Finding true Kugel-Khomskii systems

Eva Pavarini

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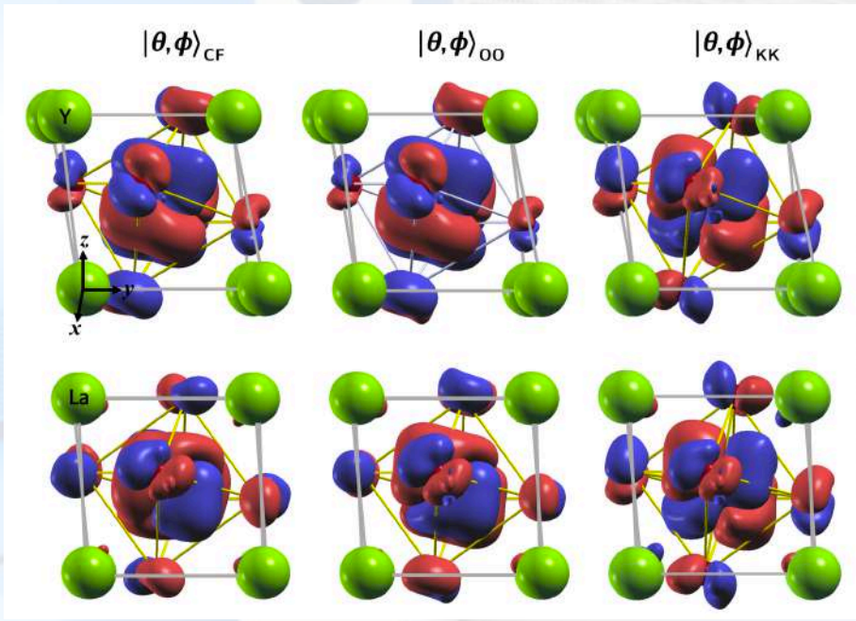

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50 years of Kugel-Khomskii model

Crystal structure and magnetic properties of substances with orbital degeneracy

$KCuF_3$

$LaMnO_3$

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.

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50 years of Kugel-Khomskii model

$$H = -\sum_{imjm'\sigma} t_{imjm'} c^{\dagger}_{im\sigma} c_{jm'\sigma} + U \sum_{im\sigma jm'\sigma'} n_{im\sigma} n_{jm'\sigma'}$$

perturbation t/U

super-exchange Hamiltonian

$J \propto t^2/U$ → $H = J_{SS} S_1 \cdot S_2 + J_{OO} \tau_1 \tau_2 + J_{SO}[\tau_1 S_2 + \tau_2 S_1]$

τ : pseudospins in orbital space

order without distortions

no static crystal-field splitting

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Kugel Khomskii 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 specific atomic site, has three attributes: charge, spin, and orbital. The orbital represents the shape of the electron cloud in solid. In transition-metal oxides with anisotropic-shaped d-orbital electrons, the Coulomb interaction between the electrons (strong electron correlation effect) is of importance for understanding their metal-insulator transitions and properties such as high-temperature superconductivity and colossal magnetoresistance. The orbital degree of freedom occasionally plays an important role in these phenomena, and its correlation and/or order-disorder transition causes a variety of phenomena through strong coupling with charge, spin, and lattice dynamics. An overview is given here on this "orbital physics," which will be a key concept for the science and technology of correlated electrons.

When more than two orbitals are involved, a variety of situations can be realized, and this quantum mechanical process depends on the orbitals (*4, 5*). In this way, the spin $\vec{S}$ and the orbital pseudospin $\vec{T}$ are coupled. In more general cases, the transfer integral t_{ij} depends on the direction of the
pair of the two orbitals
$(3z^2 - r^2)$. This gives
of the Hamiltonian in t
well as in the real sp
transfer integral betwe
Mn atoms in the cryst

[PDF] 1 Metal-Insulator Transition and Orbital Order in ... - arXiv...
arxiv.org/pdf/0811.3378 arXiv
by SAJ Kimber - 2008 - Cited by 24 - Related articles
shows a coupling of Ru4+ 4d **orbital order** to distortions from Pb2+ 6s6p orbital hybridization. The Pnma to Imma transition is an unconventional reversal of the ...

Preemptive nematic order, pseudogap, and orbital order in ...
arxiv.org › cond-mat arXiv
by RM Fernandes - 2011 - Cited by 132 - Related articles
Oct 9, 2011 - Furthermore, due to the distinct orbital character of each Fermi pocket, the nematic transition also induces **orbital order**. We compare our results ...

Exotic Spin Order due to Orbital Fluctuations

trong competition between different types of spin an
rbital phases at the crossover ...

rder in transition-metal oxides
.pdf Max Planck Society
xides. Eva Pavarini (FZ Jülich, Germany). **Orbital**
sicis of trasition-metal oxides, and yet its.

first principles study - ScienceDirect
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case for orbital ordering has been ...

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l bias induced ferroelectricity in manganites with competing charge and **orbital** r states. Fábio G. N. Figueiras, Igor K. Bdikin, Vitor B. S. Amaral and ...

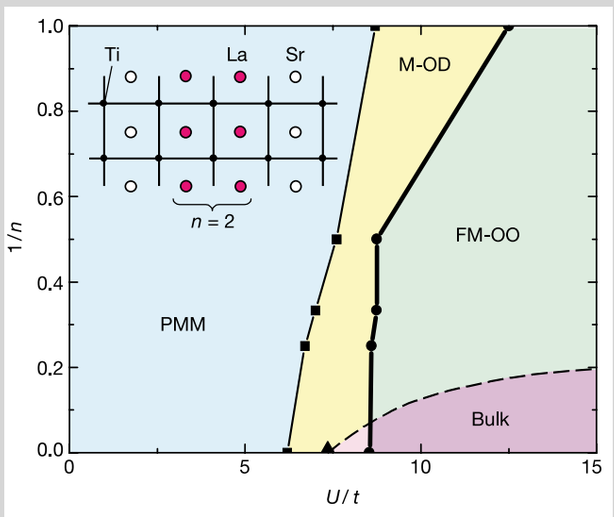
ral Charge and Orbital Order,' SIMES Seminar March 28 ...
://news.slac.stanford.edu/.../c... SLAC National Accelerator Laboratory
26, 2014 - Jasper van Wezel, a lecturer in condensed matter theory at Bristol ersity, will deliver this week's SIMES Seminar, "Chiral charge and **orbital** ...

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

Satoshi Okamoto & Andrew J. Millis

Department of Physics, Columbia University 538 West 120th Street, New York, New York 10027, USA

Surface science is an important and well-established branch of materials science involving the study of changes in material



NEWS & VIEWS

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.

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orbital liquid

ME 85, NUMBER 18 PHYSICAL REVIEW LETTERS 30 OCTO

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)

We present a theory of spin and orbital states in Mott insulator $LaTiO_3$. The spin-orbital superexchange interaction between $d^1(t_{2g})$ ions in cubic crystal suffers from a pathological degeneracy of orbital states at the classical level. Quantum effects remove this degeneracy and result in the formation of the coherent ground state, in which the orbital moment of t_{2g} level is fully quenched. We find a finite gap for orbital excitations. Such a disordered state of local degrees of freedom on unfrustrated, simple cubic lattice is highly unusual. Orbital liquid state naturally explains observed anomalies of $LaTiO_3$.

orbital fluctuations

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

Changes in pressure and magnetic field in the orbital and magnetic ordering temperatures of RVO_3 perovskites are reported; they reveal a competition between two magnetic orbitally ordered phases that have opposite preferences for the e-orbital component in the localized $^3T_{1g}$ ground state of the V^{3+} ion. This competition is shown to be biased by the $VO_{6/2}$ site distortion intrinsic to the orthorhombic structure. A remarkable enhancement of T_N with pressure is found where the competition leads to enhanced orbital critical fluctuations.

DOI: 10.1103/PhysRevLett.99.156401 PACS numbers: 71.70.Ej, 75.10.Dg, 75.30.Et, 75.50.Ee

spin-orbital entanglement

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **24** (2012) 313201 (28pp) doi:10.1088/0953-8984/24/31/313201

TOPICAL REVIEW

Fingerprints of spin–orbital entanglement in transition metal oxides

Andrzej M Oleś

Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Kraków, Poland
and
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

E-mail: a.m.oles@fkf.mpg.de

manipulation of orbitals degrees of freedom

Optical Stabilization of Fluctuating High Temperature Ferromagnetism in $YTiO_3$

A.S. Disa[1], J. Curtis[2], M. Fechner[1], A. Liu[1], A. von Hoegen[1], M. Först[1], T.F. Nova[1], P. Narang[2], A. Maljuk[3], A.V. Boris[4], B. Keimer[4], A. Cavalleri[1,5]

[1]*Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany*
[2]*John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, USA*
[3]*Leibniz Institute for Solid State and Materials Research Dresden, Germany*
[4]*Max Planck Institute for Solid State Research, Stuttgart, Germany*
[5]*Clarendon Laboratory, Department of Physics, Oxford University, Oxford, UK*

arXiv:2111.13622

In quantum materials, degeneracies and frustrated interactions can have a profound impact on the emergence of long-range order, often driving strong fluctuations that suppress functionally relevant electronic or magnetic phases. Engineering the atomic structure in the bulk or at heterointerfaces has been an important research strategy to lift these degeneracies, but these equilibrium methods are limited by thermodynamic, elastic, and chemical constraints. Here, we show that all-optical, mode-selective manipulation of the crystal lattice can be used to enhance and stabilize high-temperature ferromagnetism in $YTiO_3$, a material that exhibits only partial orbital polarization, an unsaturated low-temperature magnetic moment, and a suppressed Curie temperature, T_c = 27 K.

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50 years of Kugel-Khomskii model

Crystal structure and magnetic properties of substances with orbital degeneracy

$KCuF_3$

$LaMnO_3$

K. I. Kugel' and D. I. Khomskiĭ
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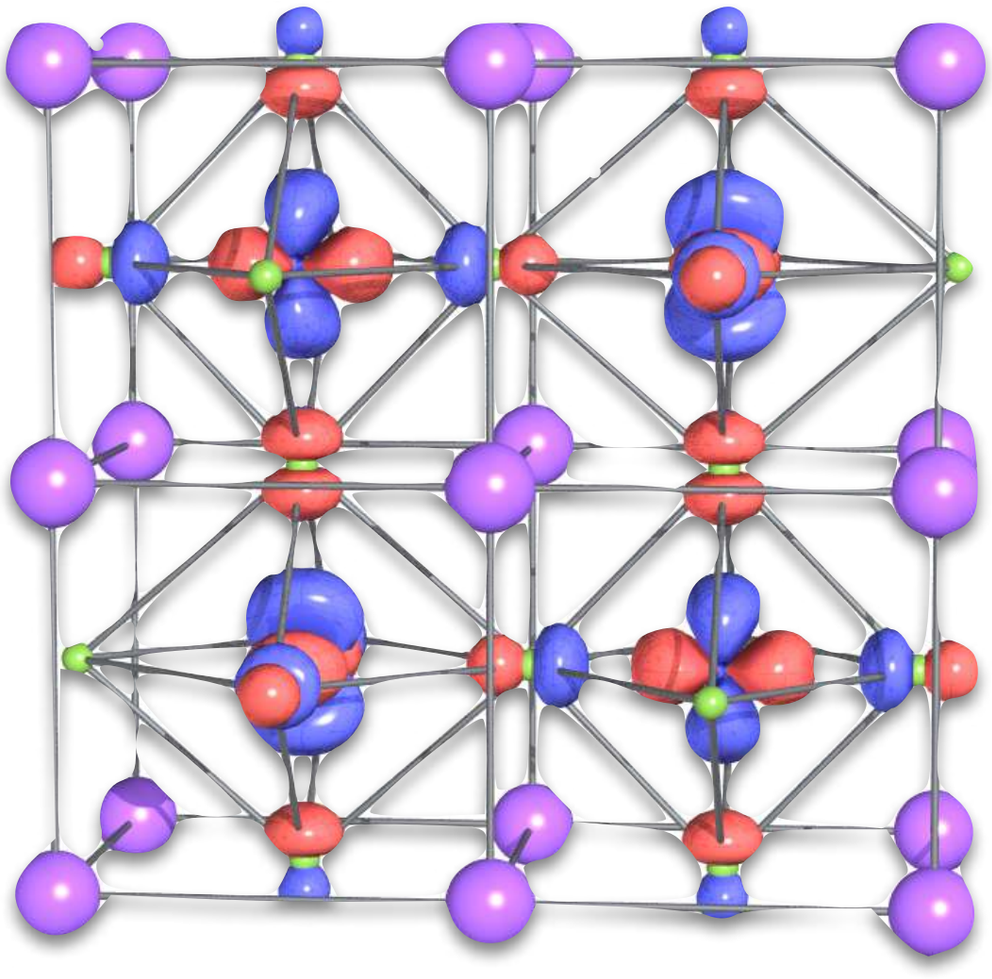
where is the evidence?

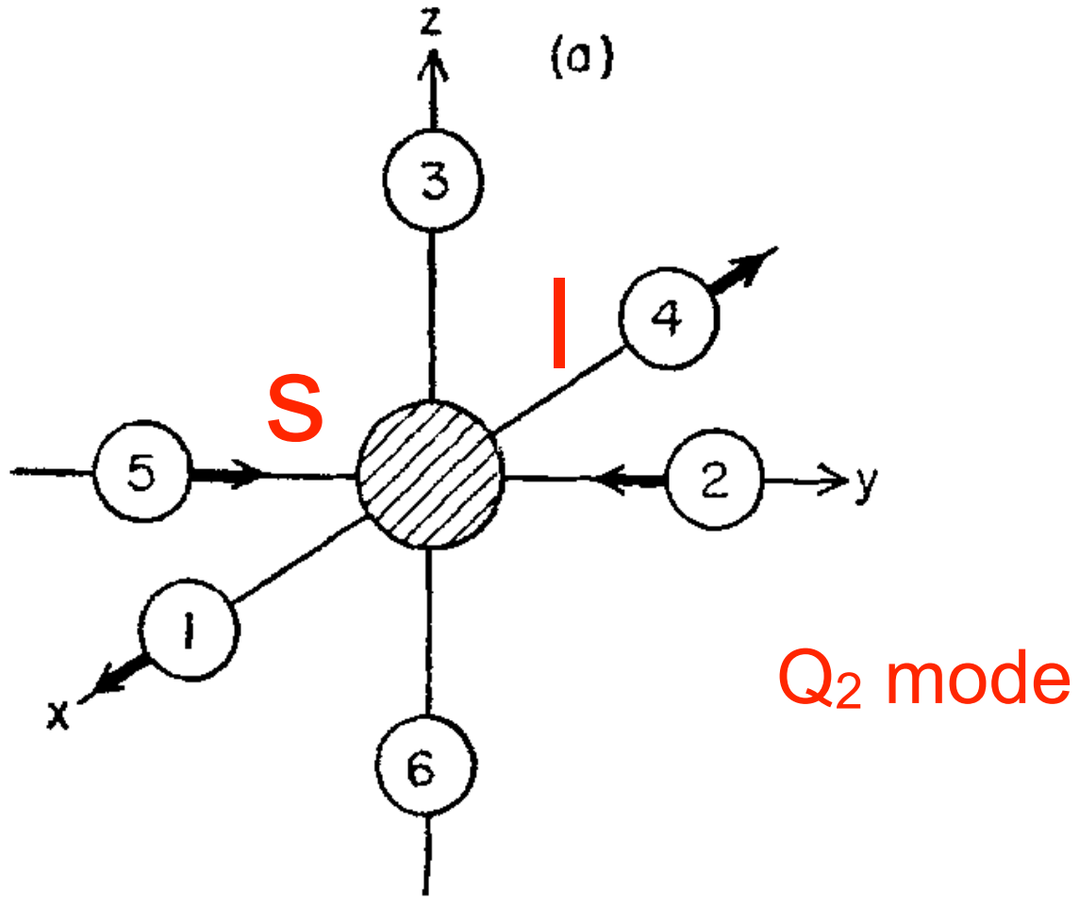
co-operative Jahn-Teller distortion

partially field e_g levels

$KCuF_3$



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



Q_2 mode

The Normal Mode
Q_2 (Q_2 >0)

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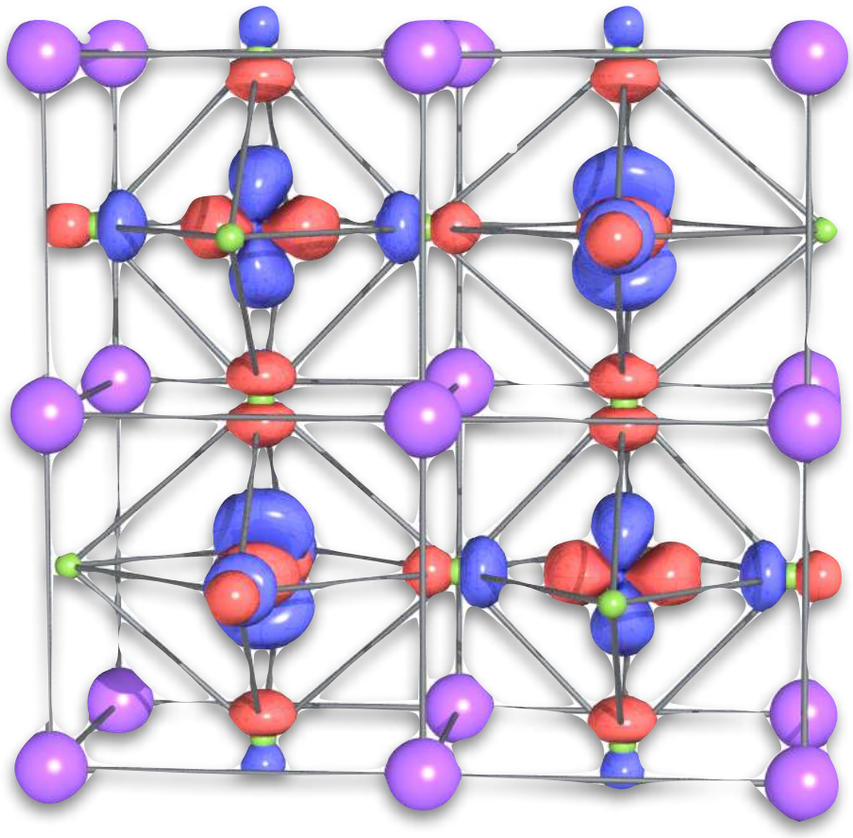
the hallmark of orbital order

co-operative Jahn-Teller distortion

partially field e_g levels

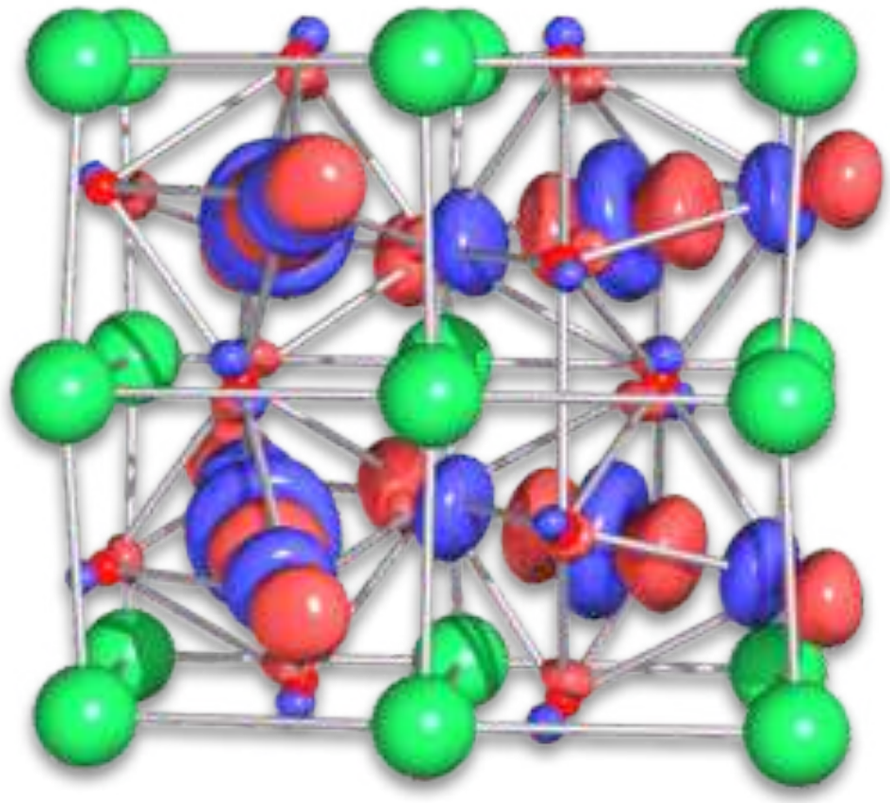
$KCuF_3$

$LaMnO_3$



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

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



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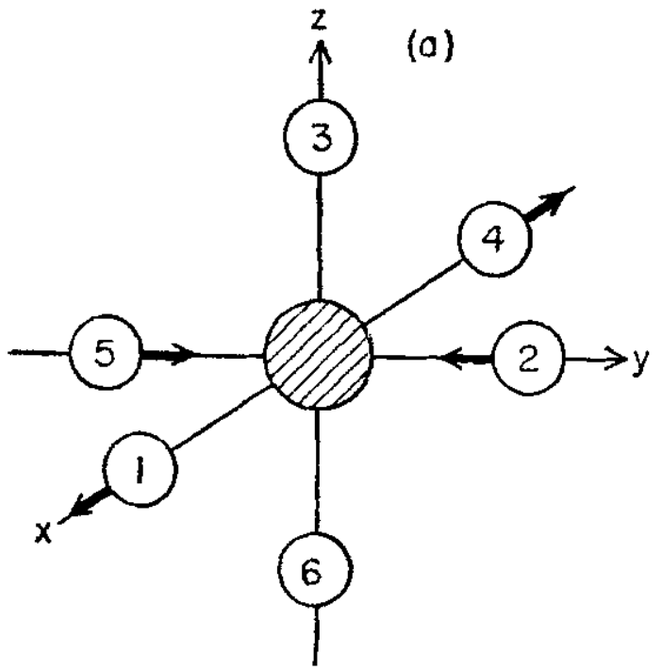
Jahn-Teller: splitting generates order

