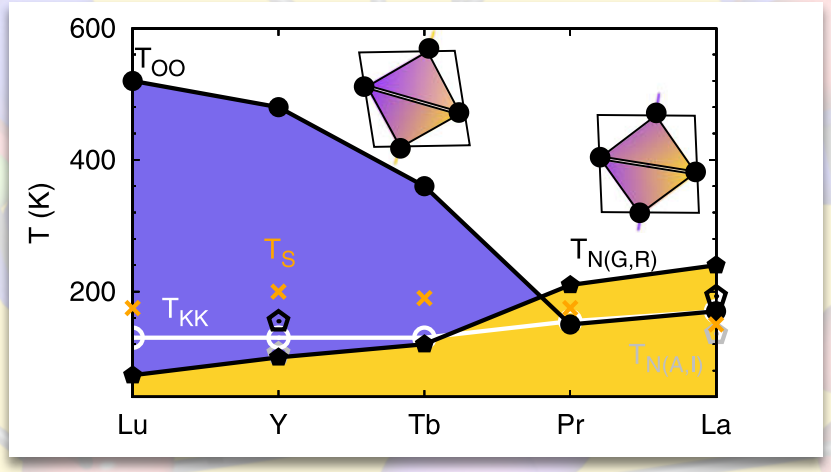
Kugel-Khomskii materials: flipping the order of transitions



Eva Pavarini

Forschungszentrum Jülich

Peter Grünberg Institute

spontaneous ordering of orbitals

Crystal structure and magnetic properties of substances with orbital degeneracy

K. I. Kugel' and D. I. Khomskiĭ
P. N. Lebedev Physics Institute
(Submitted November 13, 1972)
Zh. Eksp. Teor. Fiz. **64**, 1429-1439 (April 1973)

Exchange interaction in magnetic substances containing ions with orbital degeneracy is considered. It is shown that, among with spin ordering, superexchange also results in cooperative ordering of Jahn-Teller ion orbitals, which, generally speaking, occurs at a higher temperature and is accompanied by distortion of the lattice (which is a secondary effect here). Concrete studies are performed for substances with a perovskite structure ($KCuF_3$, $LaMnO_3$, MnF_3). The effective spin Hamiltonian is obtained for these substances and the properties of the ground state are investigated. The orbital and magnetic structures obtained in this way without taking into account interaction with the lattice are in accord with the structures observed experimentally. The approach employed also permits one to explain the strong anisotropy of the magnetic properties of these compounds and to obtain a reasonable estimate for the critical temperatures.

$KCuF_3$

$LaMnO_3$

strong Coulomb repulsion (the Hubbard U)

+ orbitals degrees of freedom

= orbital super-exchange

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orbital ordering and orbital physics

CORRELATED ELECTRON SYSTEMS

REVIEW

Orbital Physics in Transition-Metal Oxides

Y. Tokura[1,2] and N. Nagaosa[1]

An electron in a solid, that is, bound to or nearly localized on the
atomic site, has three attributes: charge, spin, and orbital. Th
represents the shape of the electron cloud in solid. In transiti
oxides with anisotropic-shaped d-orbital electrons, the Coulomb
tion between the electrons (strong electron correlation effe
importance for understanding their metal-insulator transitions a
erties such as high-temperature superconductivity and colossal
toresistance. The orbital degree of freedom occasionally plays a
tant role in these phenomena, and its correlation and/or order
transition causes a variety of phenomena through strong coupl
charge, spin, and lattice dynamics. An overview is given here
"orbital physics," which will be a key concept for the science a
nology of correlated electrons.

VOLUME 85, NUMBER 18 PHYSICAL REVIEW LETTERS 30 OCTOBER 2000

Orbital Liquid in Three-Dimensional Mott Insulator: $LaTiO_3$

G. Khaliullin[1,2] and S. Maekawa[2]

[1]*Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*
[2]*Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*

(Received 5 June 2000)

of spin and orbital states in Mott insulator $LaTiO_3$. The spin-orbital superexchange
(t_{2g}) ions in cubic crystal suffers from a pathological degeneracy of orbital states
Quantum effects remove this degeneracy and result in the formation of the coherent
the orbital moment of t_{2g} level is fully quenched. We find a finite gap for orbital
sordered state of local degrees of freedom on unfrustrated, simple cubic lattice is
al liquid state naturally explains observed anomalies of $LaTiO_3$.

Electronic reconstruction at an interface between a Mott insulator and a band in

Satoshi Okamoto & Andrew J. Millis

Department of Physics, Columbia University 538
New York 10027, USA

Surface science is an important and we
materials science involving the study

PRL **99,** 156401 (2007) PHYSICAL REVIEW LETTERS 12 OCTOBER 2007

Superexchange Interaction in Orbitally Fluctuating RVO_3

J.-S. Zhou and J. B. Goodenough
Texas Materials Institute, University of Texas at Austin, Austin, Texas 78712, USA

J.-Q. Yan
Ames Laboratory, Ames, Iowa 50011, USA

Y. Ren
Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA

(Received 18 May 2007; published 8 October 2007)

103, 067205 (2009) PHYSICAL RE

Magnetically Hidden Order of Kra

George Jackeli* and Giniyat Khaliullin
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany
(Received 10 June 2009; published 7 August 2009)

We formulate and study an effective Hamiltonian for low-energy Kramers doublets of d^1 ions on a square lattice. We find that the system exhibits a magnetically hidden order in which the expectation values of the local spin and orbital moments both vanish. The order parameter responsible for a time-reversal symmetry breaking has a composite nature and is a spin-orbital analog of a magnetic octupole. We argue that such a hidden order is realized in the layered perovskite Sr_2VO_4.

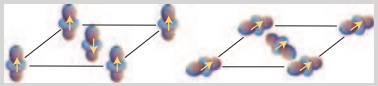
DOI: 10.1103/PhysRevLett.103.067205 PACS numbers: 75.30.Et, 71.70.Ej, 75.10.Jm

TRANSITION METAL OXIDES

Ferroelectricity driven by orbital order

The discovery that the rotation of the orbital arrangement in manganites induces ferroelectricity exposes an intriguing phase transition that could serve as a blueprint for novel applications.

BERNHARD KEIMER
is at the Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany
e-mail: B.Keimer@fkf.mpg.de



Transition metal oxides have fascinated scientists since the 1950s, when the newly developed technique of neutron diffraction was used to show that the compound $La_{1-x}Ca_xMnO_3$ exhibits a rich variety of structural and magnetic phases as the Ca concentration is tuned[1]. The fascination has increased in the wake of the discovery of high-temperature superconductivity in a chemically similar compound,

Figure 1 Possible arrangements of Mn^{3+} d-orbitals on a square lattice. The patterns are two-dimensional versions of orbitally ordered states actually observed in manganese oxides. The corresponding magnetic states are indicated by yellow arrows.

[PDF] 1 Metal-Insulator Transition and Orbital Order in ... - arXiv...

arxiv.org/pdf/0811.3378

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...ngular lattice system
...Queen et al. [Phys.
...tion-metal ...
...ifornia, Los Angeles
by Z Nussinov - Cited by 80 - Related articles
resonant X-ray scattering techniques in which the 3d **orbital order** is detected by its

ECS Journal of Solid State Science and Technology, 2022 **11** 054004
2162-8777/2022/11(5)/054004/16/$40.00 © 2022 The Electrochemical Society ("ECS"). Published on behalf of ECS by IOP Publishing Limited

CrossMark

Review—Orbital Physics: Glorious Past, Bright Future

D. I. Khomskii[z]

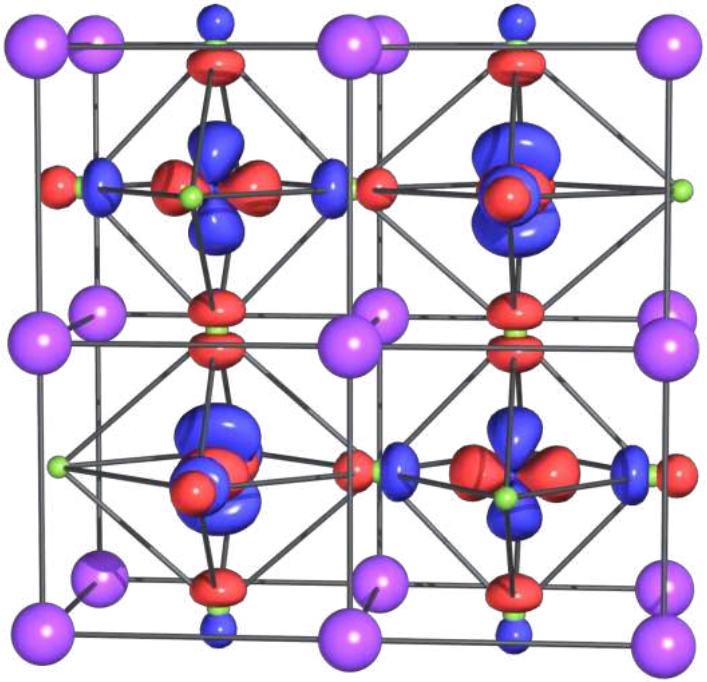
II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

Transition metal (TM) compounds present a very big class of materials with quite diverse properties. Ther
and systems with insulator–metal transitions among them; most magnetic systems are TM compounds; t
superconductors among them. Their very rich properties are largely determined by the strong interplay
freedom: charge; spin; orbital; lattice. Orbital effects play a very important role in these systems—and not o
of this field, initiated by Goodenough almost 70 years ago, turned out to be very fruitful and produced a lot
this short review I discuss the basics of orbital physics and summarize the main achievements in th
Goodenough played a pivotal role, and which are nowadays widely used to explain many properties of TM c
part of the text I discuss novel developments and perspectives in orbital physics, which is still a very a
constantly producing new surprises.

the secondary effect

co-operative Jahn-Teller-like distortion

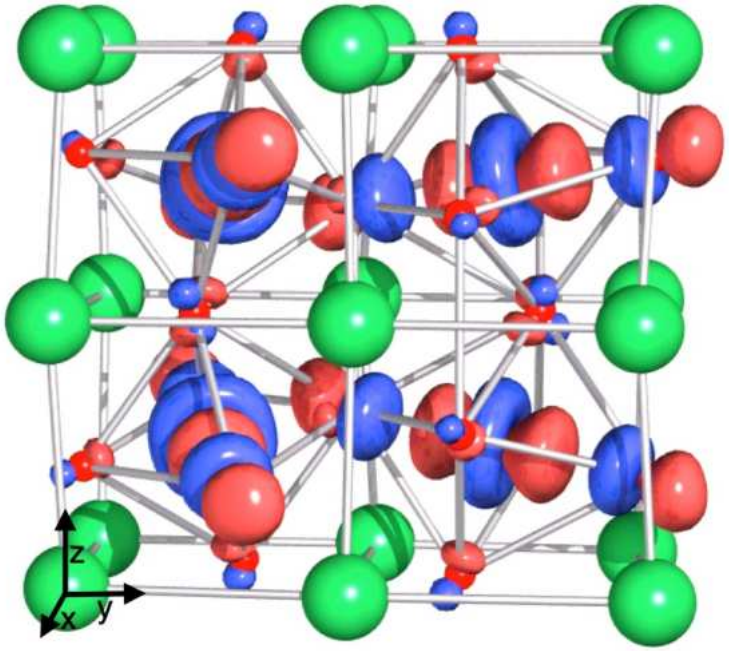
$KCuF_3$



$t_{2g}^6 e_g^3$

G-type OO

$LaMnO_3$



$t_{2g}^3 e_g^1$

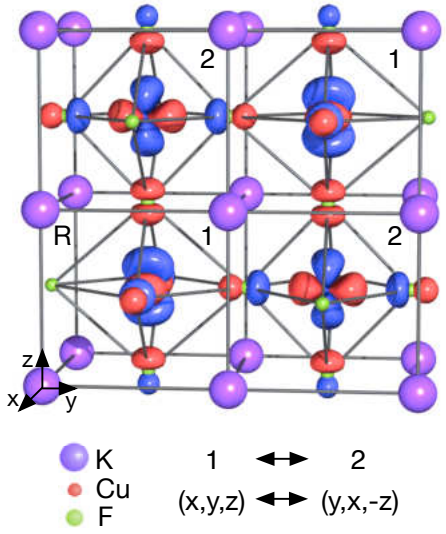
C-type OO

but there is the Jahn-Teller theorem

Crystal Distortion in Magnetic Compounds

JUNJIRO KANAMORI*
Institute for the Study of Metals, University of Chicago, Chicago 37, Illinois

The crystal distortion which arises from the Jahn-Teller effect is discussed in several examples. In the case of compounds containing Cu^{2+} or Mn^{3+} at octahedral sites, the lowest orbital level of these ions is doubly degenerate in the undistorted structure, and there is no spin-orbit coupling in this level. It is shown that, introducing a fictitious spin to specify the degenerate orbital states, we can discuss the problem by analogy with the magnetic problems. The "ferromagnetic" and "antiferromagnetic" distortions are discussed in detail. The transition from the distorted to the undistorted structure is of the first kind for the former and of the second kind for the latter. Higher approximations are discussed briefly. In compounds like FeO, CoO, and $CuCr_2O_4$, the lowest orbital level is triply degenerate, and the spin-orbit coupling is present in this level. In this case the distortion is dependent on the magnitude of the spin-orbit coupling relative to the strength of the Jahn-Teller effect term. The distortion at absolute zero temperature and its temperature dependence are discussed.

