3,5,†] Lance E. DeLong,[6] and Gang Cao[7,‡]

[1]*Anhui Province Key Laboratory of Condensed Matter Physics at Extreme Conditions, High Magnetic Field Laboratory, Chinese Academy of Sciences, Hefei 230031, China*

[2]*Science Island Branch of Graduate School, University of Science and Technology of China, Hefei 230026, China*

[3]*Institutes of Physical Science and Information Technology, Anhui University, Hefei 230601, China*

hanghai Synchrotron Radiation Facility, Shanghai Advanced Research Institute, Chinese Academy of Sciences, Shanghai 201204, China

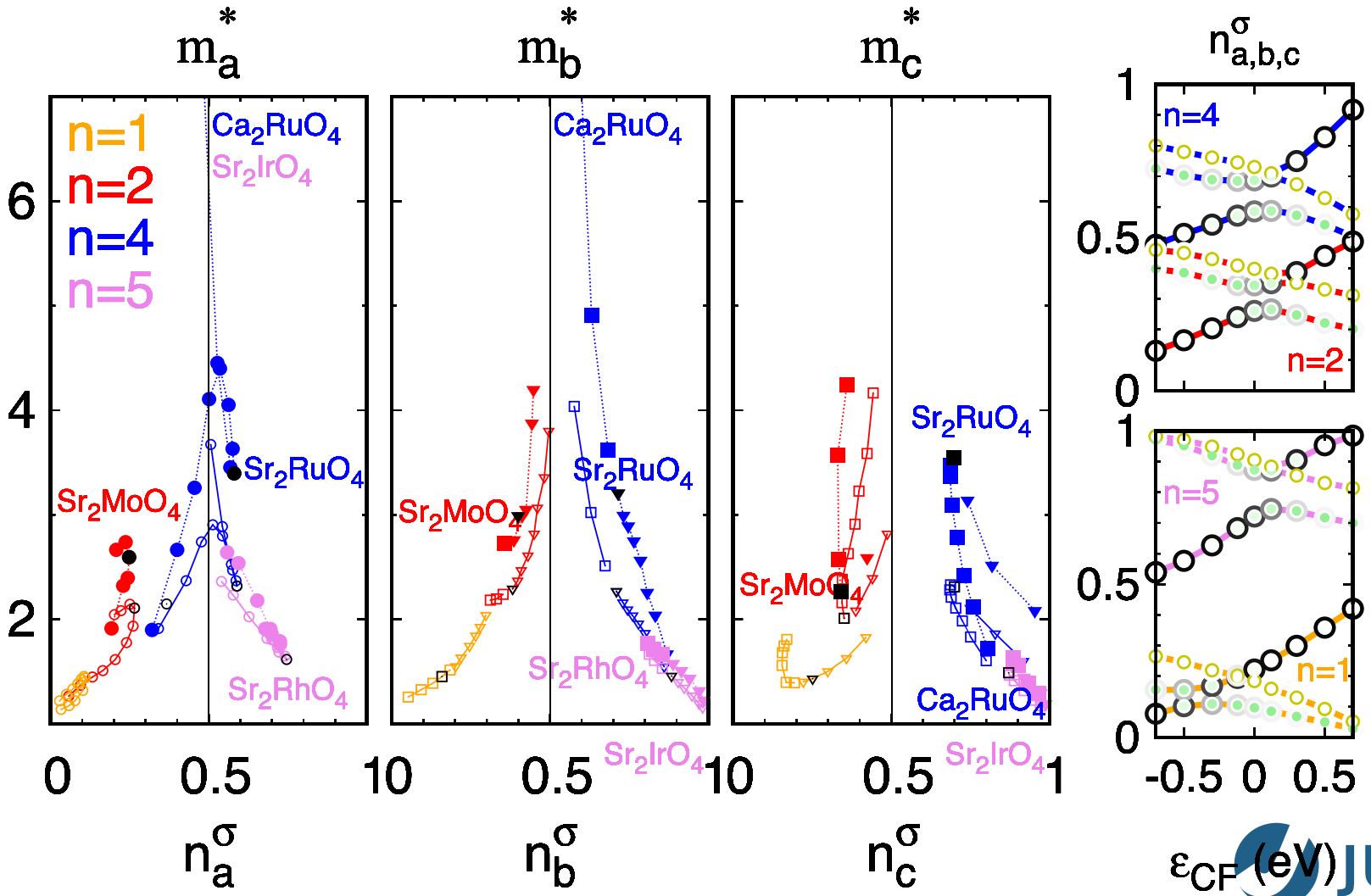
[5]*Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China*