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.

electron-phonon coupling



The Normal Mode
Q_2 (Q_2 >0)

static crystal-field splitting

$$H = -g\sqrt{C}(\tau_z Q_3 + \tau_x Q_2)$$

τ : pseudospins in orbital space

$E_0 + \Delta/2$ ——

Δ

$E_0 - \Delta/2$ —— θ

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

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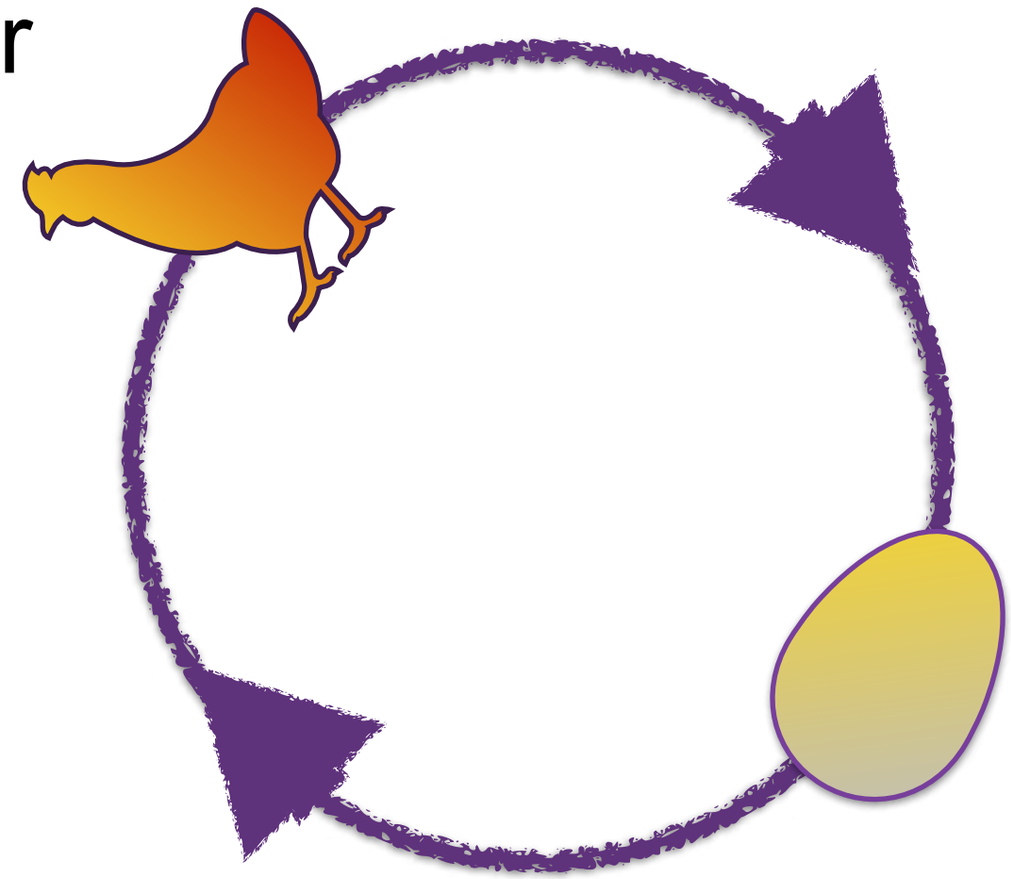
a chicken-and-egg problem

Jahn-Teller



Kugel-Khomskii

how to disentangle the two?

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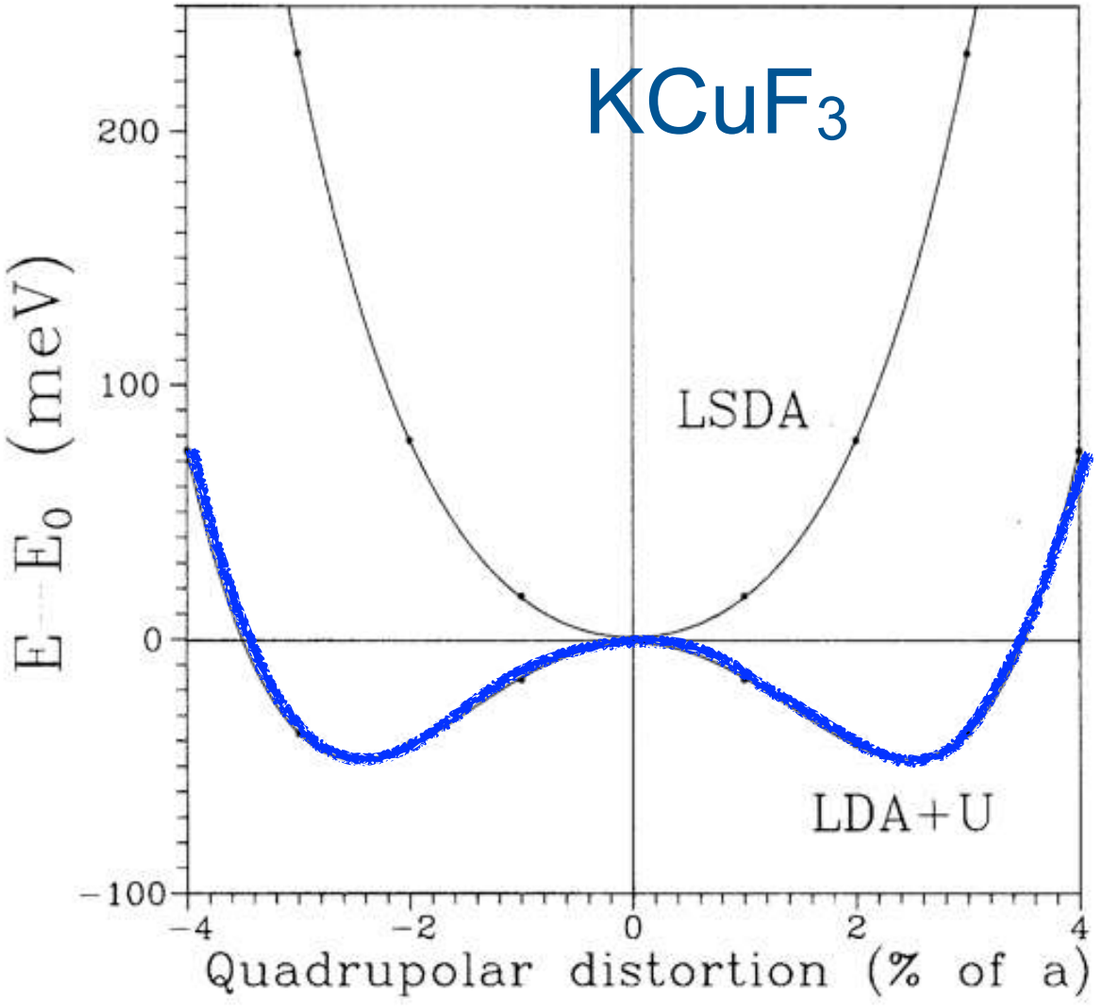
LDA+U: KK-like mechanism

Density-functional theory and strong interactions: Orbital ordering in Mott-Hubbard insulators

A. I. Liechtenstein
Max-Planck-Institut für Festkörperforschung, D-70506 Stuttgart, Germany

V. I. Anisimov
Institute of Metal Physics, GSP-170 Ekaterinburg, Russia

J. Zaanen
Lorentz Institute for the Theoretical Physics, Leiden University, Leiden, The Netherlands
(Received 15 May 1995)



The situation changes drastically if we allow for orbital polarization. Because U exceeds the bandwidth, the orbital sector is already strongly polarized (as are the spins) before the lattice is allowed to react. Overlooking some unimportant details concerning the coherence of the intermediate states, the well-known rule that electronic MFT in strong coupling maps onto the classical "spin" problem holds also in this case. In other words, we find the quadrupolar orbital-ferromagnetic spin phase to be most stable (for the same reasons as Kugel and Khomskii[6]). Obviously the cubic lattice is unstable in the presence of this orbital order parameter. In fact, despite large-scale changes in the electronic system the deformation is modest, indicating a rather weak electron-phonon coupling.

KK-like mechanism !

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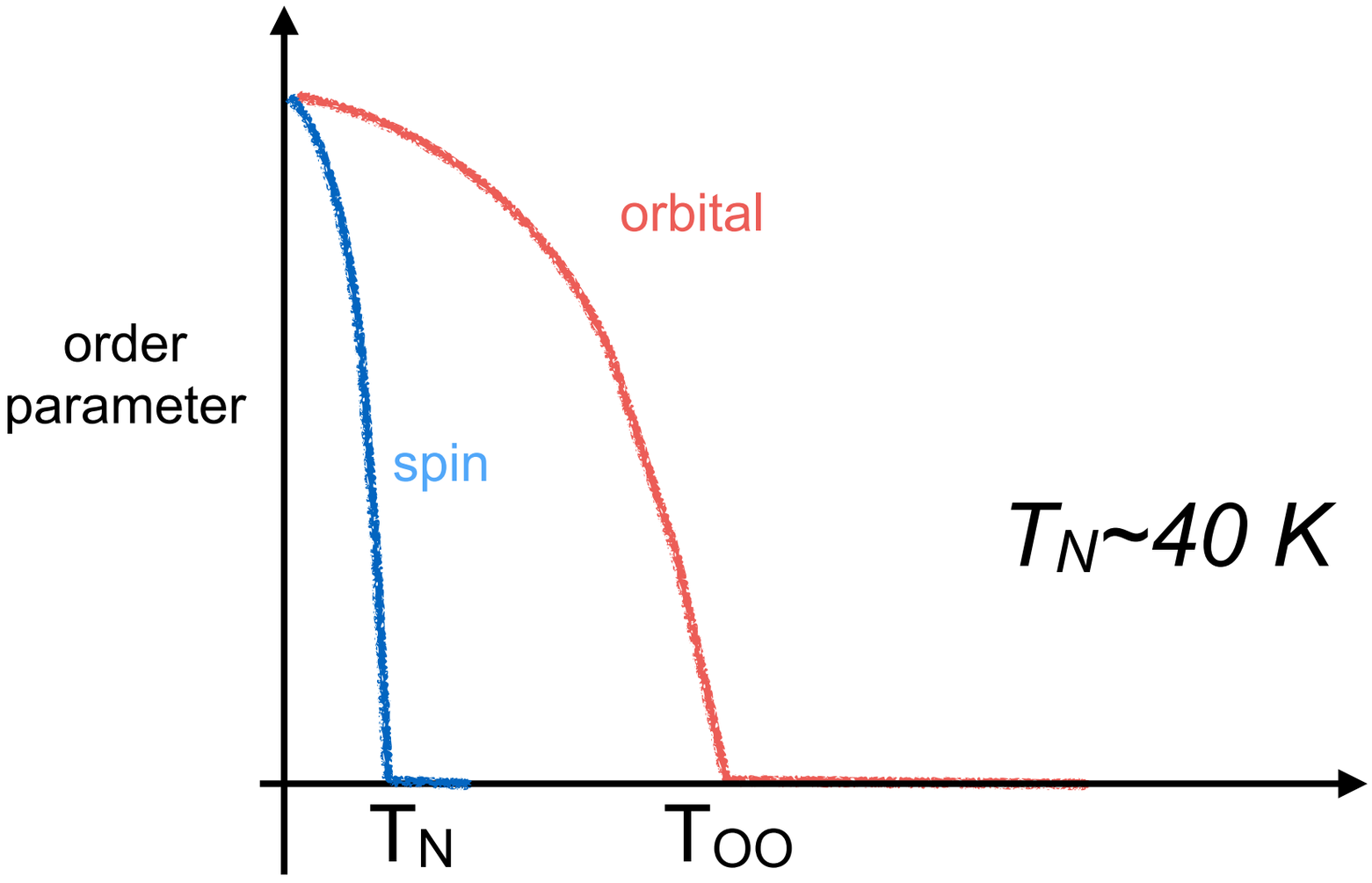
something not quite right



$KCuF_3$

$T_N \sim 40\ K \ll T_{OO} \sim 1400\ K$?

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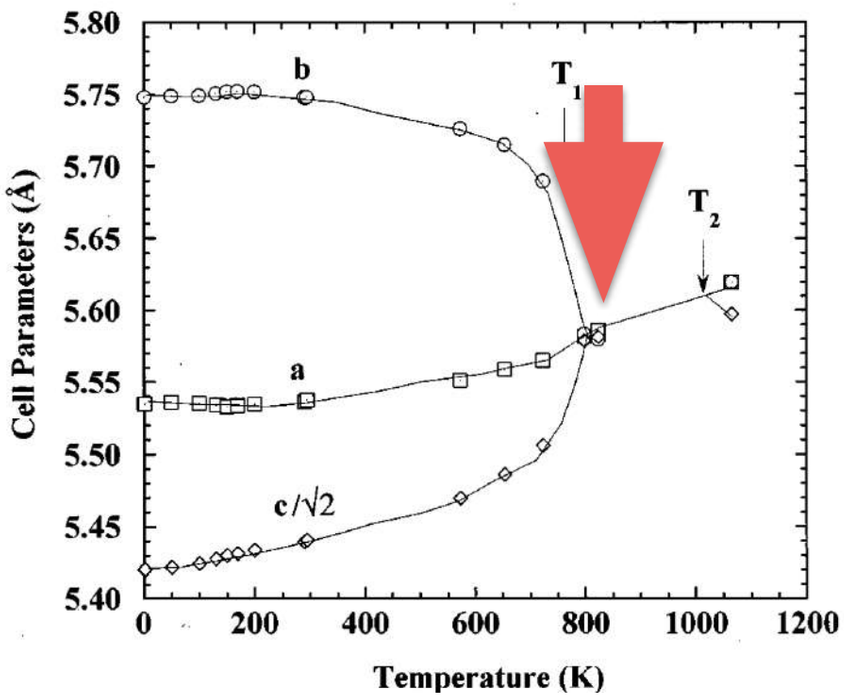
orbital-order transition at T_{OO} in $LaMnO_3$

$T_{OO} \sim 800$ K



PHYSICAL REVIEW B VOLUME 57, NUMBER 6 1 FEBRUARY 1998-II

Neutron-diffraction study of the Jahn-Teller transition in stoichiometric $LaMnO_3$

J. Rodríguez-Carvajal,* M. Hennion, F. Moussa, and A. H. Moudden
Laboratoire Léon Brillouin (CEA-CNRS), Centre d'Etudes de Saclay, 91191 Gif sur Yvette Cedex, France

L. Pinsard and A. Revcolevschi
Laboratoire de Chimie des Solides, Université Paris Sud, 91405 Orsay Cedex, France
(Received 2 September 1997)

The parent compound of the giant magnetoresistance Mn-perovskite, $LaMnO_3$, has been studied by thermal analysis and high-resolution neutron-powder diffraction. The orthorhombic *Pbnm* structure at room temperature is characterized by an antiferrodistorsive orbital ordering due to the Jahn-Teller effect. This ordering is evidenced by the spatial distribution of the observed Mn-O bond lengths. $LaMnO_3$ undergoes a structural phase transition at $T_{JT} \approx 750$ K, above which the orbital ordering disappears. There is no change in symmetry although the lattice becomes metrically cubic on the high-temperature side. The MnO_6 octahedra become nearly regular above T_{JT} and the thermal parameter of oxygen atoms increases significantly. The observed average cubic lattice is probably the result of dynamic spatial fluctuations of the underlying orthorhombic distortion. [S0163-1829(98)51706-7]

VOLUME 81, NUMBER 3 PHYSICAL REVIEW LETTERS 20 JULY 1998

Resonant X-Ray Scattering from Orbital Ordering in $LaMnO_3$

Y. Murakami,[1,2] J. P. Hill,[3] D. Gibbs,[3] M. Blume,[3] I. Koyama,[1] M. Tanaka,[1] H. Kawata,[1] T. Arima,[4] Y. Tokura,[5] K. Hirota,[2,6] and Y. Endoh[2,6]
[1]*Photon Factory, Institute of Materials Structure Science, High Energy Accelerator Research Organization, Tsukuba, 305-0801, Japan*
[2]*Core Research for Evolutional Science and Technology (CREST), Tsukuba 305-0047 Japan*
[3]*Department of Physics, Brookhaven National Laboratory, Upton, New York 11973*
[4]*Institute of Materials Science, University of Tsukuba, Tsukuba 305-8573, Japan*
[5]*Department of Applied Physics, University of Tokyo, Tokyo 113-0033, Japan and Joint Research Center for Atom Technology (JRCAT), Tsukuba 305-0046, Japan*
[6]*Department of Physics, Tohoku University, Sendai 980-8578, Japan*
(Received 22 April 1998)

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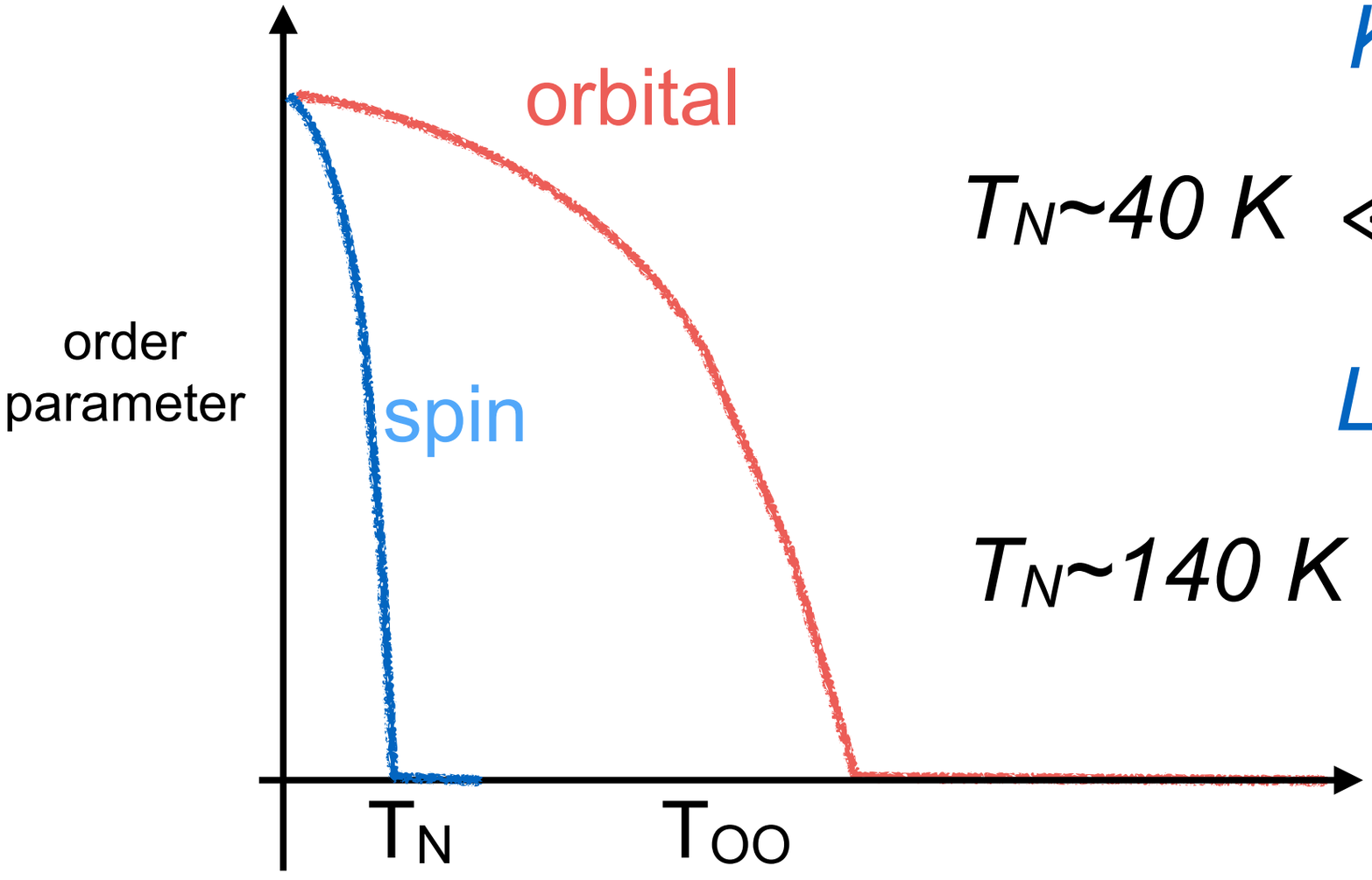
something not quite right



$KCuF_3$

T_N~40 K ≪ T_{OO} ~1400 K?

