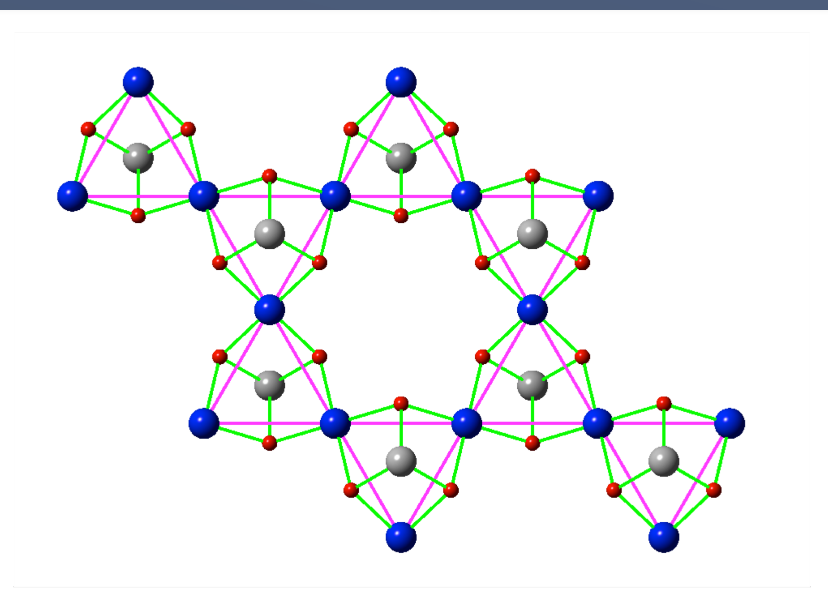
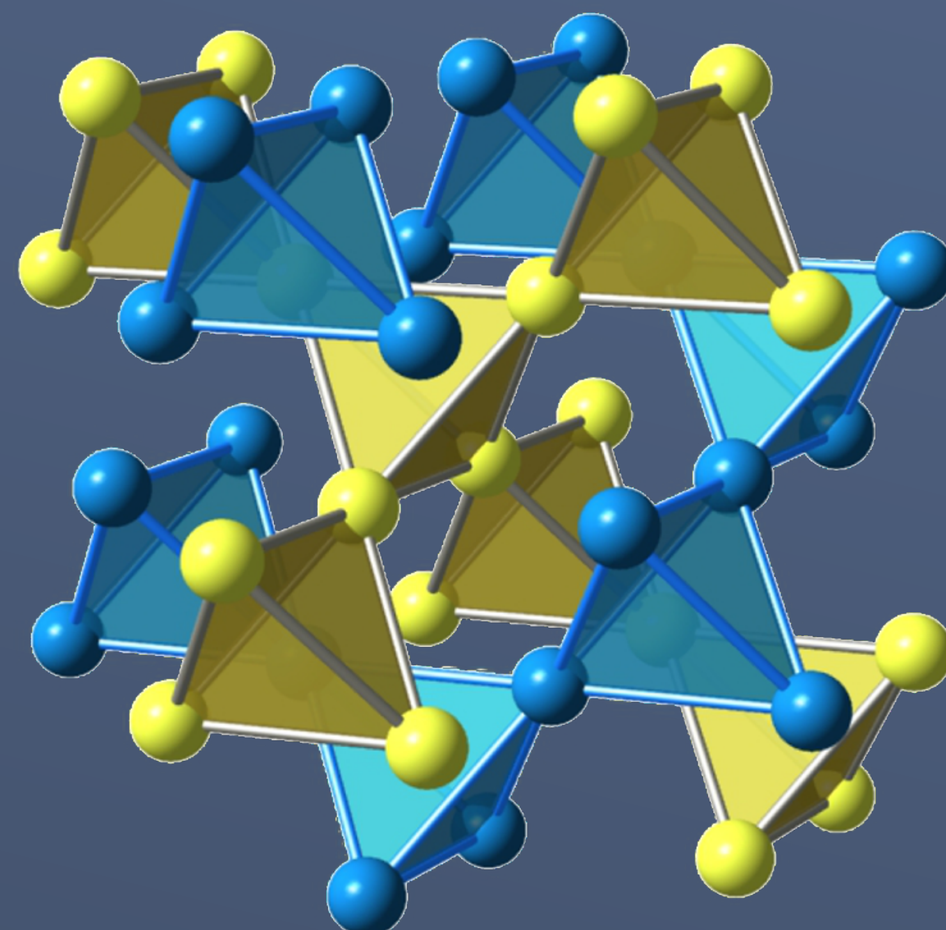
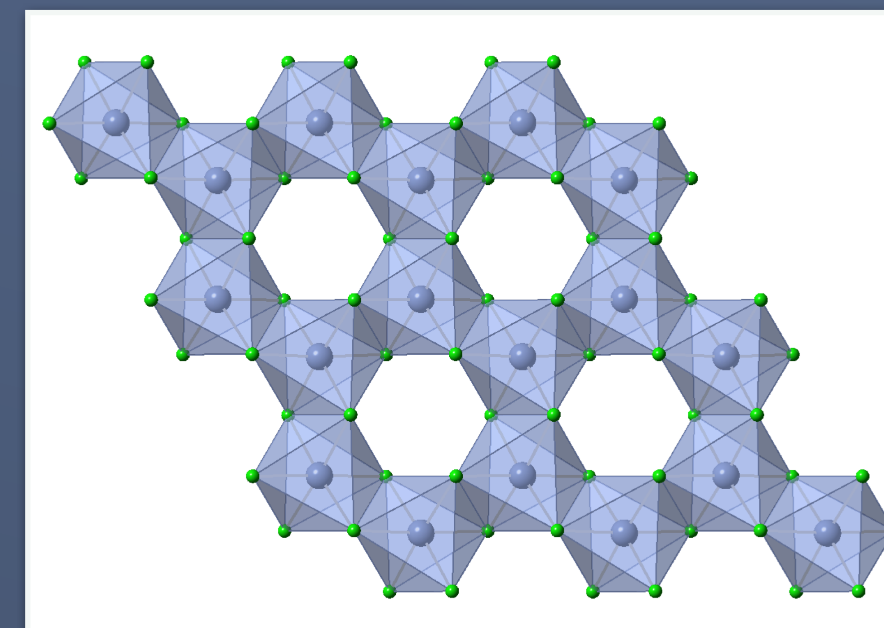
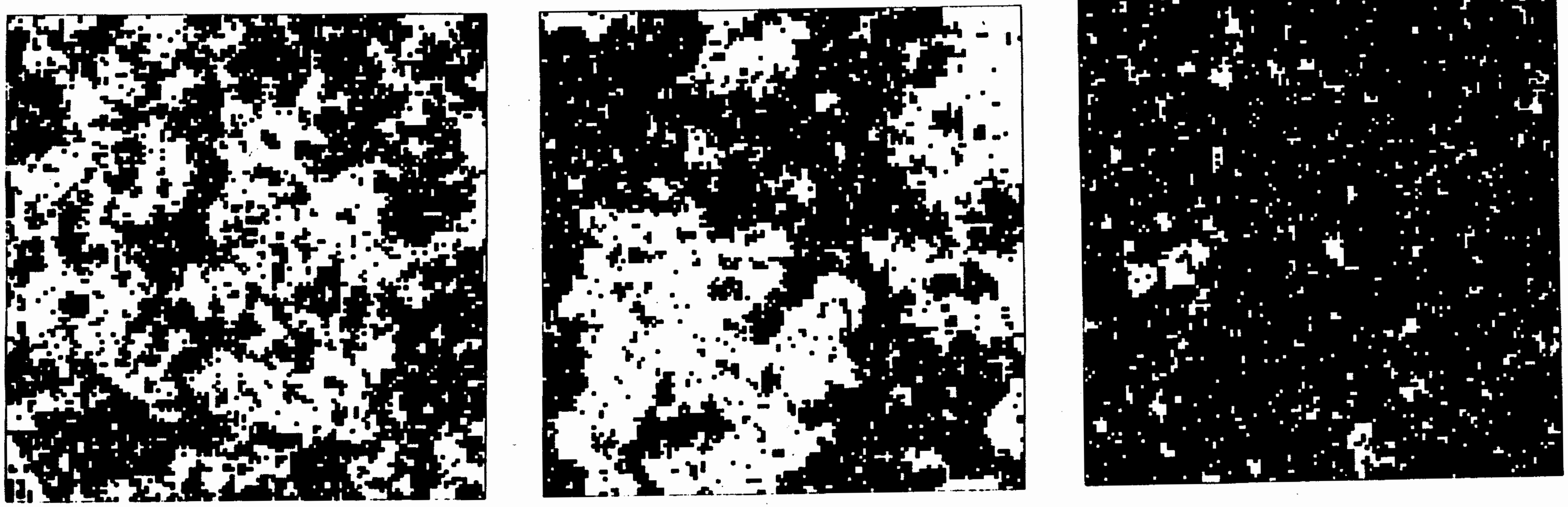
The Search for Spin Liquid Ground States in Real Materials