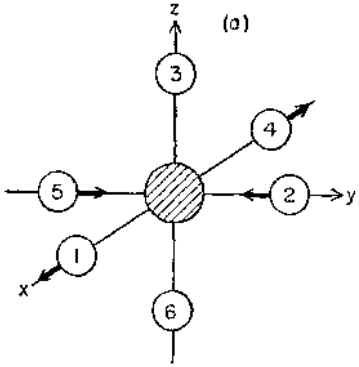


$E_0 + \Delta/2$

$E_0 - \Delta/2$

Δ_{CF}

e_g states



$$|\theta\rangle = \sin\frac{\theta}{2}|3z^2 - 1\rangle + \cos\frac{\theta}{2}|x^2 - y^2\rangle$$

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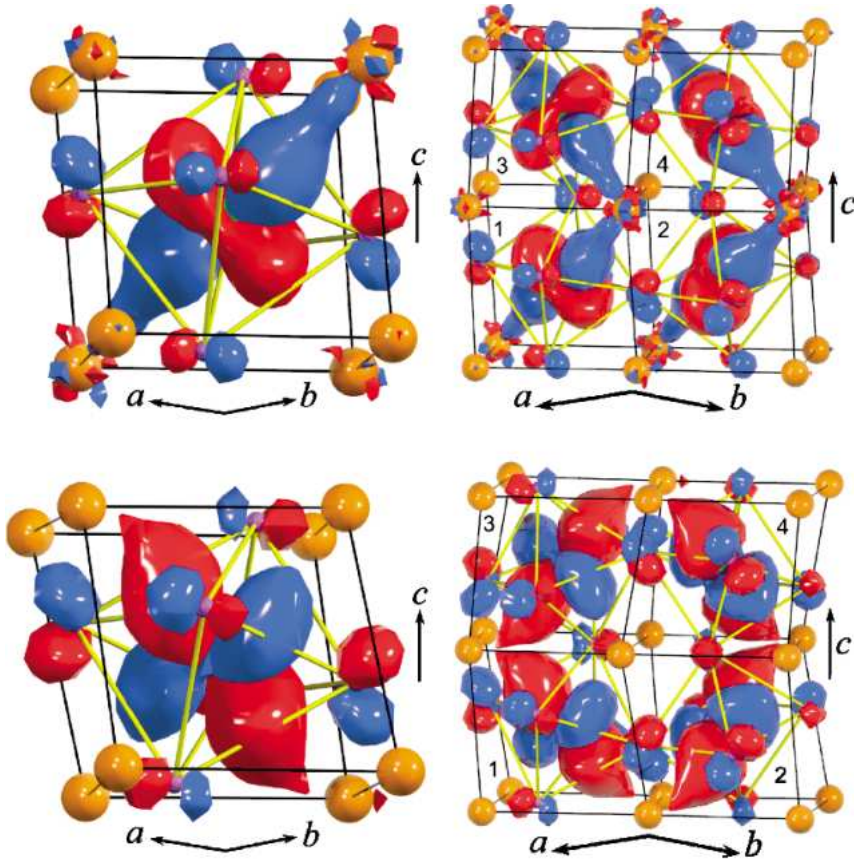
a small CF splitting can be enough!

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

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

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

$LaTiO_3$



$YTiO_3$

t_{2g}^1

CF=200-300 meV

LDA+DMFT 770 K

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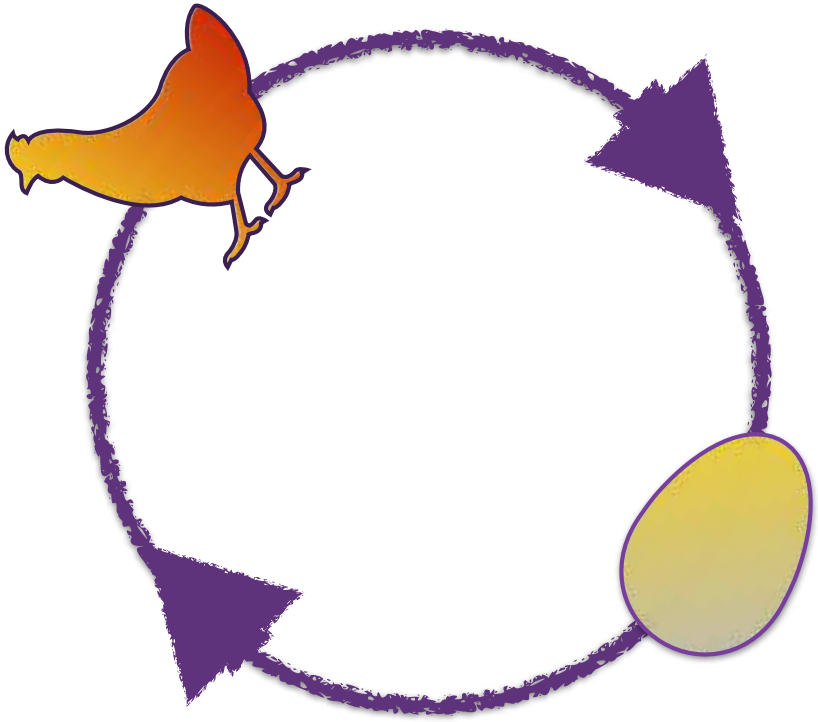
Kugel-Khomskii materials ?

a chicken-and-egg problem

distortions



orbital ordering

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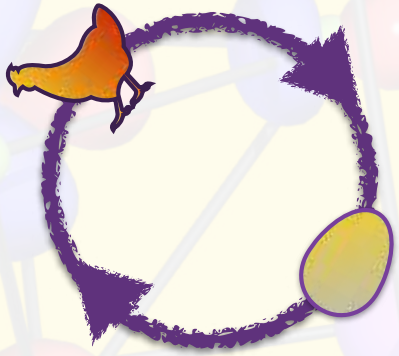
(i) are there true Kugel-Khomskii materials ?

and how do we identify them?

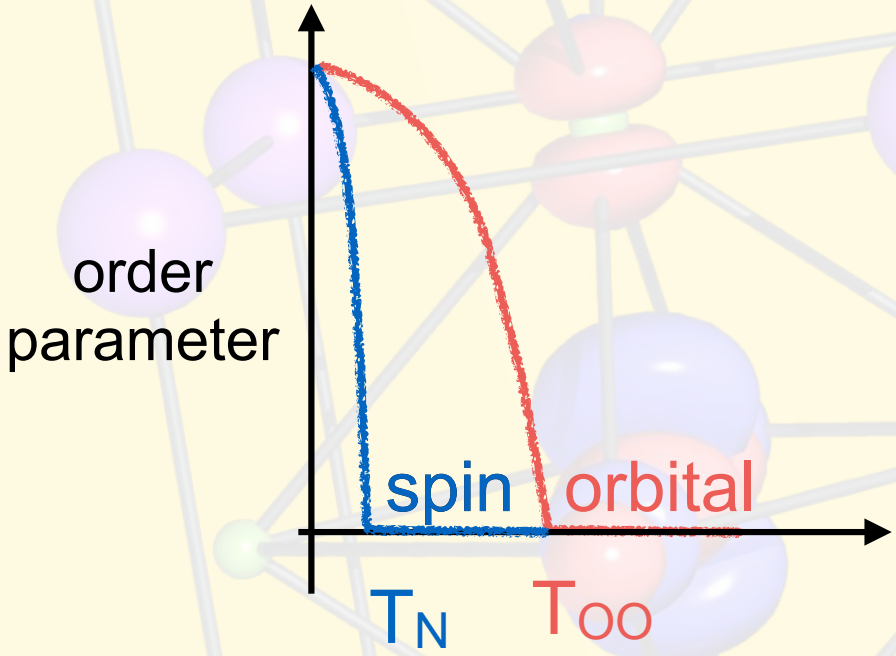
a chicken-and-egg problem



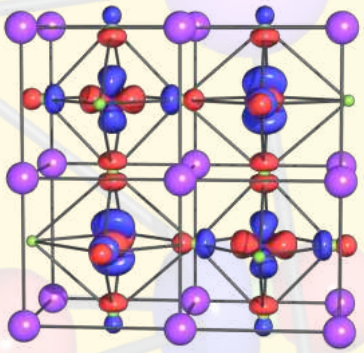
(ii) why $T_{OO}>T_N$?

can one flip the transitions?

- $T_{OO}>T_N$



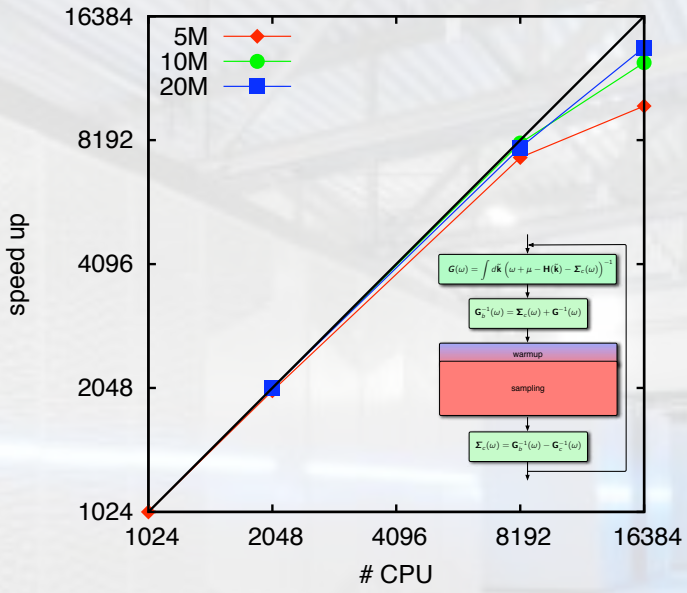
$KCuF_3$



T_N~40 K T_{OO} ~1400 K

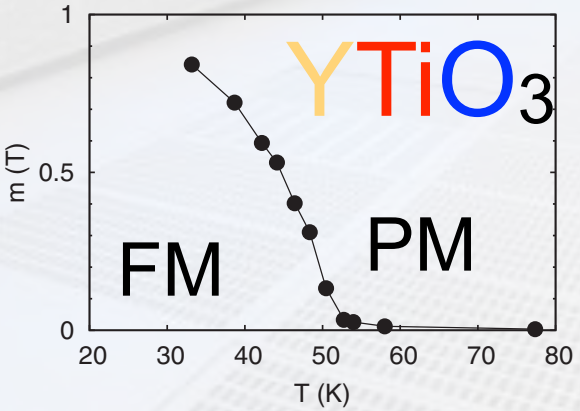
cDMFT/QMC on JURECA

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



DMFT and cDMFT
generalized QMC solvers:

- 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)



solution of chicken and egg problem

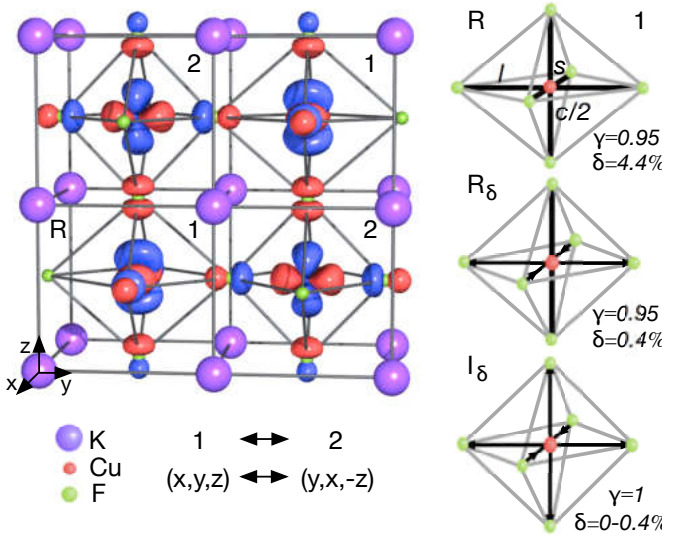
PRL **101,** 266405 (2008) PHYSICAL REVIEW LETTERS week ending 31 DECEMBER 2008

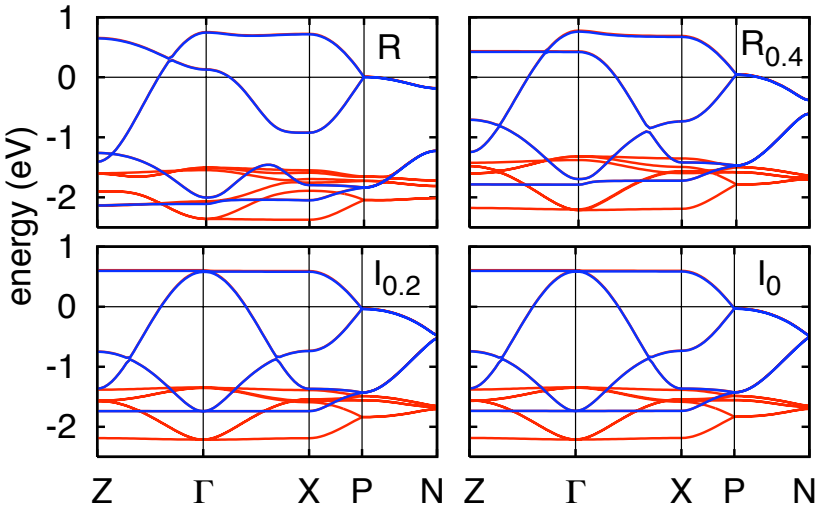
Mechanism for Orbital Ordering in $KCuF_3$

E. Pavarini,[1] E. Koch,[1] and A. I. Lichtenstein[2]

[1]*Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany*
[2]*Institute of Theoretical Physics, University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany*

(Received 18 August 2008; published 31 December 2008)





to single out KK effects:

(i) progressively reduce distortion (hence CF splitting)

(ii) calculate order parameter vs temperature

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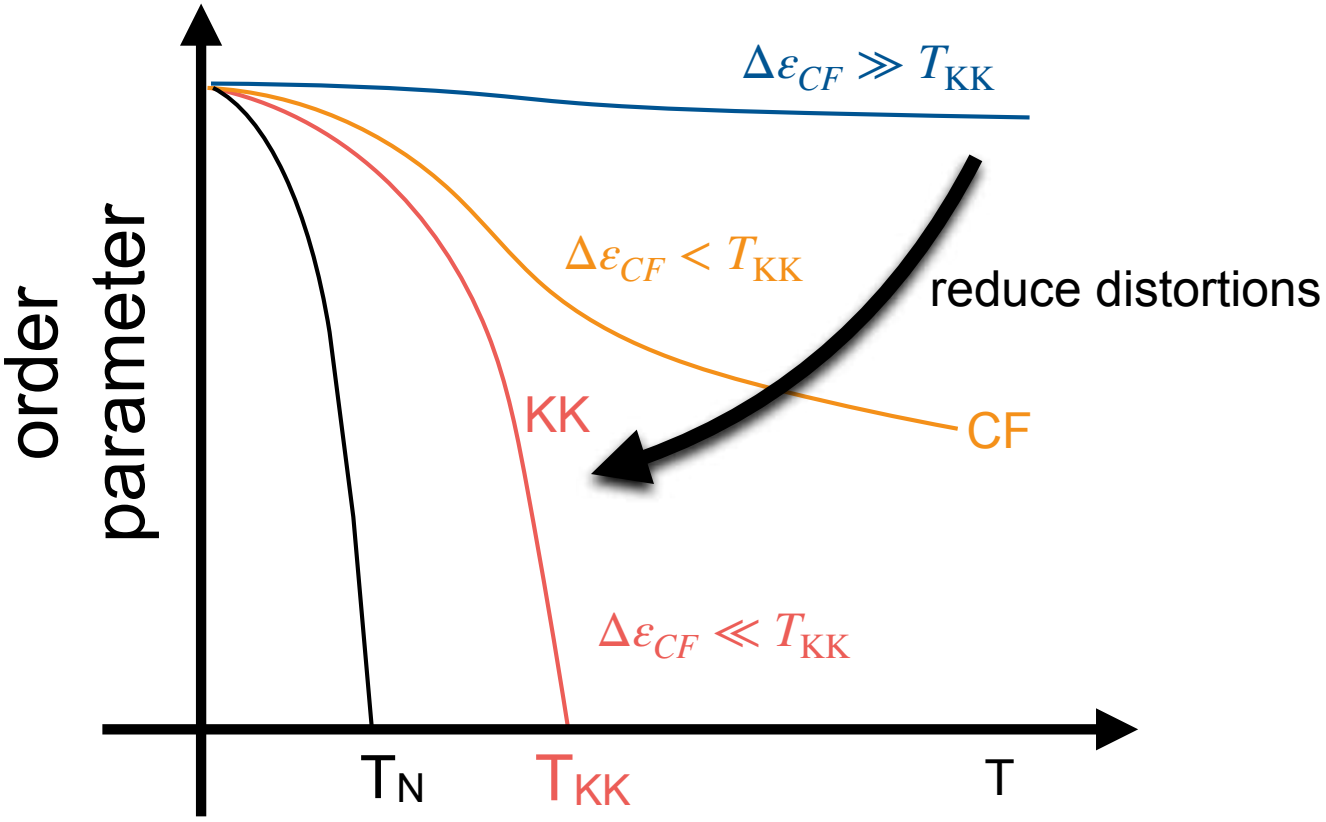
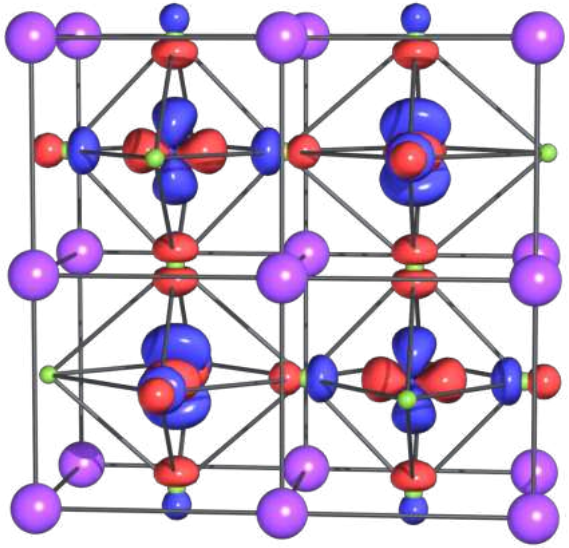
order parameter vs temperature





if KK is the mechanism: $T_{OO} \sim T_{KK}$

$KCuF_3$ $T_N \sim 40$ K $T_{OO} \sim 1400$ K

Phys. Rev. Lett. **101**, 266405 (2008)

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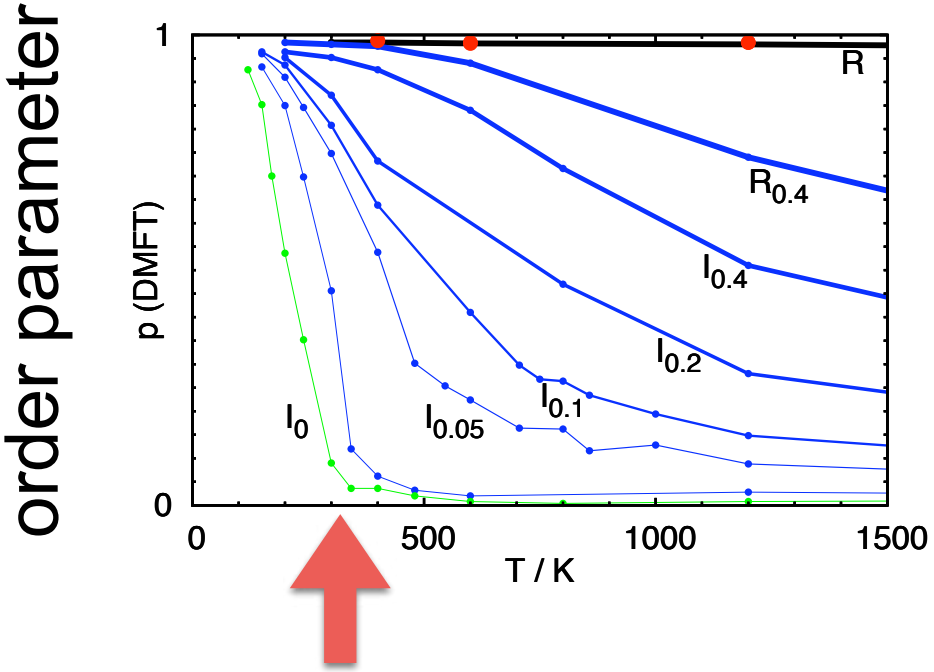
KK SE large but not sufficient alone

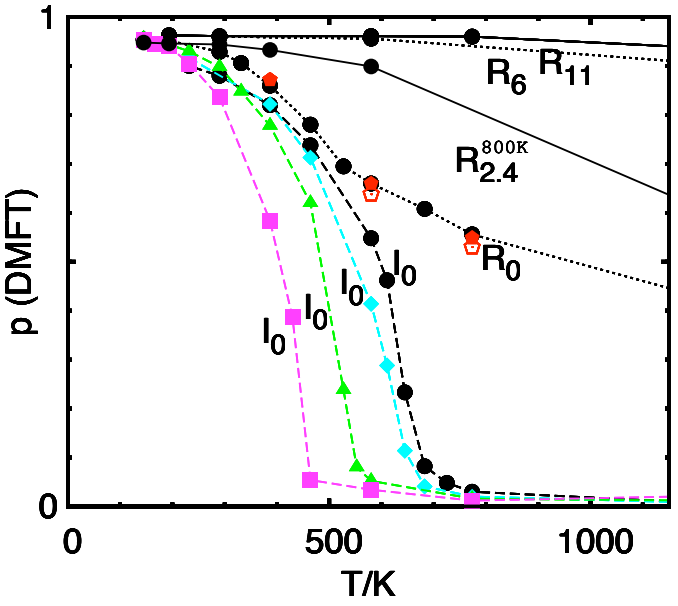
$KCuF_3$



Phys. Rev. Lett. **101**, 266405 (2008)

$T_{KK} \sim 350\ K \ll T_{OO} \sim 1400\ K$

$LaMnO_3$



Phys. Rev. Lett. **104**, 086402 (2010)

$T_{KK} \sim 600\ K \ll T_{OO} \sim 1200\ K$

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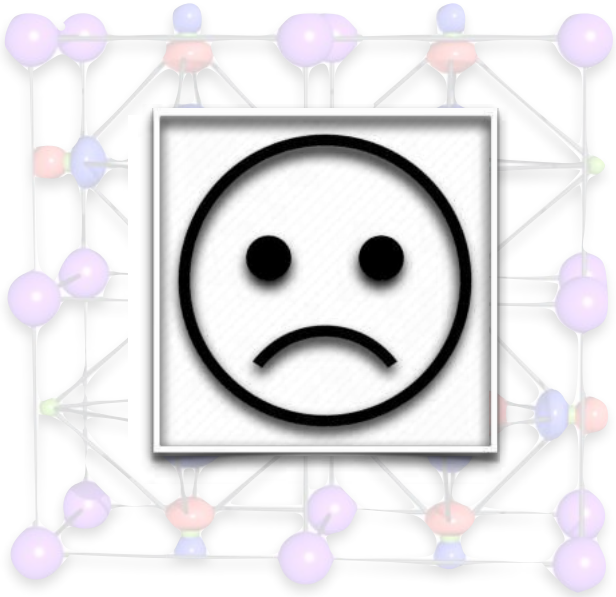
so far for e_g systems…