$LaMnO_3$

T_N~140 K ≪ T_{OO} ~ 800 K?

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50 years of Kugel and Khomskii model

$$H = -\sum_{imjm'\sigma} t_{imjm'} c^{\dagger}_{im\sigma} c_{jm'\sigma} + U \sum_{im\sigma jm'\sigma'} n_{im\sigma} n_{jm'\sigma'}$$

super-exchange Hamiltonian

perturbation t/U

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τ : pseudospins in orbital space

order without distortions

no static crystal-field splitting

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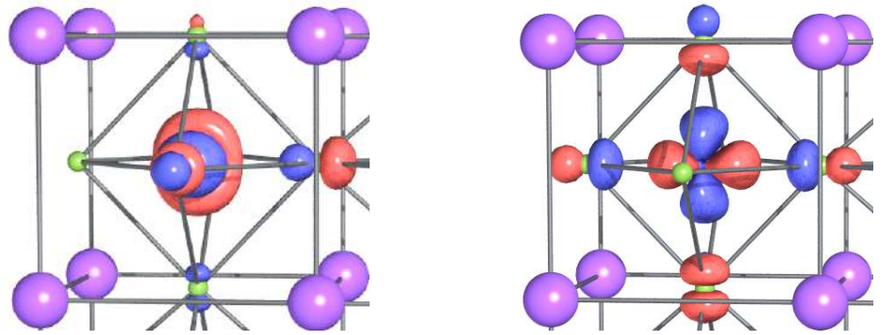
LDA+DMFT with Wannier functions

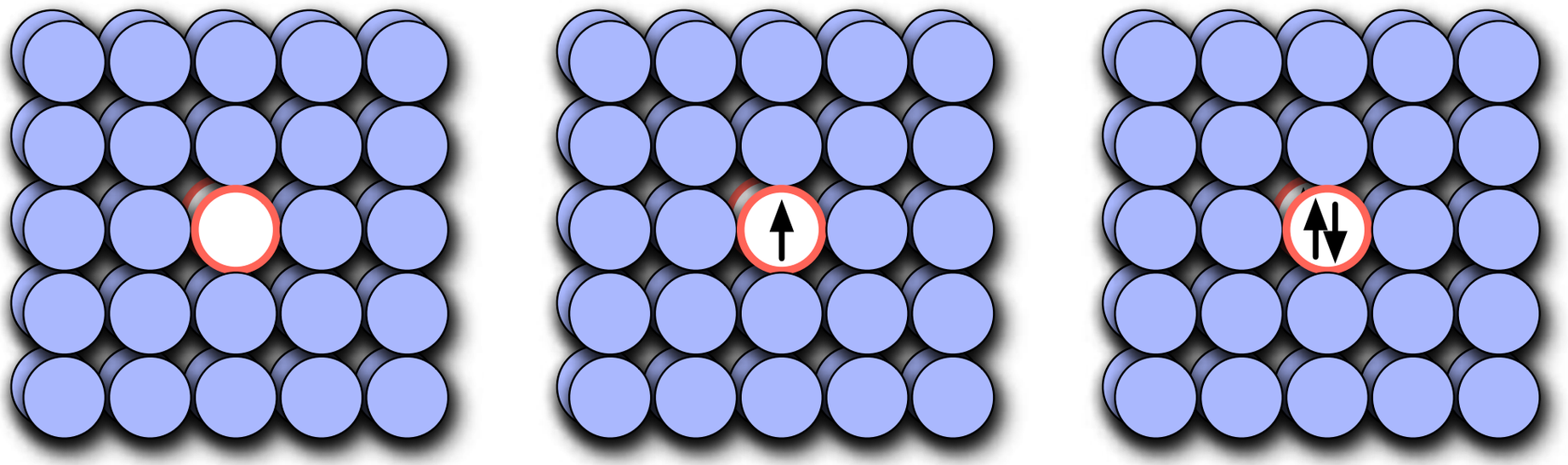
$$
\begin{aligned}
H = & - \sum_{ii'} \sum_{mm'} \sum_{\sigma} t^{ii'}_{mm'} c^{\dagger}_{im\sigma} c_{i'm'\sigma} \\
& + U \sum_{im} n_{im\uparrow} n_{im\downarrow} \\
& + \frac{1}{2} \sum_{im \neq m' \sigma\sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'} \\
& - J \sum_{m \neq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

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]





$$
G_{m,m'} = \sum_{\mathbf{k},\mathbf{n}} \left[\frac{1}{i\omega_n + \mu - \mathrm{H}_{0\mathbf{k}} - \Sigma(i\omega_n)} \right]_{m,m'}
$$

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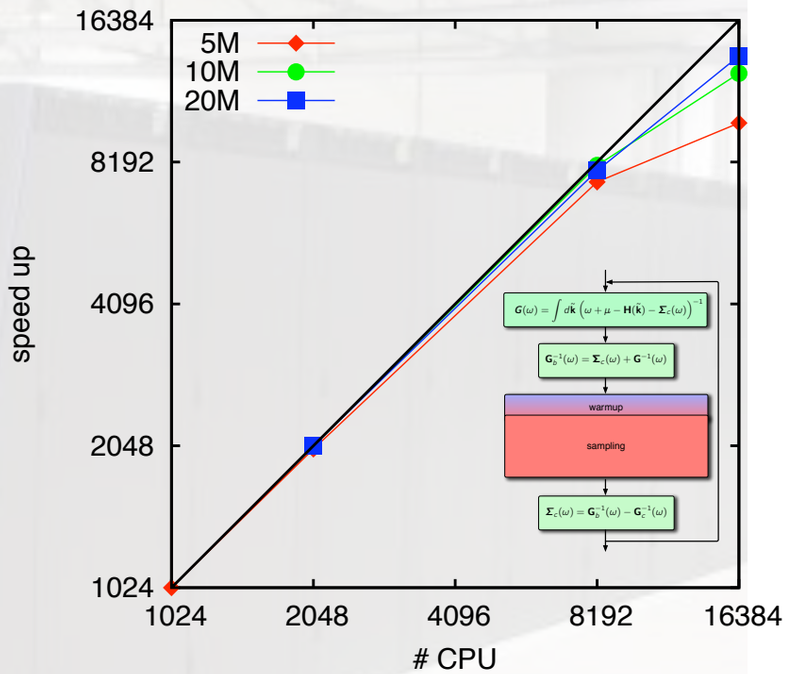
LDA+DMFT with Wannier functions

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



DMFT and cDMFT

quantum impurity solvers:

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

- A. Flesch, E. Gorelov, E. Koch and E. Pavarini
  Phys. Rev. B **87**, 195141 (2013)

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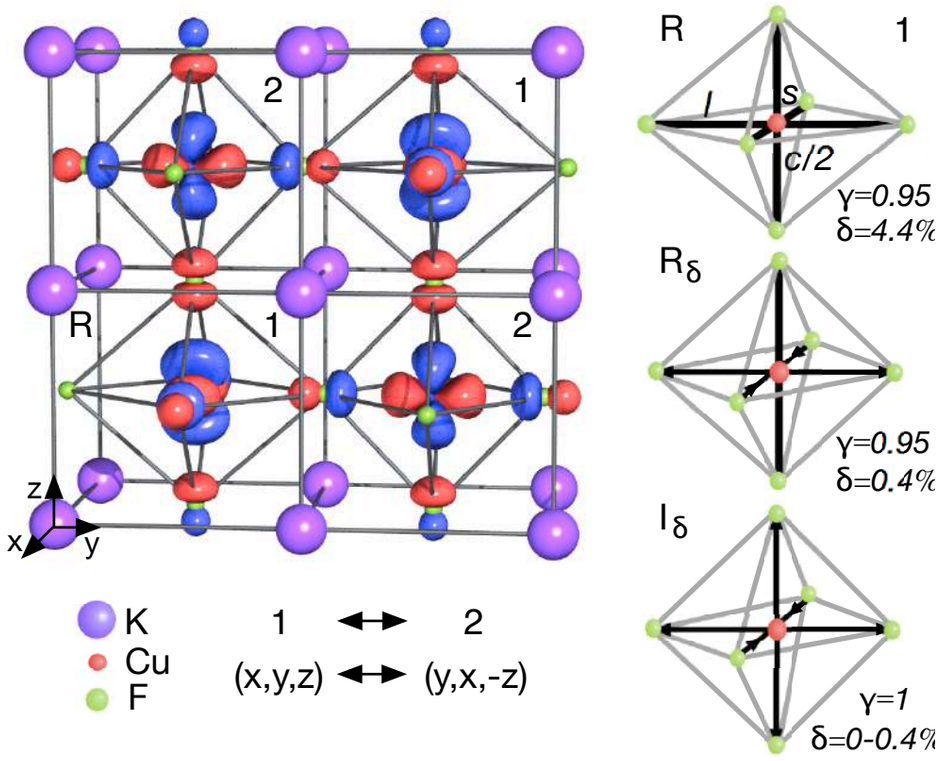
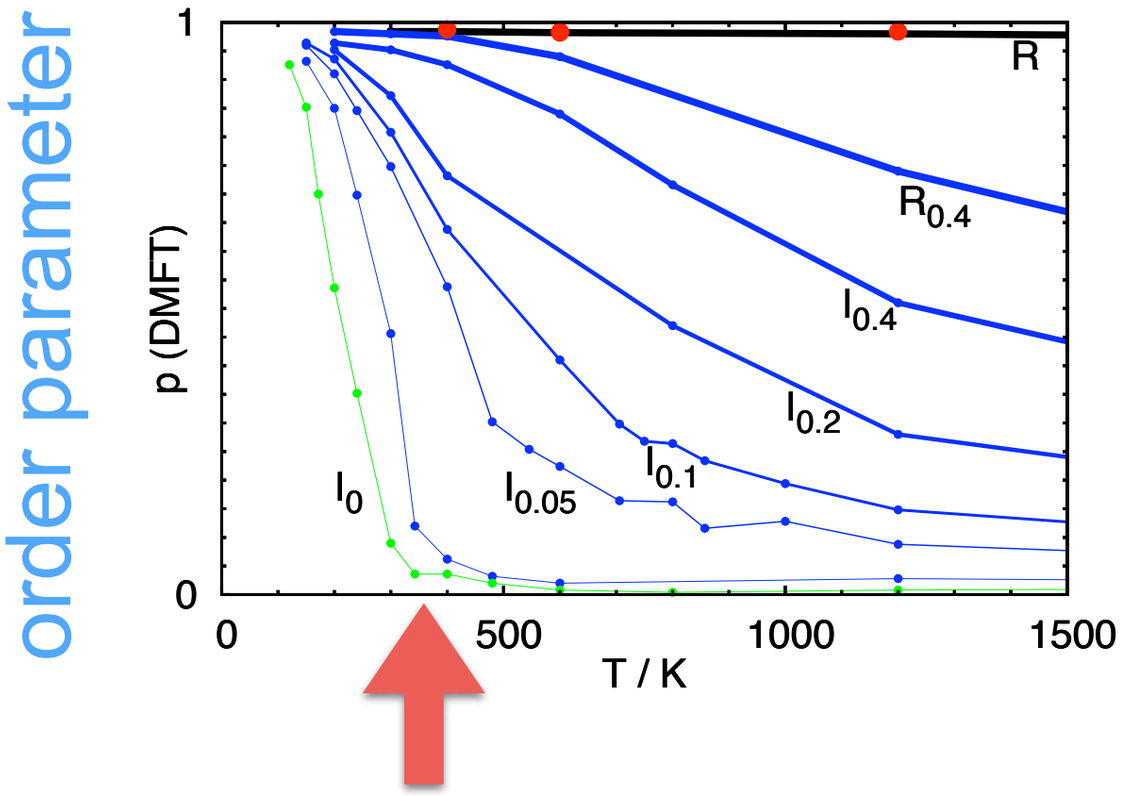
the KK mechanism in e_g^3 $KCuF_3$



$p=n_1-n_2$



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

T_{KK}~350 K

$T_{KK} \ll T_{OO} > 1400$ K

LDA+DMFT

reminder: mean field theory *overestimates* T_{KK}

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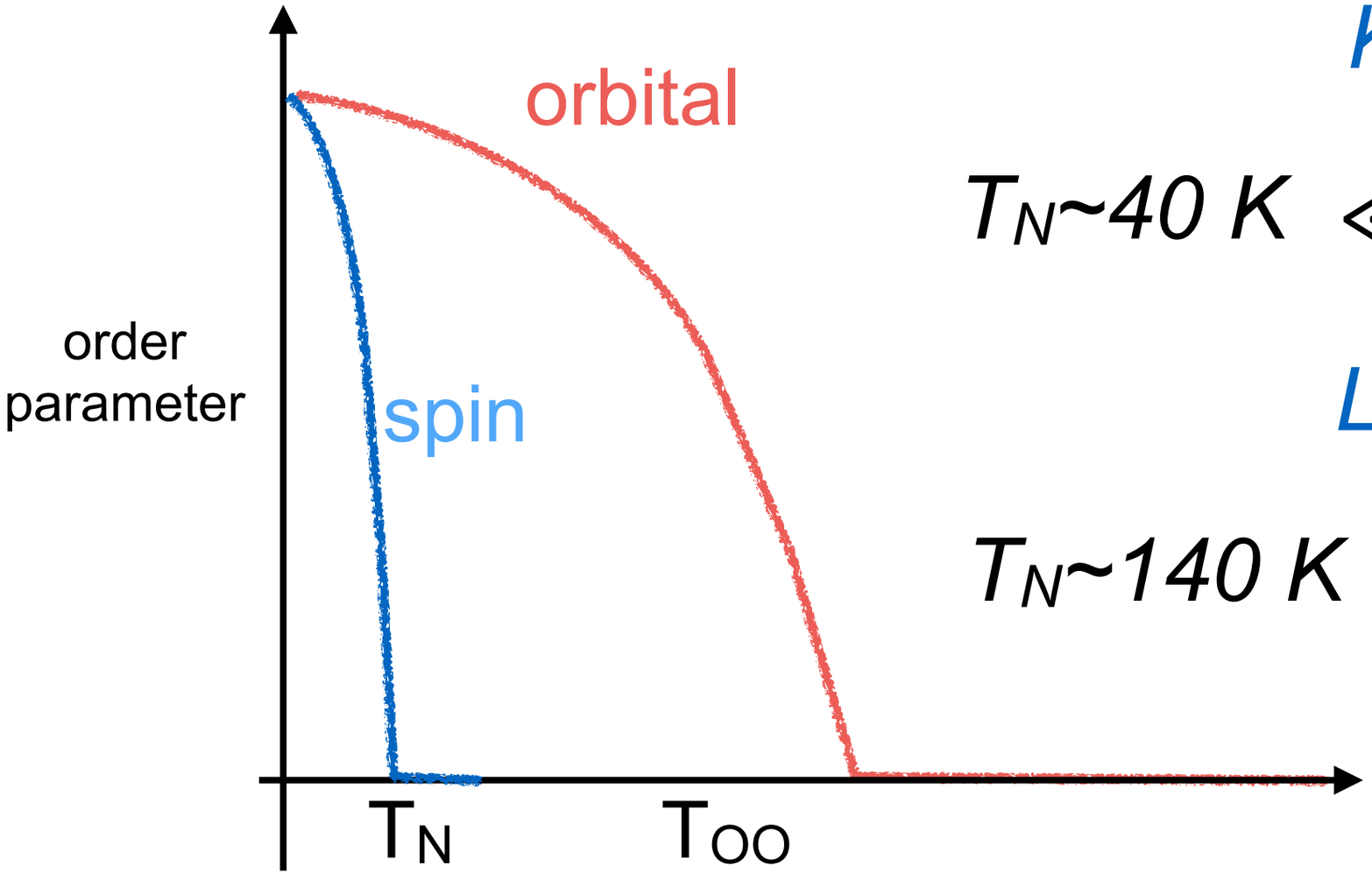
but also JT alone is not the full story



$KCuF_3$

$T_N \sim 40\ K \ll T_{OO} \sim 1400\ K?$

$LaMnO_3$

$T_N \sim 140\ K \ll T_{OO} \sim 800\ K?$

more experiments

PHYSICAL REVIEW B **87**, 014109 (2013)

Unusual structural evolution in $KCuF_3$ at high temperatures by neutron powder diffraction

Luke G. Marshall,[1] Jianshi Zhou,[1,*] Jianzhong Zhang,[2] Jiantao Han,[2] Sven C. Vogel,[2] Xiaohui Yu,[2] Yusheng Zhao,[2,3]
M. T. Fernández-Díaz,[4] Jinguang Cheng,[1] and John B. Goodenough[1]

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[2]*LANSCE Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

