Spin-Orbital Interplay in Double Perovskites

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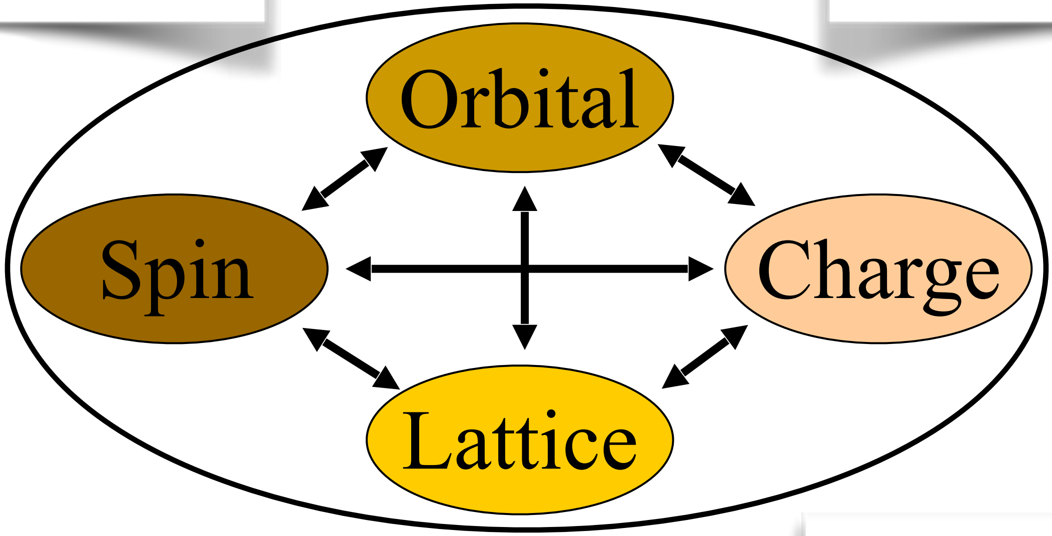
Intertwined17, KITP
Sep 26, 2017

Transition metal oxides: Plethora of Challenging Phenomena

- d- electrons are partially filled and not very extended
- Interactions dominate over kinetic energy
- Many degrees of freedom are at work

Metal to Magnetic Insulator

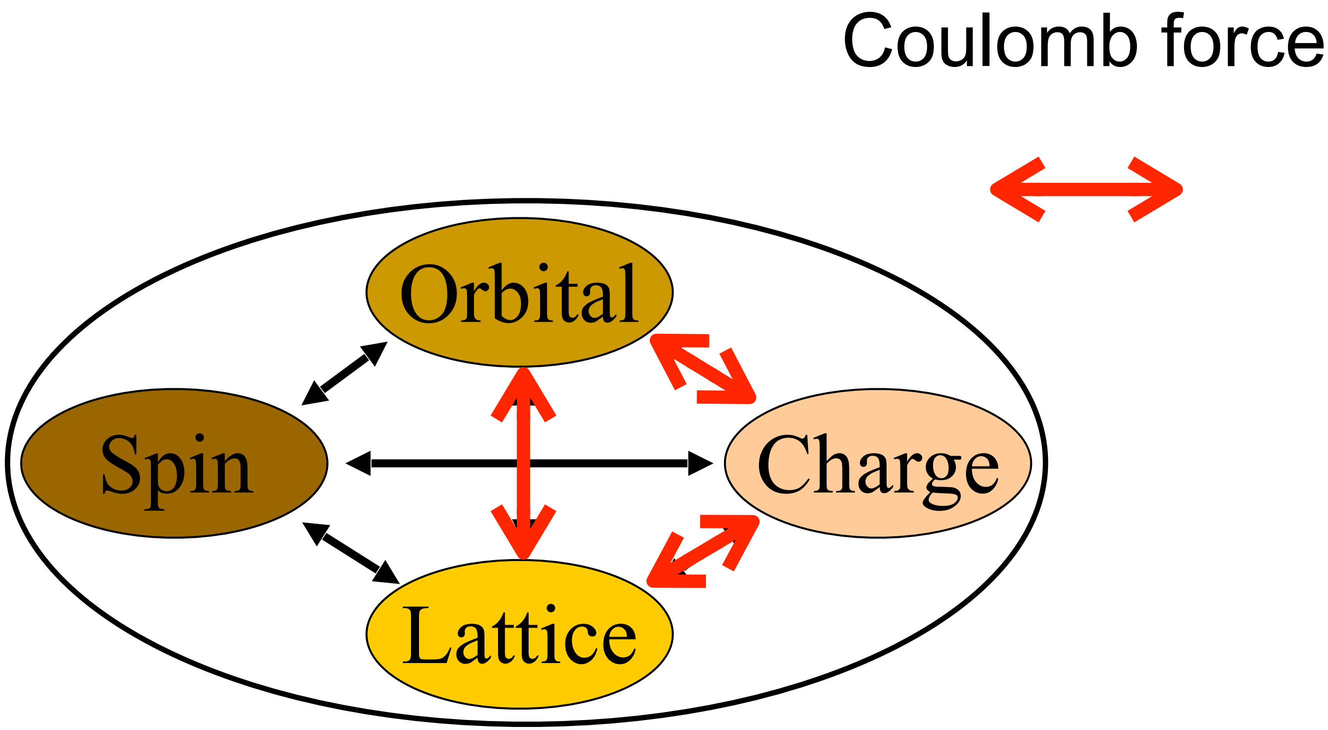
Colossal Magnetoresistance



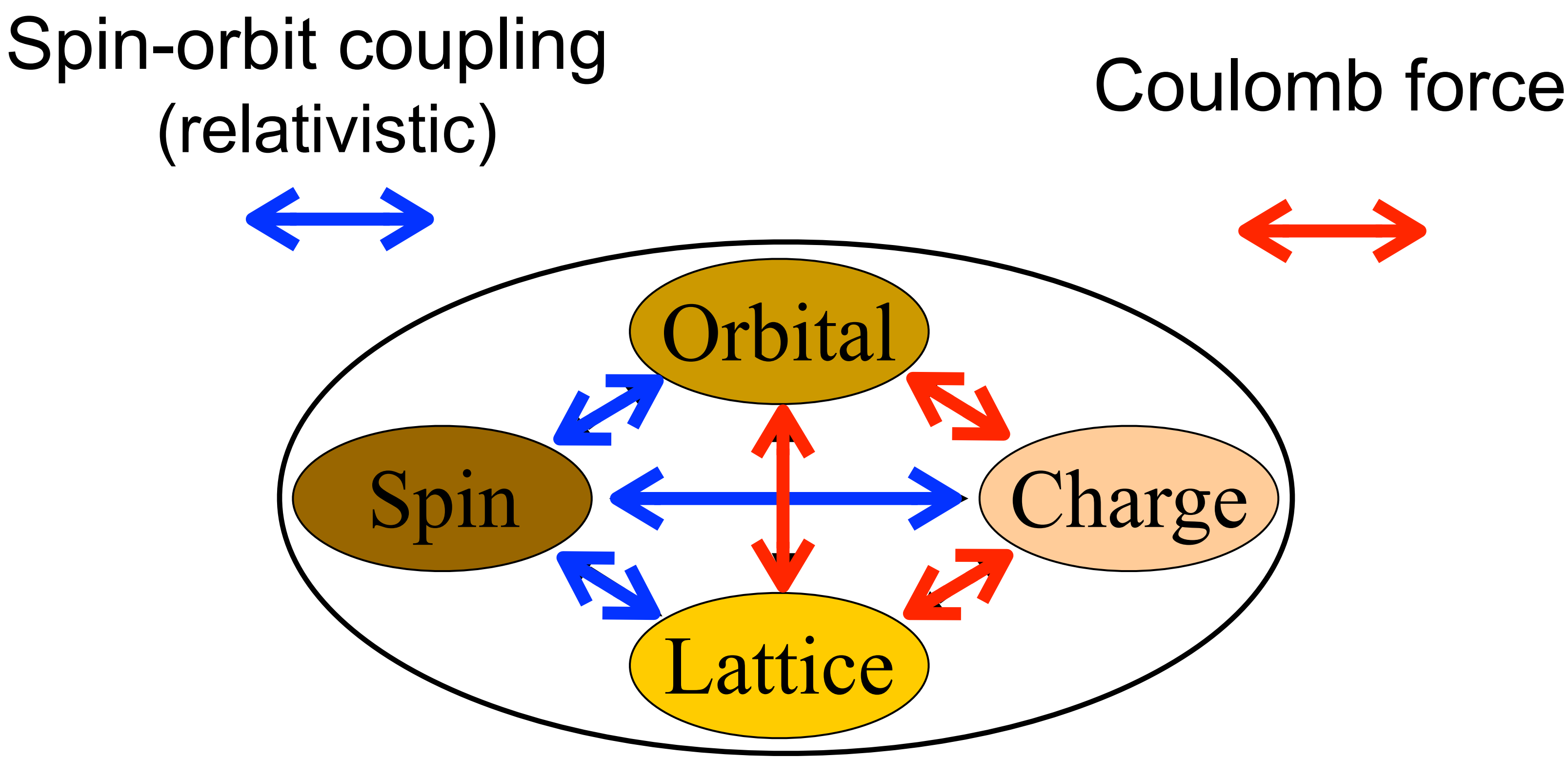
High-Tc Superconductivity

Unexpected variety of phases and transitions between them

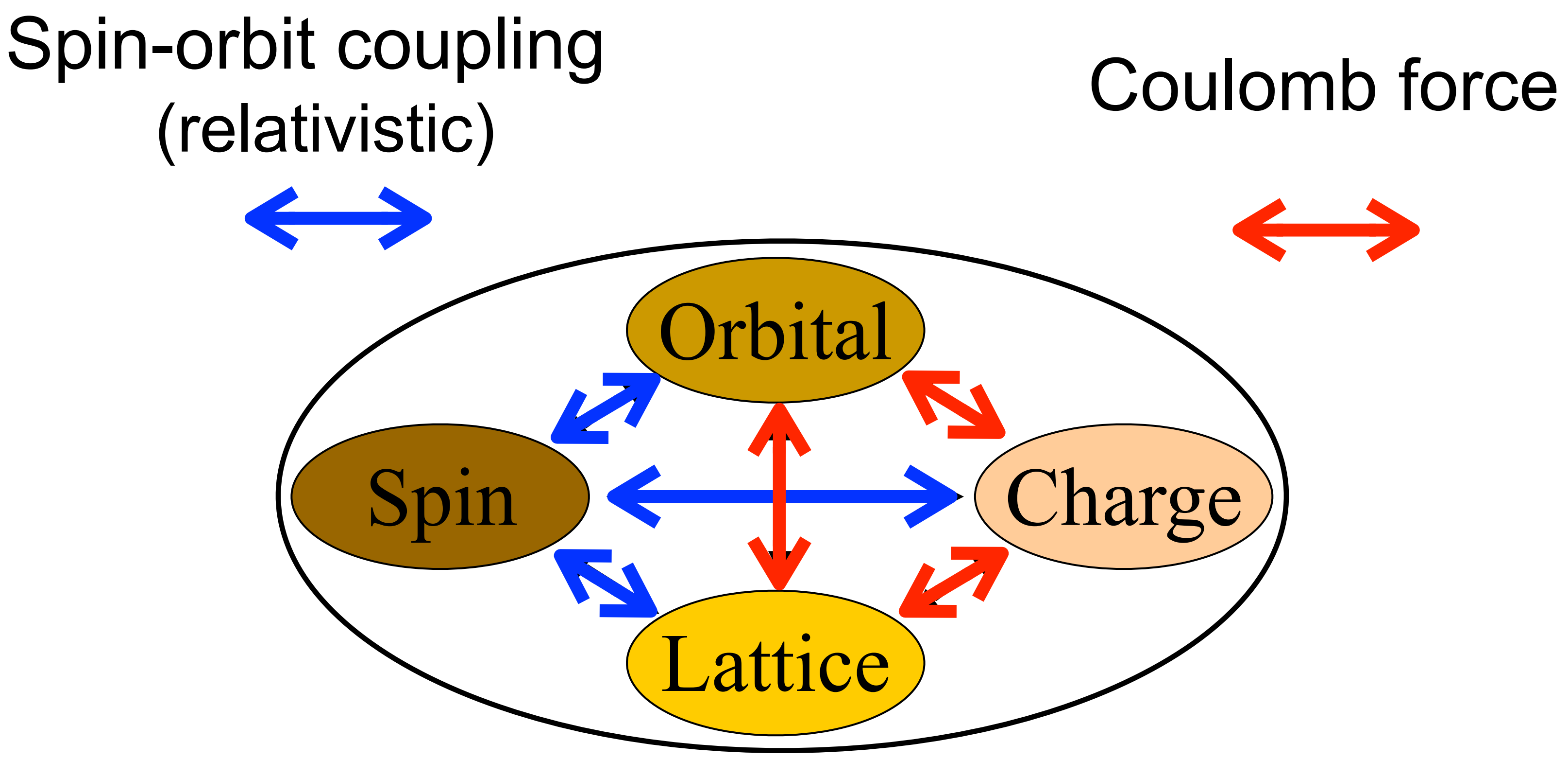
Transition metal oxides:
Plethora of Challenging Phenomena