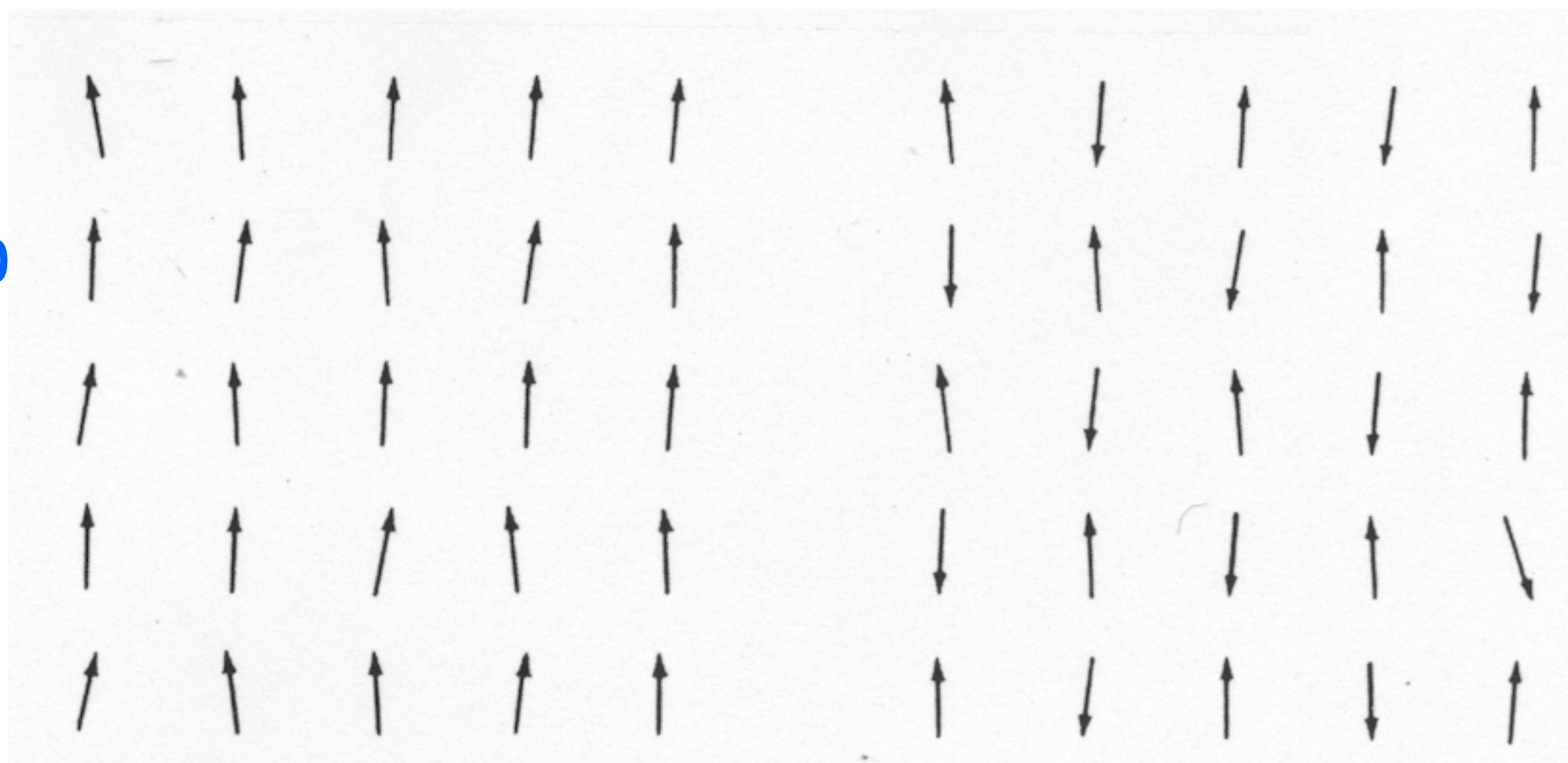


Bruce D. Gaulin
McMaster University
and LPS, U Paris-Saclay



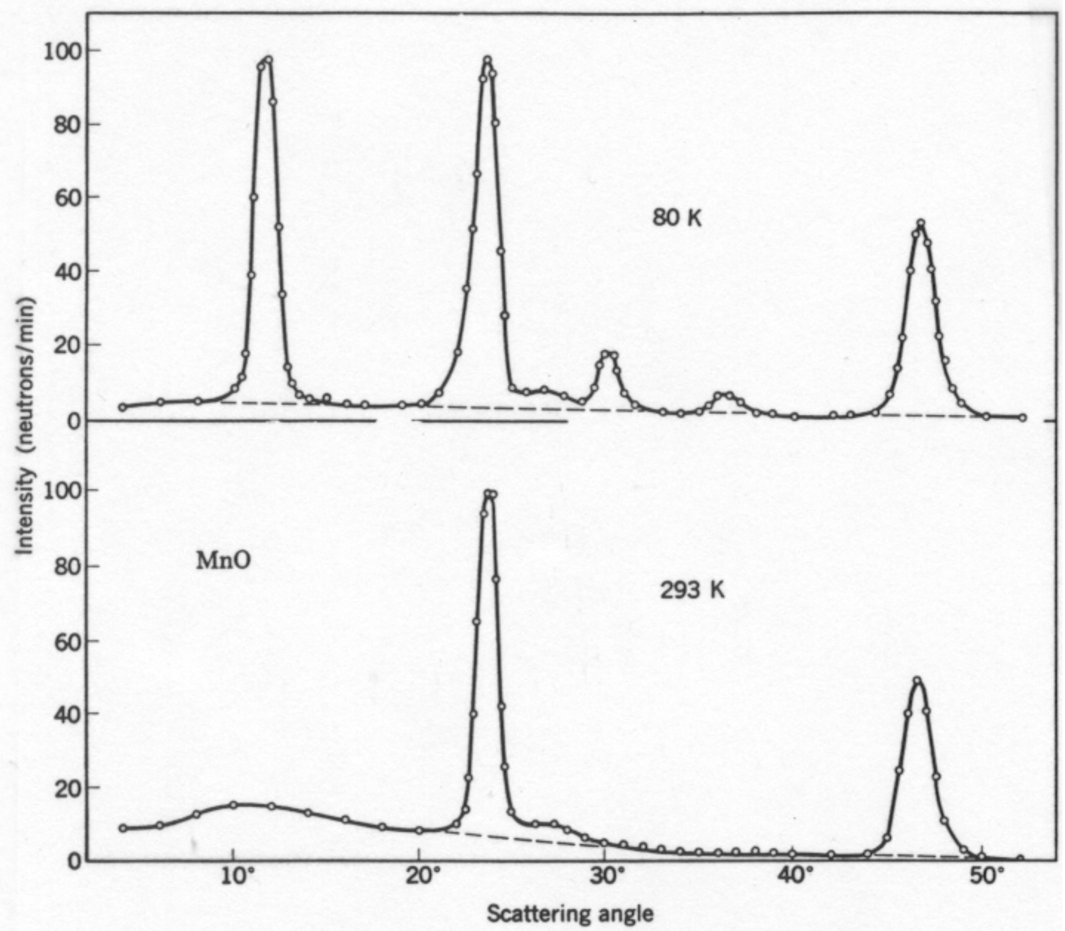
1.1 Tc   Tc   0.9 Tc

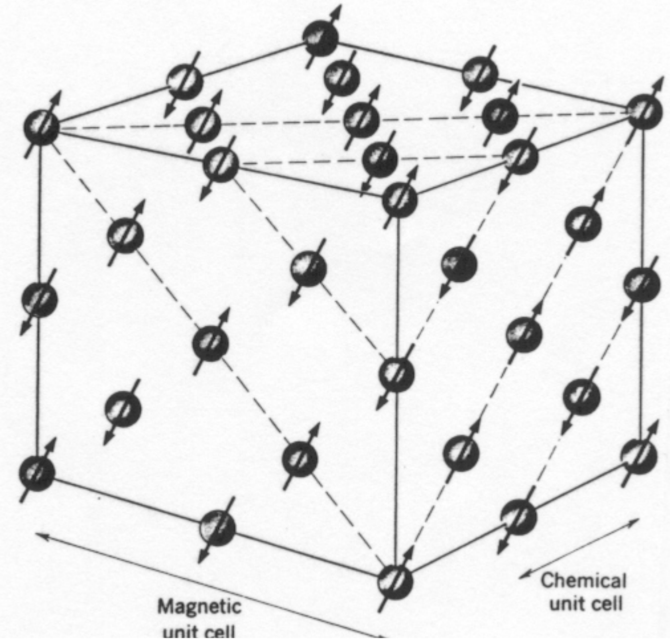
Ferromagnet



Antiferromagnet

$$H = 2J \sum_{ij} \mathbf{S_i} \cdot \mathbf{S_j}$$





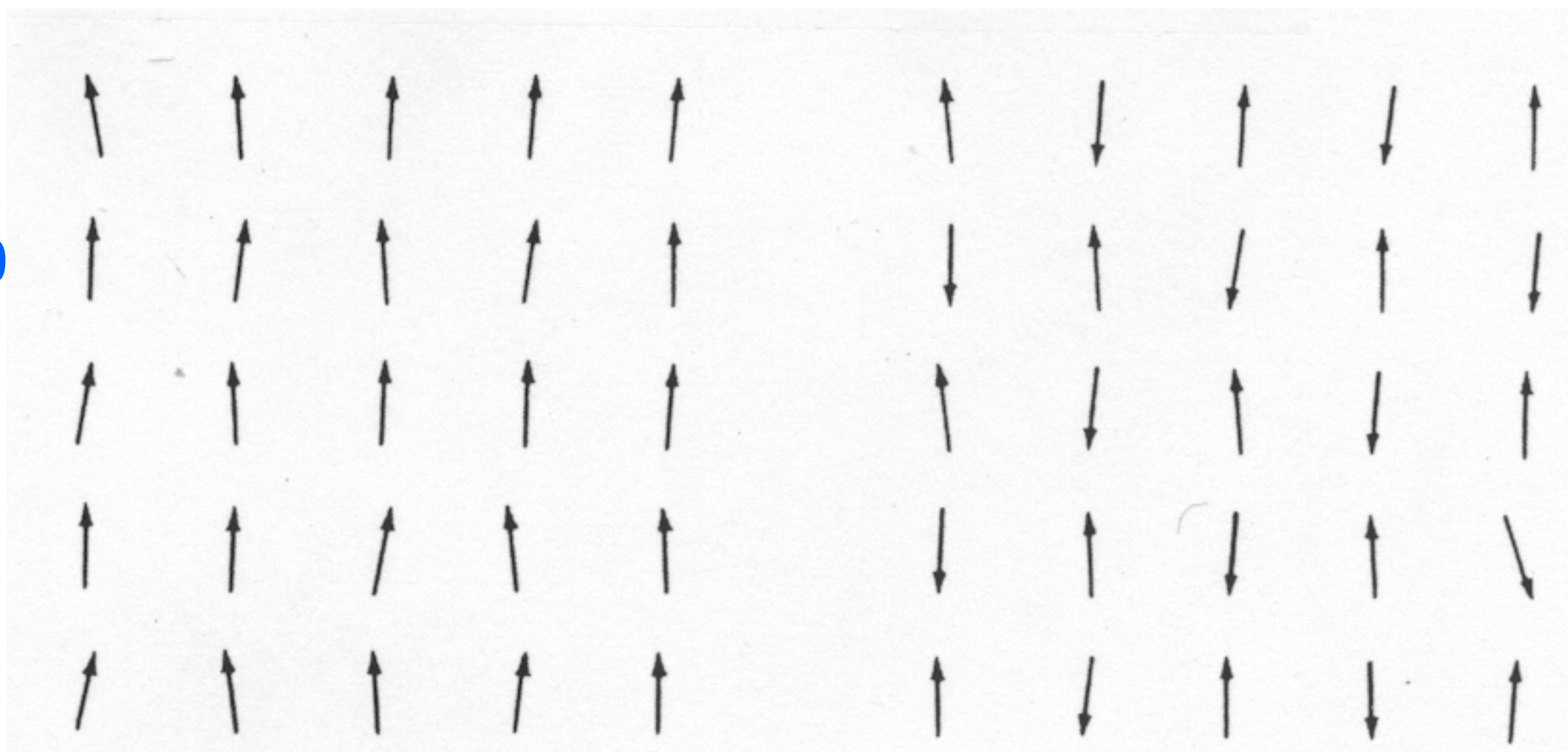
Detection of Antiferromagnetism by Neutron Diffraction*

C. G. Shull
Oak Ridge National Laboratory, Oak Ridge, Tennessee
AND
J. Samuel Smart
Naval Ordnance Laboratory, White Oak, Silver Spring, Maryland

August 29, 1949

Clifford G. Shull, MIT, Camebridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.

Ferromagnet



Antiferromagnet

about 400 cal. at 45°.

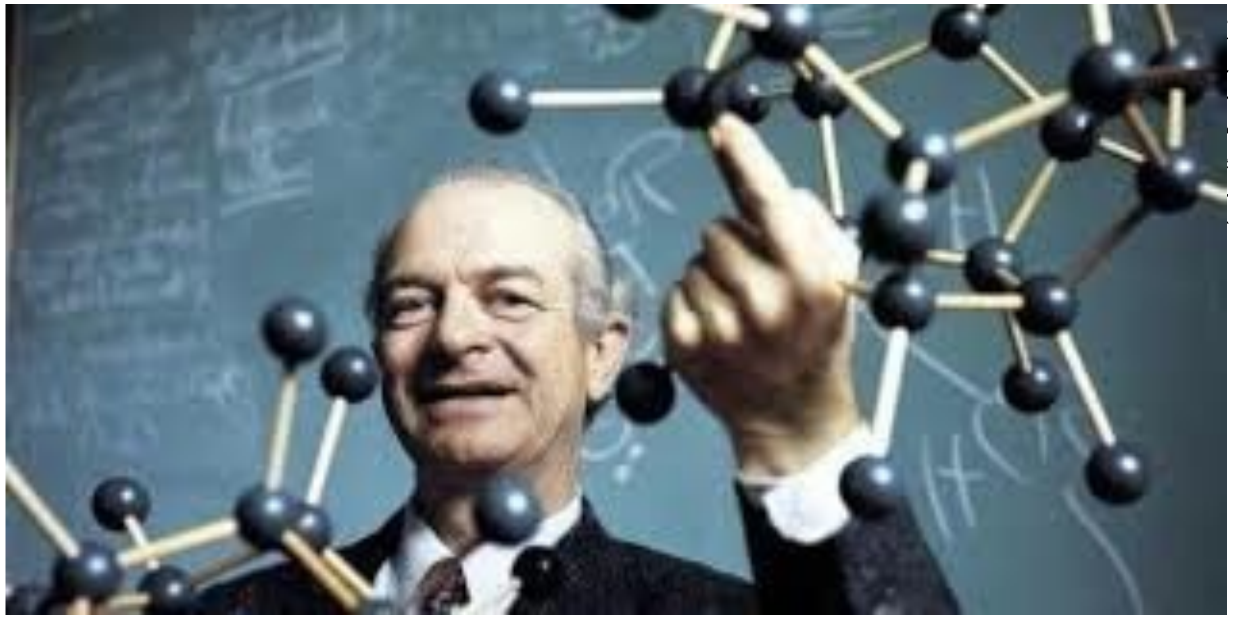
New York, N. Y. Received August 15, 1935

1935

[Contribution from the Gates Chemical Laboratory, California Institute of Technology, No. 506]

The Structure and Entropy of Ice and of Other Crystals with Some Randomness of Atomic Arrangement

By Linus Pauling



PHYSICAL REVIEW VOLUME 102, NUMBER 4 MAY 15, 1956

Ordering and Antiferromagnetism in Ferrites

1956

P. W. Anderson
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received January 9, 1956)

The octahedral sites in the spinel structure form one of the anomalous lattices in which it is possible to achieve essentially perfect short-range order while maintaining a finite entropy. In such a lattice nearest-neighbor forces alone can never lead to long-range order, while calculations indicate that even the long-range Coulomb forces are only 5% effective in creating long-range order. This is shown to have many possible consequences both for antiferromagnetism in "normal" ferrites and for ordering in "inverse" ferrites.