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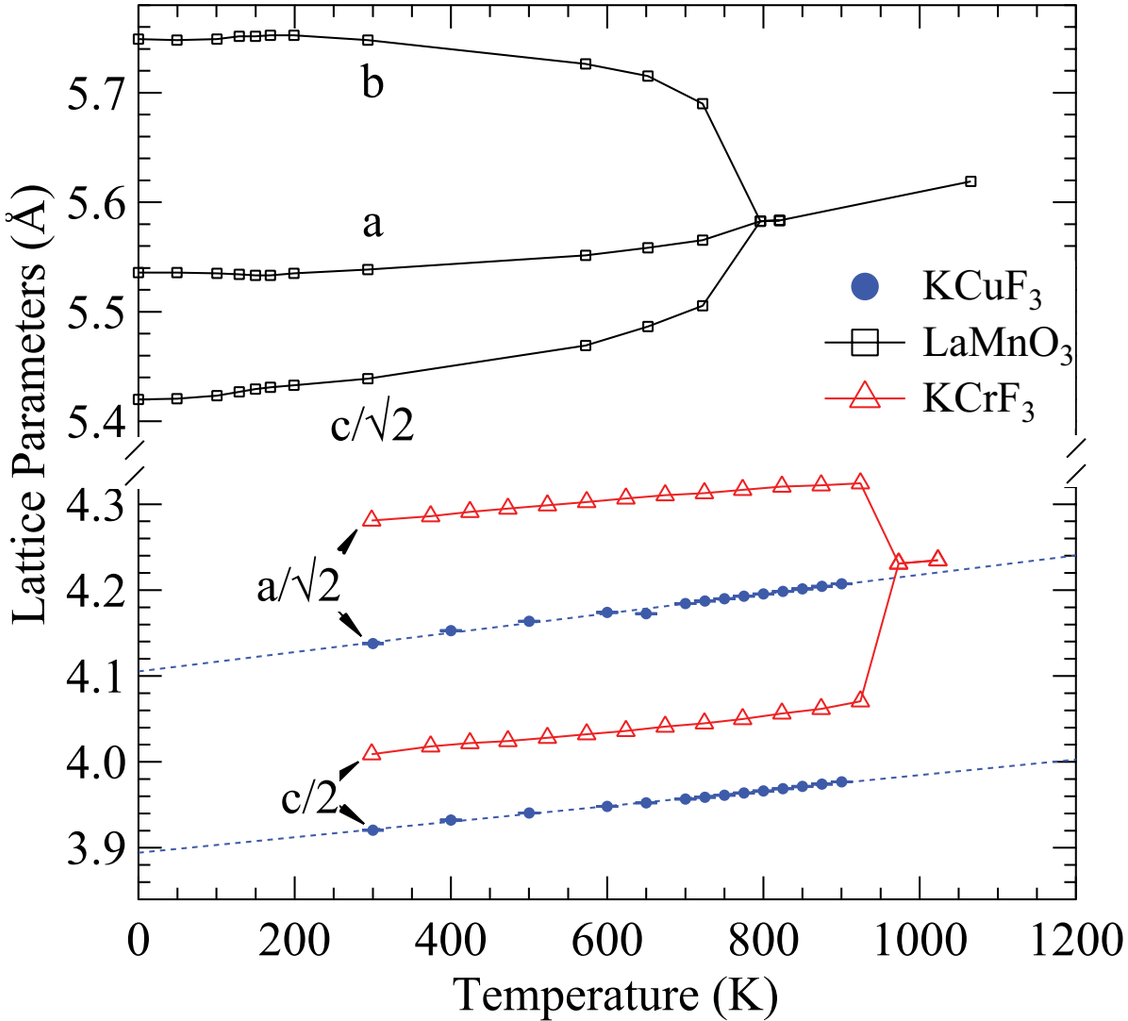
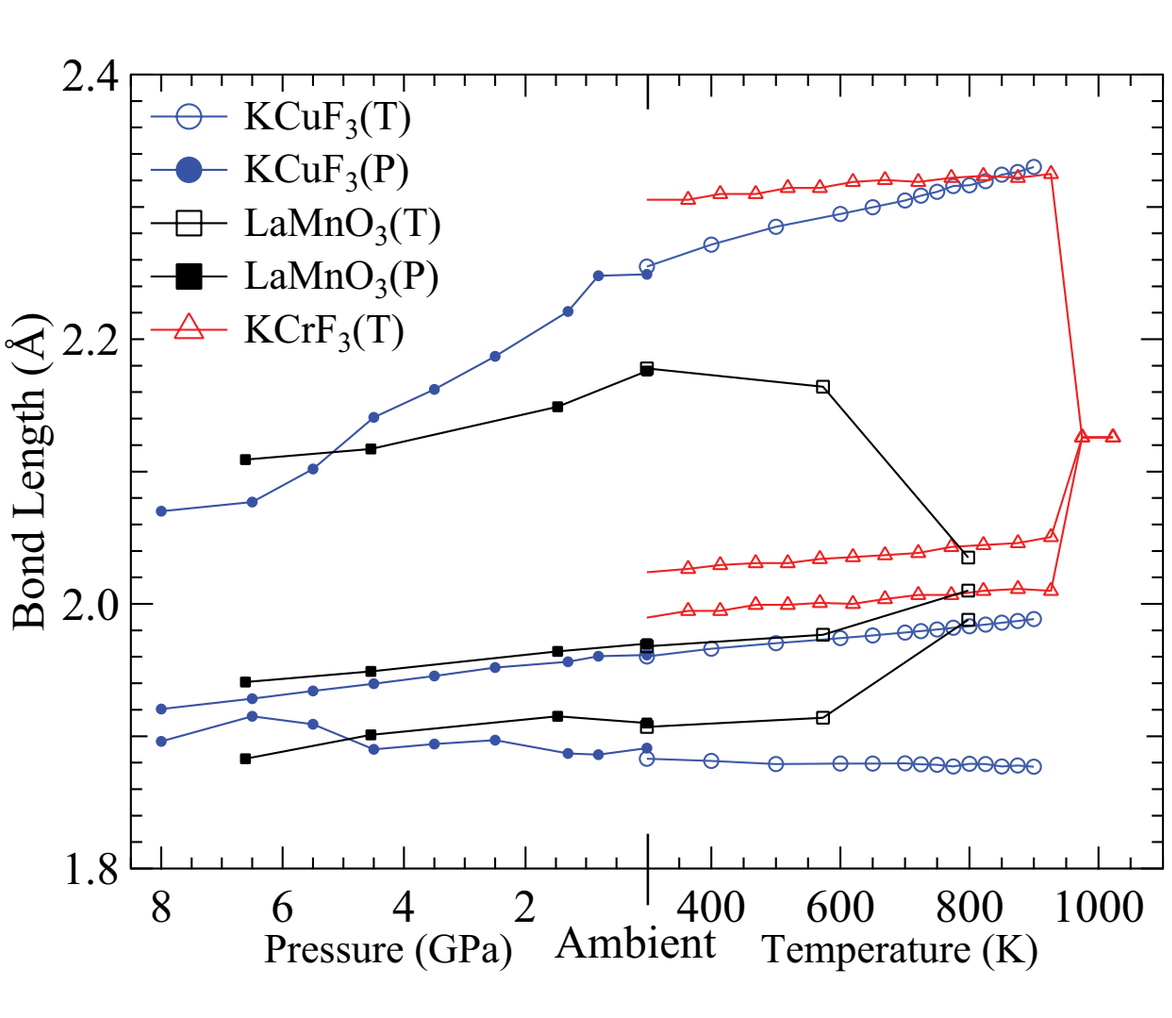
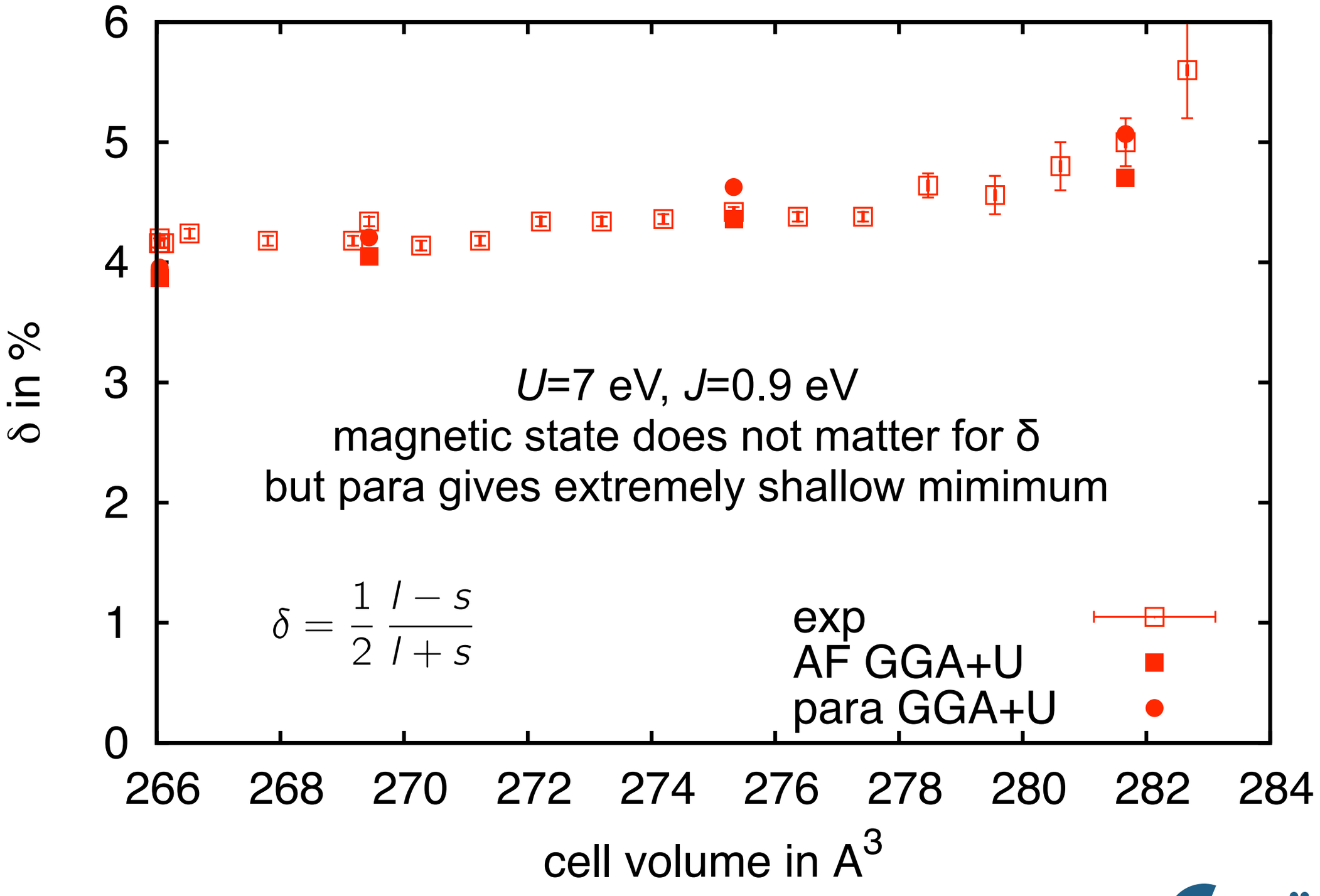
(Received 21 July 2012; revised manuscript received 22 November 2012; published 22 January 2013)





excellent agreement with GGA+U



(same result of GGA+DMFT)

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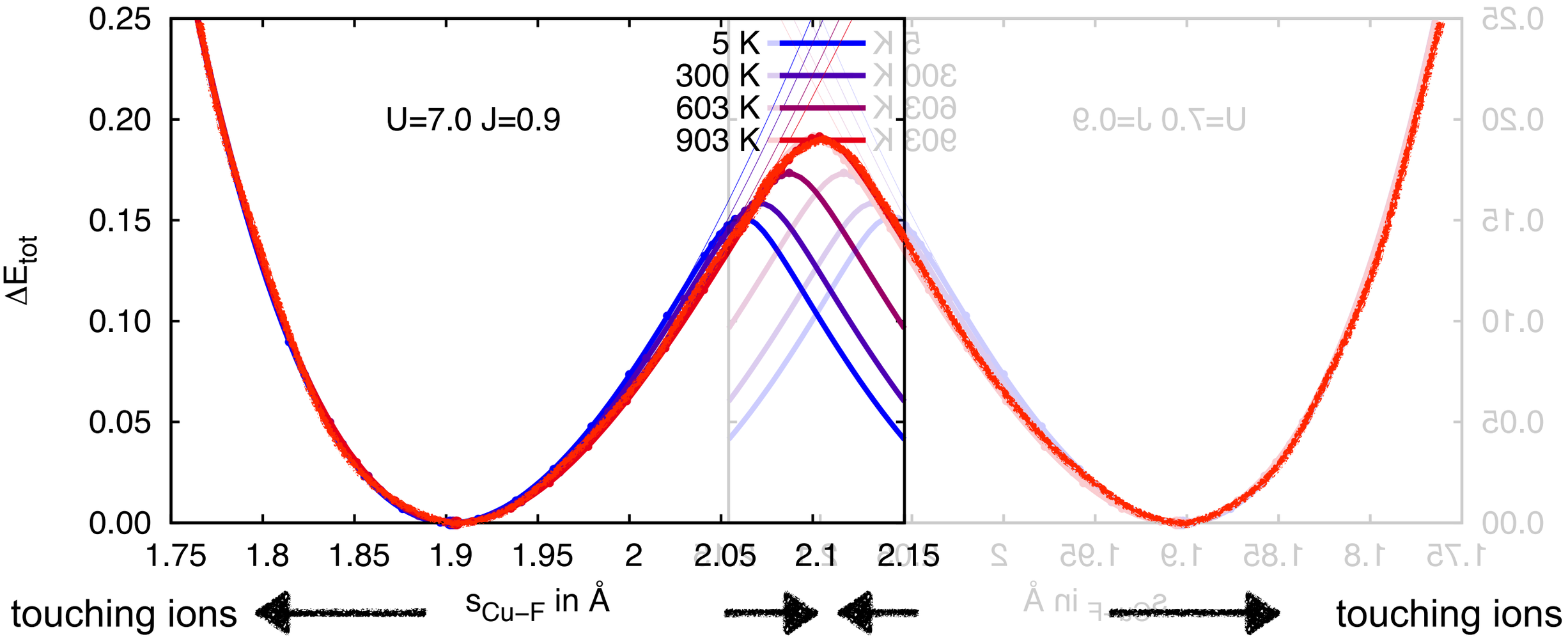
GGA+U energy curve



(same result of GGA+DMFT)

effects of distortion: a simple model

change in e_g crystal-field splitting

change in Ewald term

$$E_{\mathrm{ionJT}}(\Delta) = \Gamma - \sqrt{\Gamma^2 + (g\Delta)^2} - C_{\mathrm{Ewald}}\Delta^2/2$$
$$+ 2Be^{-a/\rho 2\sqrt{2}}[\cosh(\Delta/\rho) - 1],$$

Born-Mayer potential

the T-dependence is via the lattice constant!

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

Thermally assisted ordering in Mott insulators

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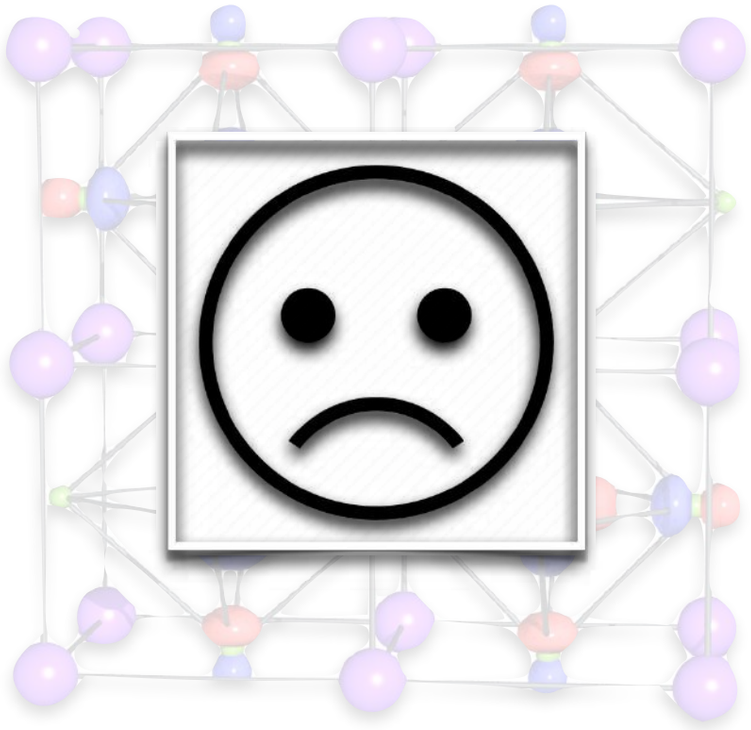
(Received 16 November 2016; revised manuscript received 19 July 2017; published 8 August 2017)

Landau theory describes phase transitions as the competition between energy and entropy: The ordered phase has lower energy, while the disordered phase has larger entropy. When heating the system, ordering is reduced entropically until it vanishes at the critical temperature. This picture implicitly assumes that the energy difference between the ordered and disordered phases does not change with temperature. We show that for orbital ordering in the Mott insulator $KCuF_3$, this assumption fails qualitatively: entropy plays a negligible role, while thermal expansion energetically stabilizes the orbitally ordered phase to such an extent that no phase transition is observed. To understand this strong dependence on the lattice constant, we need to take into account the Born-Mayer repulsion between the ions. It is the latter, and not the Jahn-Teller elastic energy, which determines the magnitude of the distortion. This effect will be seen in all materials where the distortion expected from the Jahn-Teller mechanism is so large that the ions would touch. Our mechanism explains not only the absence of a phase transition in $KCuF_3$, but even suggests the possibility of an *inverted* transition in closed-shell systems, where the ordered phase emerges only at high temperatures.