KK super-exchange large but not sufficient to explain ordering at high temperature

$KCuF_3$

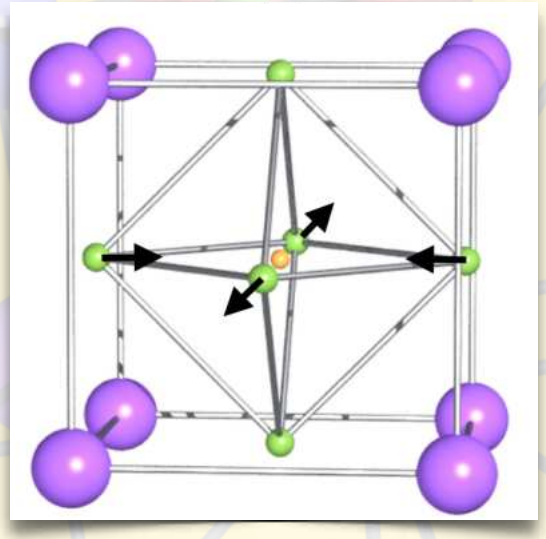


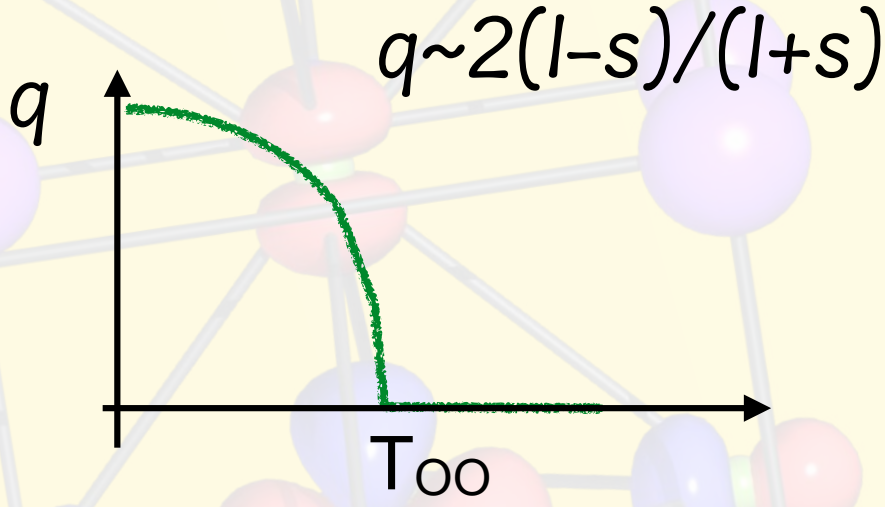
$LaMnO_3$

(and many more systems)

$KCuF_3$ not a true KK material

… but also not a true Jahn-Teller system!





l= long CuF bond

s= short CuF bond

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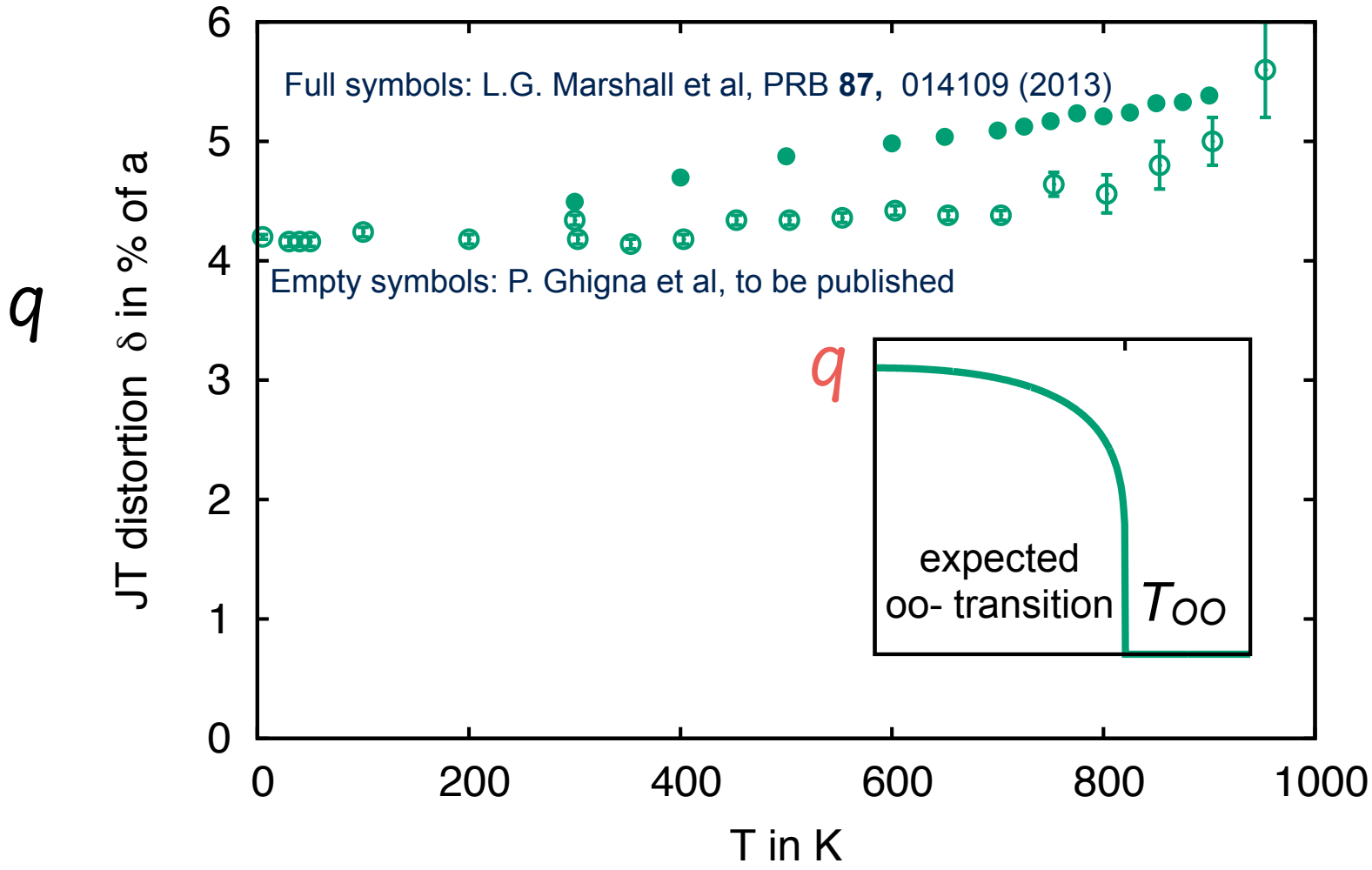
experiments: q increases with temperature

theory reproduce this behavior

PRB **96**, 054107 (2017)

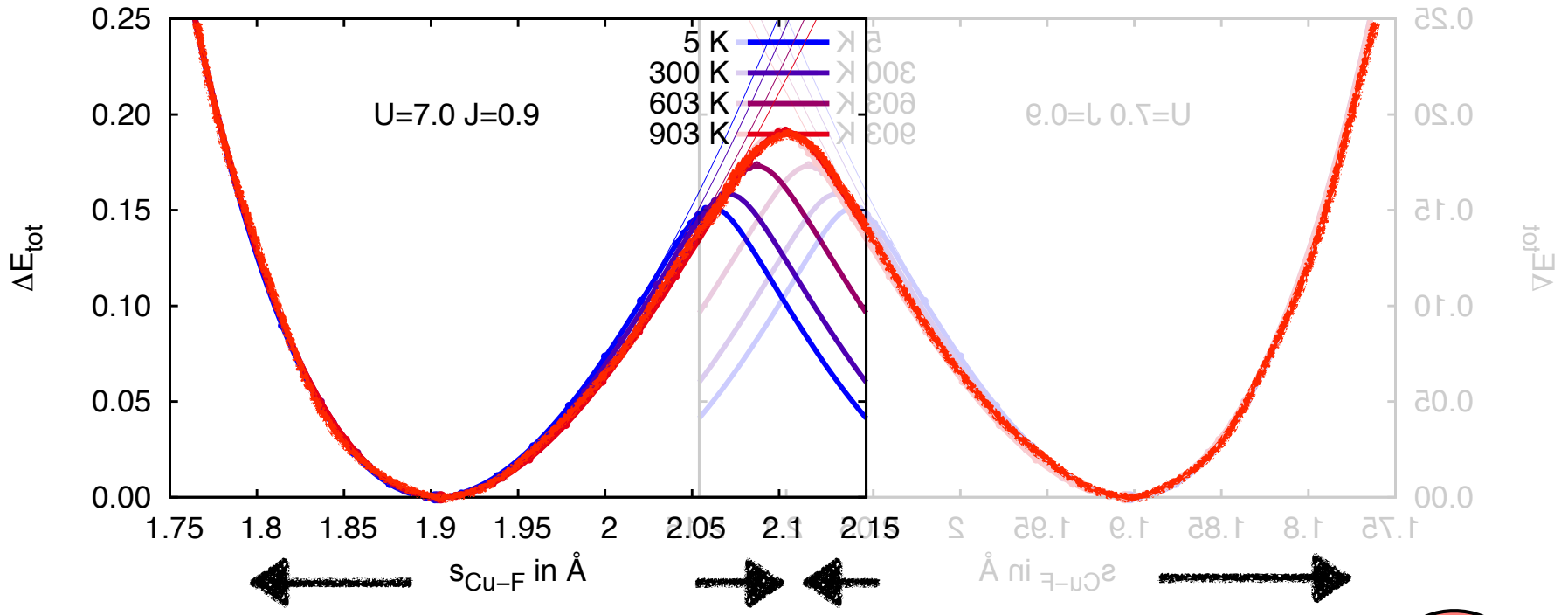


the *T*-dependence is via the lattice constant!

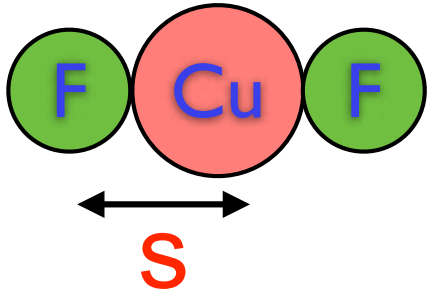
PHYSICAL REVIEW B **96**, 054107 (2017)

Thermally assisted ordering in Mott insulators

Hunter Sims,[1] Eva Pavarini,[2,3] and Erik Koch[1,2,3,*]



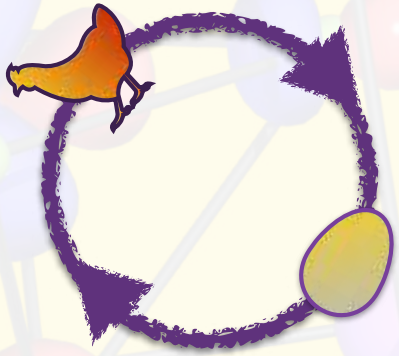
touching ions!