Exotic magnetism was of interest from the beginning!

PHYSICAL REVIEW VOLUME 79, NUMBER 2 JULY 15, 1950

Antiferromagnetism. The Triangular Ising Net

G. H. Wannier
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received February 11, 1950)

1950

Z. Physik B 33, 31 – 42 (1979)

Zeitschrift für Physik B

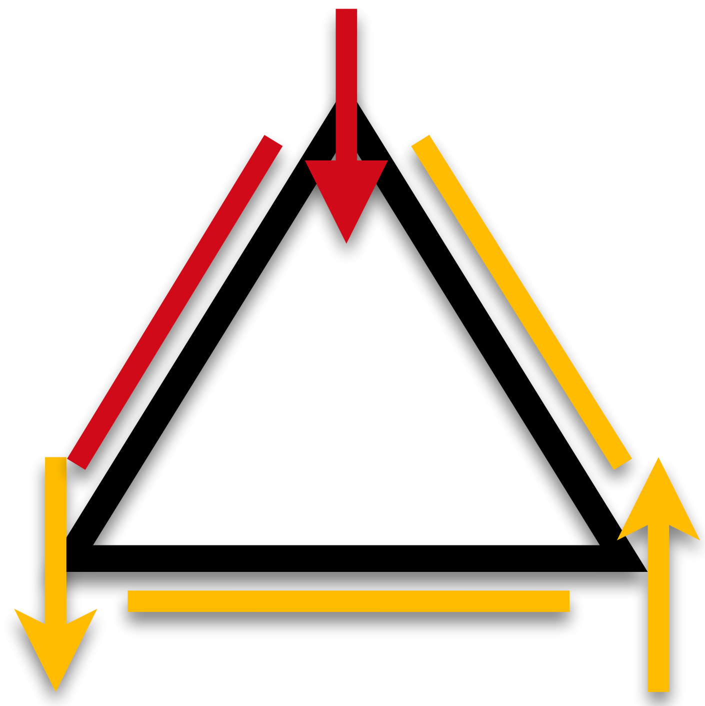
Insulating Spin Glasses

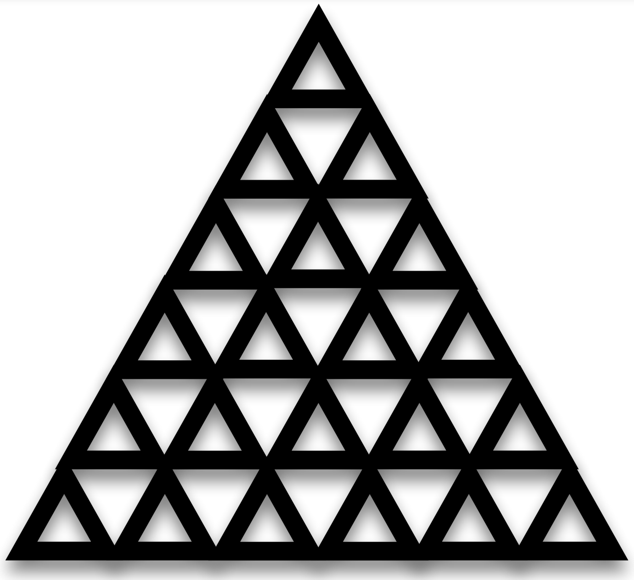
1979

Jacques Villain
Département de Recherche Fondamentale, Laboratoire de Diffraction Neutronique, Centre d'Etudes Nucléaires de Grenoble, Grenoble, France