Transition metal oxides: Plethora of Challenging Phenomena



Transition metal oxides:
Plethora of Challenging Phenomena



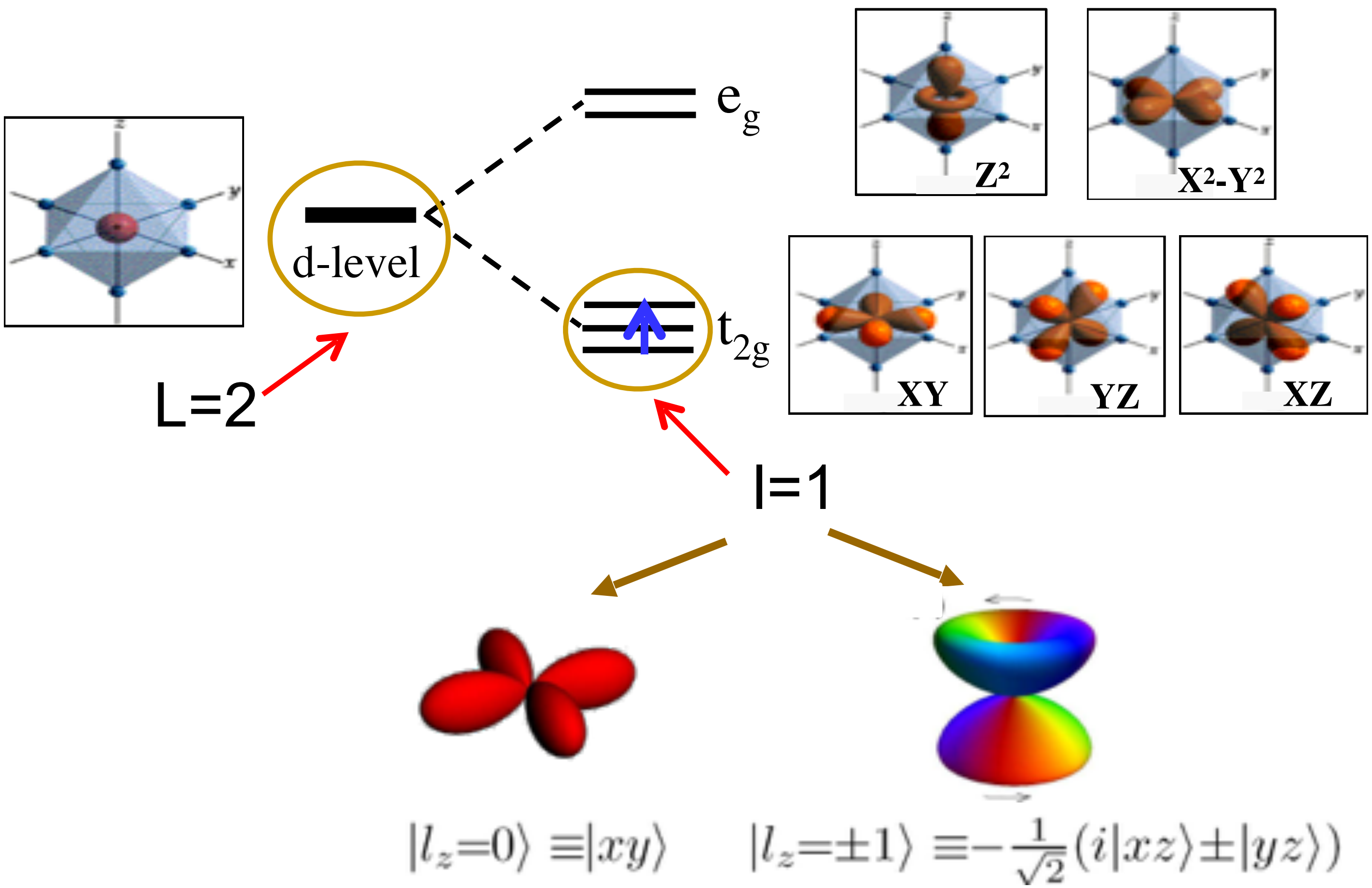
Enhanced interplay by going to heavier TM compounds:
a possible route to Novel Collective States & Phenomena

correlations

21 **Sc** 44.9559 Scandium	22 **Ti** 47.867 Titanium	23 **V** 50.9415 Vanadium	24 **Cr** 51.9961 Chromium	25 **Mn** 54.938 Manganese	26 **Fe** 55.845 Iron	27 **Co** 58.9332 Cobalt	28 **Ni** 58.6934 Nickel	29 **Cu** 63.546 Copper	30 **Zn** 65.4089 Zinc
39 **Y** 88.9058 Yitrium	40 **Zr** 91.224 Zirconium	41 **Nb** 92.9064 Niobium	42 **Mo** 85.94 Molybdenum	43 **Tc** 98 Technetium	44 **Ru** 101.07 Ruthenium	45 **Rh** 102.9055 Rbodium	46 **Pd** 106.42 Palladium	47 **Ag** 107.8682 Silver	48 **Cd** 112.411 Cadmium
71 **Lu** 174.967 Lutetium	72 **Hf** 178.49 Hafnium	73 **Ta** 180.9497 Tantalum	74 **W** 183.84 Tungsten	75 **Re** 186.207 Rhenium	76 **Os** 190.23 Osmium	77 **Ir** 192.217 Iridium	78 **Pt** 195.084 Platinum	79 **Au** 196.9666 Gold	80 **Hg** 200.59 Mercury

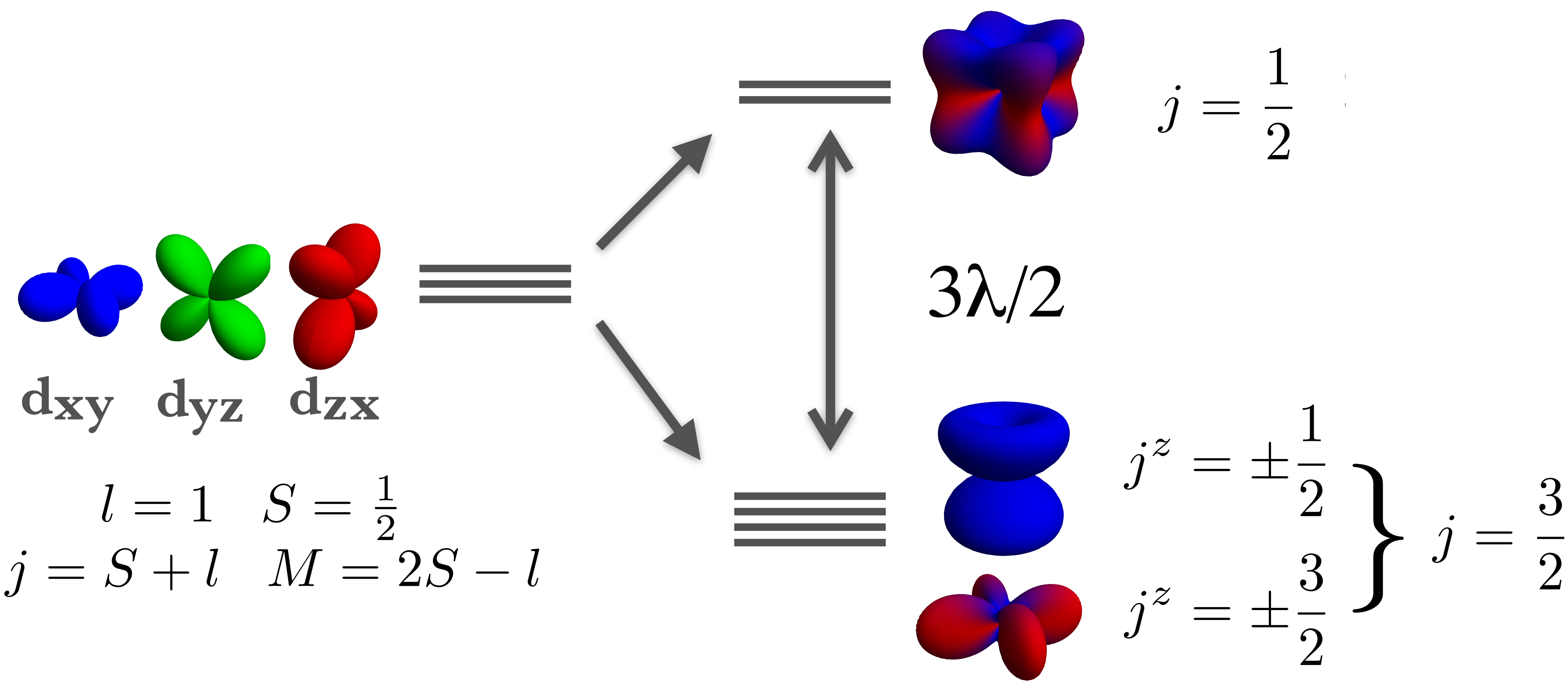
spin-orbit

Angular momentum in t_{2g} shell



Spin-orbit coupling in t_{2g} shell

A. Abragam and B. Bleaney, "EPR of Transition Ions" (1970)



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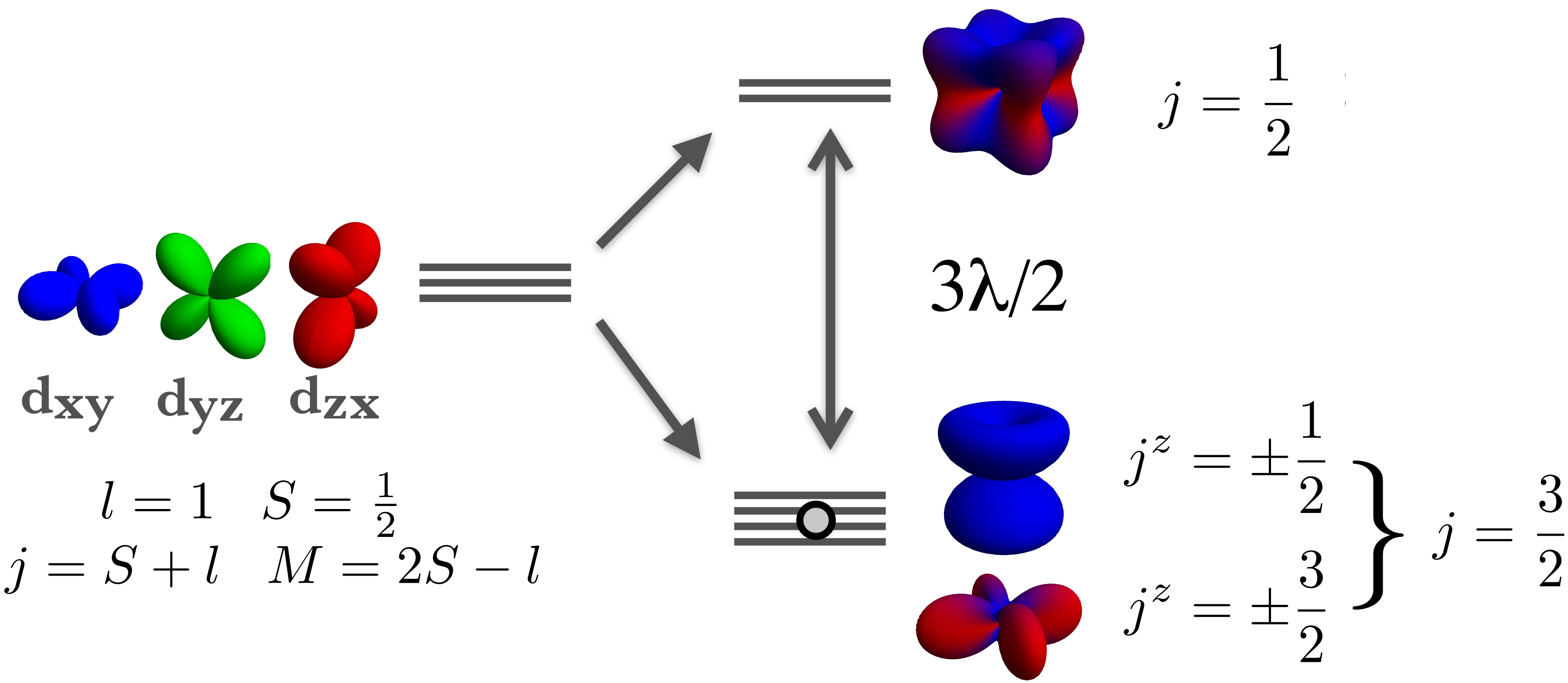

d^1 (Mo^{5+}, Os^{7+}…) *g=0*

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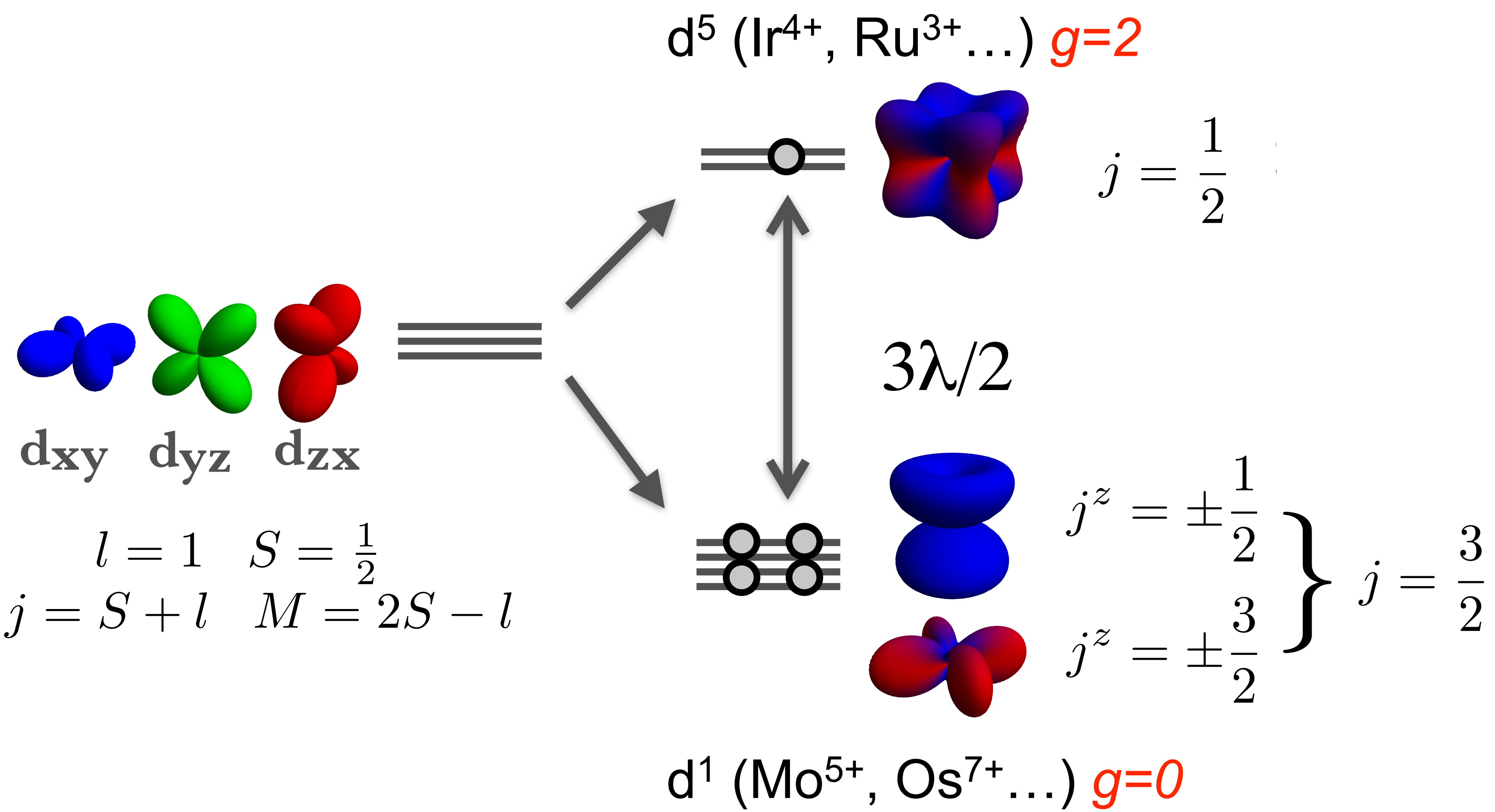
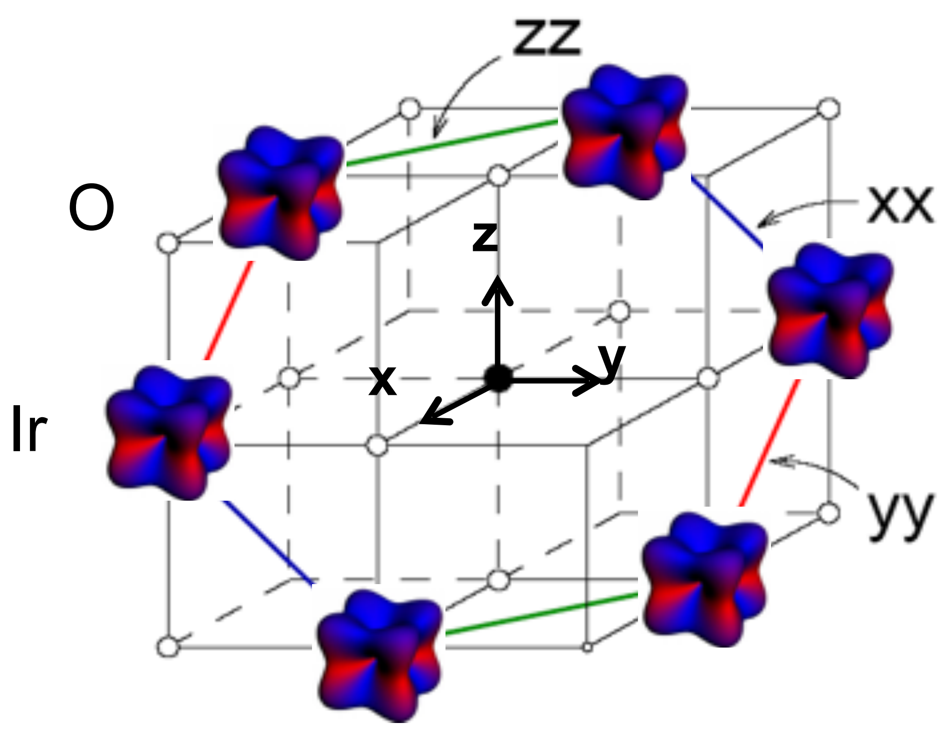