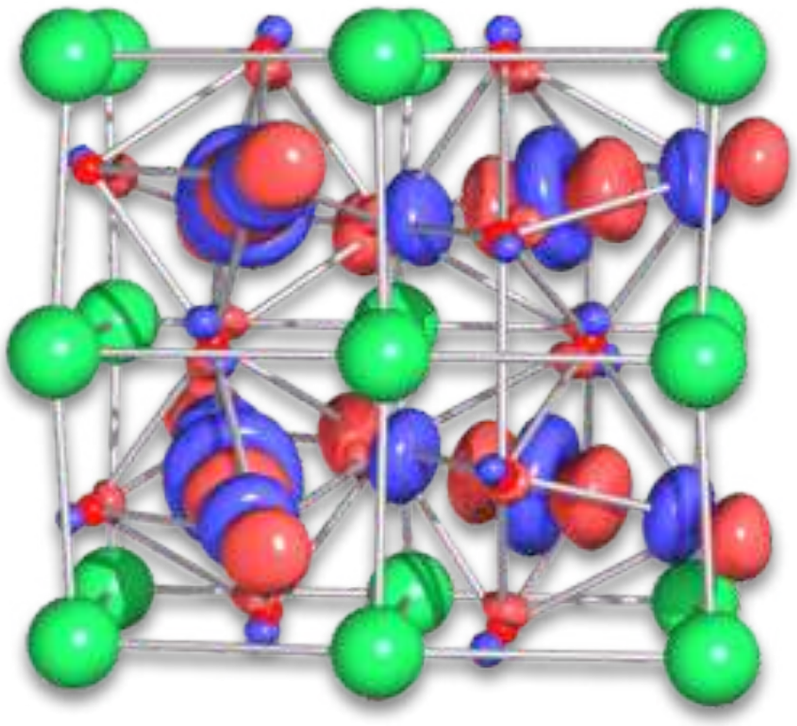
Kugel-Khomskii candidates

$KCuF_3$

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



$LaMnO_3$



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

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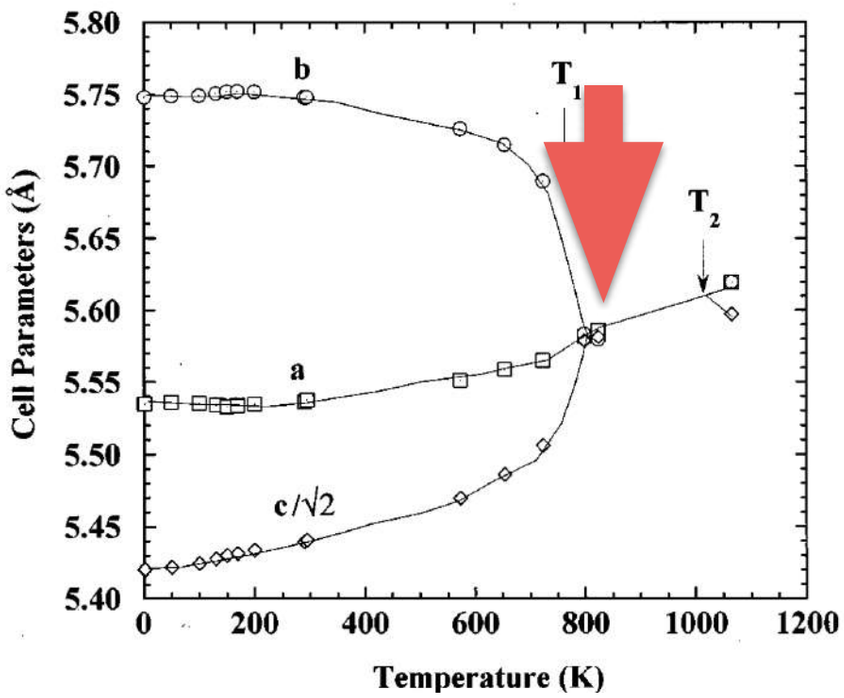
orbital-order transition at T_{OO} in $LaMnO_3$

$T_{OO} \sim 800$ K



PHYSICAL REVIEW B VOLUME 57, NUMBER 6 1 FEBRUARY 1998-II

Neutron-diffraction study of the Jahn-Teller transition in stoichiometric $LaMnO_3$

J. Rodríguez-Carvajal,* M. Hennion, F. Moussa, and A. H. Moudden
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L. Pinsard and A. Revcolevschi
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(Received 2 September 1997)

The parent compound of the giant magnetoresistance Mn-perovskite, $LaMnO_3$, has been studied by thermal analysis and high-resolution neutron-powder diffraction. The orthorhombic *Pbnm* structure at room temperature is characterized by an antiferrodistorsive orbital ordering due to the Jahn-Teller effect. This ordering is evidenced by the spatial distribution of the observed Mn-O bond lengths. $LaMnO_3$ undergoes a structural phase transition at $T_{JT} \approx 750$ K, above which the orbital ordering disappears. There is no change in symmetry although the lattice becomes metrically cubic on the high-temperature side. The MnO_6 octahedra become nearly regular above T_{JT} and the thermal parameter of oxygen atoms increases significantly. The observed average cubic lattice is probably the result of dynamic spatial fluctuations of the underlying orthorhombic distortion. [S0163-1829(98)51706-7]

VOLUME 81, NUMBER 3 PHYSICAL REVIEW LETTERS 20 JULY 1998

Resonant X-Ray Scattering from Orbital Ordering in $LaMnO_3$

Y. Murakami,[1,2] J. P. Hill,[3] D. Gibbs,[3] M. Blume,[3] I. Koyama,[1] M. Tanaka,[1] H. Kawata,[1] T. Arima,[4] Y. Tokura,[5] K. Hirota,[2,6] and Y. Endoh[2,6]
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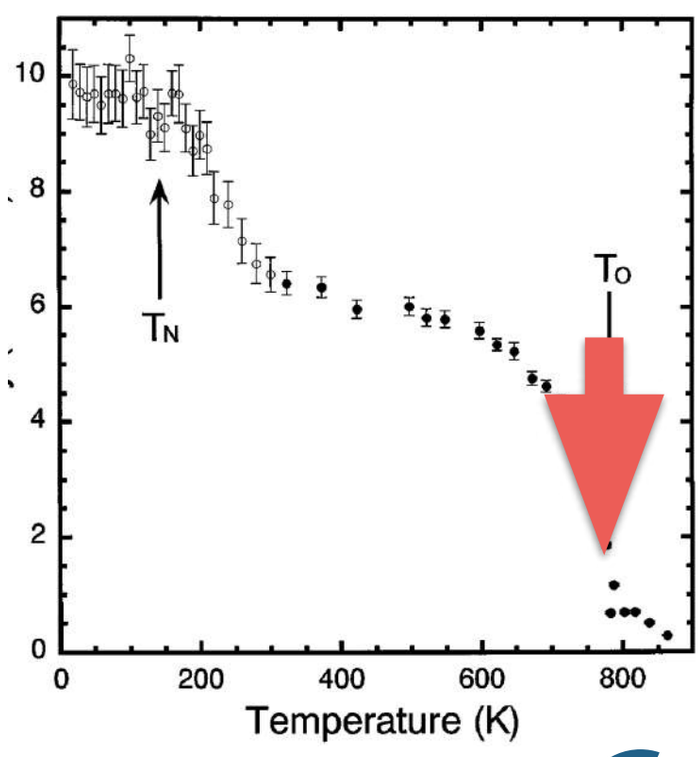
[5]*Department of Applied Physics, University of Tokyo, Tokyo 113-0033, Japan and Joint Research Center for Atom Technology (JRCAT), Tsukuba 305-0046, Japan*
[6]*Department of Physics, Tohoku University, Sendai 980-8578, Japan*
(Received 22 April 1998)



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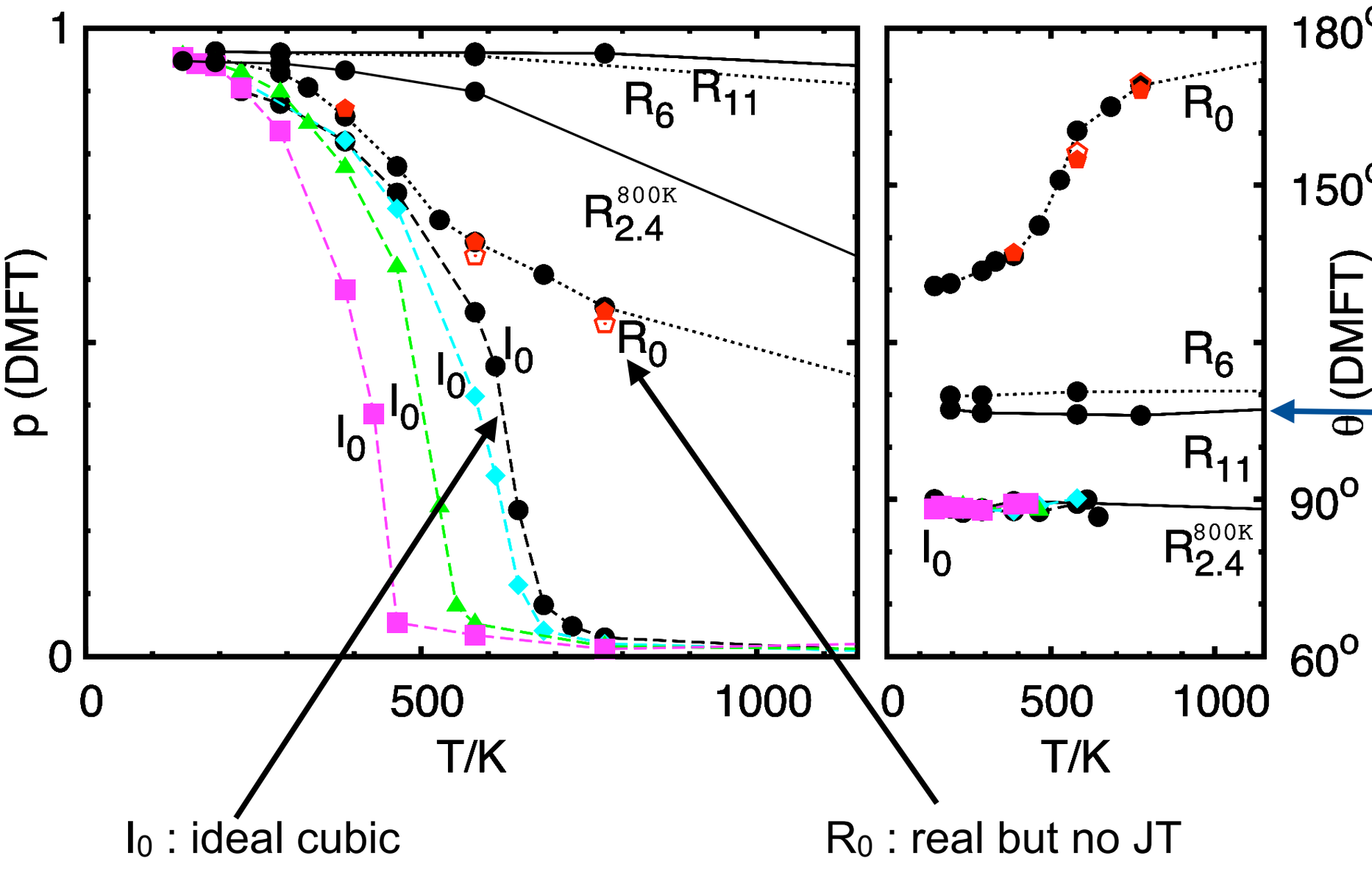
$LaMnO_3$: T_{KK} ~ 600 K !!

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



non-JT crystal-field

red: cDMFT 4 sites

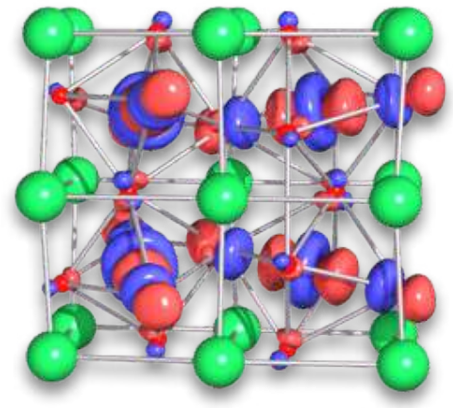
black: DMFT

experiments

super-exchange

I_0 : ideal cubic

R_0 : real but no JT



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

T_{OO}: orbital order-to-disorder transition

$T_{OO} \sim 800$ K

PRL **94,** 177203 (2005) PHYSICAL REVIEW LETTERS week ending 6 MAY 2005

Orbital Correlations in the Pseudocubic *O* and Rhombohedral *R* Phases of $LaMnO_3$

Xiangyun Qiu,[1] Th. Proffen,[2] J. F. Mitchell,[3] and S. J. L. Billinge[1]

[1]*Department of Physics and Astronomy, Michigan State University, E. Lansing, Michigan 48824, USA*
[2]*Los Alamos National Laboratory, LANSCE-12, MS H805, Los Alamos, New Mexico 87545, USA*
[3]*Material Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA*

(Received 12 August 2004; revised manuscript received 24 February 2005; published 5 May 2005)

The local and intermediate structure of stoichiometric $LaMnO_3$ has been studied in the pseudocubic and rhombohedral phases at high temperatures (300–1150 K). Neutron powder diffraction data were collected and a combined Rietveld and high real space resolution atomic pair distribution function analysis was carried out. The nature of the Jahn-Teller (JT) transition around 750 K is confirmed to be orbital order to disorder. In the high-temperature orthorhombic (*O*) and rhombohedral (*R*) phases, the MnO_6 octahedra are still fully distorted locally. More importantly, the intermediate structure suggests the presence of local ordered clusters of diameter ~16 Å (~4 MnO_6 octahedra) implying strong nearest-neighbor JT antiferrodistortive coupling. These clusters persist well above the JT transition temperature even into the high-temperature *R* phase.

DOI: 10.1103/PhysRevLett.94.177203 PACS numbers: 75.47.Lx, 61.12.−q, 75.47.Gk

$T_{JT} > 1150$ K

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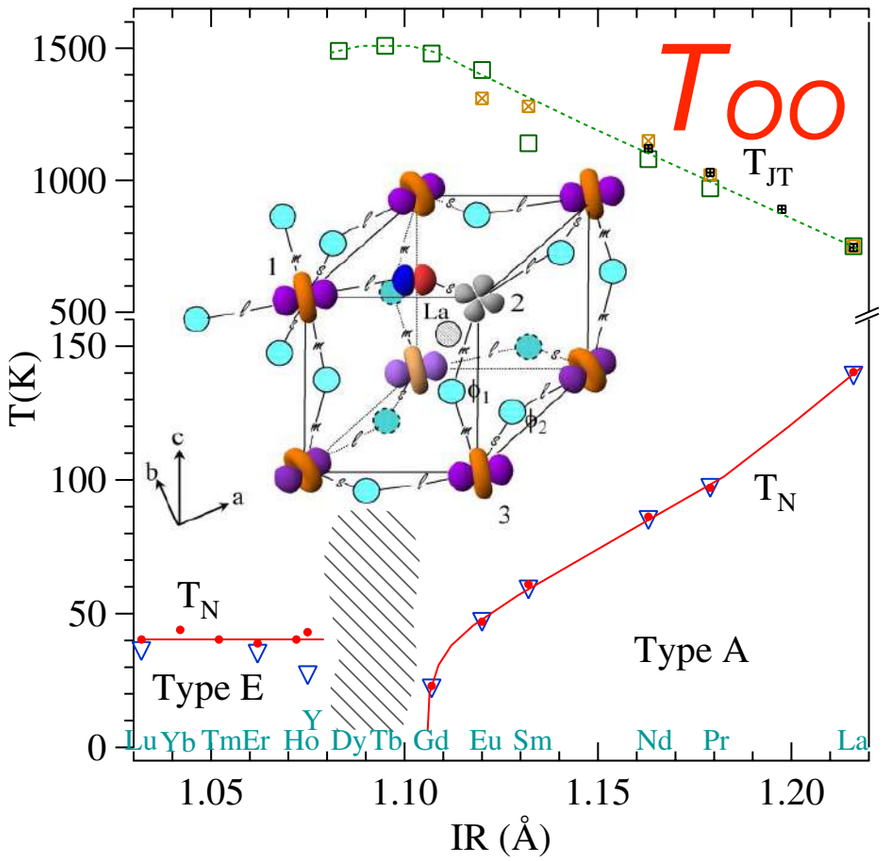
orbital order melting in $ReMnO_3$

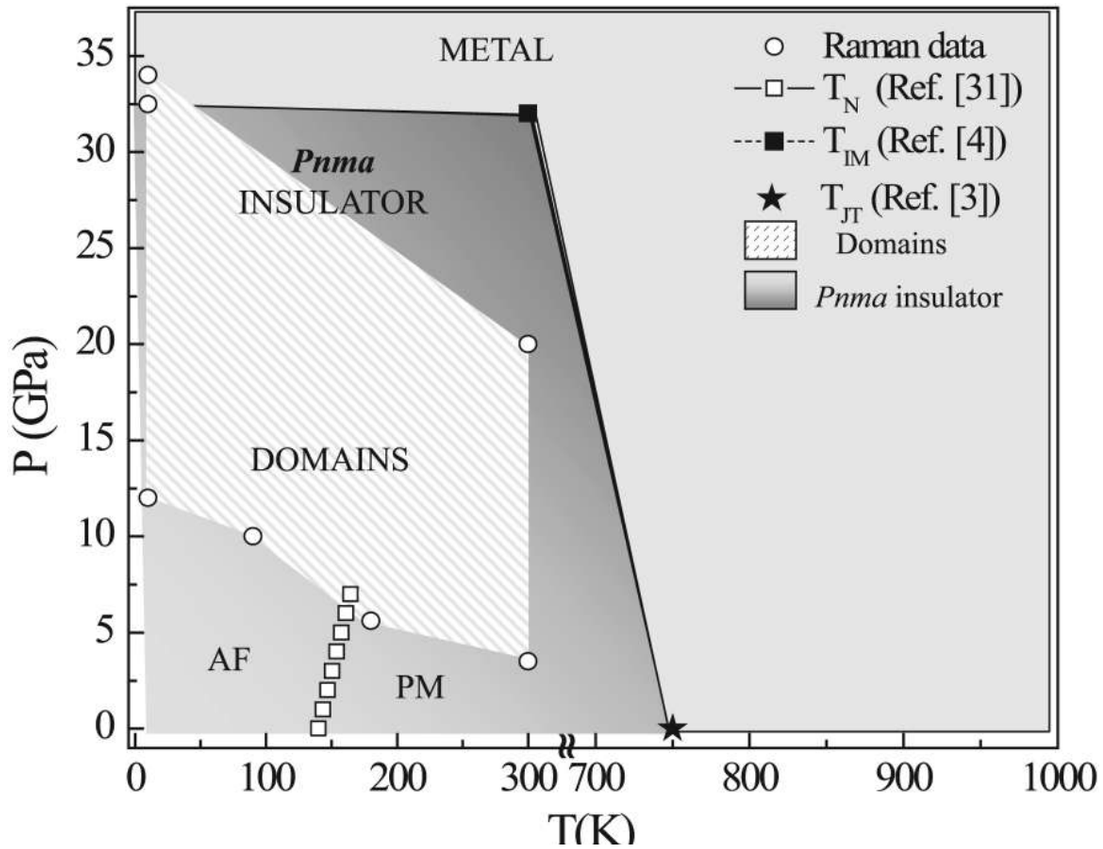
Unusual Evolution of the Magnetic Interactions versus Structural Distortions in $RMnO_3$ Perovskites

J.-S. Zhou and J. B. Goodenough



Persistence of Jahn-Teller Distortion up to the Insulator to Metal Transition in $LaMnO_3$

M. Baldini,[1,2] V. V. Struzhkin,[3] A. F. Goncharov,[3] P. Postorino,[4,5] and W. L. Mao[1,2,6]



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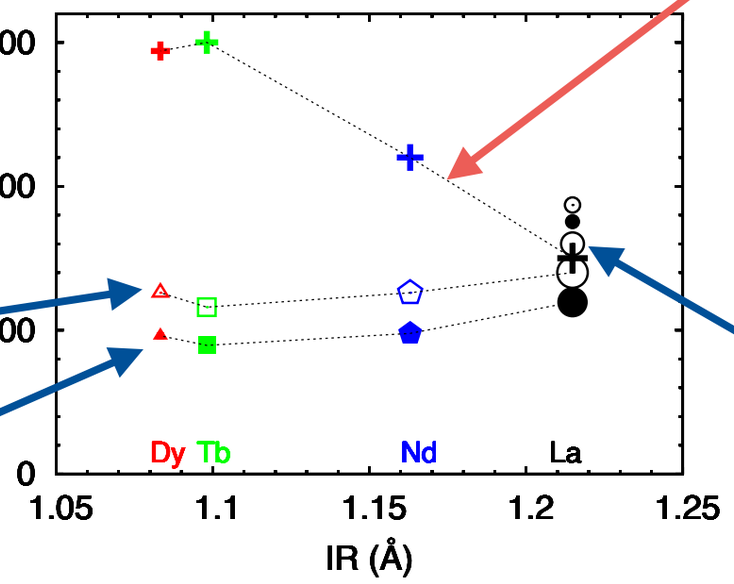
KK critical temperatures

T_{KK} decreases with IR

T_{OO} in experiments

T_{KK}
from orbital polarization

T_{KK}
from total energy



$KCuF_3$

$KCrF_3$

$LaMnO_3$
under pressure

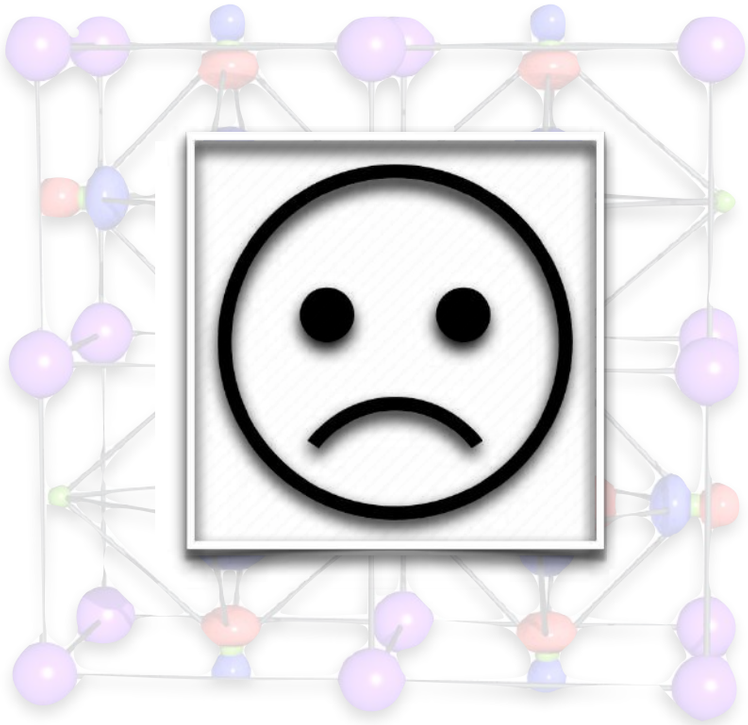
Phys. Rev. B **85**, 035124 (2012)

Phys. Rev. B **87**, 195141 (2013)

Kugel-Khomskii candidates

e_g systems

$KCuF_3$



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

$LaMnO_3$

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

$KCrF_3$

$ReMnO_3$

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perhaps we looked in the wrong place..

t_{2g} titanates at low temperature?