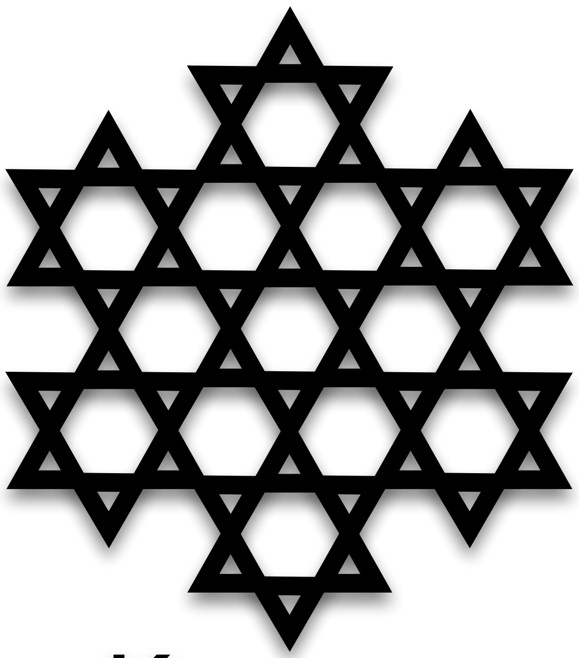
Received September 21, 1978

Physics of Frustration in 2D on Triangles

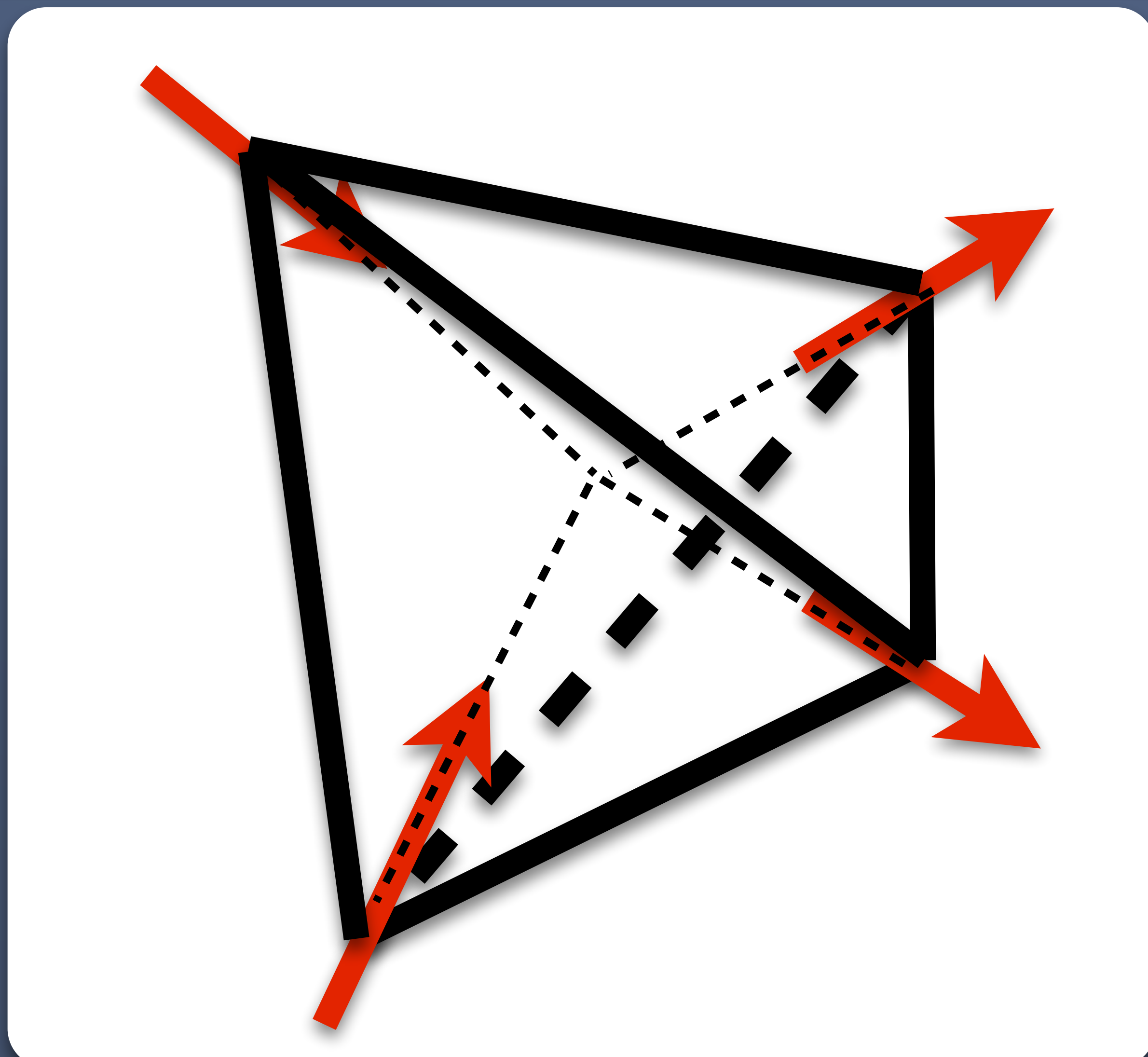


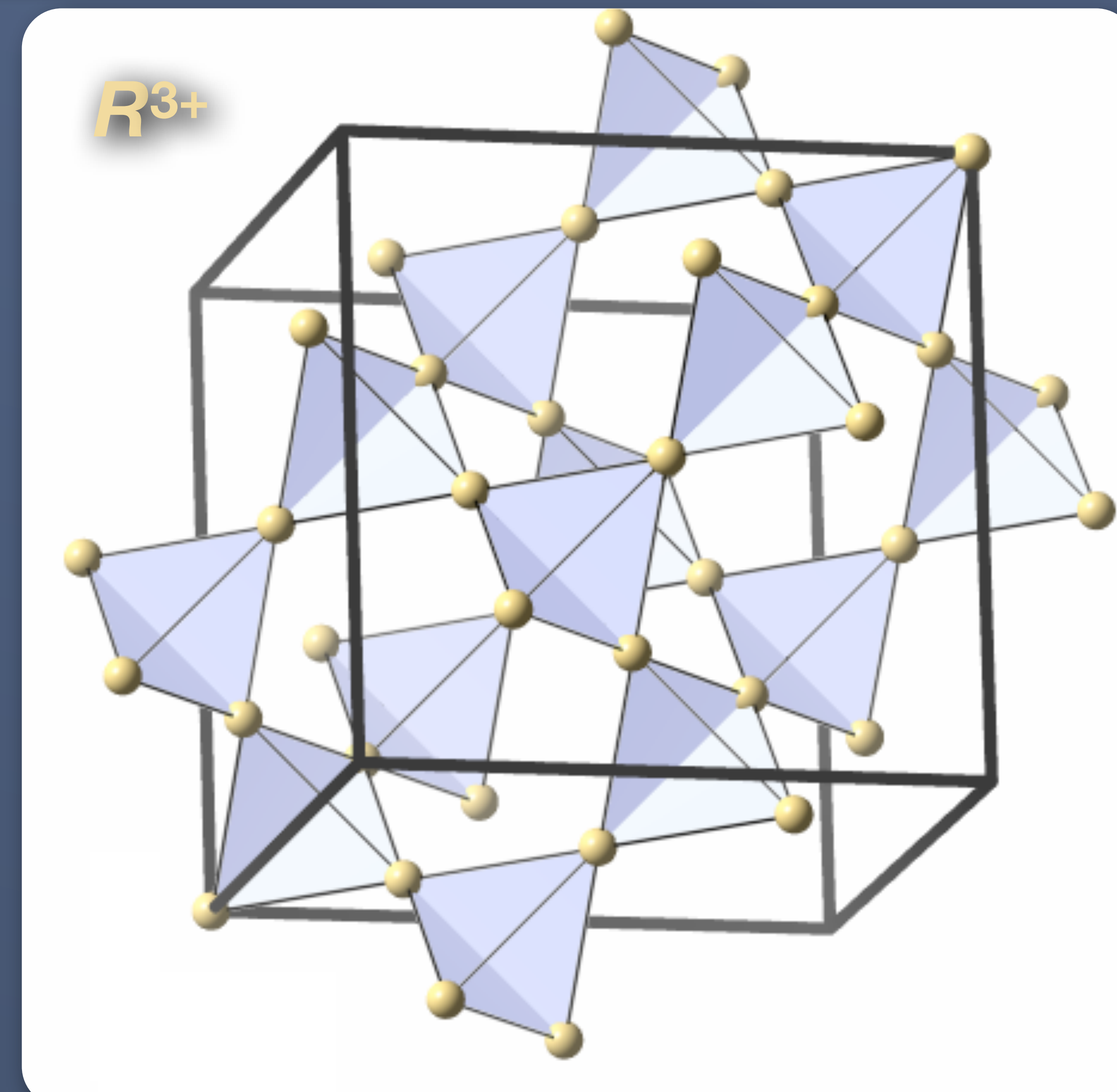


Antiferromagetism on a triangle:
↑↓ alignment energetically preferred,
but 1 of 3 "bonds" must be ↑↑