[6]*Department of Physics and Astronomy, University of Kentucky, Lexington, Kentucky 40506, USA*

[7]*Department of Physics, University of Colorado at Boulder, Boulder, Colorado 80309, USA*

position in the map

j_{eff}=1/2 orbital order is stable



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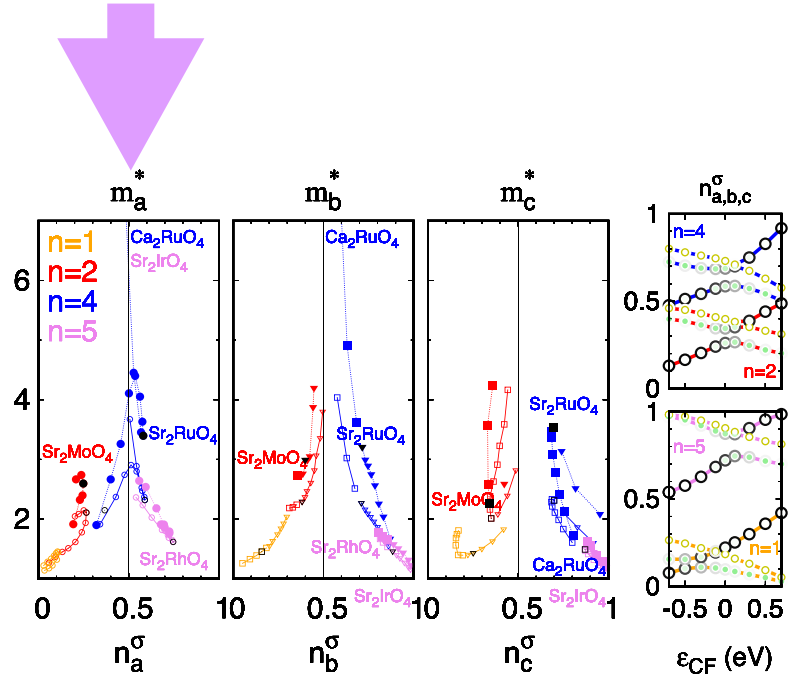
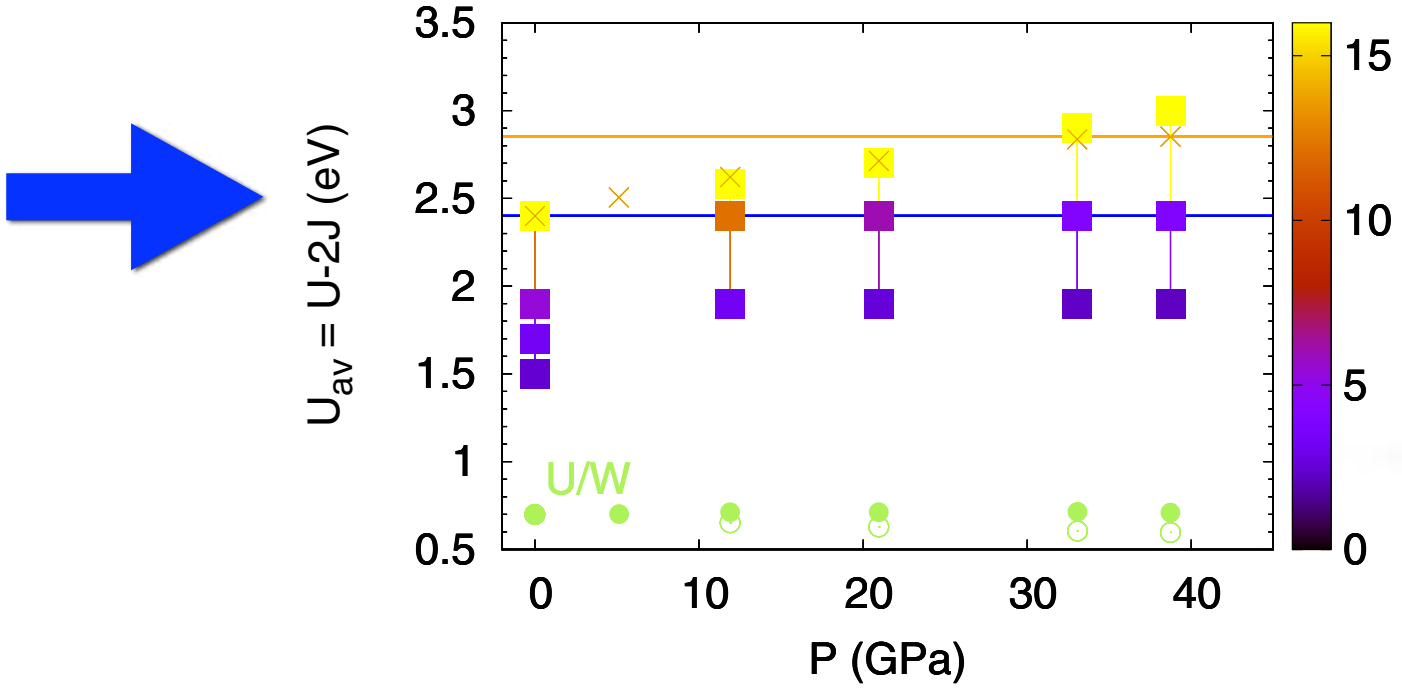
W increases but slowed down by rotations