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

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orbital liquid?

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)

We present a theory of spin and orbital states in Mott insulator $LaTiO_3$. The spin-orbital superexchange interaction between $d^1(t_{2g})$ ions in cubic crystal suffers from a pathological degeneracy of orbital states at the classical level. Quantum effects remove this degeneracy and result in the formation of the coherent ground state, in which the orbital moment of t_{2g} level is fully quenched. We find a finite gap for orbital excitations. Such a disordered state of local degrees of freedom on unfrustrated, simple cubic lattice is highly unusual. Orbital liquid state naturally explains observed anomalies of $LaTiO_3$.

d^1 electronic configuration

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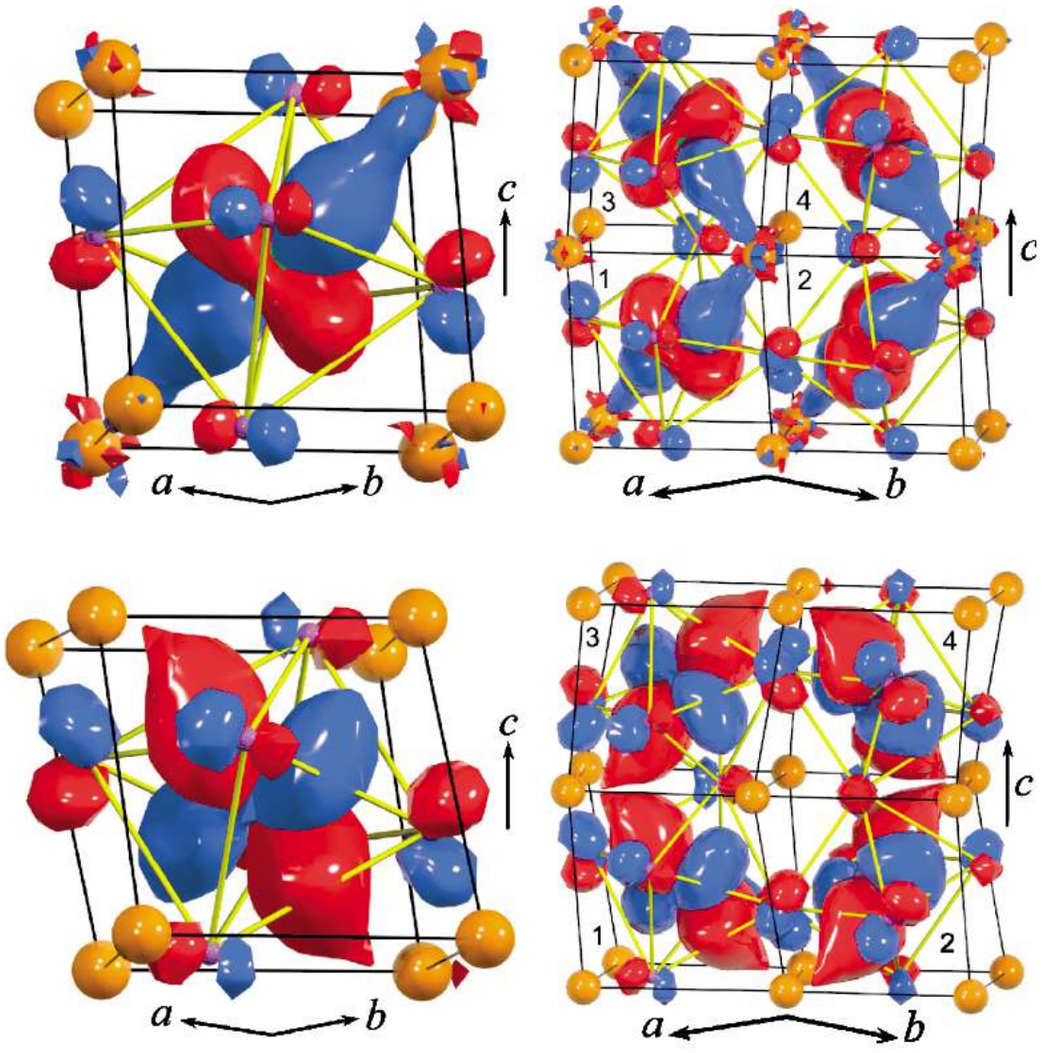
Coulomb-enhanced crystal field

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

LDA+DMFT 770 K

Δ=200-300 meV

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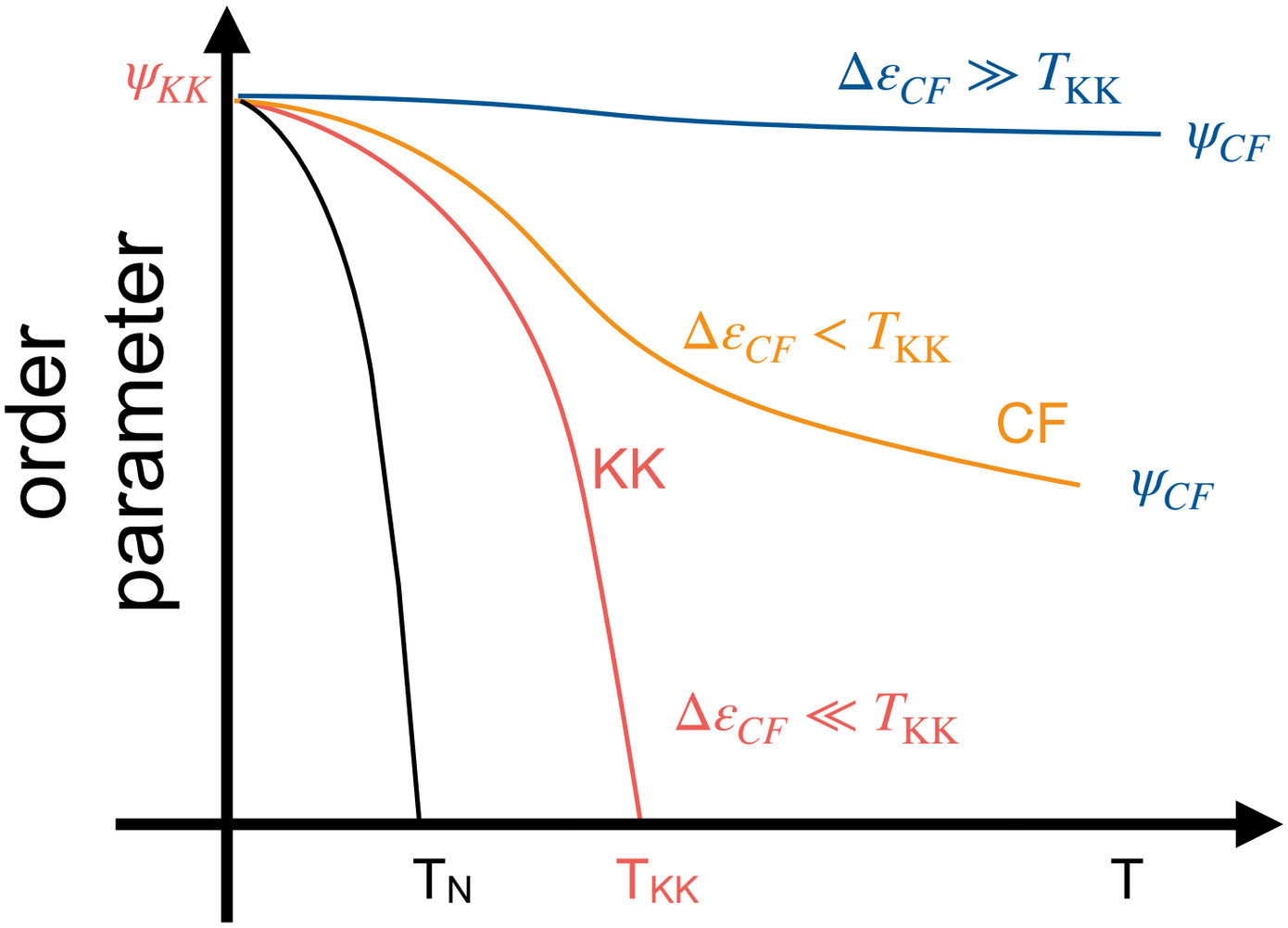
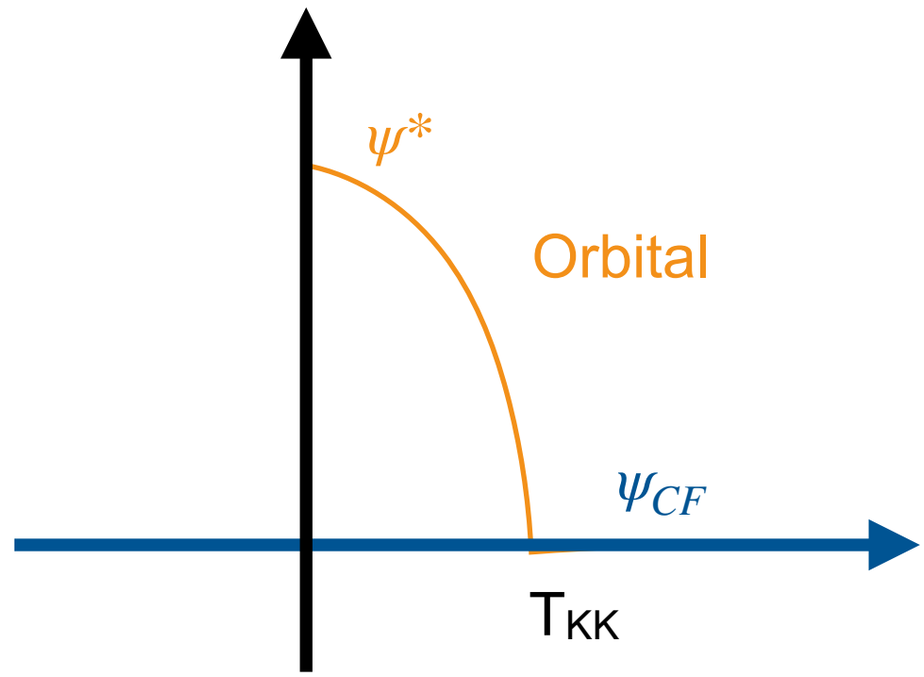
but what about low T, right above T_N?

change of orbitals at low T?





ψ = occupied orbital

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General Super Exchange 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 Hamiltonian for the t_{2g}^1 configuration, we show that the $GdFeO_3$-type distortion plays a key part in enhancing T_{KK} to about 300 K. Still, orbital ordering above 300 K can be ascribed only to the presence of a static crystal-field splitting.

General Super Exchange Hamiltonians

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 based on *ab initio* hopping parameters and realistic screened Coulomb interactions and allows for a systematic exploration of superexchange energy surfaces in a realistic context.

DOI: 10.1103/PhysRevB.105.115104

derivation

II. FORMALISM

The superexchange Hamiltonian has the form:

$$\hat{H}_{\mathrm{SE}} = \frac{1}{2}\sum_{ij}\hat{H}^{ij}_{\mathrm{SE}}, \tag{1}$$

where i and j are neighboring sites coupled via hopping integrals. This Hamiltonian acts in the subspace of states with $|n_i, n_j\rangle$, where n_i and n_j are the site occupations with the constraint $n_i{+}n_j = N = 2n$, where n is the number of electrons per site. From strong-coupling second-order perturbation theory, Eq. (1) can be written as

$$\hat{H}_{\mathrm{SE}} = -\hat{H}_{\mathrm{T}}(\hat{H}_U - E_0)^{-1}\hat{H}_{\mathrm{T}},$$

so that

$$\hat{H}^{ij}_{\mathrm{SE}} = -\hat{H}_{\mathrm{T}}(\hat{P}_{ij} + \hat{P}_{ji})\hat{H}_{\mathrm{T}}.$$

Here, $\hat{P}_{ij}$ is an operator which projects, with an energy denominator, to atomic excited states of type $|n_i{+}1, n_j{-}1\rangle$, and $\hat{H}_{\mathrm{T}}$ is the hopping part of the Hubbard Hamiltonian from which the superexchange interaction is derived, while $\hat{H}_U$ is the electron-electron repulsion.

Let us start from the well-known case of magnetic exchange for the single-band Hubbard model:

$$\hat{H} = \underbrace{-\sum_{\sigma}\sum_{i,j} t^{i,j} c^{\dagger}_{i\sigma} c_{j\sigma}}_{\hat{H}_{\mathrm{T}}} + \underbrace{U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}}_{\hat{H}_U}, \tag{2}$$

where $\hat{n}_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$, $t^{i,j}$ is the hopping integral and U the screened Coulomb parameter. Since the atomic limit of the half-filled Hubbard Hamiltonian has only spin degrees of freedom, one can write the associated exchange Hamiltonian in an irreducible tensor basis as

$$\hat{H}^{ij}_{\mathrm{SE}} = \sum_{qq'}\sum_{\nu\nu'}\hat{s}^{q,\nu}_i D^{ij}_{q\nu,q'\nu'}\hat{s}^{q',\nu'}_j, \tag{3}$$

where $q = 0, 1$ is the rank of the operators and ν the associated components. For $q = 0$, the only component is $\nu = s$, while for $q = 1$, we have instead $\nu = x, y, z$ in the real harmonics representation. For convenience, we normalize the tensors such that

$$\sum_{\sigma}\langle 0|c_{i\sigma}\left(\hat{s}^{q,\nu}_i\right)^2 c^{\dagger}_{i\sigma}|0\rangle = 1. \tag{4}$$

With this convention, the irreducible tensors are

$$\hat{s}^{0,s}_i = \frac{1}{\sqrt{2}}\sum_{\sigma} c^{\dagger}_{i\sigma}c_{i\sigma}, \tag{5}$$

$$\hat{s}^{1,\nu}_i = \frac{1}{\sqrt{2}}\sum_{\sigma\sigma'} c^{\dagger}_{i\sigma}\langle\sigma|\hat{\sigma}^{\nu}|\sigma'\rangle c_{i\sigma'}, \tag{6}$$

where $\hat{\sigma}_\nu$ is the $\nu = x, y, z$ Pauli matrix. At half-filling ($n_i = n_j = 1$), we define the projectors as

$$\hat{P}_{ij} = \sum_{\alpha_+\alpha_-}\frac{|\alpha_+\rangle_i|\alpha_-\rangle_j\,{}_j\langle\alpha_-|\,{}_i\langle\alpha_+|}{E_{\alpha_+}{+}E_{\alpha_-}{-}2E_0}, \tag{7}$$

where $|\alpha_\pm\rangle_i$ are atomic (site i) multiplets with $n_i \pm 1$ electrons, quantum number $\alpha_\pm$ and energy $E_{\alpha_\pm}$. In the case of the single-band Hubbard model, $|\alpha_+\rangle_i$ and $|\alpha_-\rangle_i$ are, respectively, the doubly occupied and the vacuum state; in general, however, α_+ and α_- will label several excited states with different energies. Here, E_0 is the energy of the ground state with $N = n_i + n_j = 2$ electrons in the atomic limit, here, $E_0 = 0$. The tensor elements in Eq. (3) are obtained using the orthogonality properties of irreducible tensors. To this end, we multiply by a pair of irreducible operators, one for site i and one for site j, and trace over all states in the atomic ground multiplet. This yields

$$\begin{aligned} D^{ij}_{0s,0s} &= -\frac{\mathrm{Tr}\left[\hat{s}^{0,s}_i\hat{s}^{0,s}_j\hat{H}_{\mathrm{T}}(\hat{P}_{ij}+\hat{P}_{ji})\hat{H}_{\mathrm{T}}\right]}{\mathrm{Tr}\left[\left(\hat{s}^{0,s}_i\right)^2\left(\hat{s}^{0,s}_j\right)^2\right]} \\ &= -2\frac{|t^{i,j}|^2}{U}, \end{aligned}$$

and

$$\begin{aligned} D^{ij}_{1\nu,1\nu'} &= -\frac{\mathrm{Tr}\left[\hat{s}^{1,\nu}_i\hat{s}^{1,\nu'}_j\hat{H}_{\mathrm{T}}(\hat{P}_{ij}+\hat{P}_{ji})\hat{H}_{\mathrm{T}}\right]}{\mathrm{Tr}\left[\left(\hat{s}^{1,\nu}_i\right)^2\left(\hat{s}^{1,\nu'}_j\right)^2\right]} \\ &= 2\frac{|t^{i,j}|^2}{U}\delta_{\nu,\nu'}. \end{aligned}$$

irreducible tensor decomposition

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

$$\hat{H}^{ij}_{\mathrm{SE}} = \sum_{rr'}\sum_{\mu\mu'} \hat{\tau}^{r,\mu}_{i} D^{ij}_{r\mu,r'\mu'} \hat{\tau}^{r',\mu'}_{j}$$

$\mathcal{W}_0 = f_{-3}+\frac{5}{9}f_{-1}+\frac{1}{9}f_2 = \frac{w_1+4w_2}{3}$,			$\mathcal{V}_0 = \frac{8}{9}f_{-3}+\frac{10}{9}f_0+\frac{2}{3}f_2 = \frac{4(v_1+v_2)}{3}$
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$\mathcal{W}_2 = \frac{3}{4}f_{-3}-\frac{1}{12}f_{-1}-\frac{1}{6}f_2 = \frac{2w_2-w_1}{2}$,			$\mathcal{V}_2 = \frac{2}{3}f_{-3}+\frac{1}{12}f_0-\frac{1}{4}f_2 = \frac{2v_2-v_1}{2}$
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$\tilde{\mathcal{W}}_1 = \frac{1}{8}f_{-3}-\frac{11}{24}f_{-1}-\frac{1}{6}f_2$,			$\tilde{\mathcal{V}}_1 = -\frac{1}{6}f_{-3}-\frac{1}{3}f_0-\frac{1}{2}f_2$
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$\tilde{\mathcal{W}}_3 = \frac{1}{4}f_{-3}+\frac{5}{12}f_{-1}-\frac{1}{6}f_2$,			$\tilde{\mathcal{V}}_3 = \frac{1}{3}f_{-3}+\frac{5}{12}f_0-\frac{1}{4}f_2$