(i) are there true Kugel-Khomskii materials ?

and how do we identify them?

a chicken-and-egg problem



let us change perspective

focus on electronic effects only

candidates: t_{2g} systems

larger orbital degeneracy, smaller electron-lattice coupling, smaller crystal-field coupling

augment DMFT with general SE Hamiltonians

PHYSICAL REVIEW B **102**, 035113 (2020)

Origin of orbital ordering in $YTiO_3$ and $LaTiO_3$

Xue-Jing Zhang, Erik Koch, and Eva Pavarini
Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

(Received 14 April 2020; accepted 15 June 2020; published 6 July 2020)

The origin of orbital order in correlated transition-metal compounds is strongly debated. For the paradigmatic e_g systems $KCuF_3$ and $LaMnO_3$, it has been shown that the electronic Kugel'-Khomskii mechanism alone is not sufficient to drive the orbital-ordering transition up to the high temperatures at which it is experimentally observed. In the case of t_{2g} compounds, however, the role played by the superexchange interaction remains unclear. Here we investigate this question for two representative systems, the $3d\ t_{2g}^1$ Mott insulators $LaTiO_3$ and $YTiO_3$. We show that the Kugel'-Khomskii superexchange transition temperature T_{KK} is unexpectedly large, comparable to the value for the e_g^3 fluoride $KCuF_3$. By deriving the general form of the orbital superexchange

PHYSICAL REVIEW B **105**, 115104 (2022)

General superexchange Hamiltonians for magnetic and orbital physics in e_g and t_{2g} systems

Xue-Jing Zhang,[1] Erik Koch,[1,2] and Eva Pavarini[1,2,*]
[1]*Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany*
[2]*JARA High-Performance Computing, 52062 Aachen, Germany.*

(Received 6 December 2021; accepted 16 February 2022; published 3 March 2022)

Material-specific super-exchange Hamiltonians are the key to studying spin and orbital physics in strongly correlated materials. Recently, via an irreducible-tensor operator representation, we derived the orbital superexchange Hamiltonian for t_{2g}^1 perovskites and successfully used it, in combination with many-body approaches, to explain orbital physics in these systems. Here, we generalize our method to e_g^n and t_{2g}^n systems at arbitrary integer filling n, including both spin and orbital interactions. The approach is suitable for numerical implementations

multipolar super-exchange expansion

$$\hat{H}_{\mathrm{SE}}^{i,j} = \sum_{qq'} \sum_{\nu\nu'} \sum_{rr'} \sum_{\mu\mu'} \hat{\tau}_i^{r\mu;q\nu} D_{r\mu,r'\mu'}^{ij;q\nu} \hat{\tau}_j^{r'\mu';q\nu}$$

r: orbital rank q:spin rank

orbital monopolar (r=r'=0)

orbital multipolar (r+r'>1)

$$\hat{H}_{\mathrm{SE}}^{i,j} = \hat{H}_{C_{ij}} + \hat{H}_{O_iO_j} + \hat{H}_{S_iS_j} + \hat{H}_{S_iS_jO_iO_j}$$

spin monopolar (q=q'=0)

spin dipolar (q=q'=1)

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irreducible tensor decomposition

$$\hat{H}^{i,j}_{\mathrm{SE}} = \sum_{qq'}\sum_{\nu\nu'}\sum_{rr'}\sum_{\mu\mu'} \hat{\tau}_i^{r\mu;q\nu} D^{ij;q\nu}_{r\mu,r'\mu'} \hat{\tau}_j^{r'\mu';q\nu}$$

$r\ \mu$	$r'\ \mu'$	t^1_{2g}	t^2_{2g}		$D^{ij}_{r\mu,r'\mu'} \times U/2$
0 s	0 s	$-\mathcal{W}_0$	$-\mathcal{V}_0$		$(t^2_{xz,xz}+t^2_{yz,yz}+t^2_{xy,xy})$
0 s	1 z	$-\mathcal{W}_1$	$-\mathcal{V}_1$	$\frac{\sqrt{3}}{\sqrt{3}}$	$(t^2_{xz,xz}-t^2_{yz,yz})$
0 s	2 z^2	$-\mathcal{W}_1$	$-\mathcal{V}_1$	$\frac{\sqrt{3}}{3}$	$(t^2_{xz,xz}+t^2_{yz,yz}-2t^2_{xy,xy})$
1 z	1 z	$+\mathcal{W}_2$	$+\mathcal{V}_2$		$(t^2_{xz,xz}+t^2_{yz,yz})$
1 z	2 z^2	$+\mathcal{W}_2$	$+\mathcal{V}_2$	$\frac{1}{\sqrt{3}}$	$(t^2_{xz,xz}-t^2_{yz,yz})$
2 z^2	2 z^2	$+\mathcal{W}_2$	$+\mathcal{V}_2$	$\frac{1}{3}$	$(t^2_{xz,xz}+t^2_{yz,yz}+4t^2_{xy,xy})$
1 x	1 x	$+\mathcal{W}_2$	$+\mathcal{V}_2$		$(t_{xz,xz}+t_{yz,yz})t_{xy,xy}$
2 xz	2 xz	$+\mathcal{W}_2$	$+\mathcal{V}_2$		$(t_{xz,xz}+t_{yz,yz})t_{xy,xy}$
1 x	2 xz	$+\mathcal{W}_2$	$+\mathcal{V}_2$		$(t_{xz,xz}-t_{yz,yz})t_{xy,xy}$
2 x^2-y^2	2 x^2-y^2	$+\mathcal{W}_2$	$+\mathcal{V}_2$		$2t_{xz,xz}t_{yz,yz}$
1 y	1 y	$+\mathcal{W}_3$	$+\mathcal{V}_3$		$(t_{xz,xz}+t_{yz,yz})t_{xy,xy}$
2 yz	2 yz	$+\mathcal{W}_3$	$+\mathcal{V}_3$		$(t_{xz,xz}+t_{yz,yz})t_{xy,xy}$
2 xy	2 xy	$+\mathcal{W}_3$	$+\mathcal{V}_3$		$2t_{xz,xz}t_{yz,yz}$
1 y	2 yz	$+\mathcal{W}_3$	$+\mathcal{V}_3$		$(t_{xz,xz}-t_{yz,yz})t_{xy,xy}$

$\mathcal{W}_0 = f_{-3}+\frac{5}{9}f_{-1}+\frac{1}{9}f_2 = \frac{w_1+4w_2}{3}$, $\mathcal{V}_0 = \frac{8}{9}f_{-3}+\frac{10}{9}f_0+\frac{2}{3}f_2 = \frac{4(v_1+v_2)}{3}$

$\mathcal{W}_1 = \frac{3}{8}f_{-3}+\frac{11}{24}f_{-1}+\frac{1}{6}f_2 = \frac{w_1+w_2}{2}$, $\mathcal{V}_1 = -\frac{1}{3}f_{-3}+\frac{1}{3}f_0+\frac{1}{2}f_2 = \frac{2v_1-v_2}{2}$

$\mathcal{W}_2 = \frac{3}{4}f_{-3}-\frac{1}{12}f_{-1}-\frac{1}{6}f_2 = \frac{2w_2-w_1}{2}$, $\mathcal{V}_2 = \frac{2}{3}f_{-3}+\frac{1}{12}f_0-\frac{1}{4}f_2 = \frac{2v_2-v_1}{2}$

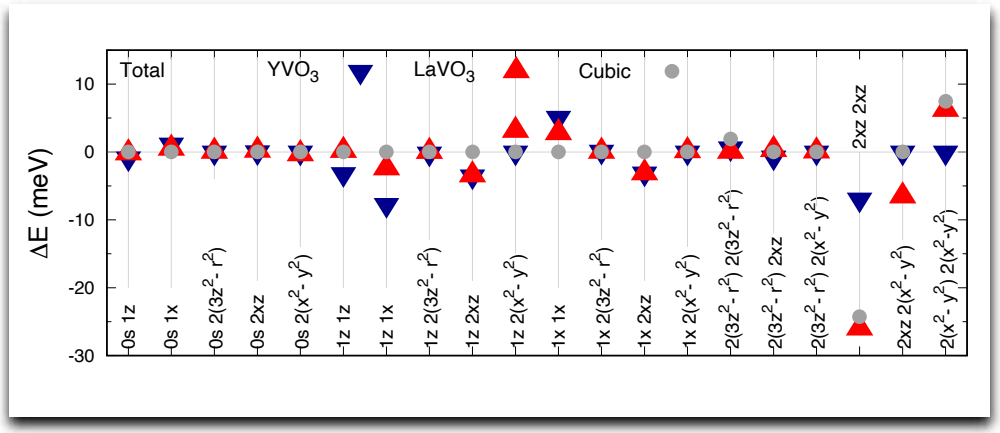
$\mathcal{W}_3 = \frac{3}{4}f_{-3}-\frac{5}{12}f_{-1}+\frac{1}{6}f_2 = \frac{w_0+w_3}{2}$, $\mathcal{V}_3 = \frac{2}{3}f_{-3}-\frac{5}{12}f_0+\frac{1}{4}f_2 = \frac{v_0+v_3}{2}$

$\tilde{\mathcal{W}}_0 = \frac{1}{3}f_{-3}-\frac{5}{9}f_{-1}-\frac{1}{9}f_2$, $\tilde{\mathcal{V}}_0 = \frac{4}{9}f_{-3}-\frac{10}{9}f_0-\frac{2}{3}f_2$

$\tilde{\mathcal{W}}_1 = \frac{1}{8}f_{-3}-\frac{11}{24}f_{-1}-\frac{1}{6}f_2$, $\tilde{\mathcal{V}}_1 = -\frac{1}{6}f_{-3}-\frac{1}{3}f_0-\frac{1}{2}f_2$

$\tilde{\mathcal{W}}_2 = \frac{1}{4}f_{-3}+\frac{1}{12}f_{-1}+\frac{1}{6}f_2$, $\tilde{\mathcal{V}}_2 = \frac{1}{3}f_{-3}-\frac{1}{12}f_0+\frac{1}{4}f_2$

$\tilde{\mathcal{W}}_3 = \frac{1}{4}f_{-3}+\frac{5}{12}f_{-1}-\frac{1}{6}f_2$, $\tilde{\mathcal{V}}_3 = \frac{1}{3}f_{-3}+\frac{5}{12}f_0-\frac{1}{4}f_2$



analytic & numerical

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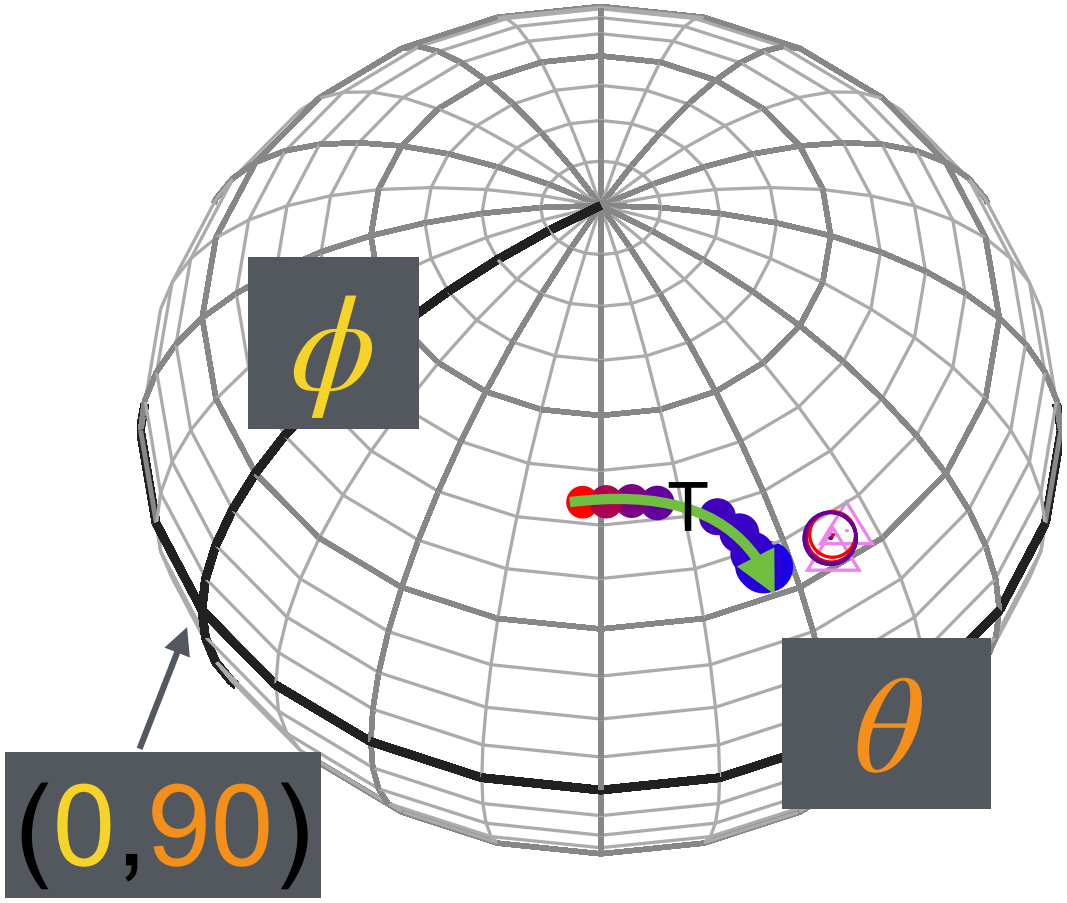
representation of orbital