metal already at 12 GPa

color map:
effective mass



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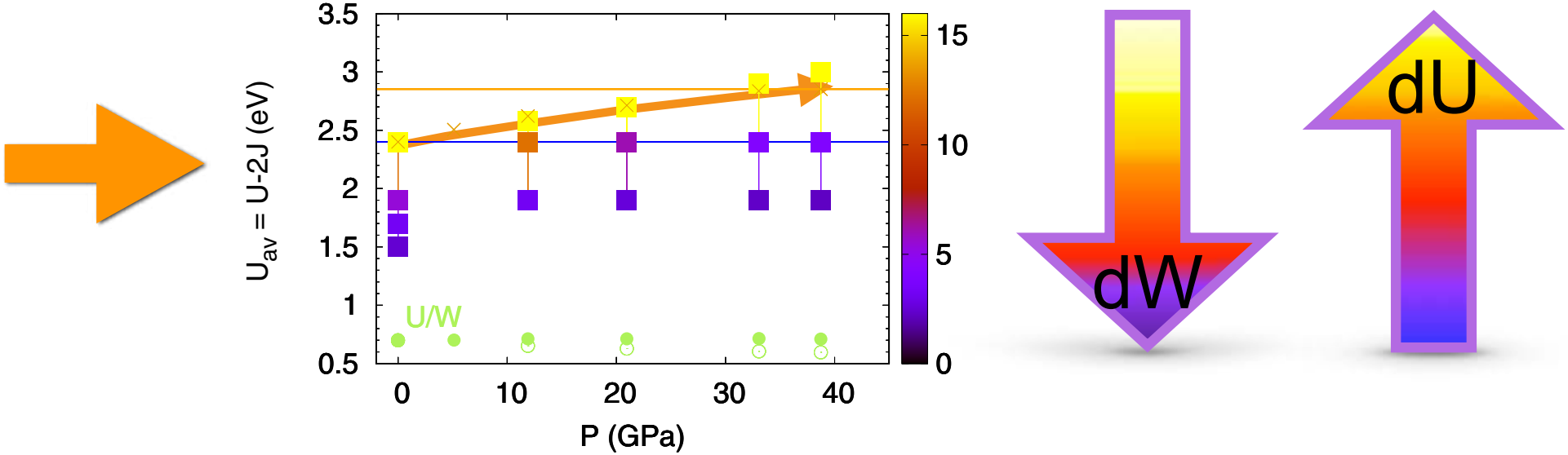
however W/U~constant

screened U (cRPA) also increases



PHYSICAL REVIEW B **111**, L121101 (2025)