Pseudospins on a Honeycomb layer of A_2IrO_3

GJ & Khaliullin, PRL (2009)



A. Kitaev, Ann. Phys'06

$$\mathcal{H}_{ij}^{(\gamma)} = J S_i^\gamma S_j^\gamma$$

Honeycomb-based Compounds do show LRO

but NON of them in Neel state

discussion on QSL

18th Aug Intertwined17@KITP

Honeycomb-based Compounds do show LRO

'Mere goodness can achieve
little against
the power of nature.'

Georg Wilhelm Friedrich HEGEL

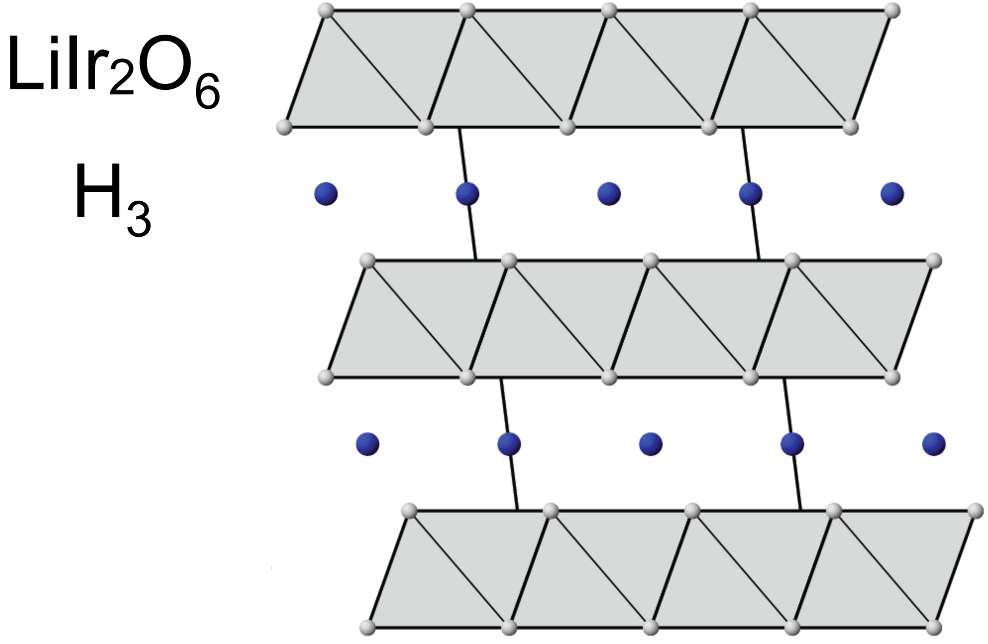
Honeycomb-based Compounds do show LRO

'Nothing great in the world
has ever been
accomplished without passion.'

Georg Wilhelm Friedrich HEGEL

$H_3LiIr_2O_6$

(Takagi's Group)



No sign of long-range order down to 50 mK

Susceptibility, NMR, Heat capacity

$H_3LiIr_2O_6$

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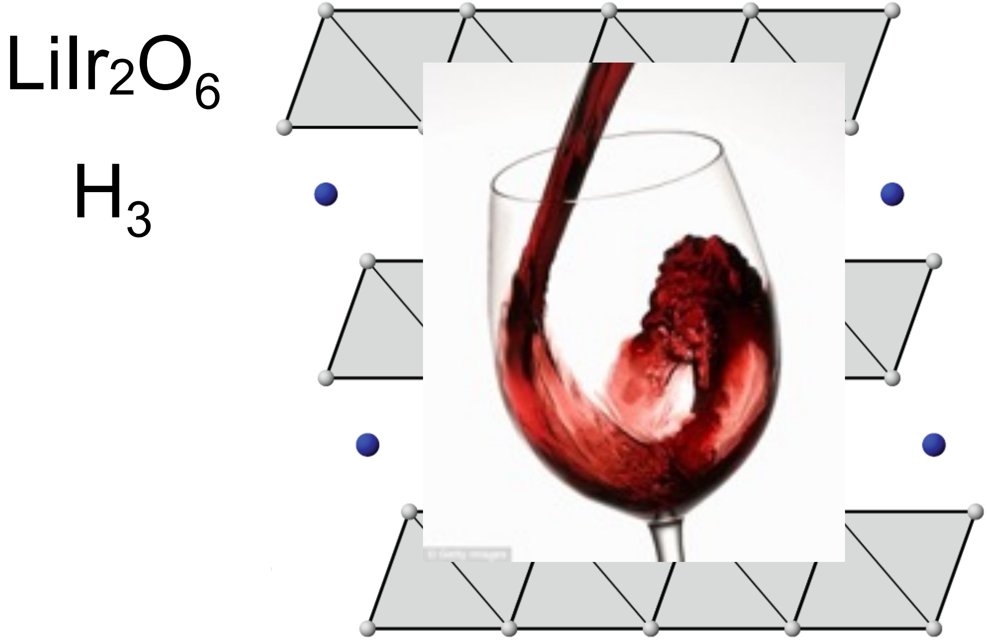

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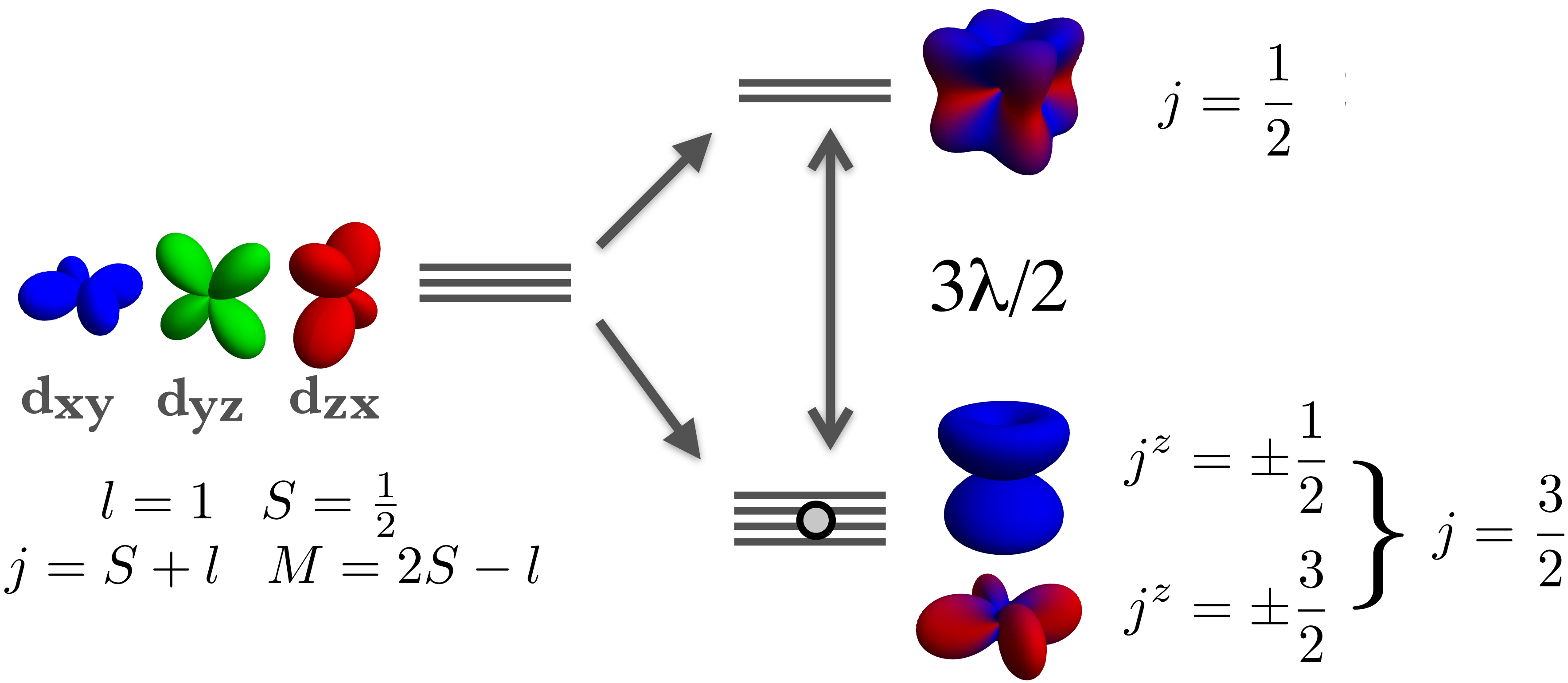

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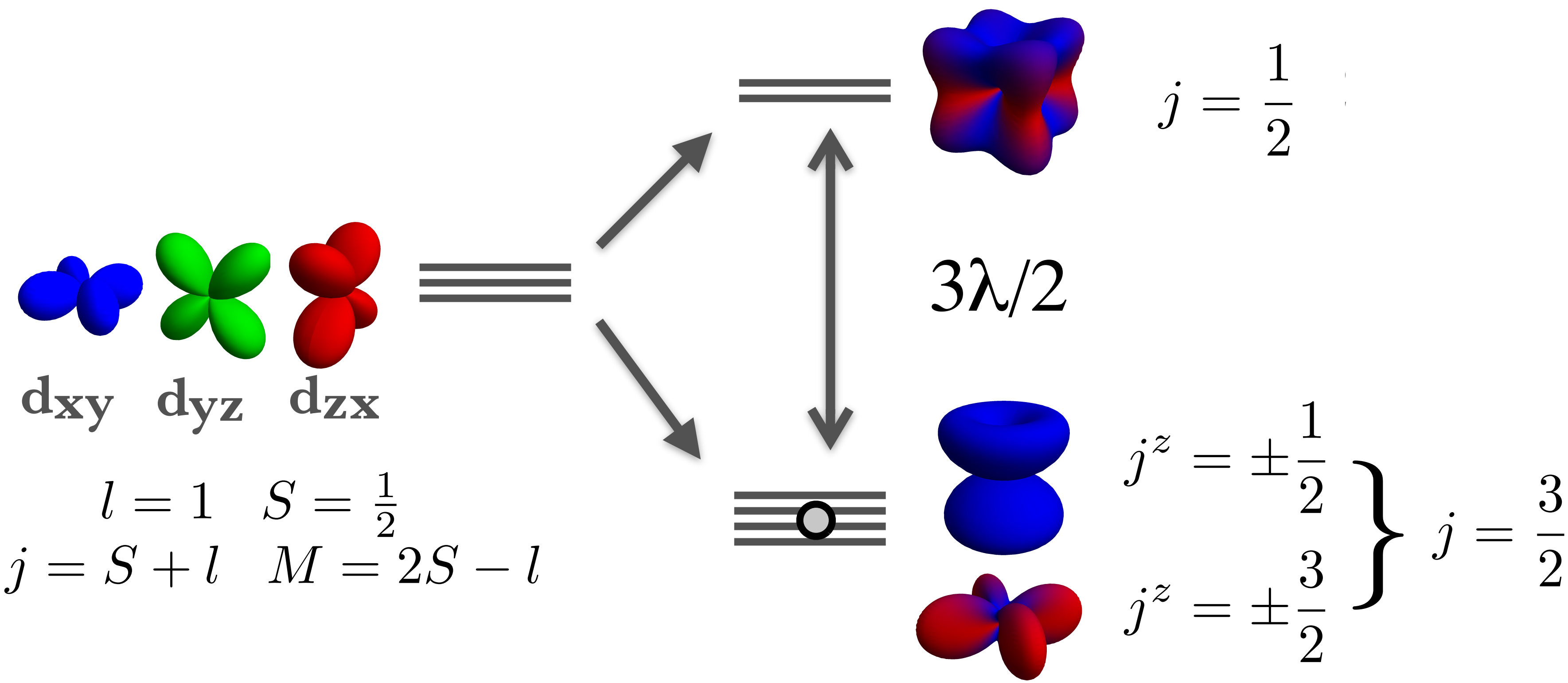