$$|\theta, \phi\rangle = -|\pi - \theta, \phi \pm \pi\rangle$$
$$= \sin\theta\cos\phi|xz\rangle + \cos\theta|xy\rangle + \sin\theta\sin\phi|yz\rangle$$



empty: with CF

no T depends if CF dominates

full: only KK SE

orbital rapidly changes at T_{KK}

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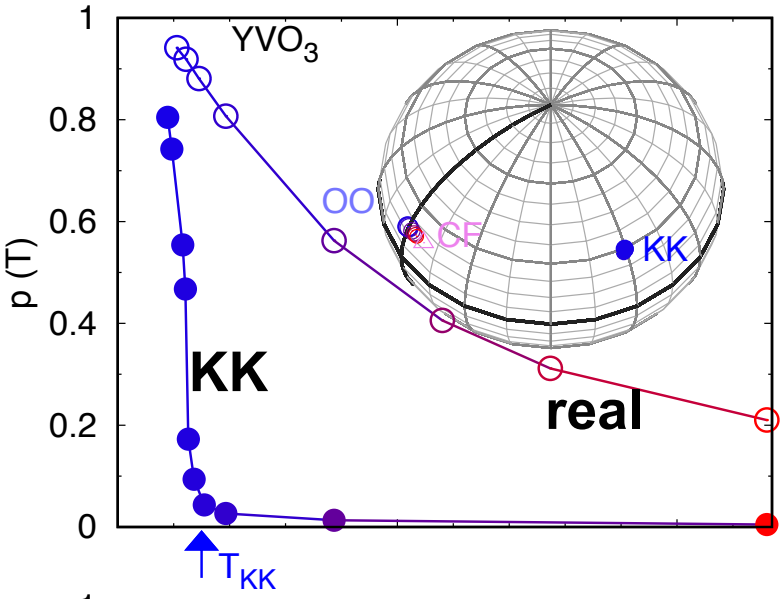
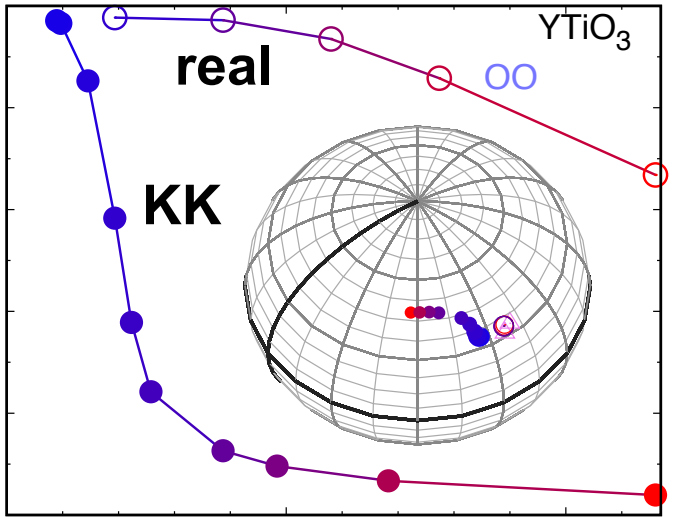
t_{2g}^2: T_{KK}~200 K but also smaller CF

R_I small

t_{2g}^2

YVO_3



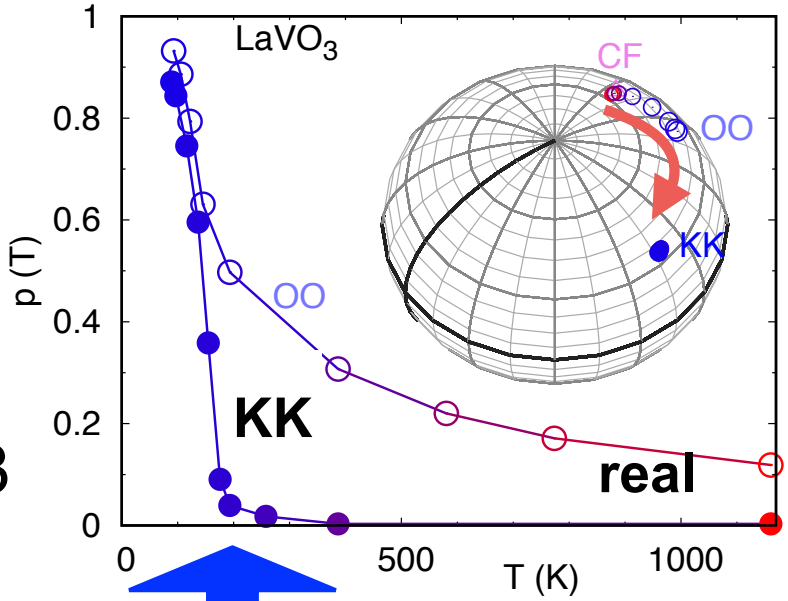


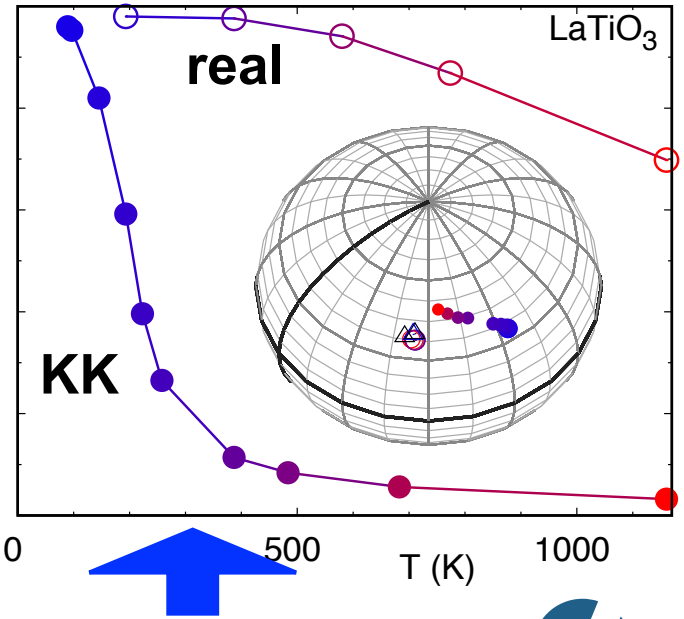
t_{2g}^1

R_I large

t_{2g}^2

$LaVO_3$





t_{2g}^1

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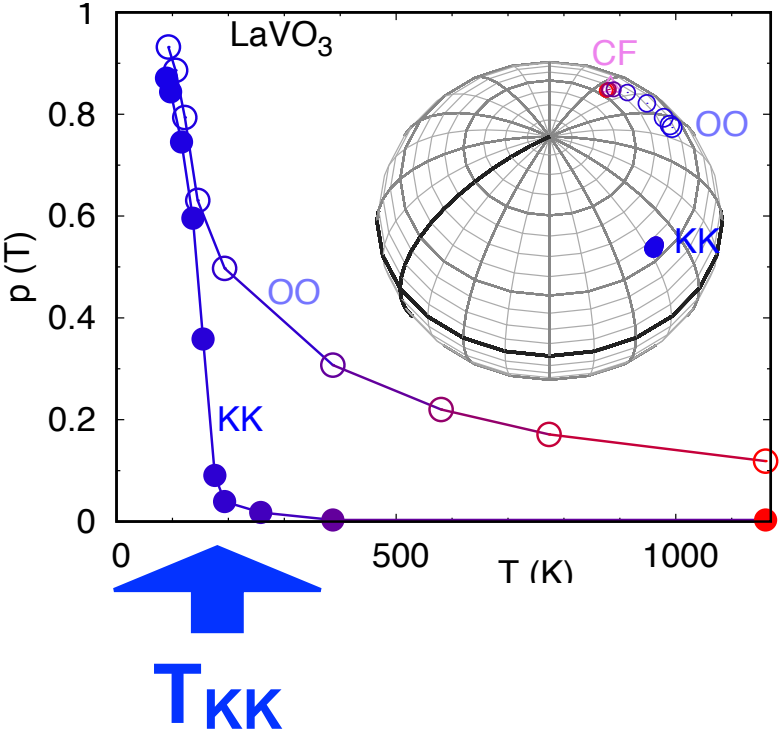
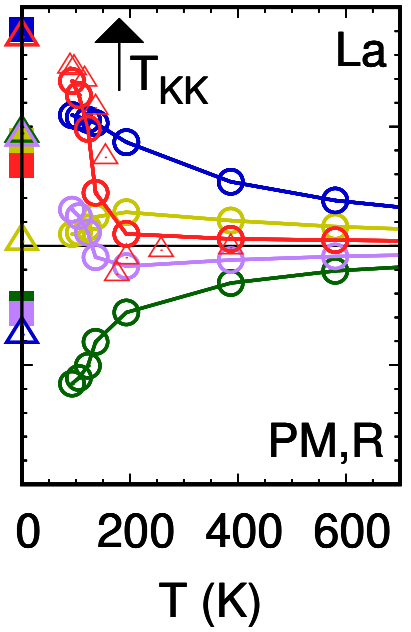
orbital channels decomposition

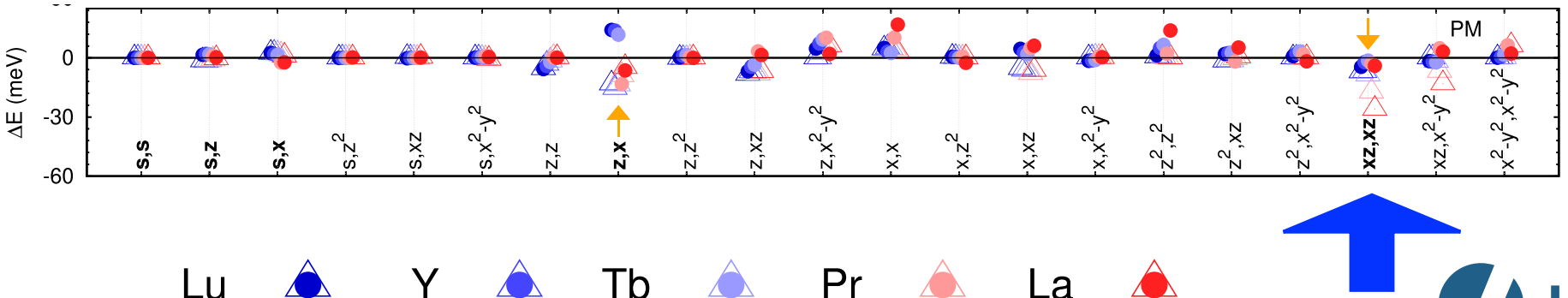


$\langle \tau_i^{r,\mu} \rangle$

z, x, $3z^2$-r^2, xz, x^2-y^2



$\langle \tau_i^{2,xz} \rangle$



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RVO_3, t_{2g}^2 : a unique series

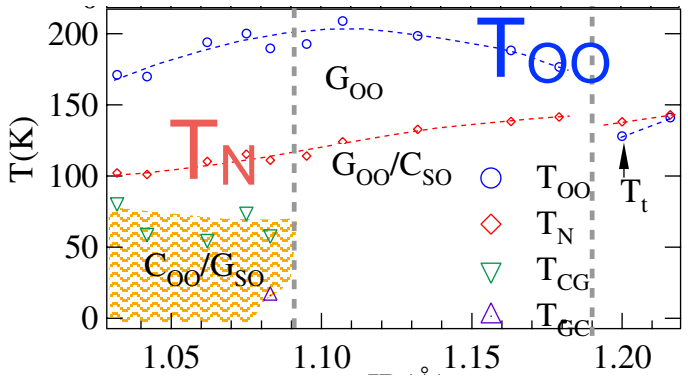
PRL **99,** 156401 (2007) PHYSICAL REVIEW LETTERS week ending 12 OCTOBER 2007