Letter

Nature of the high-pressure insulating state in Sr_2IrO_4: Mott picture

Guoren Zhang,[1,2,3] Hanif Hadipour,[4] and Eva Pavarini[3]

[1]*School of Physics and Technology, Nantong University, Nantong 226019, People's Republic of China*
[2]*Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, People's Republic of China*
[3]*Peter Grünberg Institute, Forschungszentrum Jülich, D-52425 Jülich, Germany*
[4]*Department of Physics, University of Guilan, Rasht 41335-1914, Iran*

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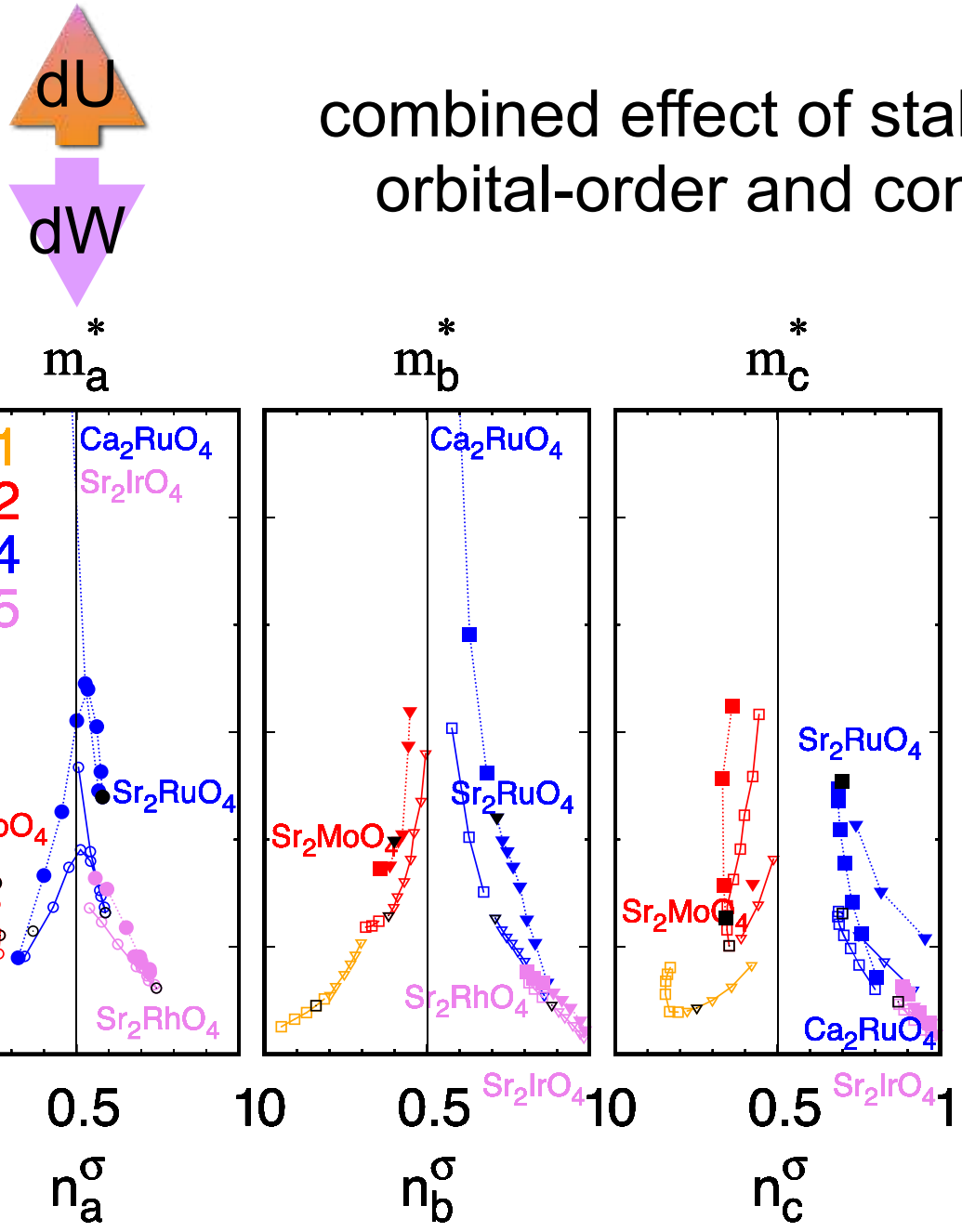
very close to MIT under high pressure!