Magnetic field mixes j=1/2 with 3/2
and induces van Vleck magnetism

Ba_2BMoO_6 (B=Y, Lu)
valence bond glass

correlations ↑

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spin-orbit ↓

Ba_2BOsO_6 (B=Na, Li)
unusual ‘spin’ textures

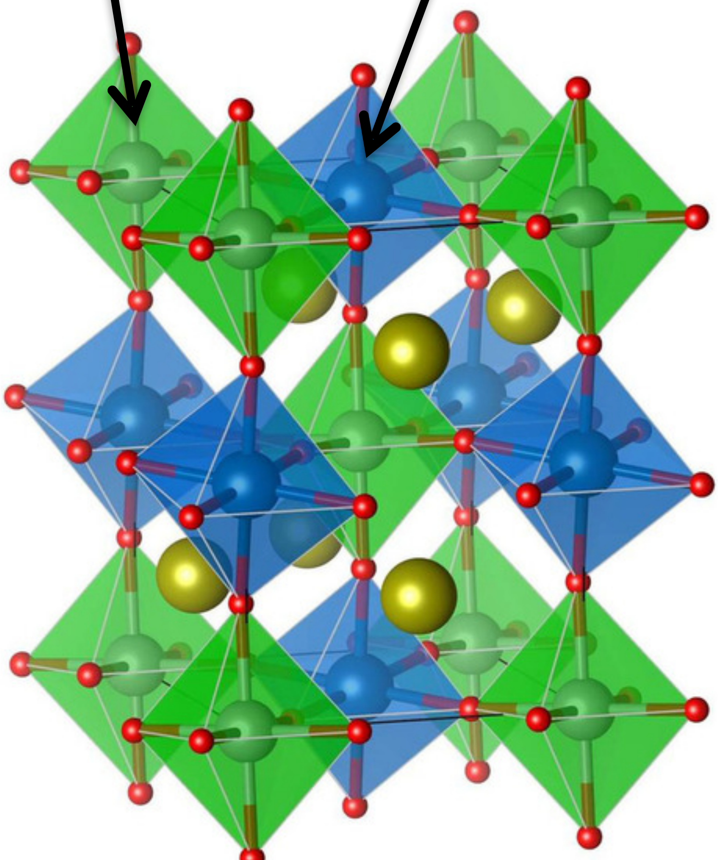
In collaboration with

Judit Romhanyi
(MPI -> OIST)

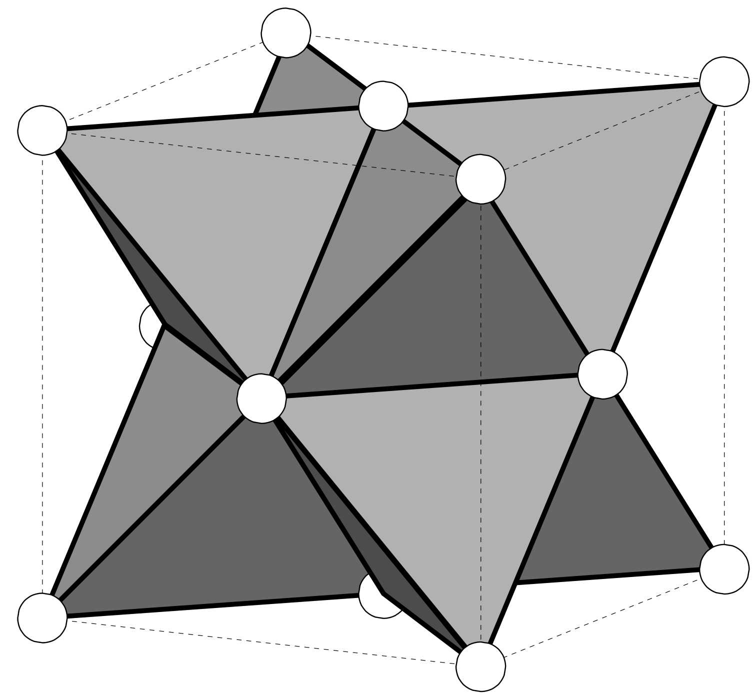
Leon Balents
(KITP)

J. Romhanyi, L. Balents & GJ, PRL (2017)

double perovskites $A_2BB'O_6$



each sublattice forms FCC



Exotic phases induced by strong spin-orbit coupling in ordered double perovskites

Gang Chen
Physics Department, University of Colorado, Boulder, Colorado 80309, USA
and Physics Department, University of California, Santa Barbara, California 93106, USA

Rodrigo Pereira
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and Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA

Leon Balents
Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA
(Received 26 September 2010; published 29 November 2010)

Compound	B' config.	Crystal structure	Θ_{CW} (K)	μ_{eff} (μ_B)	Magnetic transition	Frustration para. f	Ref
Ba_2YMoO_6	$Mo^{5+}(4d^1)$	Cubic	−91	1.34	PM down to 2 K	$f \gtrsim 45$	11
Ba_2YMoO_6	$Mo^{5+}(4d^1)$	Cubic	−160	1.40	PM down to 2 K	$f \gtrsim 80$	12
Ba_2YMoO_6	$Mo^{5+}(4d^1)$	Cubic	−219	1.72	PM down to 2 K	$f \gtrsim 100$	13
La_2LiMoO_6	$Mo^{5+}(4d^1)$	Monoclinic	−45	1.42	Short-range AFM $T_N \sim 20$ K	$f \gtrsim 2$	13
Sr_2MgReO_6	$Re^{6+}(5d^1)$	Tetragonal	−426	1.72	Spin glass, $T_G \sim 50$ K	$f \gtrsim 8$	14
Sr_2CaReO_6	$Re^{6+}(5d^1)$	Monoclinic	−443	1.659	Spin glass, $T_G \sim 14$ K	$f \gtrsim 30$	15
Ba_2CaReO_6	$Re^{6+}(5d^1)$	Cubic to tetragonal (at $T \sim 120$ K)	−38.8	0.744	AFM T_N=15.4 K	$f \sim 2$	16
Ba_2LiOsO_6	$Os^{7+}(5d^1)$	Cubic	−40.48	0.733	AFM $T_N \sim 8$ K	$f \gtrsim 5$	17
Ba_2NaOsO_6	$Os^{7+}(5d^1)$	Cubic	−32.45	0.677	FM $T_N \sim 8$ K	$f \gtrsim 4$	17
Ba_2NaOsO_6	$Os^{7+}(5d^1)$	Cubic	∼−10	∼0.6	FM T_N=6.8 K	$f \gtrsim 4$	18

PHYSICAL REVIEW B **82**, 174440 (2010)

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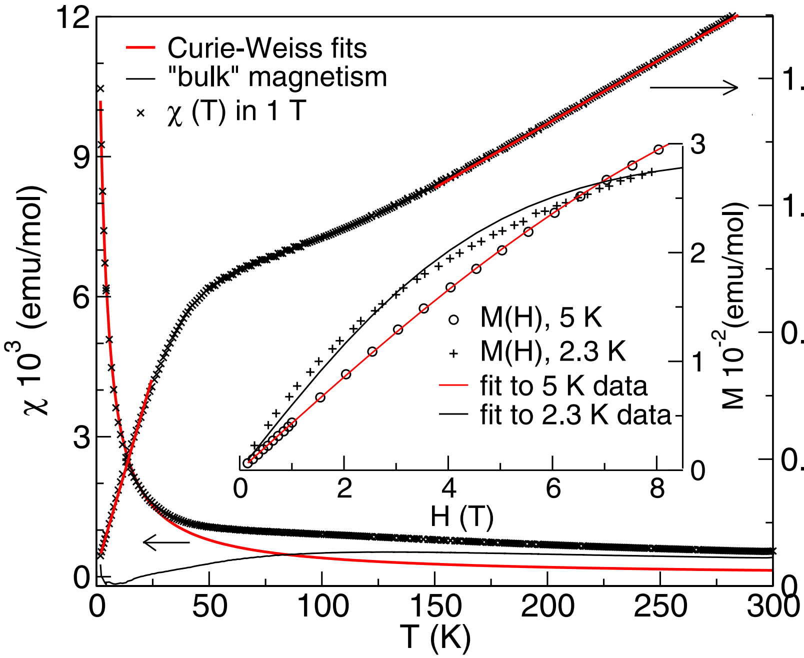
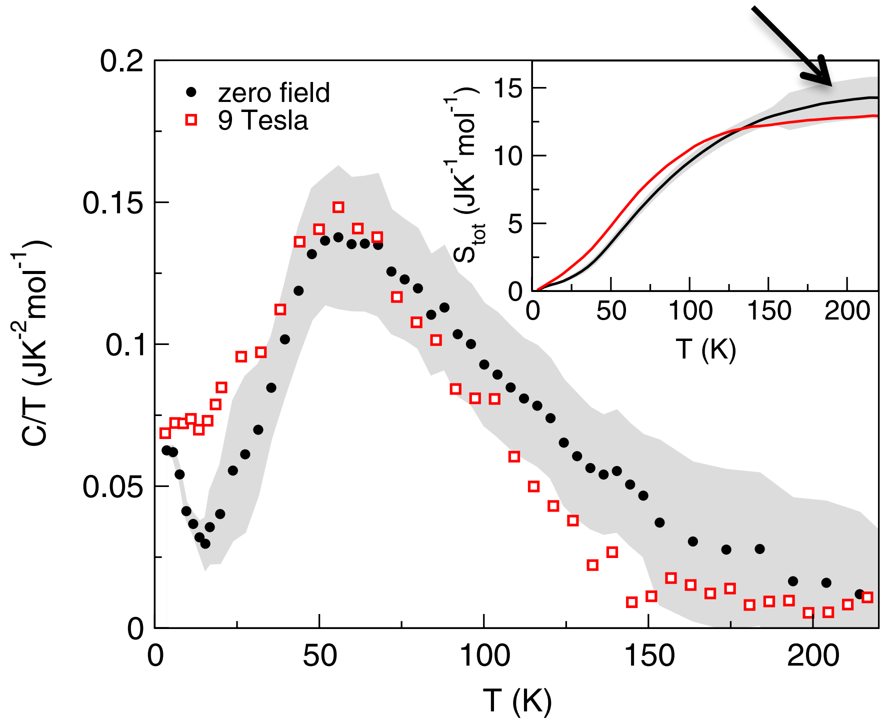
Valence Bond Glass on an fcc Lattice in the Double Perovskite Ba_2YMoO_6

M. A. de Vries,[1,2,*] A. C. Mclaughlin,[3] and J.-W. G. Bos[4,5]



*R*ln4



M(H) at 5 (2.3)K: fit Brillouin func,

accounting for 7 (2)% of the Mo s=1/2.

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PRL 104, 177202 (2010) PHYSICAL REVIEW LETTERS week ending 30 APRIL 2010

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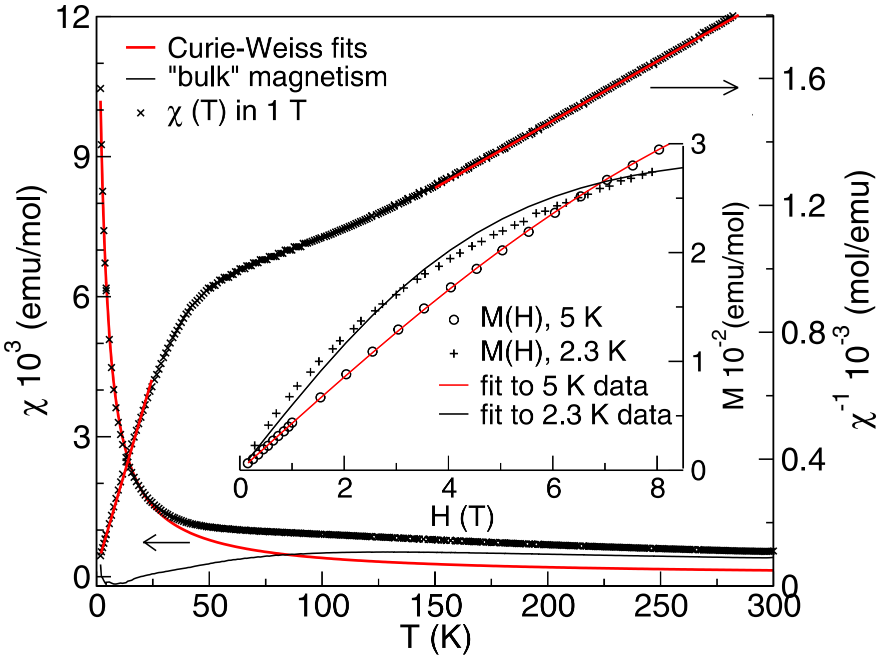

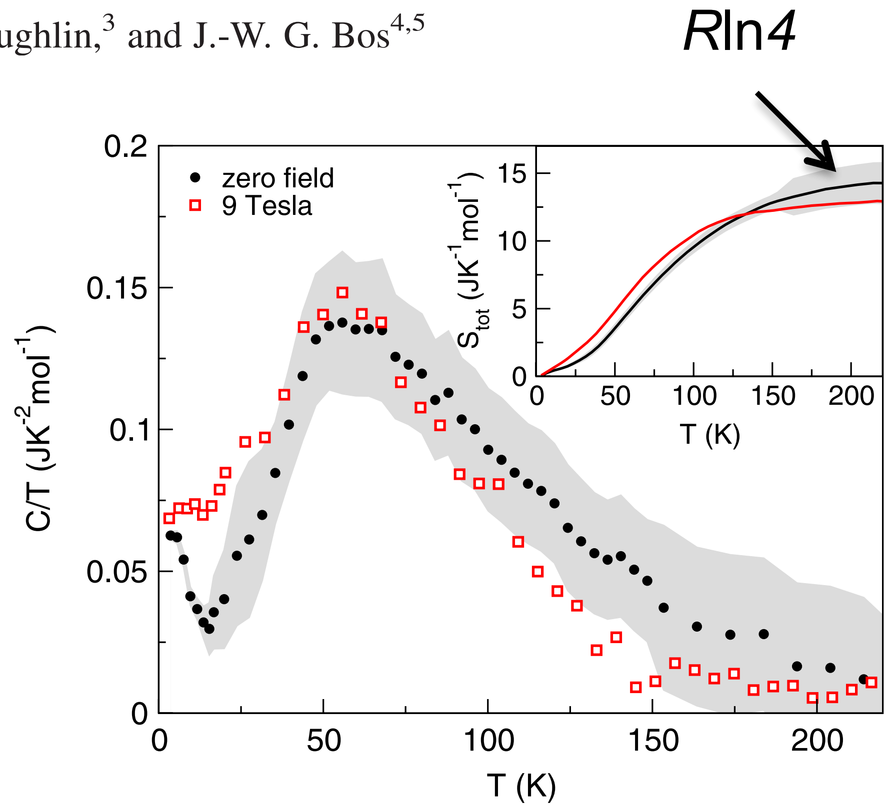

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,

similar behaviour seen also in Ba_2LuMoO_6

PHYSICAL REVIEW B **81**, 224409 (2010)

Magnetic properties of the geometrically frustrated $S=\frac{1}{2}$ antiferromagnets, La_2LiMoO_6 and Ba_2YMoO_6, with the B-site ordered double perovskite structure: Evidence for a collective spin-singlet ground state

Tomoko Aharen,[1] John E. Greedan,[1,2] Craig A. Bridges,[1] Adam A. Aczel,[3] Jose Rodriguez,[3] Greg MacDougall,[3] Graeme M. Luke,[2,3,4] Takashi Imai,[2,3,4] Vladimir K. Michaelis,[5] Scott Kroeker,[5] Haidong Zhou,[6] Chris R. Wiebe,[6,7] and Lachlan M. D. Cranswick[8]

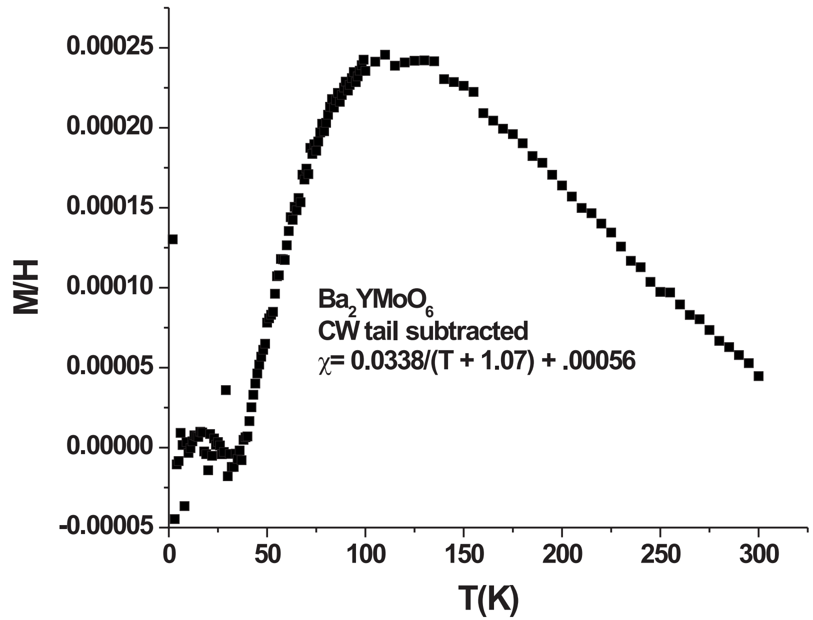


FIG. 17. The Curie-tail subtracted bulk susceptibility of Ba_2YMoO_6.