Superexchange Interaction in Orbitally Fluctuating *R*VO_3

J.-S. Zhou and J. B. Goodenough
Texas Materials Institute, University of Texas at Austin, Austin, Texas 78712, USA

J.-Q. Yan
Ames Laboratory, Ames, Iowa 50011, USA

Y. Ren
Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439, USA
(Received 18 May 2007; published 8 October 2007)



$LaVO_3$

R_I =ionic radius

inversion of T_N and T_{OO}

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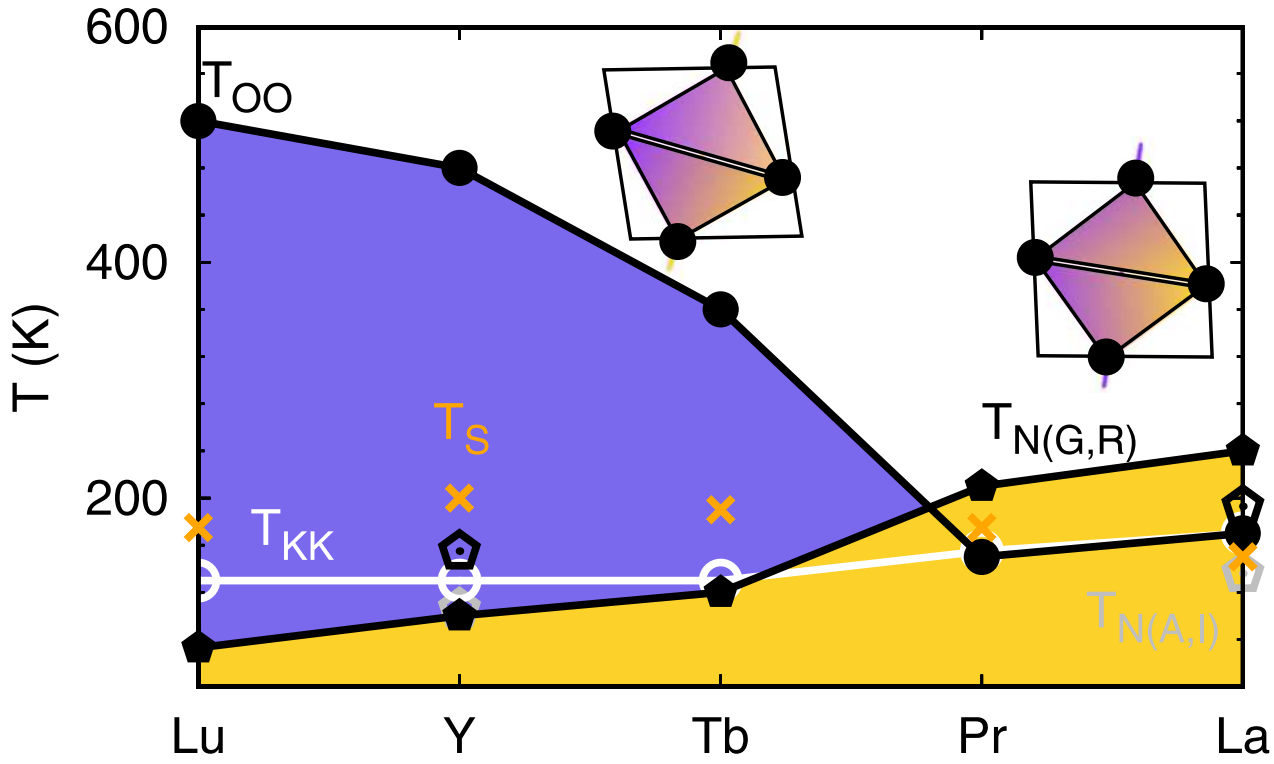
can we explain the inversion?

yes! theoretical phase diagram:



$T_{OO} >> T_{KK}$ R_I =ionic radius $T_{OO} \sim T_{KK}$

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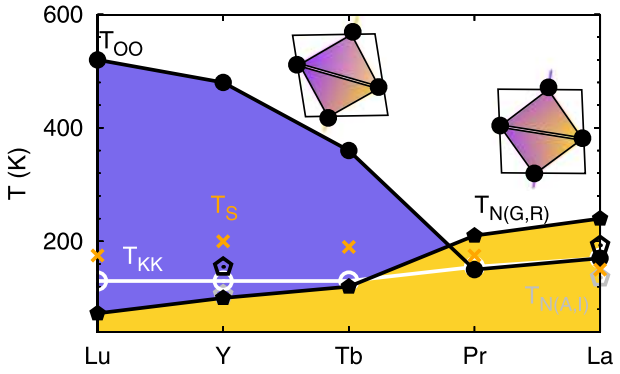
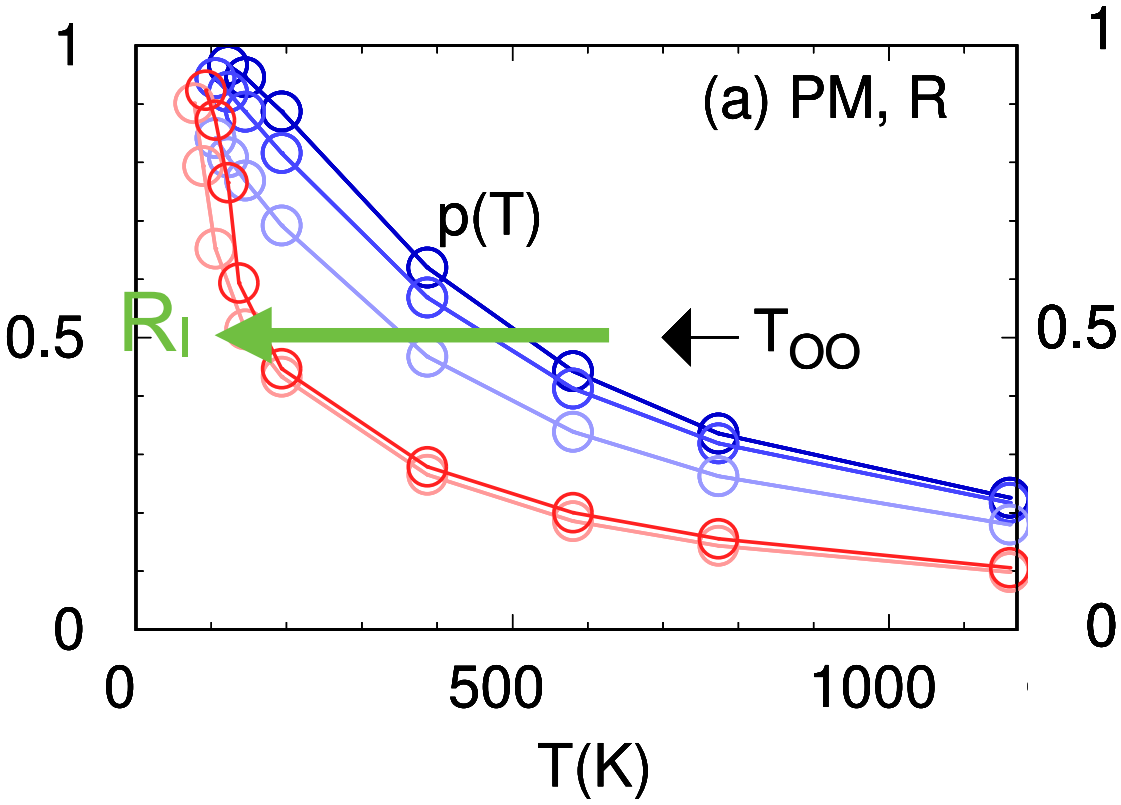
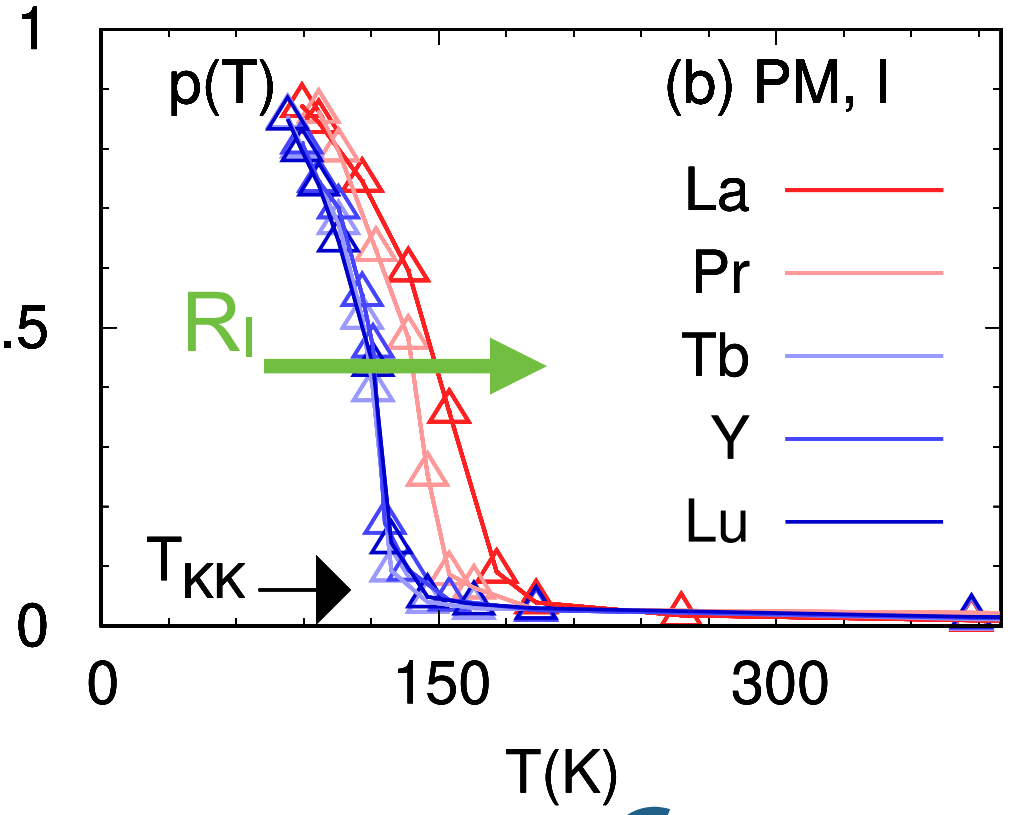
T_{OO}: evolution with R_I