Physics of Frustration in 3D on Tetrahedra



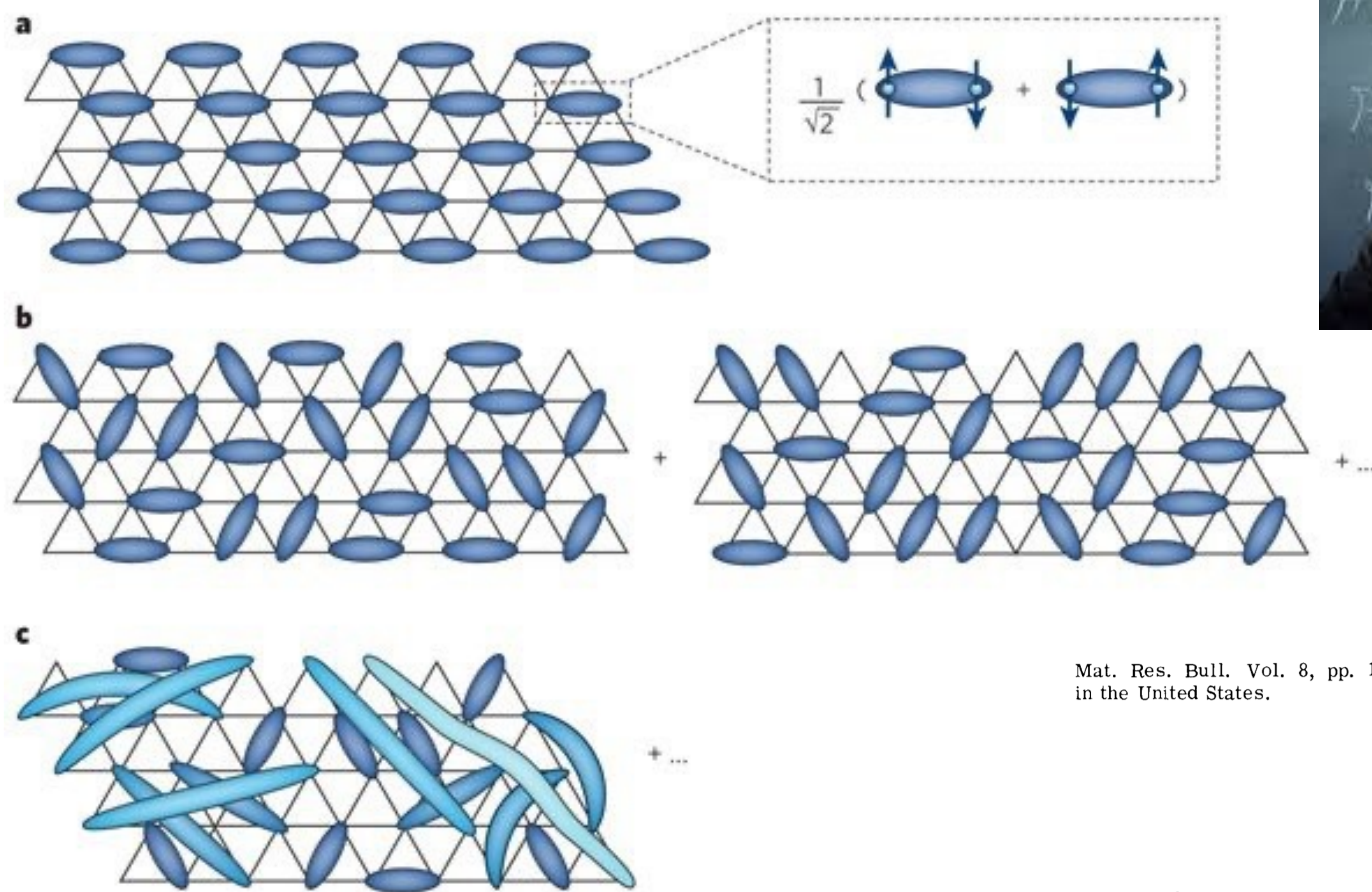


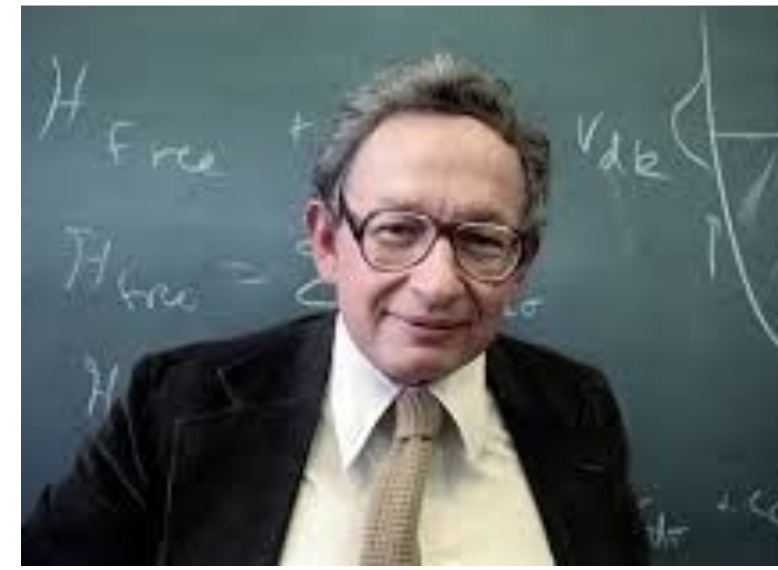
Cubic Pyrochlore Lattice

Spin Ice**:** Ferromagnetic interactions combined with local Ising anisotropy leads to 6-fold degeneracy on a single tetrahedron - macroscopic degeneracy on 3D crystal

M.J. Harris, S.T. Bramwell, D.F. McMorrow, T. Zeiske, and K.W. Godfrey, PRL 79 2554 (1997)

P.W. Anderson and the Resonating Valence Bond Model 1973





Mat. Res. Bull. Vol. 8, pp. 153-160, 1973. Pergamon Press, Inc. Printed in the United States.

RESONATING VALENCE BONDS: A NEW KIND OF INSULATOR ?*

P. W. Anderson
Bell Laboratories, Murray Hill, New Jersey 07974
and
Cavendish Laboratory, Cambridge, England

$$\mathcal{H}=J\boldsymbol{S}_i.\boldsymbol{S}_j,\ J>0$$

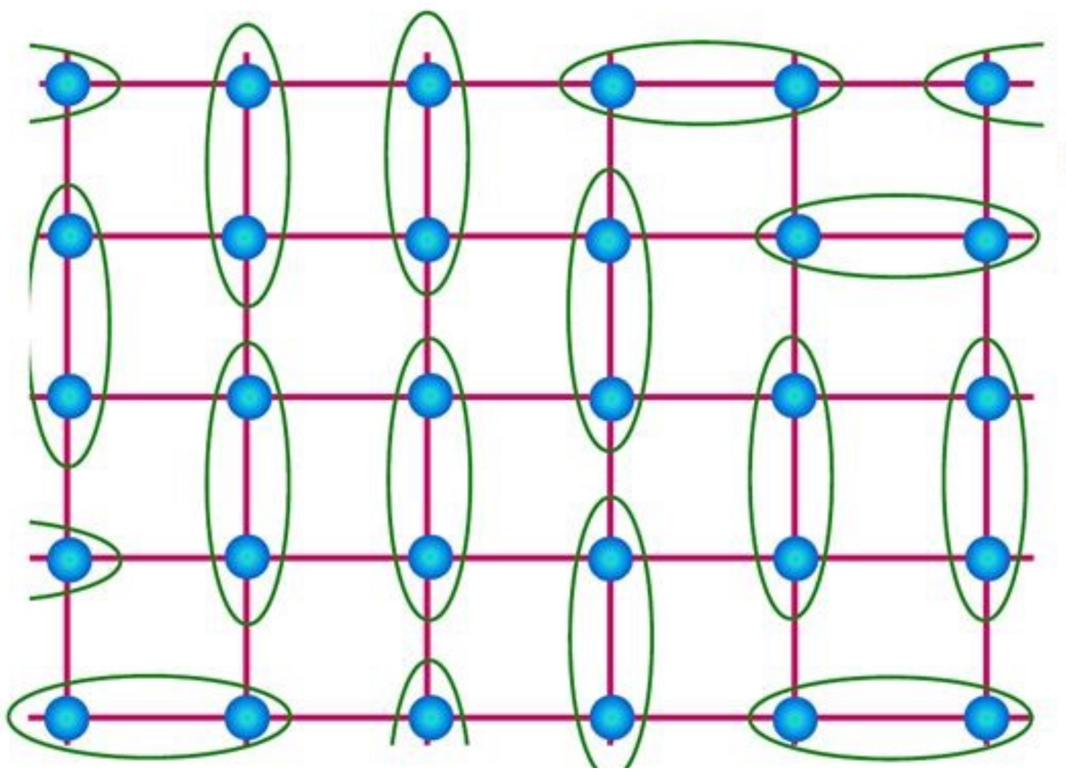
P.W. Anderson and the Resonating Valence Bond Model 1987

Science

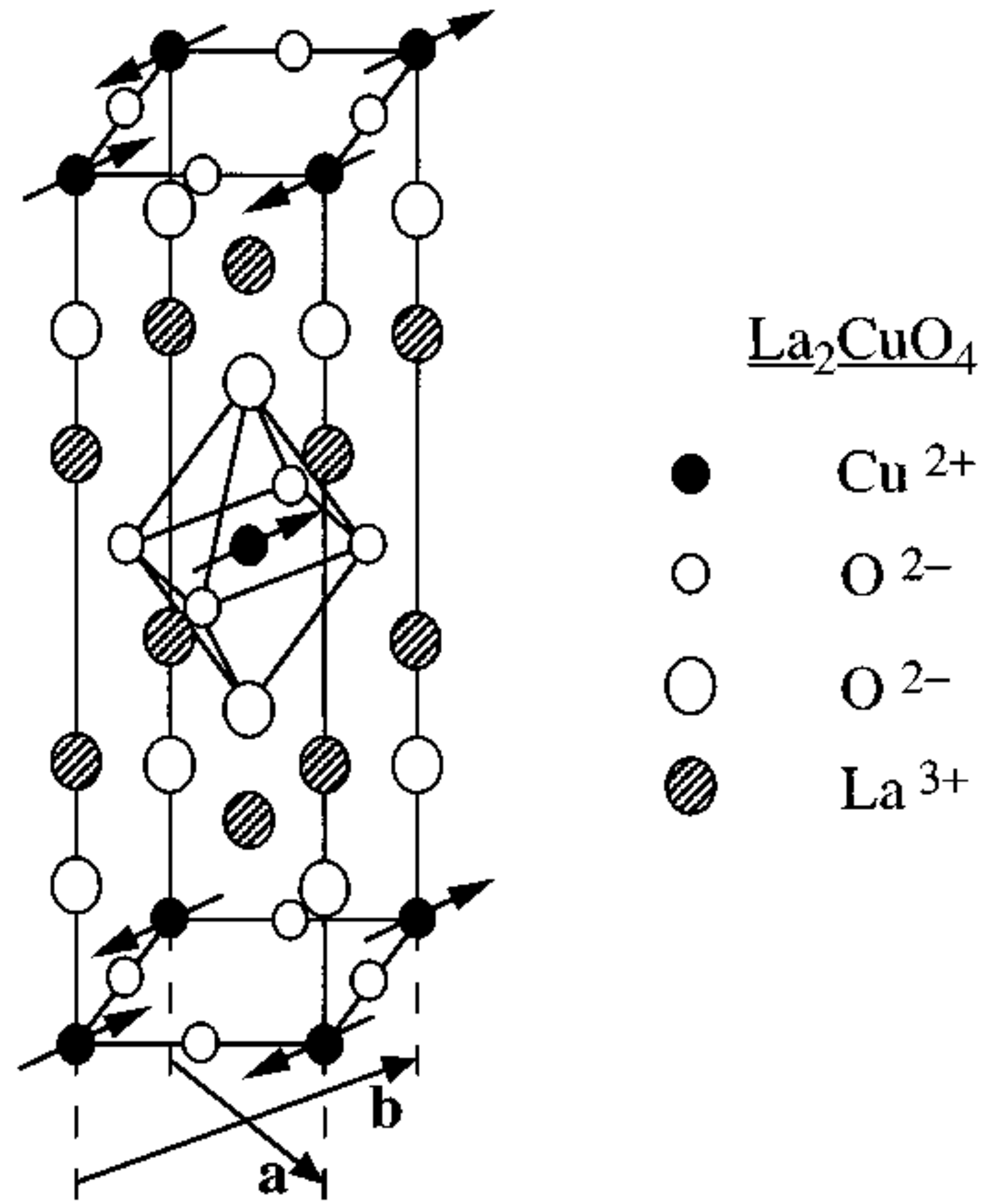
The Resonating Valence Bond State in La_2CuO_4 and Superconductivity