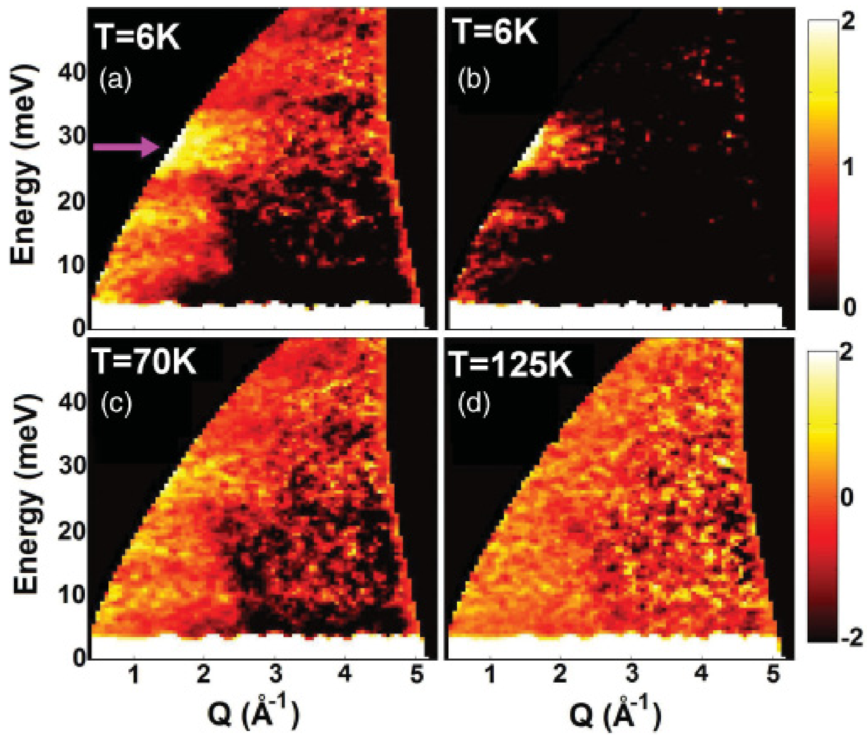
NMR $1/T_1$ - two component response:

paramagnetic & gapped (~ 140 K)

PHYSICAL REVIEW B **84**, 100404(R) (2011)

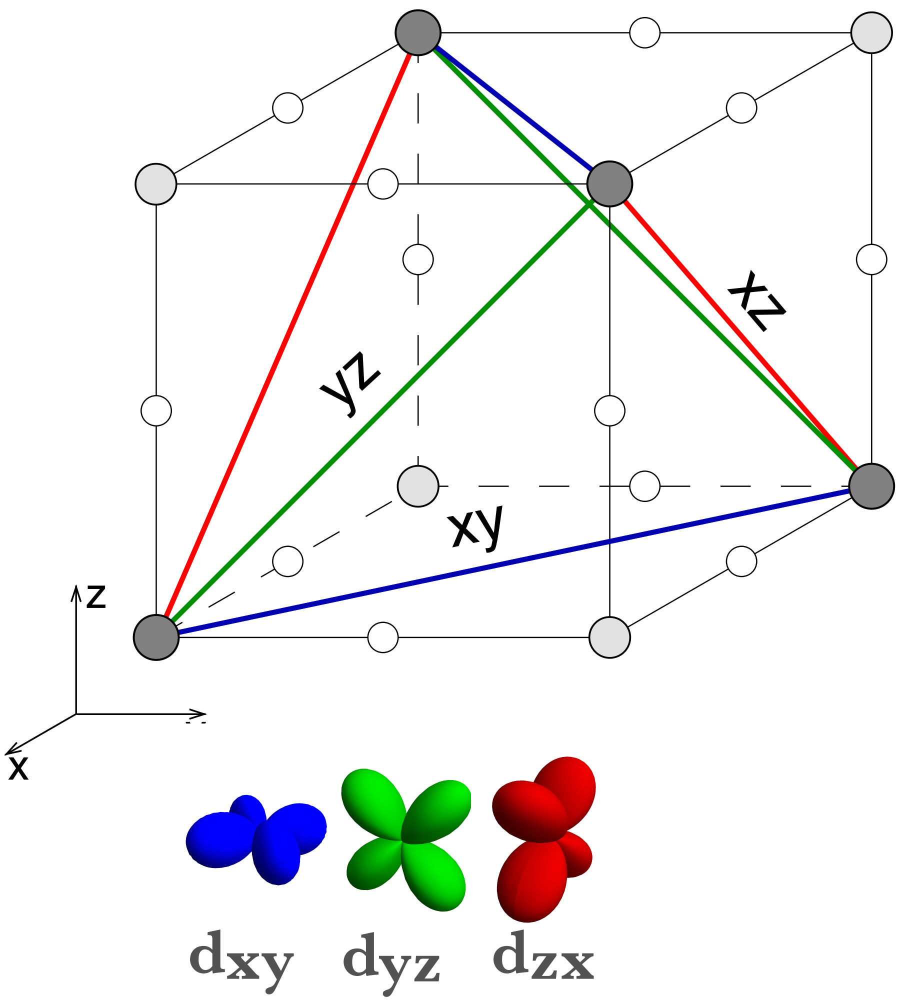
Triplet and in-gap magnetic states in the ground state of the quantum frustrated fcc antiferromagnet Ba_2YMoO_6

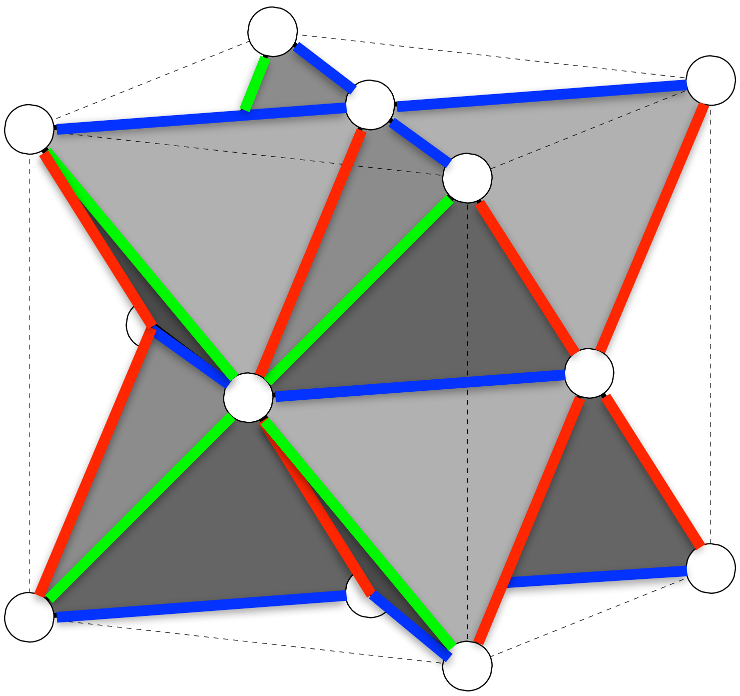
J. P. Carlo,[1,2,*] J. P. Clancy,[1] T. Aharen,[3] Z. Yamani,[2] J. P. C. Ruff,[1] J. J. Wagman,[1] G. J. Van Gastel,[1] H. M. L. Noad,[1] G. E. Granroth,[4] J. E. Greedan,[3,5] H. A. Dabkowska,[5] and B. D. Gaulin[1,5,6]



broad gapped mode ~ 28 meV (bandwidth ~4 meV)
in-gap continuum 9-17 mev

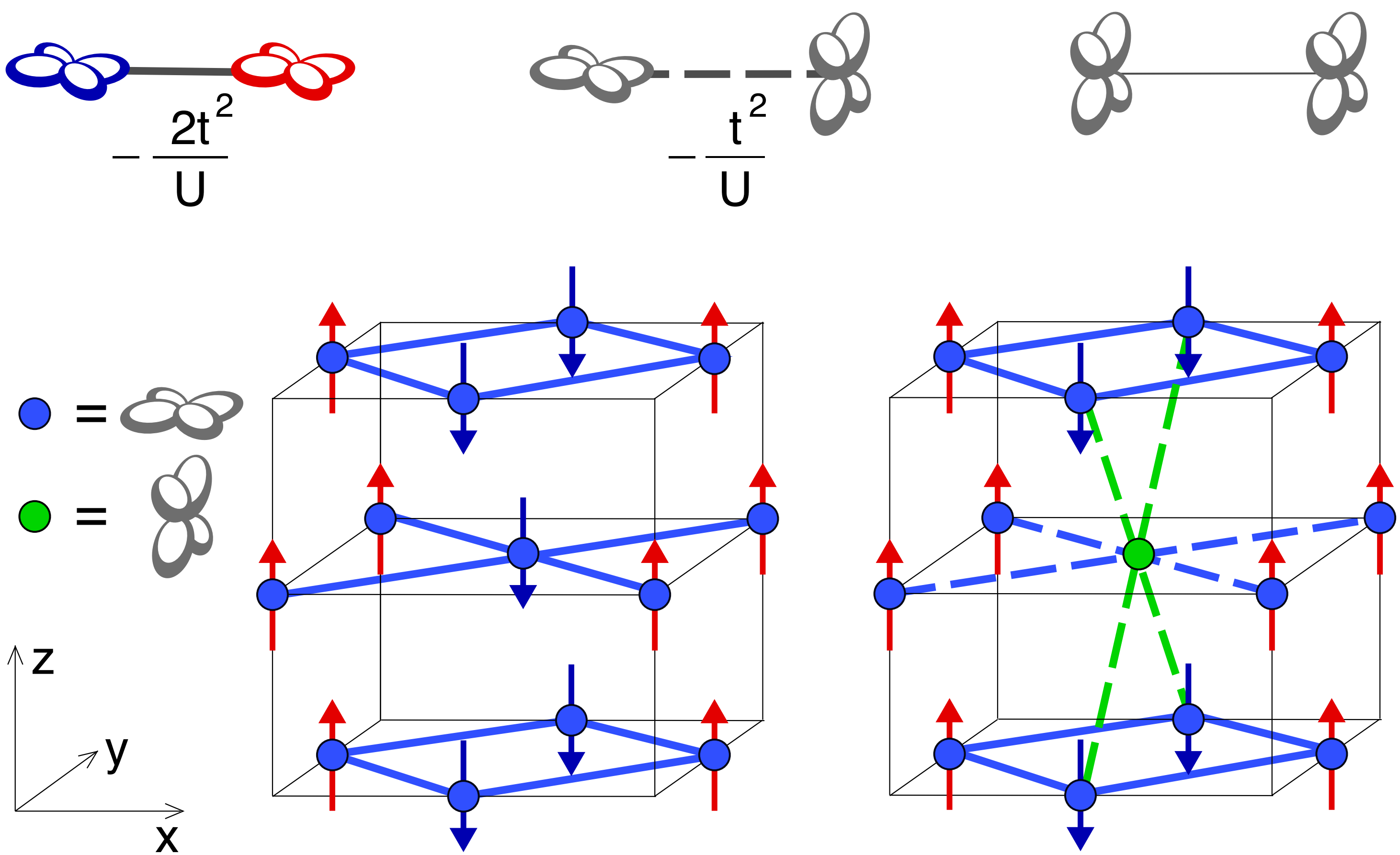
Overlap of Mo - Mo t_{2g} orbitals





Superexchange Spin-Orbital Model

$$\mathcal{H}_{\mathrm{ex}} = J \sum_{\langle i,j \rangle} \sum_{\alpha\beta} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \frac{1}{4} \right) n_{i\alpha\beta} n_{j\alpha\beta}$$