$T_{OO} >> T_{KK}$ $\xrightarrow{R_I}$ $T_{OO} \sim T_{KK}$







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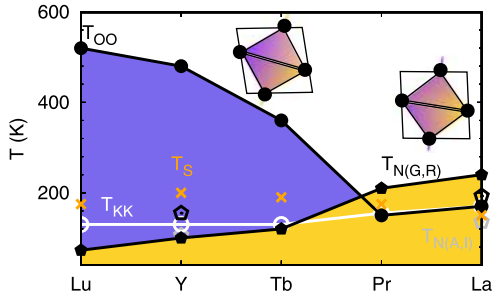
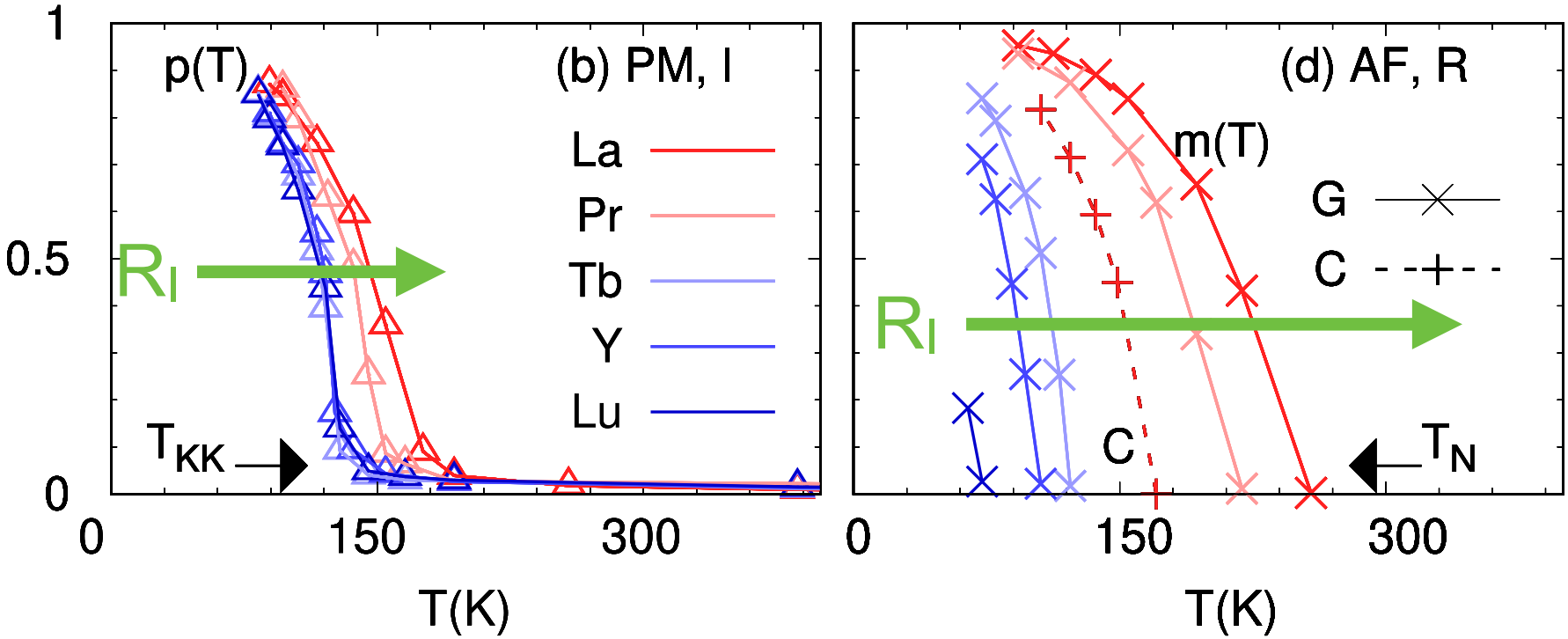
T_{KK} and T_N: evolution with R_I

$T_{OO} >> T_{KK}$ $\xrightarrow{R_I}$ $T_{OO} \sim T_{KK}$





$T_N < T_{KK}$ $\xrightarrow{R_I}$ $T_N \sim T_{KK}$

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wonderful, *but, why?*

$$\hat{H}_{\mathrm{SE}}^{i,j} = \sum_{qq'} \sum_{\nu\nu'} \sum_{rr'} \sum_{\mu\mu'} \hat{\tau}_i^{r\mu;q\nu} D_{r\mu,r'\mu'}^{ij;q\nu} \hat{\tau}_j^{r'\mu';q\nu}$$

r: orbital rank q:spin rank

orbital monopolar (r=r'=0)

orbital multipolar (r+r'>1)

$$\hat{H}_{\mathrm{SE}}^{i,j} = \hat{H}_{C_{ij}} + \hat{H}_{O_iO_j} + \hat{H}_{S_iS_j} + \hat{H}_{S_iS_jO_iO_j}$$

spin monopolar (q=q'=0)

spin dipolar (q=q'=1)

S_iS_j term main contribution to T_N!

$S_iS_jO_iO_j$ term does the rest

spin-orbit $S_iS_jO_iO_j$ channels

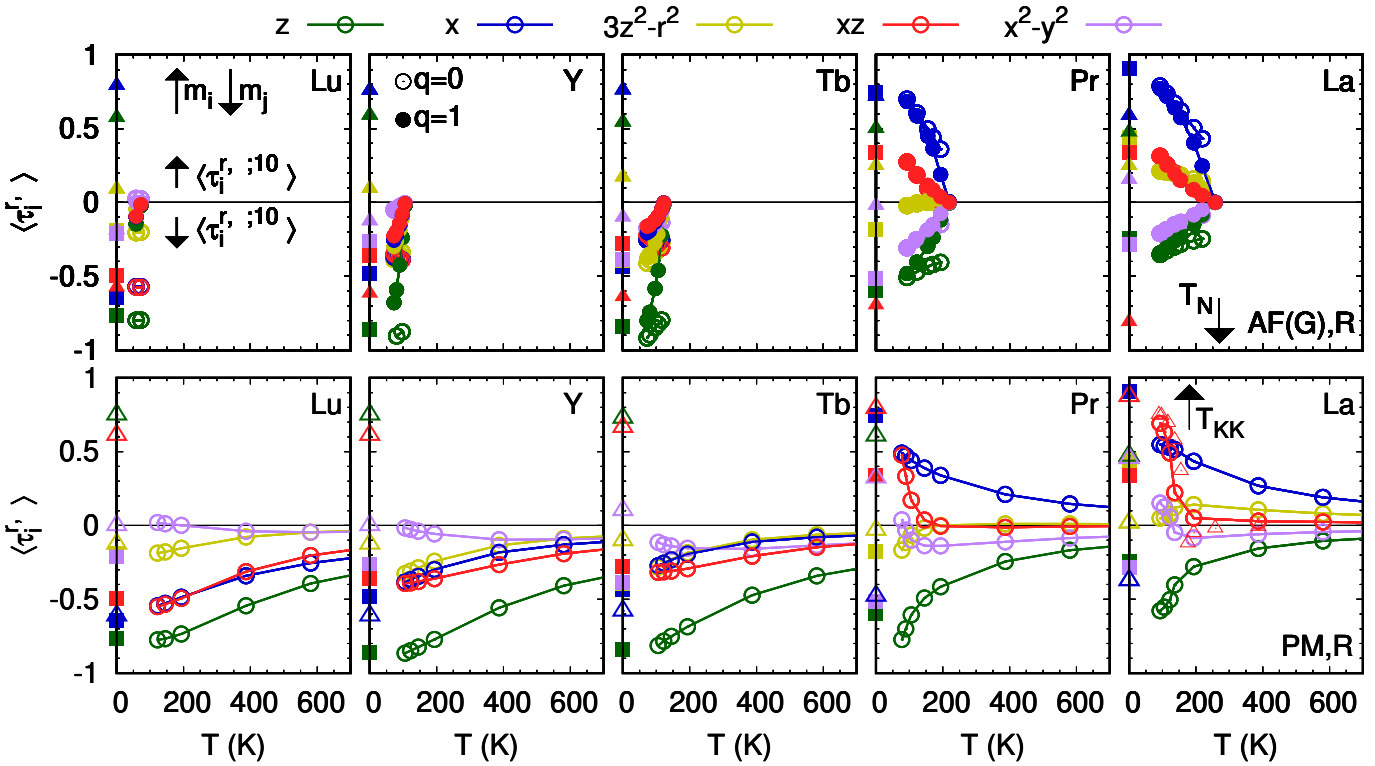
○ q=0 spin monopolar ● q=1 spin dipolar

r=s, z, x, $3z^2$-r^2, xz, x^2-y^2

m_i

AF

PM



r+r'>1 cancellation!

xz-xz

R_I

strong spin-orbital entanglement

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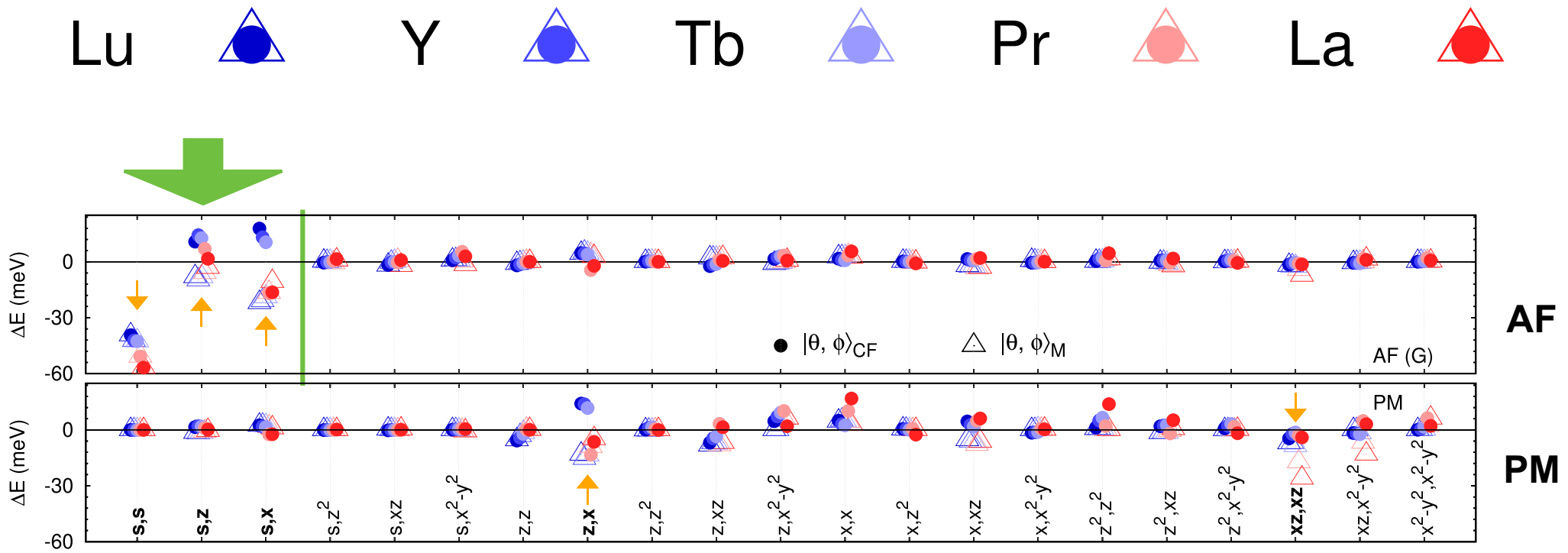
idealized magnetic state



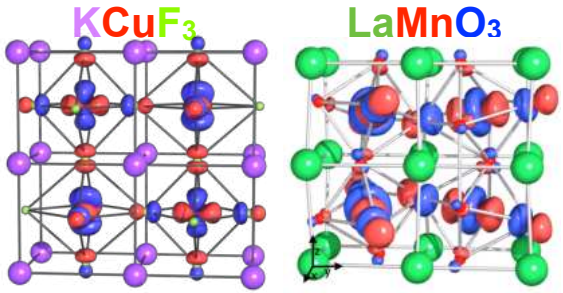
AF: orbital “Zeeman” term dominate

conclusions

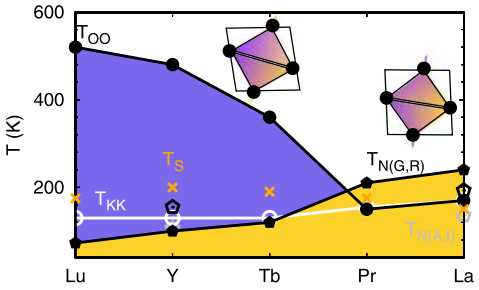
(i) are there true Kugel-Khomskii materials ?

Yes ! t_{2g} systems better than e_g
signatures are electronic

(ii) why (usually) $T_{OO}>T_N$?



in most systems $T_{OO}>>T_{KK}$



but if T_{KK}~T_{OO}, T_N and T_{KK}~T_{OO} can be flipped
G-type magnetic ordering is better

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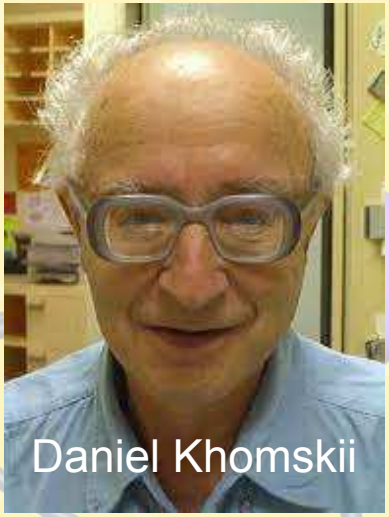
Erik Koch,
Alexander Lichtenstein,
Andreas Flesch,
Hunter Sims,
Evgeni Gorelov,
Guoren Zhang,
Xue-Jing Zhang,
Amit Chauhan


Daniel Khomskii

thank you!