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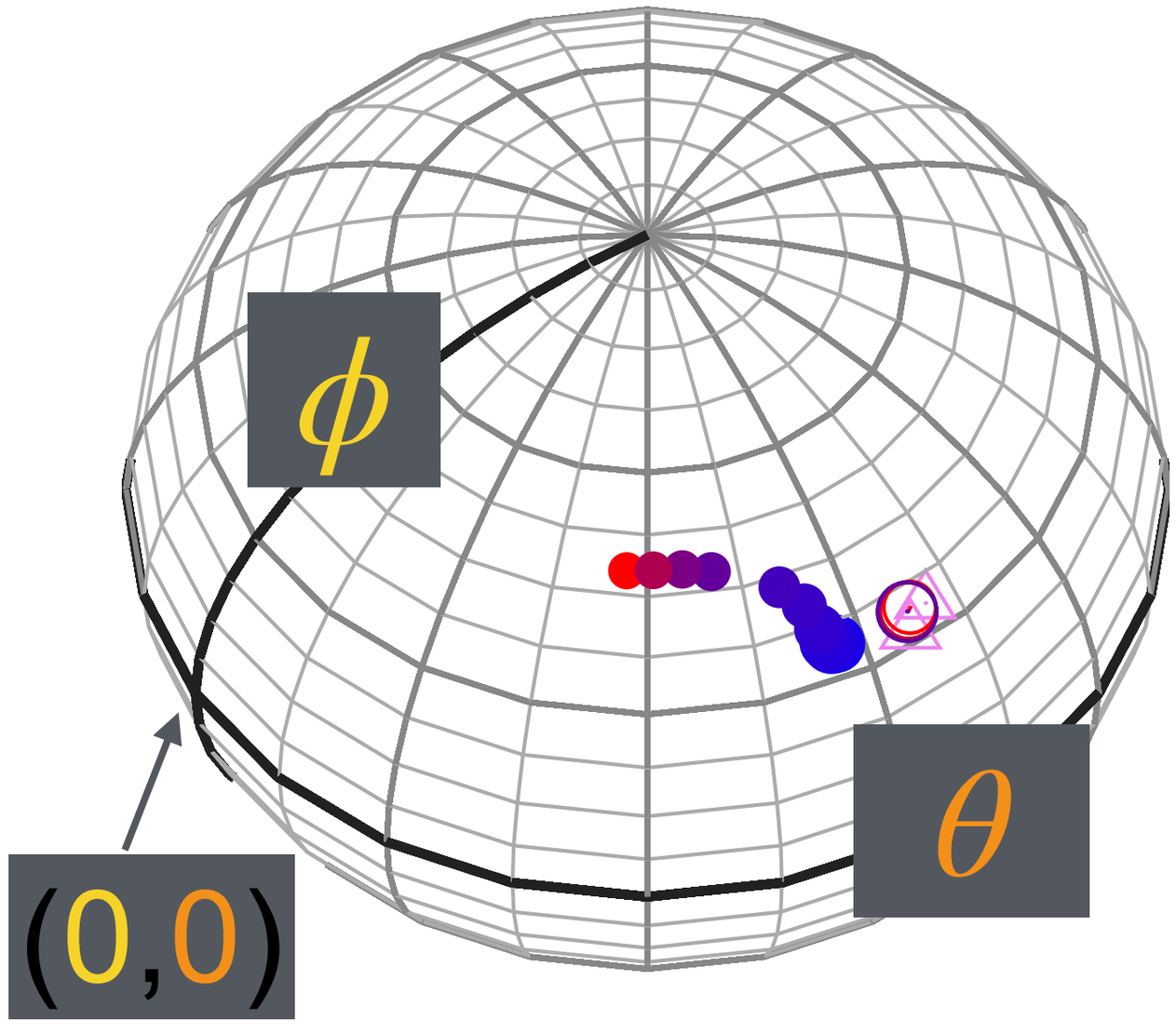
representation of orbital



$$|\theta, \phi\rangle = -\,|\pi - \theta, \phi \pm \pi\rangle$$

$$= \sin\theta\cos\phi|xz\rangle + \cos\theta|xy\rangle + \sin\theta\sin\phi|yz\rangle.$$

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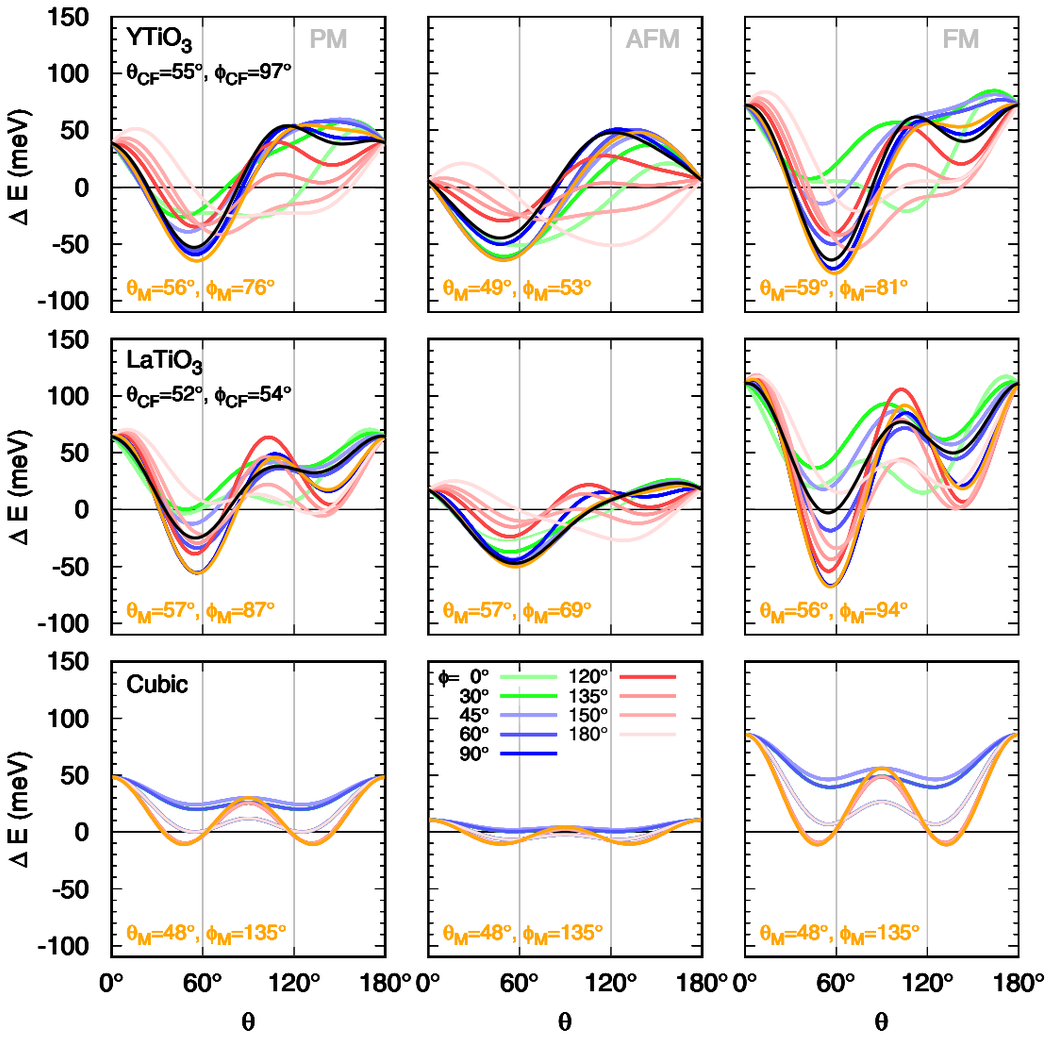
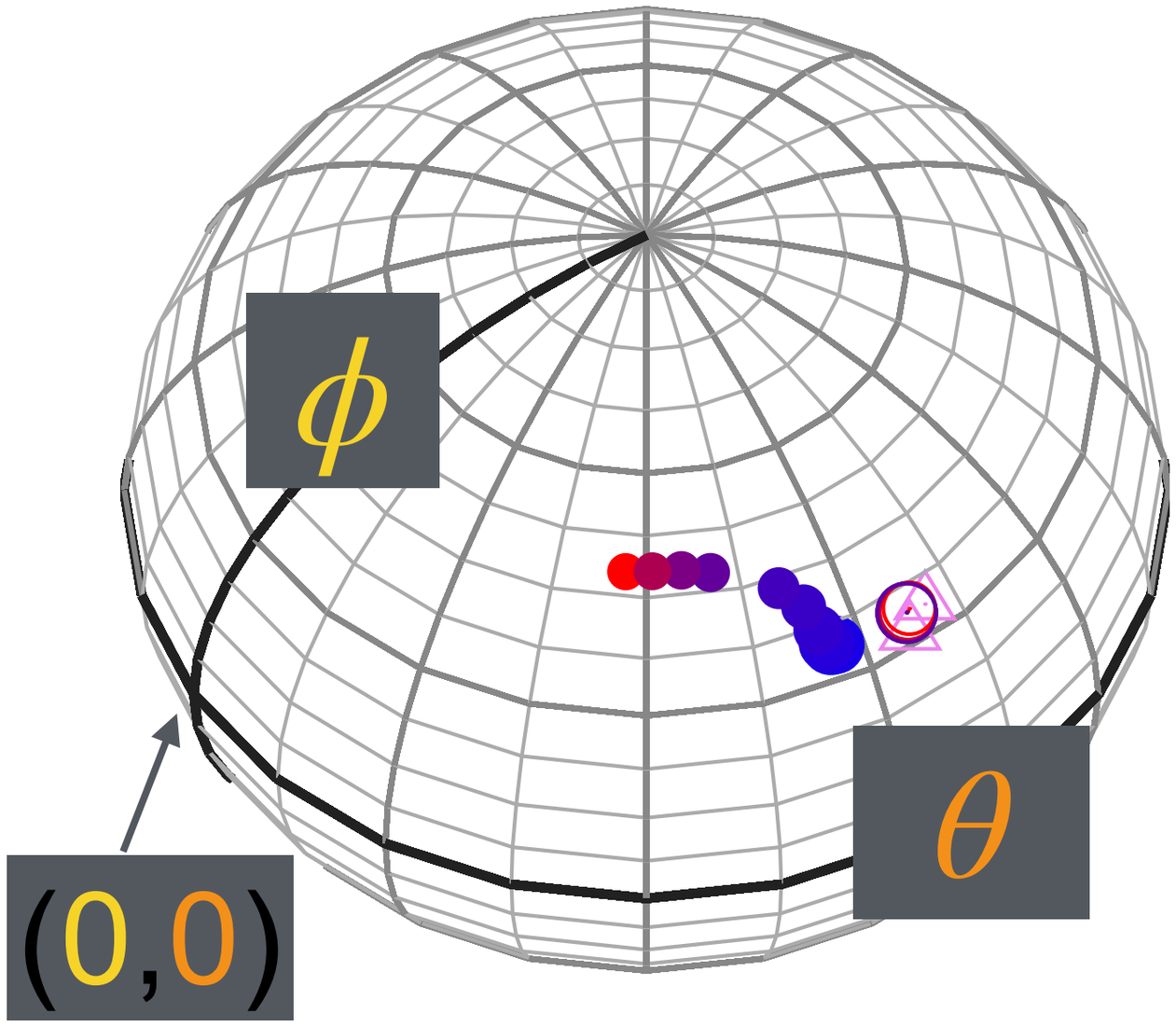
representation of orbital





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$$= \sin\theta\cos\phi|xz\rangle + \cos\theta|xy\rangle + \sin\theta\sin\phi|yz\rangle$$

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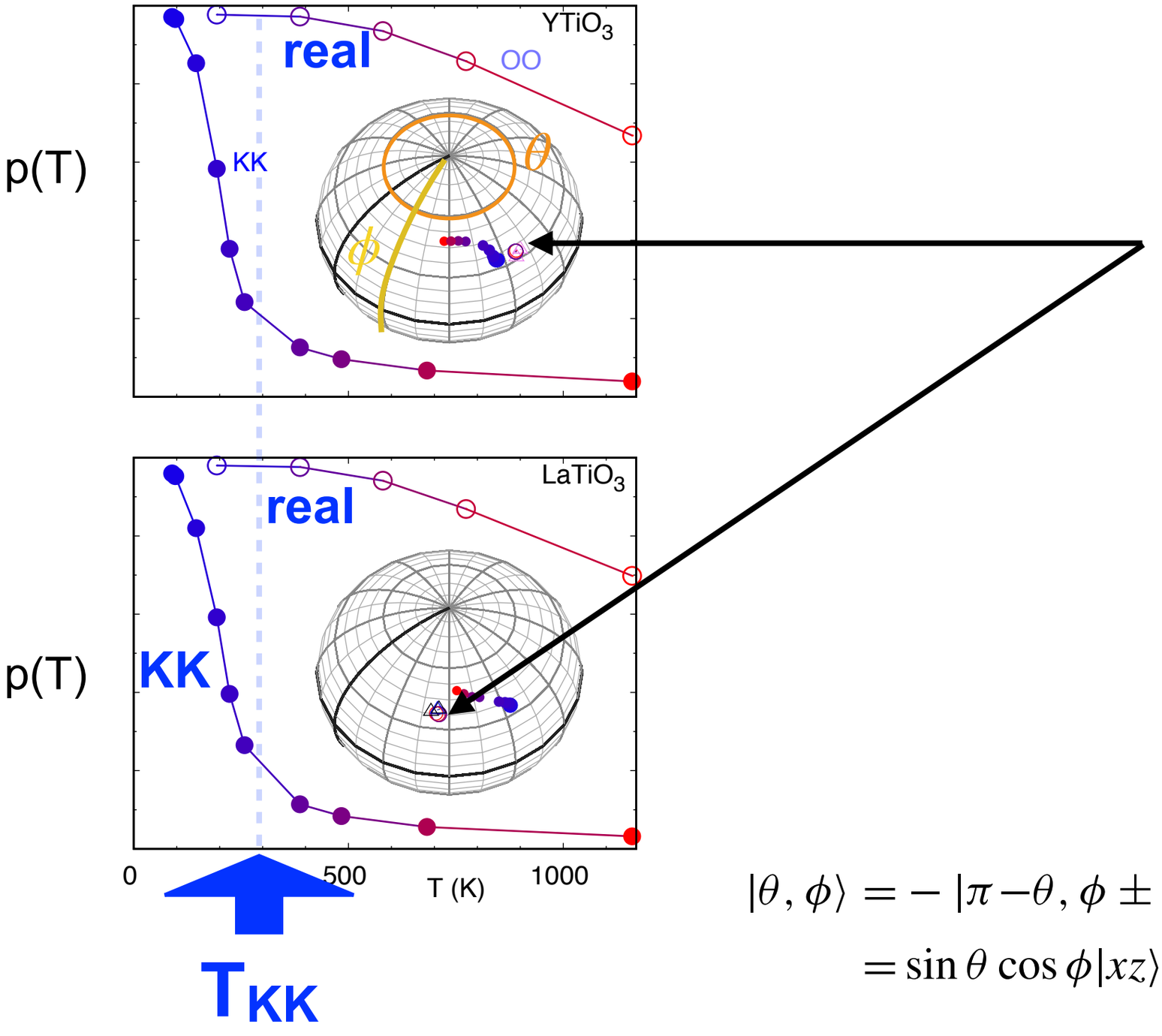
titanates: T_{KK}~300 K



same of CF-orbital

occupied state temperature-independent!

$$|\theta,\phi\rangle = -\,|\pi-\theta,\phi\pm\pi\rangle$$
$$= \sin\theta\cos\phi|xz\rangle + \cos\theta|xy\rangle + \sin\theta\sin\phi|yz\rangle. \quad (58)$$

nothing changes at T_{KK}!

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50 years of Kugel and Khomskii

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.

— Kugel-Khomskii systems — where are they?

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irreducible tensor decomposition

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

$$\hat{H}^{ij}_{\mathrm{SE}} = \sum_{rr'}\sum_{\mu\mu'} \hat{\tau}^{r,\mu}_{i} D^{ij}_{r\mu,r'\mu'} \hat{\tau}^{r',\mu'}_{j}$$

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$\tilde{\mathcal{W}}_0 = \frac{1}{3}f_{-3}-\frac{5}{9}f_{-1}-\frac{1}{9}f_2$,			$\tilde{\mathcal{V}}_0 = \frac{4}{9}f_{-3}-\frac{10}{9}f_0-\frac{2}{3}f_2$
$\tilde{\mathcal{W}}_1 = \frac{1}{8}f_{-3}-\frac{11}{24}f_{-1}-\frac{1}{6}f_2$,			$\tilde{\mathcal{V}}_1 = -\frac{1}{6}f_{-3}-\frac{1}{3}f_0-\frac{1}{2}f_2$
$\tilde{\mathcal{W}}_2 = \frac{1}{4}f_{-3}+\frac{1}{12}f_{-1}+\frac{1}{6}f_2$,			$\tilde{\mathcal{V}}_2 = \frac{1}{3}f_{-3}-\frac{1}{12}f_0+\frac{1}{4}f_2$
$\tilde{\mathcal{W}}_3 = \frac{1}{4}f_{-3}+\frac{5}{12}f_{-1}-\frac{1}{6}f_2$,			$\tilde{\mathcal{V}}_3 = \frac{1}{3}f_{-3}+\frac{5}{12}f_0-\frac{1}{4}f_2$

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what about vandatates?

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

Superexchange Interaction in Orbitally Fluctuating RVO_3

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Texas Materials Institute, University of Texas at Austin, Austin, Texas 78712, USA

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

Changes in pressure and magnetic field in the orbital and magnetic ordering temperatures of RVO_3 perovskites are reported; they reveal a competition between two magnetic orbitally ordered phases that have opposite preferences for the e-orbital component in the localized $^3T_{1g}$ ground state of the V^{3+} ion. This competition is shown to be biased by the $VO_{6/2}$ site distortion intrinsic to the orthorhombic structure. A remarkable enhancement of T_N with pressure is found where the competition leads to enhanced orbital critical fluctuations.

DOI: 10.1103/PhysRevLett.99.156401 PACS numbers: 71.70.Ej, 75.10.Dg, 75.30.Et, 75.50.Ee

suppression of orbital fluctuations

Orbital Fluctuations in the Different Phases of $LaVO_3$ and YVO_3

M. De Raychaudhury,[1,2] E. Pavarini,[3,4] and O. K. Andersen[1]

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[2]*S. N. Bose National Centre for Basic Sciences, Kolkata 700098, India*
[3]*Institut für Festkörperforschung, Forschungzentrum Jülich, D-52425 Jülich, Germany*
[4]*CNISM-Dipartimento di Fisica "A. Volta", Università di Pavia, Via Bassi 6, I-27100 Pavia, Italy*