Exact ground state manifold: spanned by spin-singlet dimer coverings

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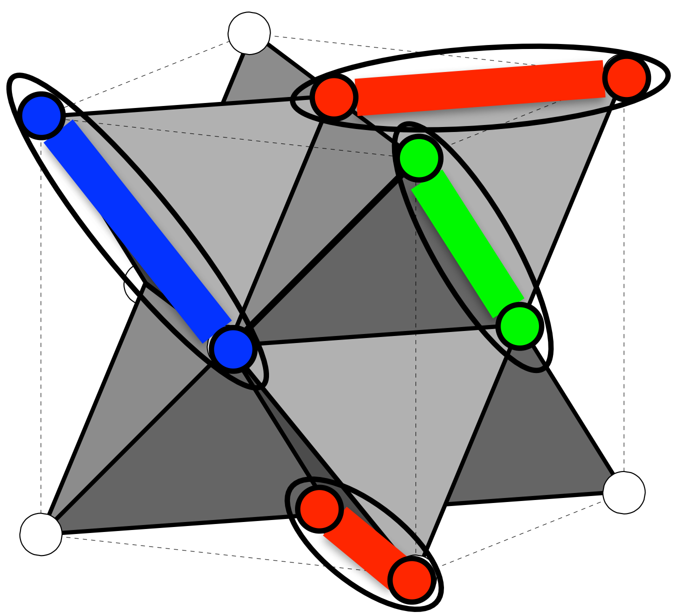
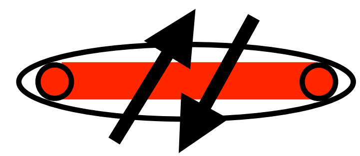
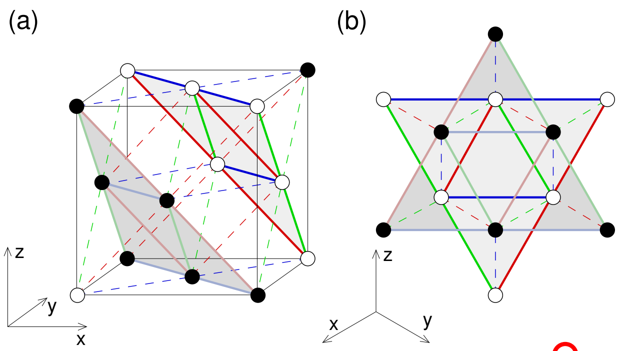
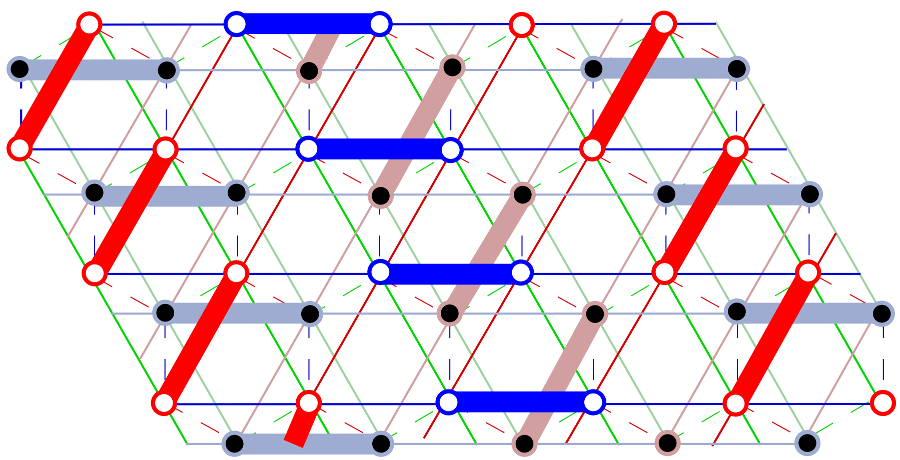




Constraint: No neighbouring dimers can lie in the same plane

Extensive orientational degeneracy: infinitely many ways of covering





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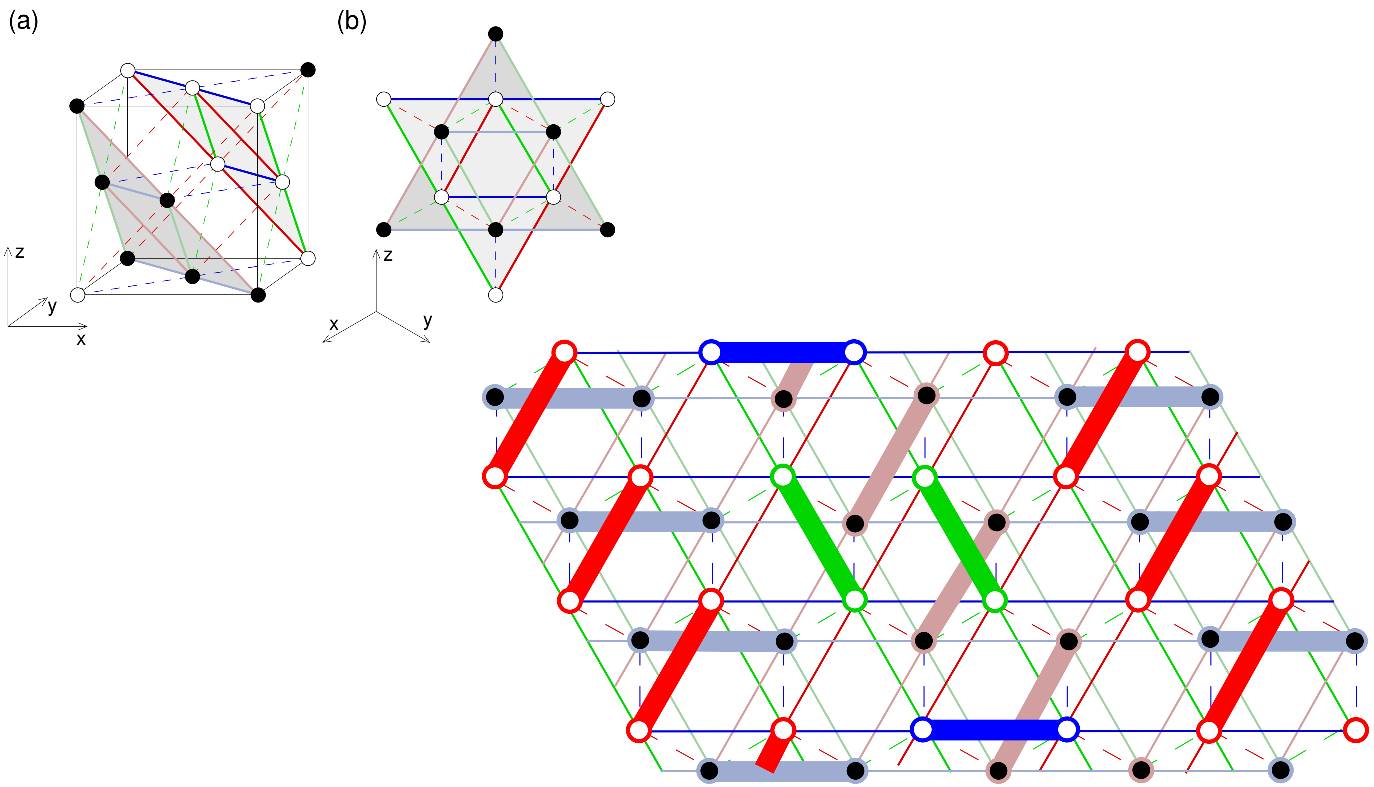

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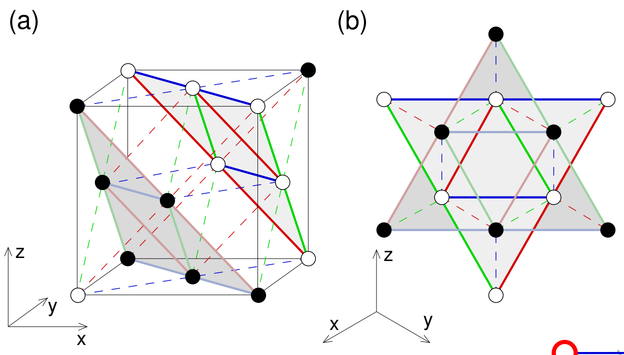
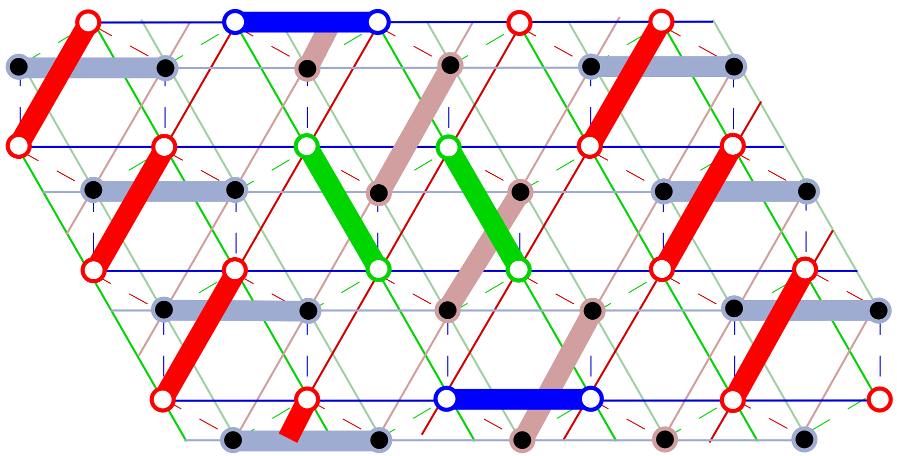
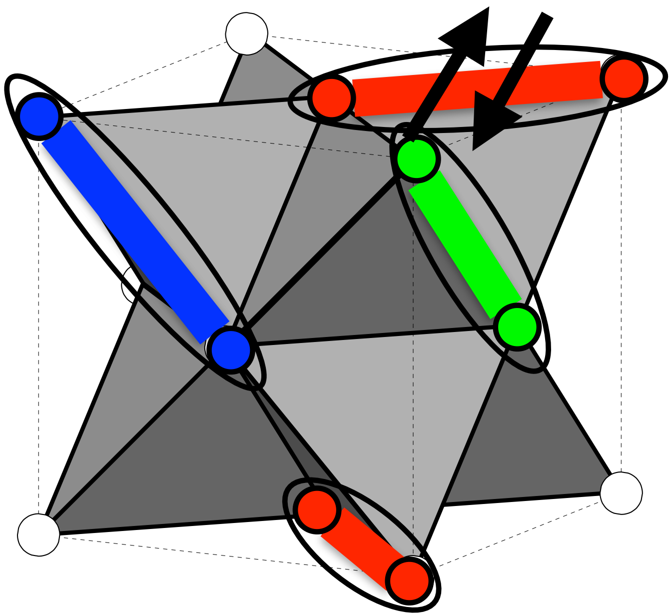




Still massively degenerate: all covering have same energy
Mis-site disorder will, most likely, choose a random pattern:
spin-orbit dimer 'glass'

Low energy excitations & defects,



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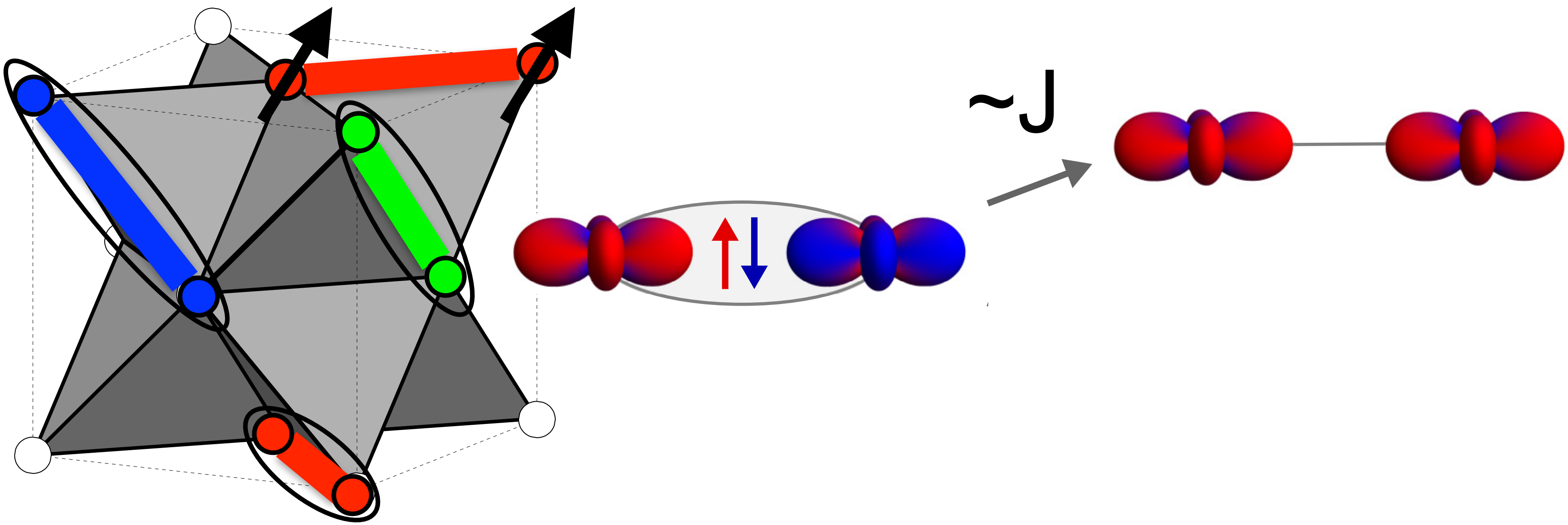

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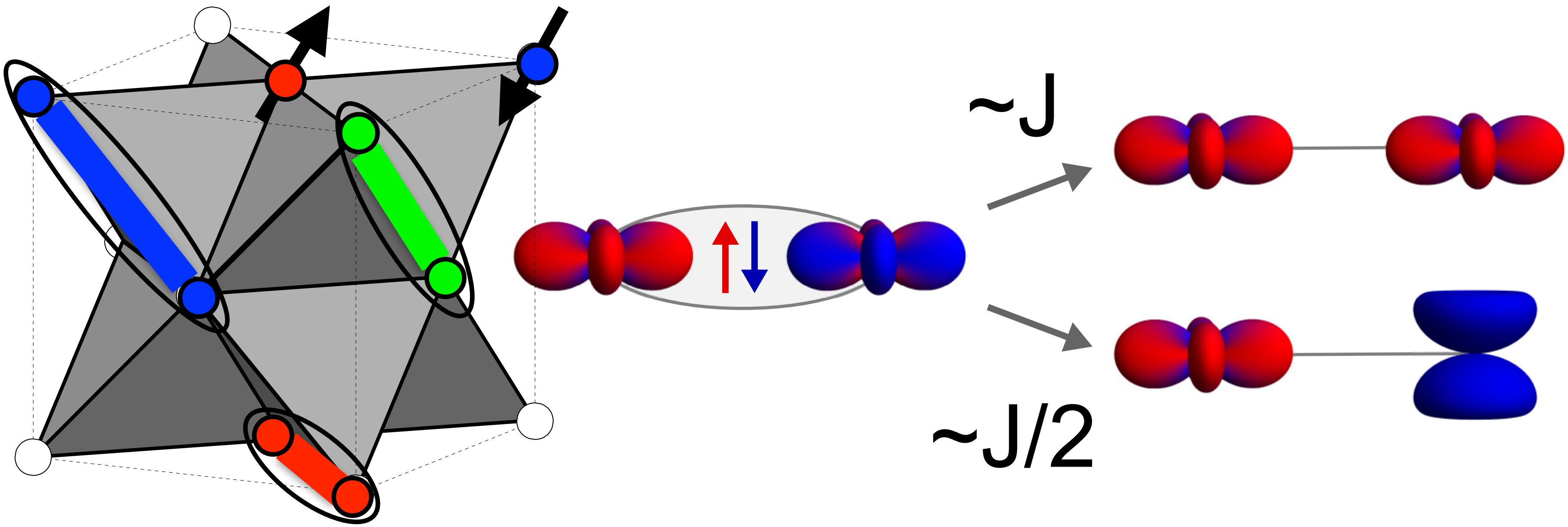