P. W. Anderson

The oxide superconductors, particularly those recently discovered that are based on La_2CuO_4, have a set of peculiarities that suggest a common, unique mechanism: they tend in every case to occur near a metal-insulator transition into an odd-electron insulator with peculiar magnetic properties. This insulating phase is proposed to be the long-sought "resonating-valence-bond" state or "quantum spin liquid" hypothesized in 1973. This insulating magnetic phase is favored by low spin, low dimensionality, and magnetic frustration. The preexisting magnetic singlet pairs of the insulating state become charged superconducting pairs when the insulator is doped sufficiently strongly. The mechanism for superconductivity is hence predominantly electronic and magnetic, although weak phonon interactions may favor the state. Many unusual properties are predicted, especially of the insulating state.

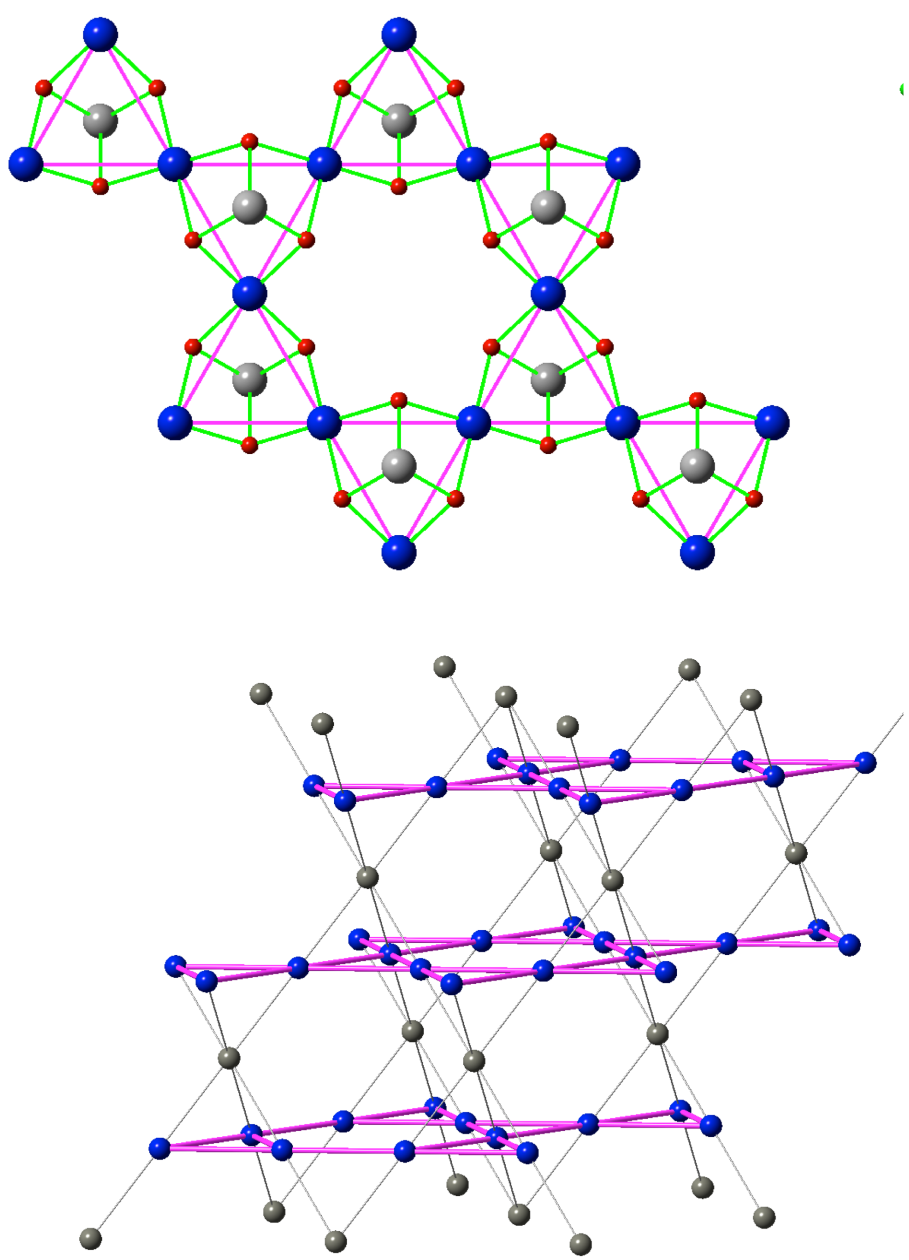


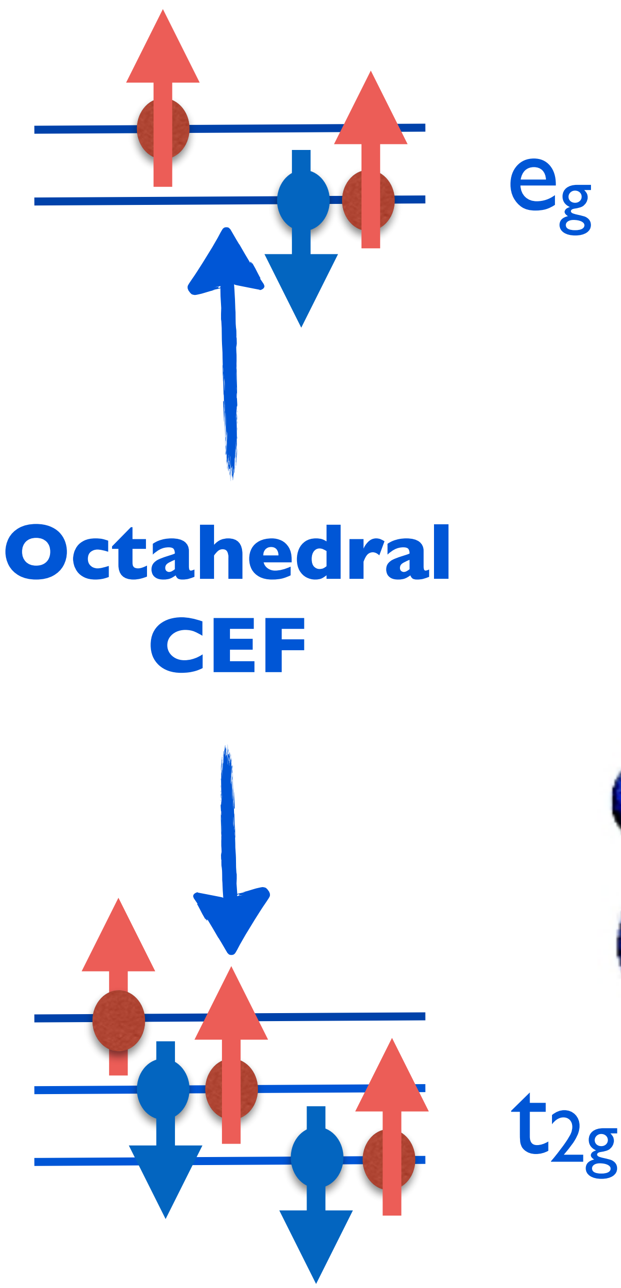
+ . . .