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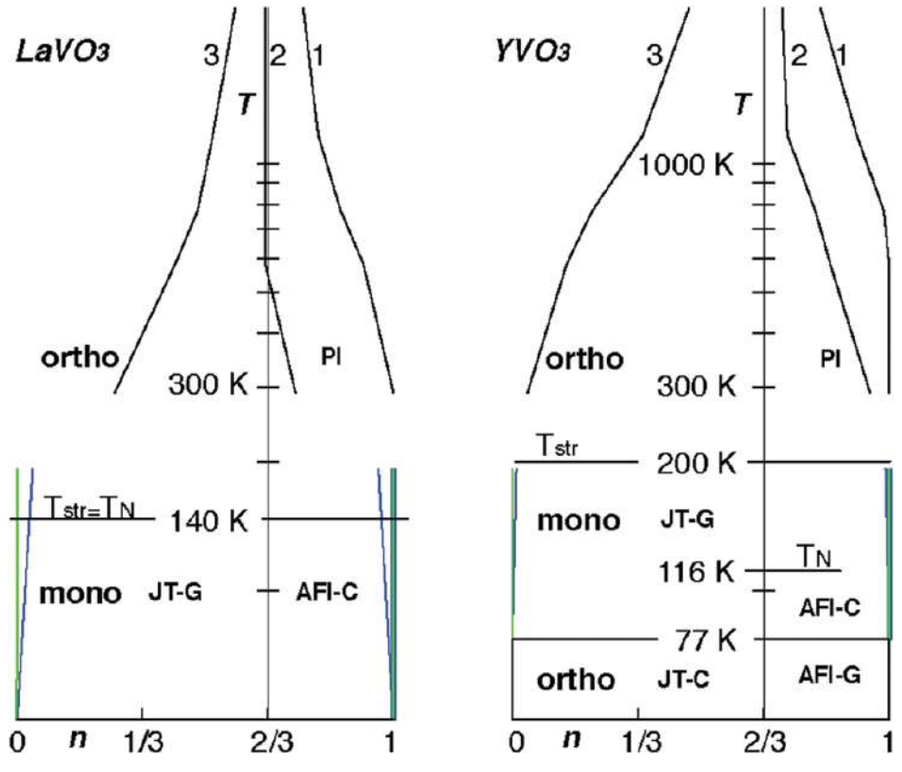
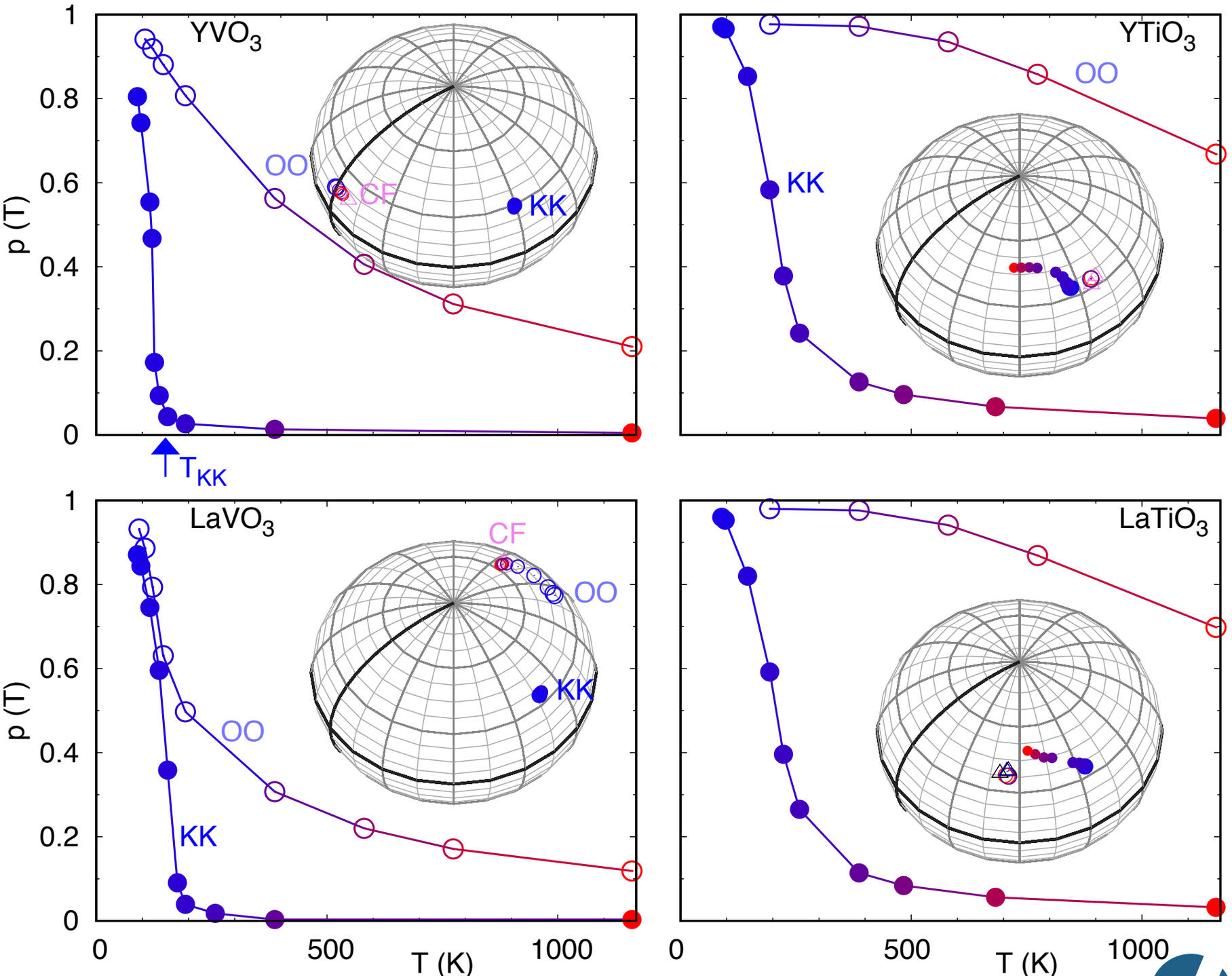


FIG. 1 (color). Temperature-dependent structural and magnetic phases of $LaVO_3$ and YVO_3. The lines show LDA + DMFT (quantum Monte Carlo [21]) results for the occupations, n, of the three t_{2g} crystal-field orbitals, 1, 2, and 3 (Table I). Black lines: orthorhombic phases. Green and blue lines: monoclinic, sites 1 and 3 (see Fig. 2). For each structure we calculated the occupations down the temperature at which the orbital

what about vanadates?



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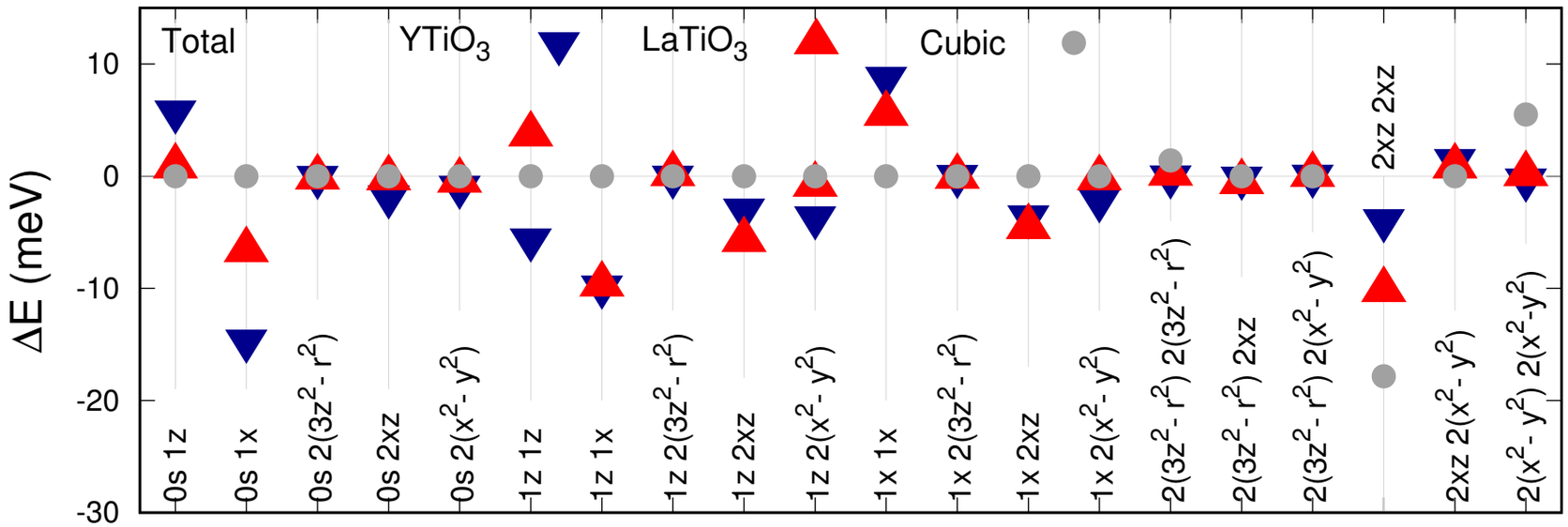
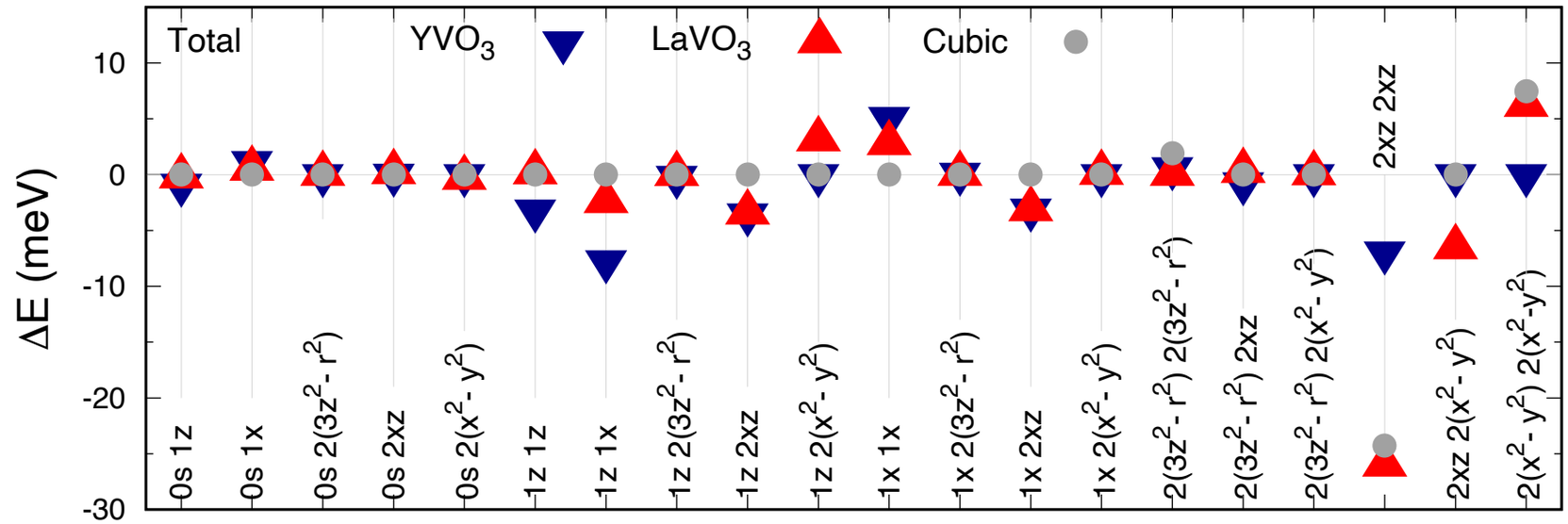
$LaVO_3$ — similar to cubic!





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we should find magnetic fluctuations..

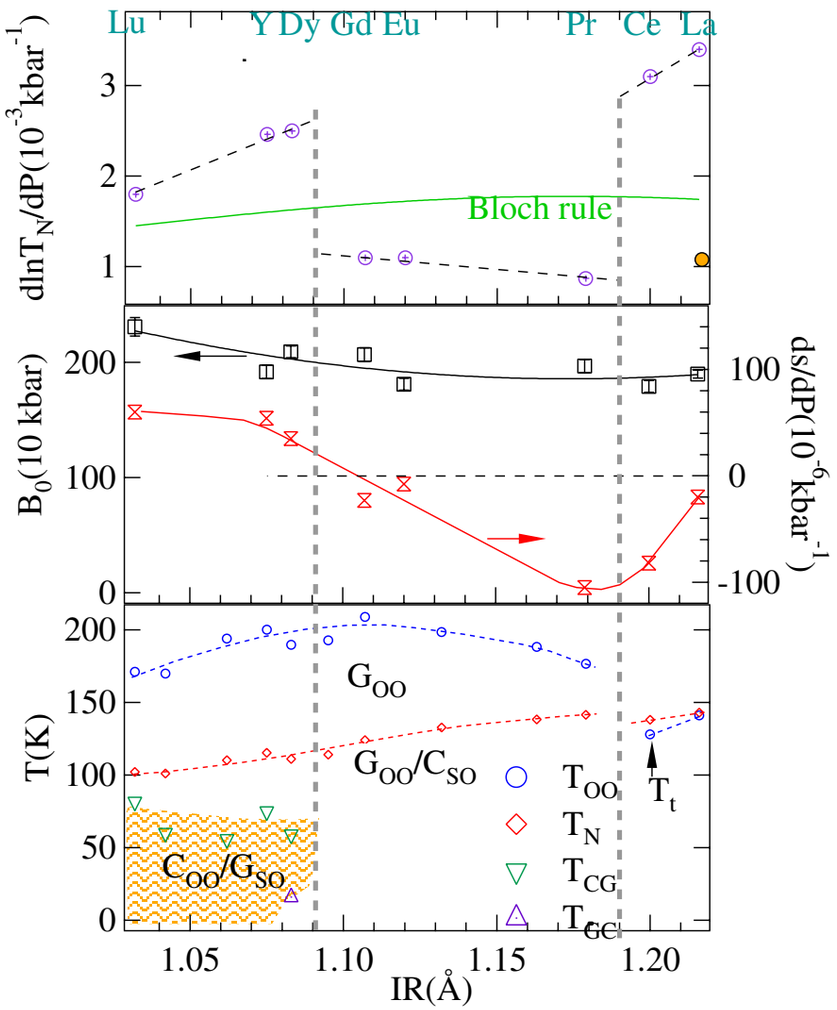

FIG. 3 (color online). Top: the IR dependence of the coefficient $d\ln T_N/dP$ for the $R\mathrm{VO}_3$. T_N is determined in the ZFC measurement. The solid symbol for LaVO_3 is obtained in the FC measurement. Middle: the IR dependence of bulk modulus B_0 and the coefficient ds/dP for the $R\mathrm{VO}_3$. Bottom: the phase diagram of transition temperatures versus IR for $R\mathrm{VO}_3$, data from Ref. [8].

shortening the bond length. This extra gain of T_N under pressure is turned off sharply for the phase in $1.10\text{Å} < IR < 1.19$ Å. In order to identify the possible mechanism responsible for the extra gain of T_N, we will elaborate the pressure effect on the structure and the structural evolution versus IR for these regions of IR. For $IR < 1.10$ Å, the orbitals undergo G-type ordering at T_{OO} and an orbital-flipping transition to C-type ordering at T_{CG}. In both types of orbital ordering, the long axis of the octahedra alternates direction within the (001) planes; there are changes from out-of-phase in the type-G to in-phase in type-C orbital order along the c axis and structural symmetry from $P2_1$ to $Pbnm$ [10,14]. Therefore, an abrupt volume change of the octahedra at T_{CG} cannot be explained by a simple switching from the in-phase to the out-of-phase configuration. The octahedral-site volume in the G_{OO} phase larger than that in the C_{OO} phase obtained from the structural studies [10] suggests a larger percentage of e orbital is present in the ${}^3T_{1g}$ ground state in the G_{OO} phase. More interestingly, the intrinsic component of the site distortion, which can be well-resolved in the orbitally disordered phase and in the G_{OO} phase, disappears in the C_{OO} phase of smaller volume where each $\mathrm{VO}_{6/2}$ site has one long and two equally short V-O bonds. It is clear, therefore, that the orbital-flipping transition results from a competition between a spin-orbital interaction and the structural bias. Pressure favors the C_{OO} phase since it has a smaller cell volume and a smaller octahedral-site distortion, which explains the giant pressure dependence of T_{CG} in Fig. 2. As for the phase with $IR > 1.19$ Å, the orbital-ordering temperature T_t to the G_{OO} phase drops below T_N [8,15]. It is important to note

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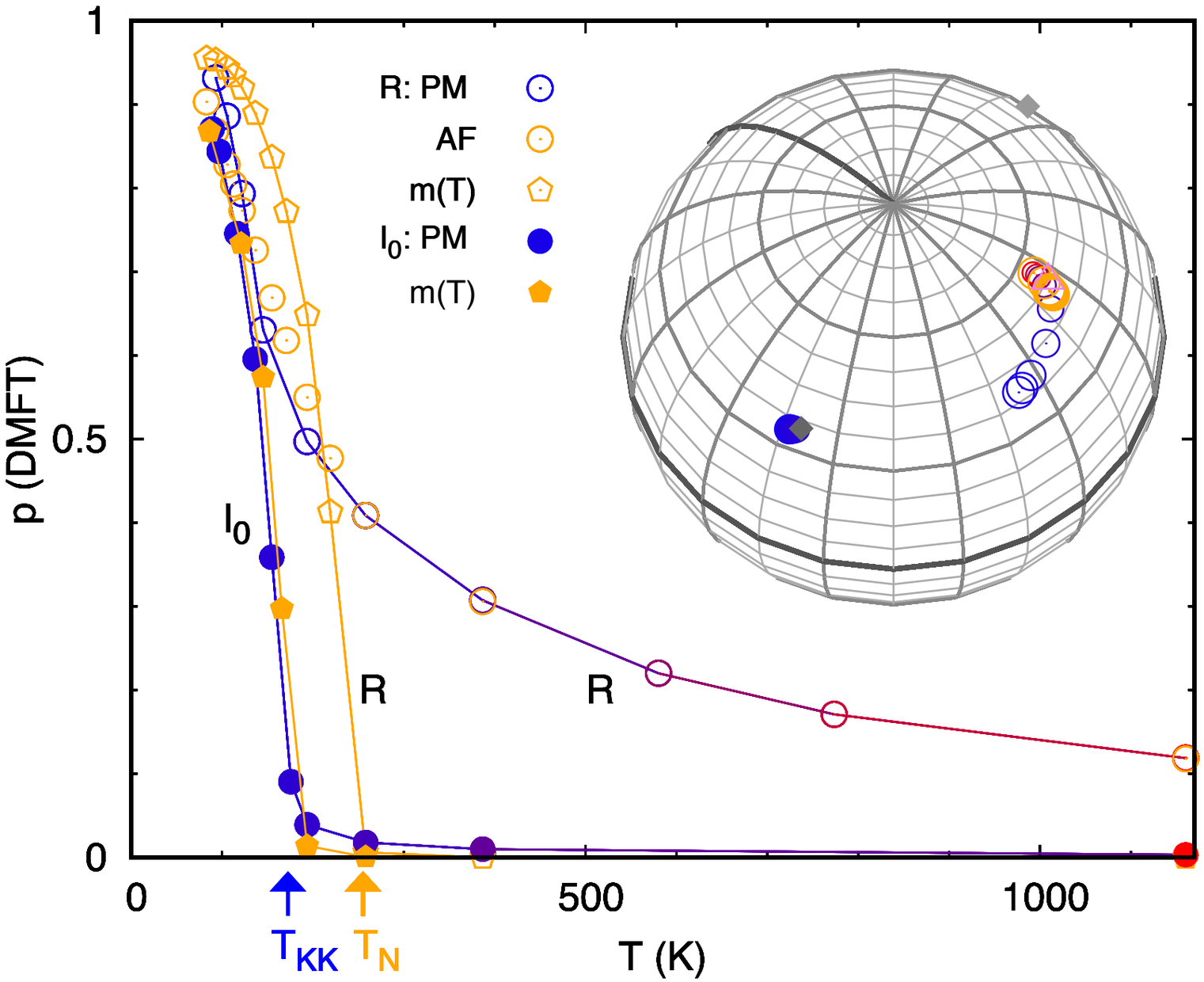
yes, $T_N > T_{KK}$!



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50 years of Kugel-Khomskii model

Crystal structure and magnetic properties of substances with orbital degeneracy

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the first clear case: $LaVO_3$

X.-J. Zhang, E. Koch and E. Pavarini, under review

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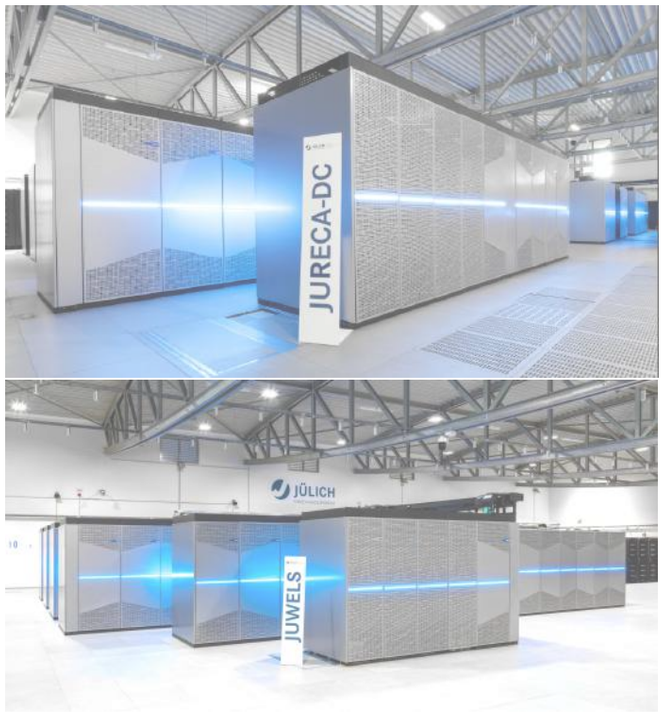
Institute for Advanced Simulation, Forschungszentrum Jülich

Juelich Supercomputing Centre



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thank you!