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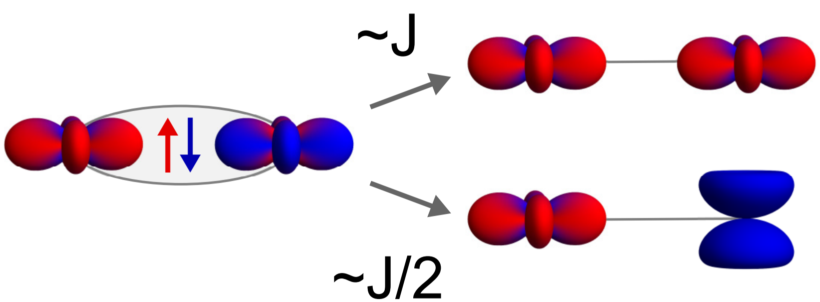

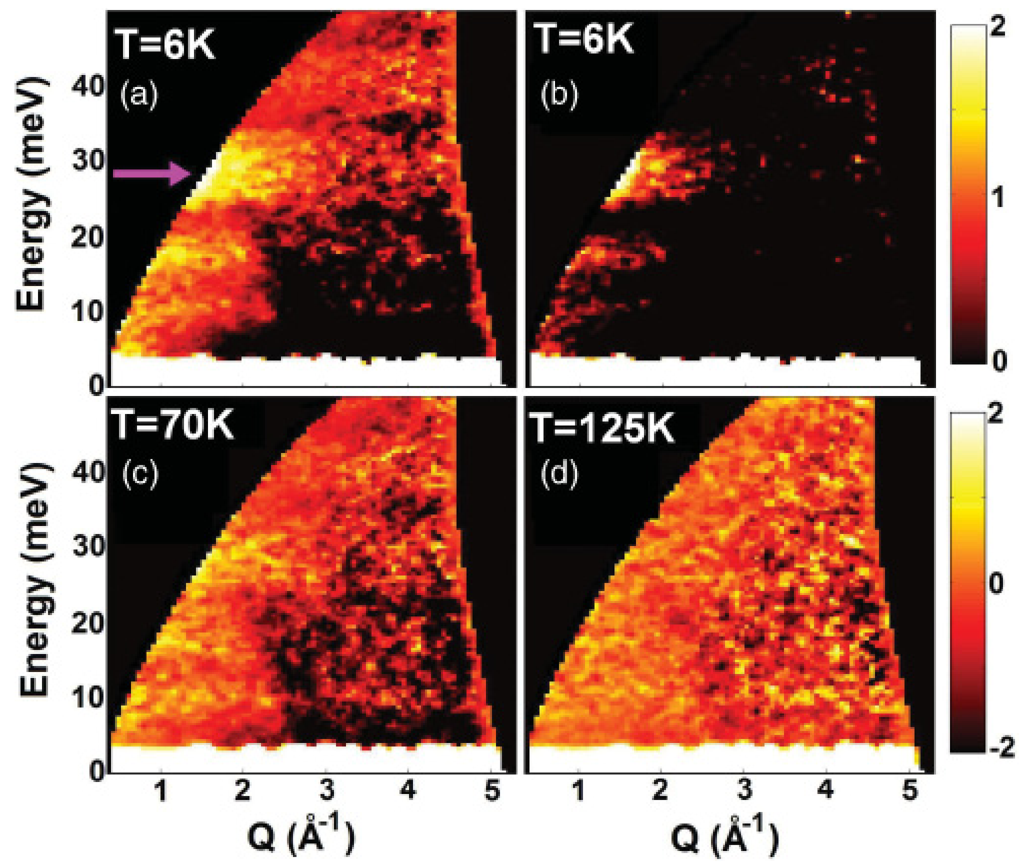

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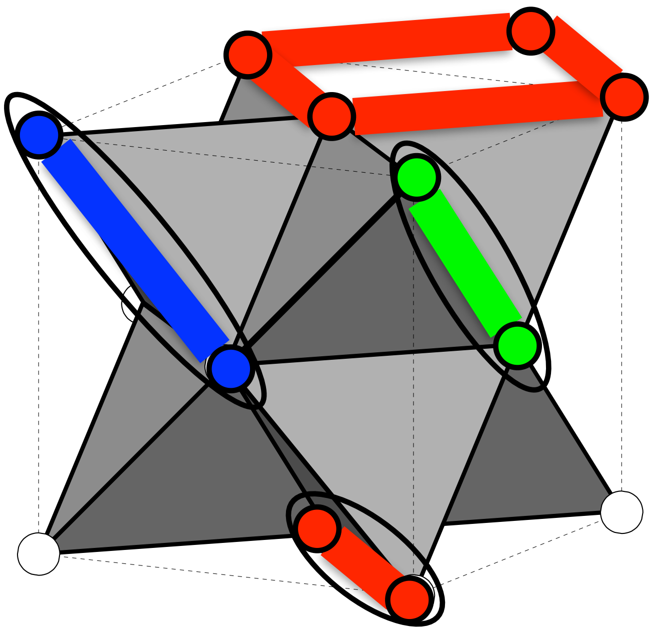
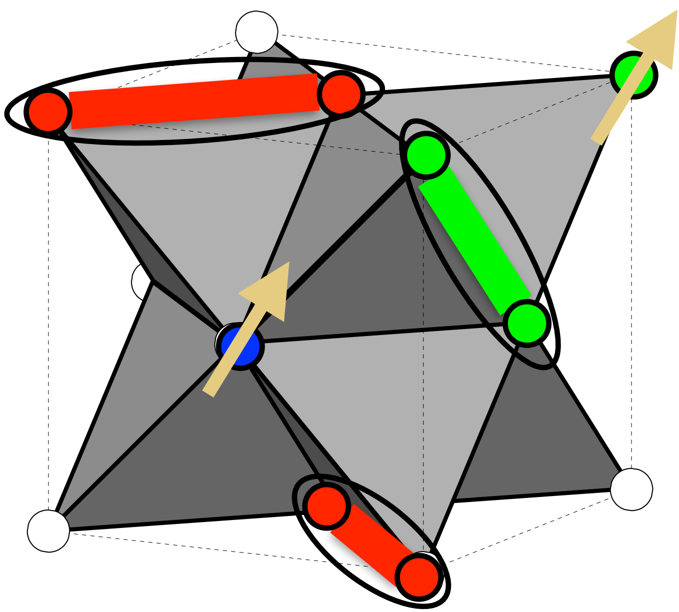


- local singlet to triplet exc: J
- local SO exc: J/2
- non-local SO exc: <J/2

Pseudogap rather than a Hard Gap

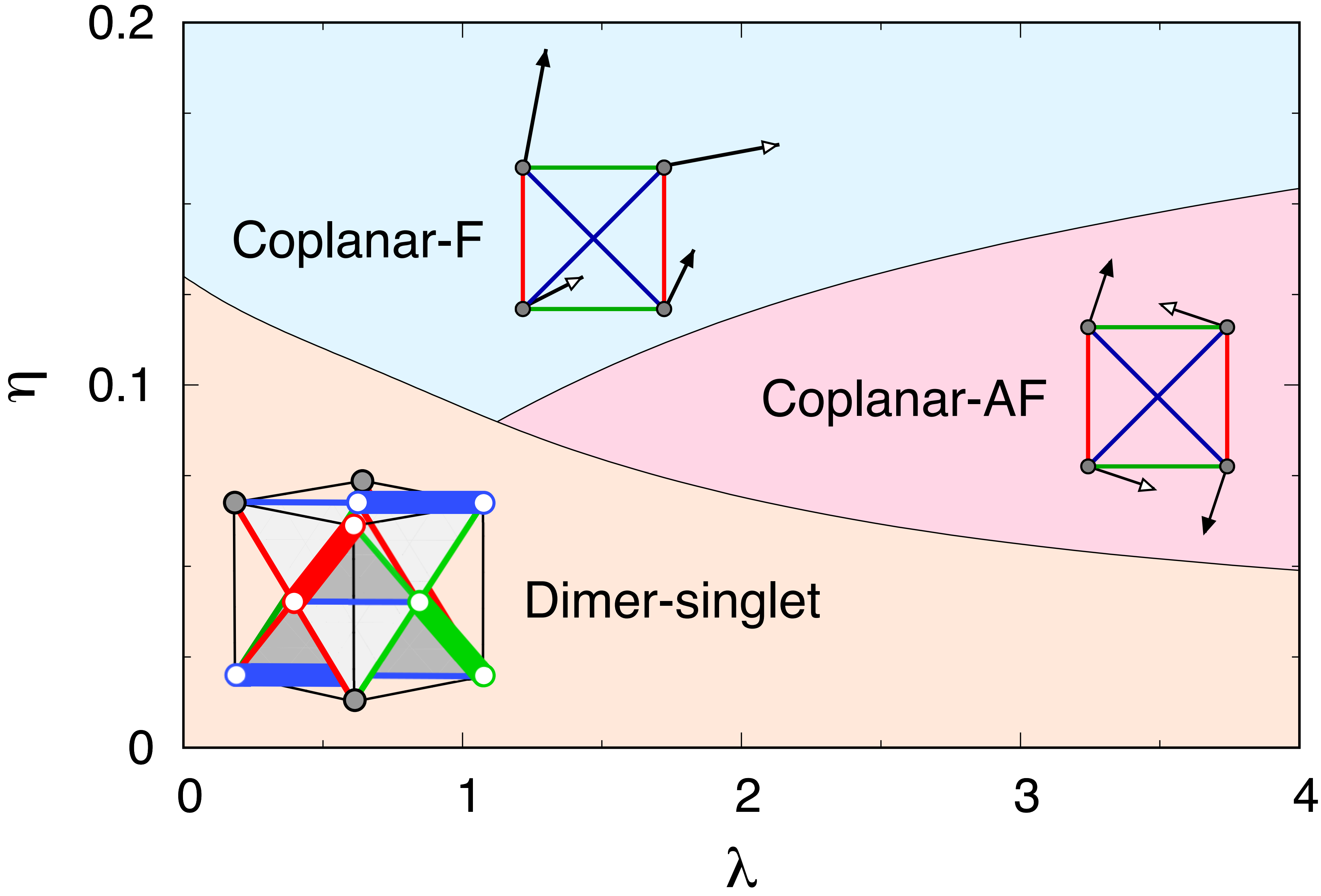
Low energy excitations & defects,



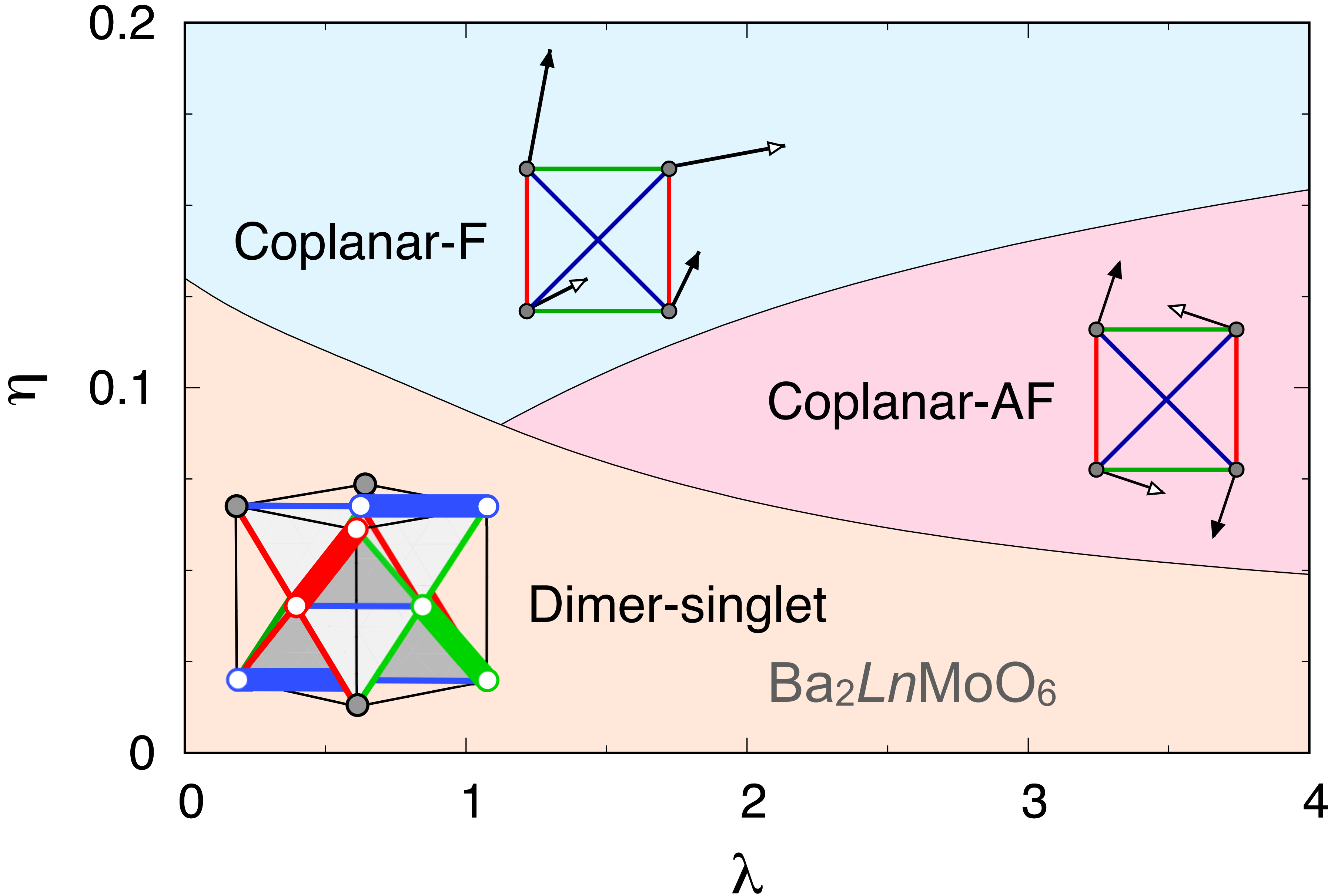
- ☐ local singlet to triplet exc: J
- ☐ local SO exc: J/2
- ☐ non-local SO exc: <J/2