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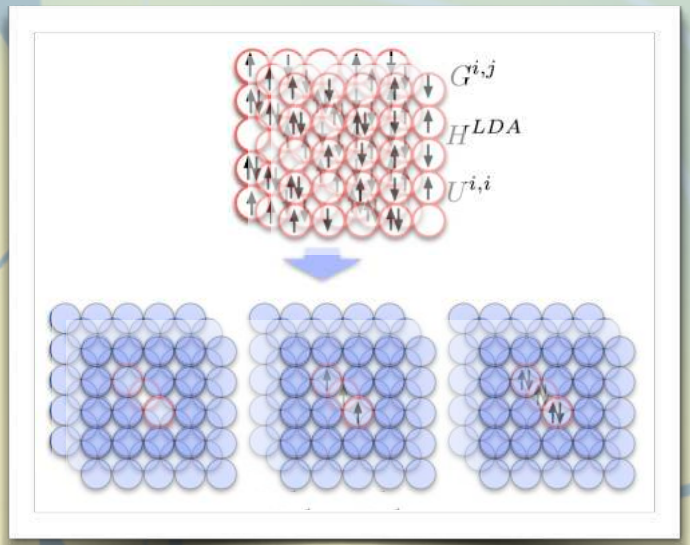
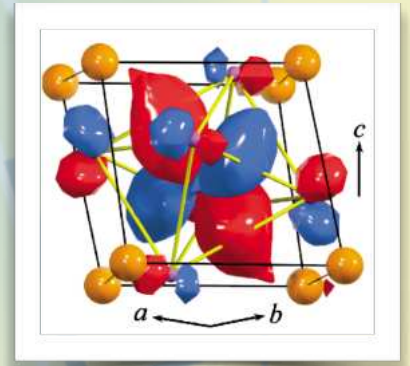
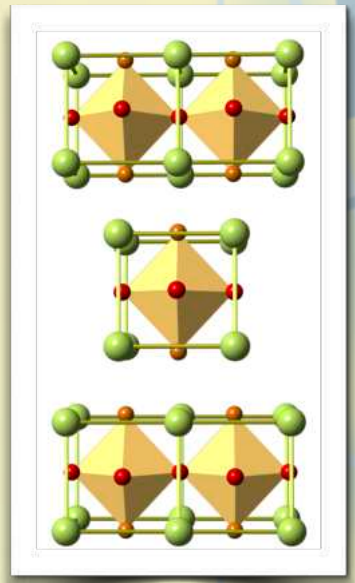
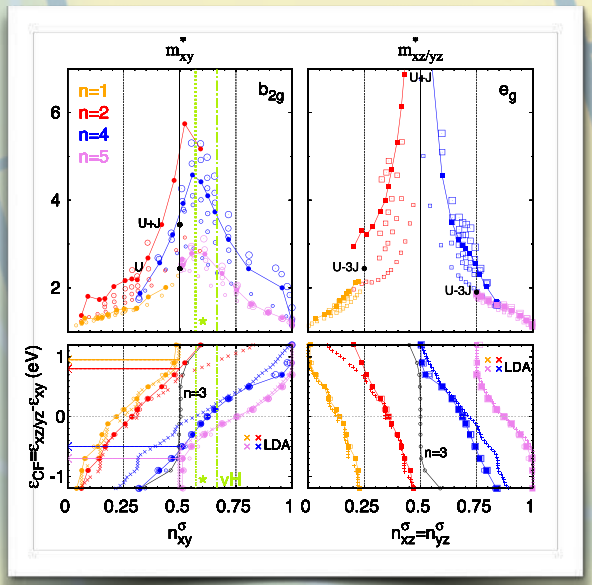
conclusions

- correlated materials
- DFT+DMFT









- Sr_2RuO_4 and its family
- disentangle complexity via an unifying map

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thank you!

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