Pseudogap rather than a Hard Gap

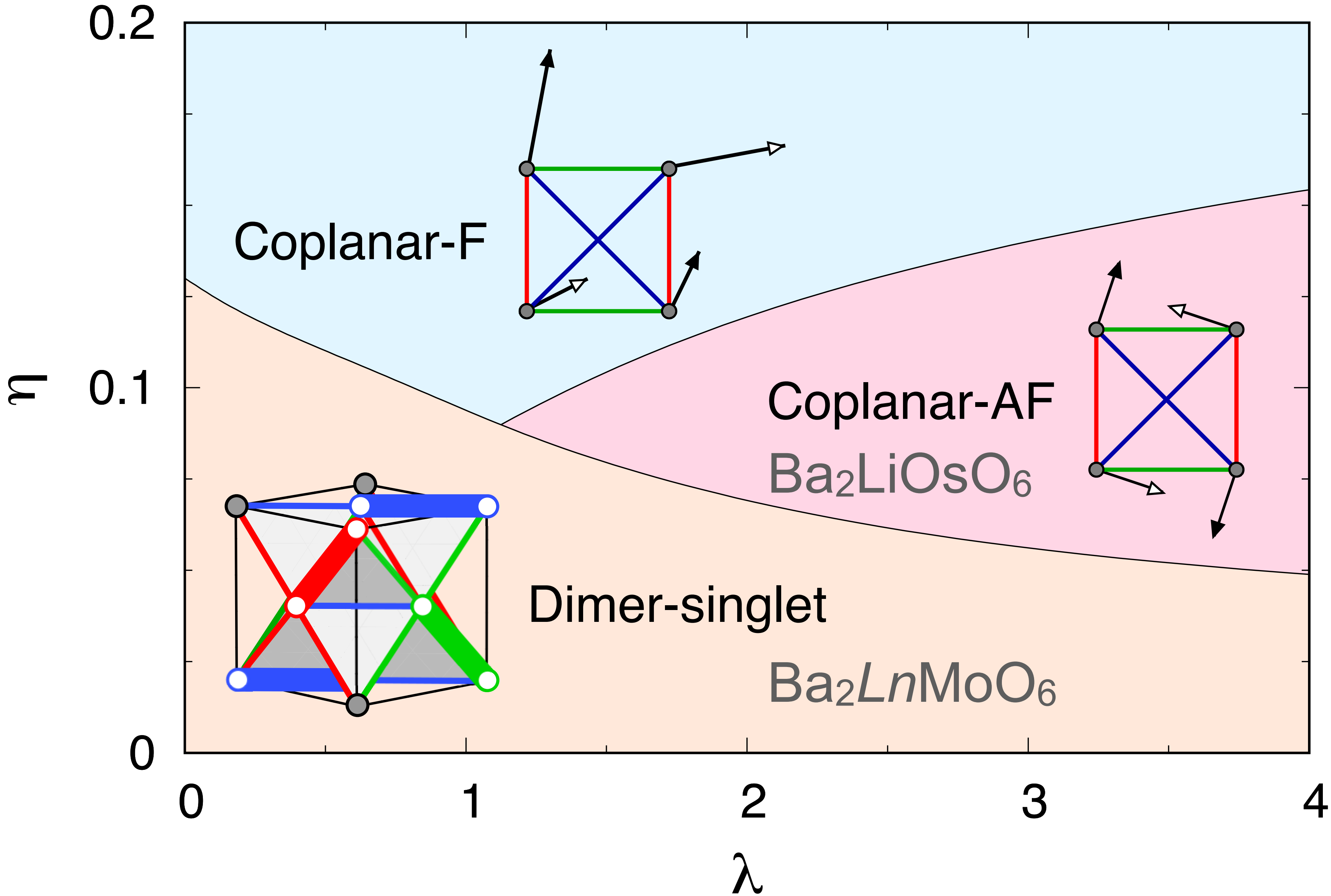
J. Romhanyi, L. Balents & GJ, PRL (2017)



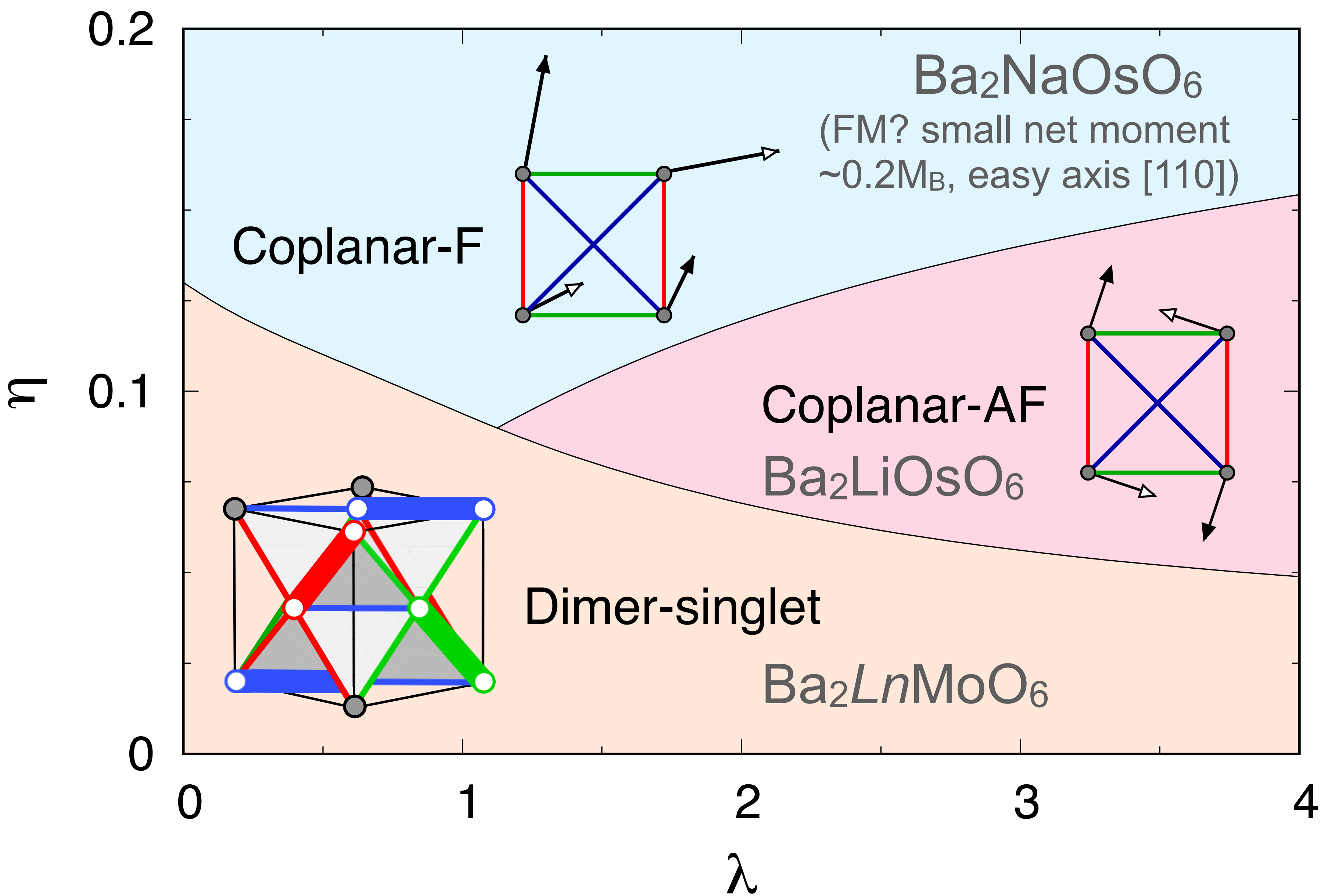
J. Romhanyi, L. Balents & GJ, PRL (2017)



J. Romhanyi, L. Balents & GJ, PRL (2017)

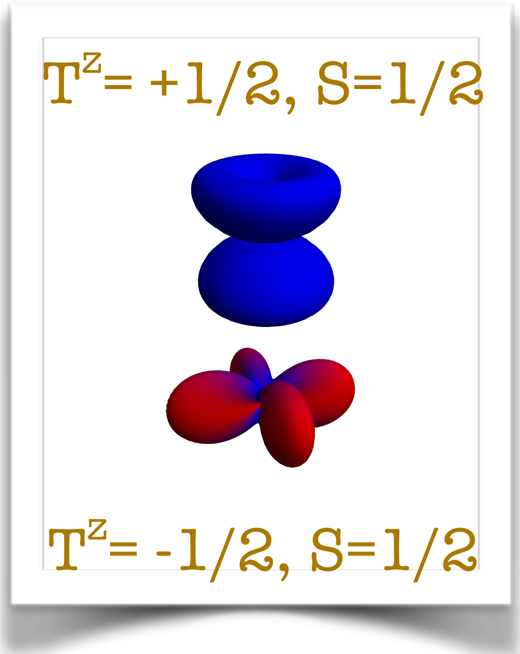


J. Romhanyi, L. Balents & GJ, PRL (2017)



Emergent SU(4) Symmetry and More

M.G. Yamada, M. Oshikawa, & GJ, arXiv:1709.05252



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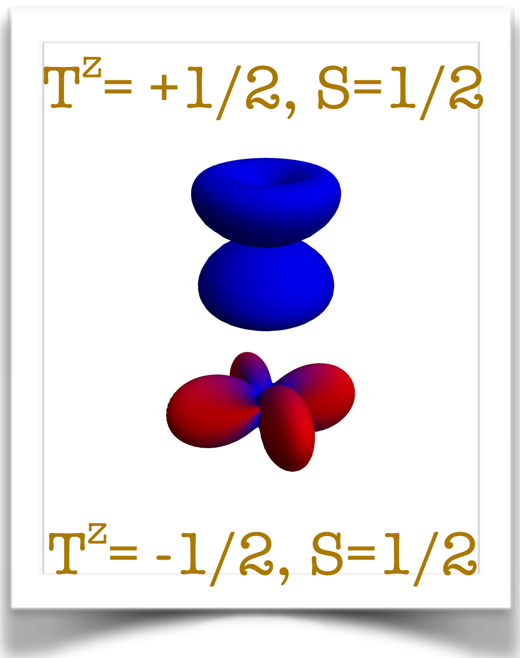

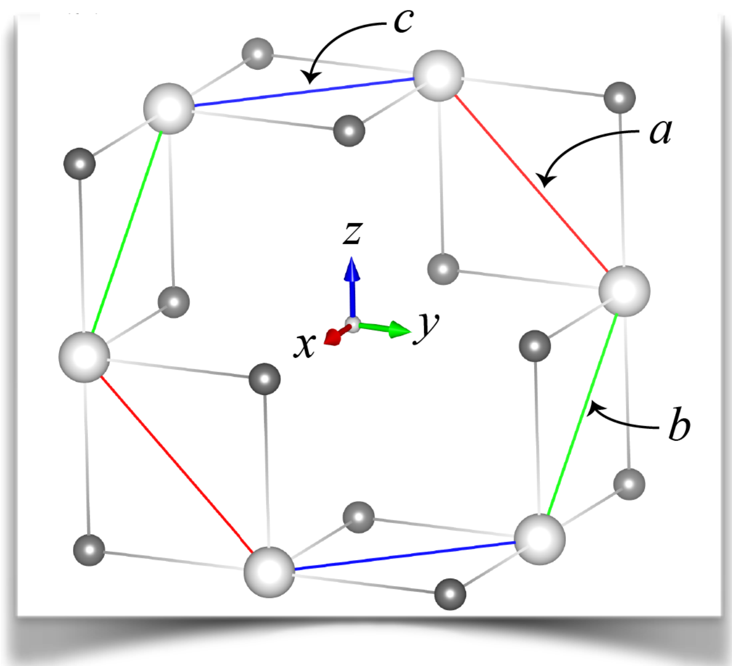

Emergent SU(4) Symmetry and More

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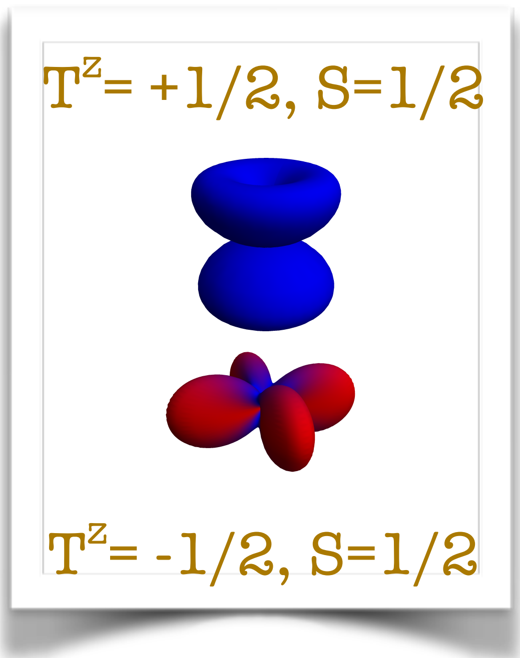

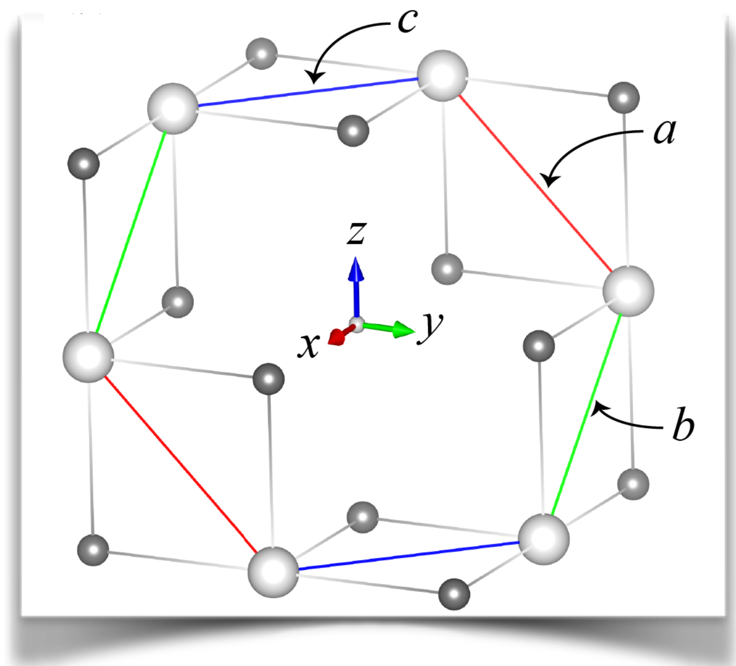

$$H_{\text{eff}} = J \sum_{\langle ij \rangle} \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \frac{1}{4} \right) \left(\boldsymbol{T}_i \cdot \boldsymbol{T}_j + \frac{1}{4} \right)$$

Thank You For Listening