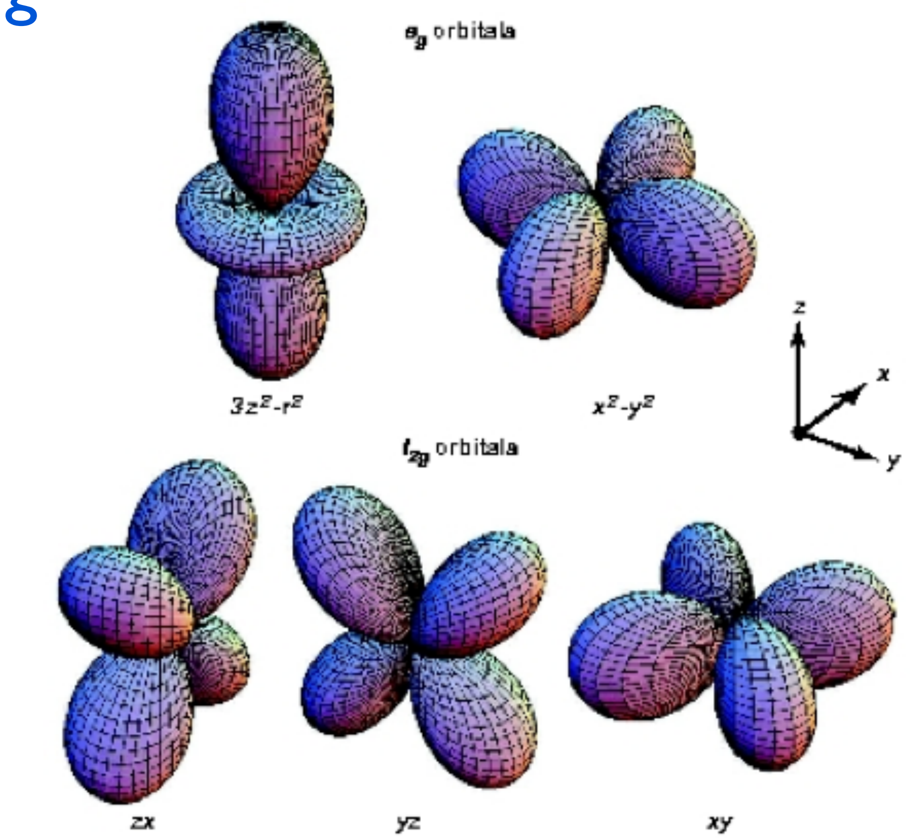


2D Heisenberg S=1/2 Kagome AF

(b) $ZnCu_3(OH)_6Cl_2$

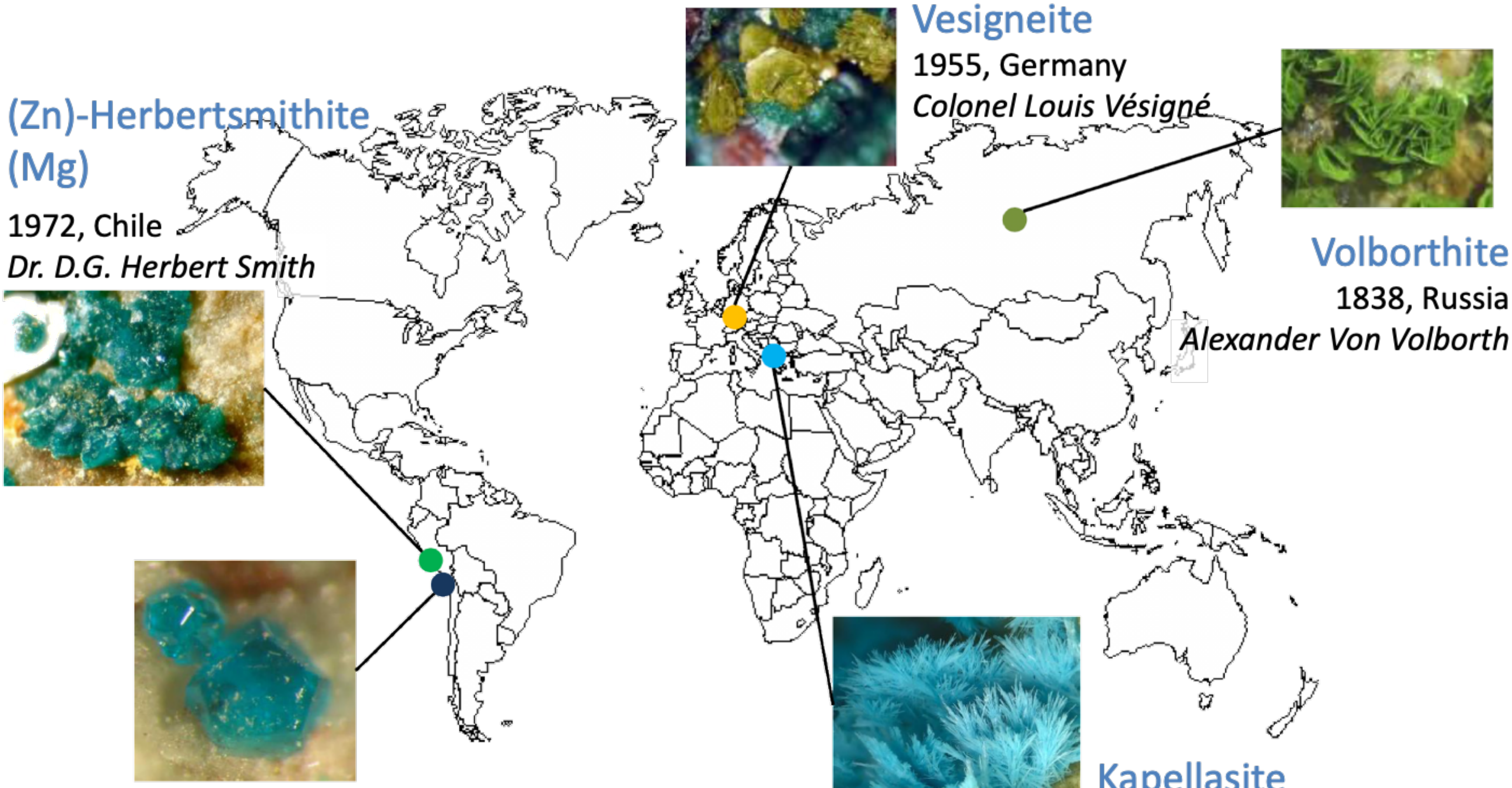




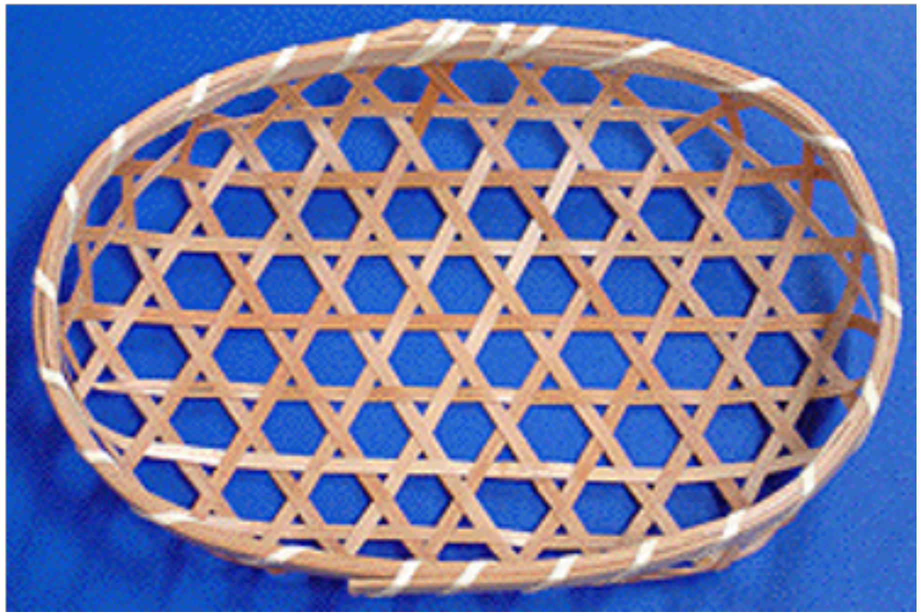


Cu^{2+} $3d^9$ S=1/2

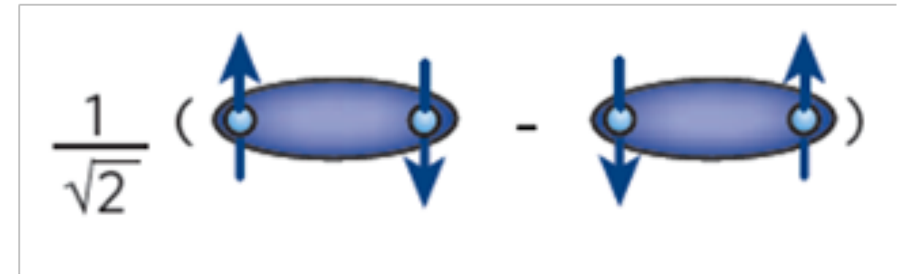
A World of Kagome Minerals

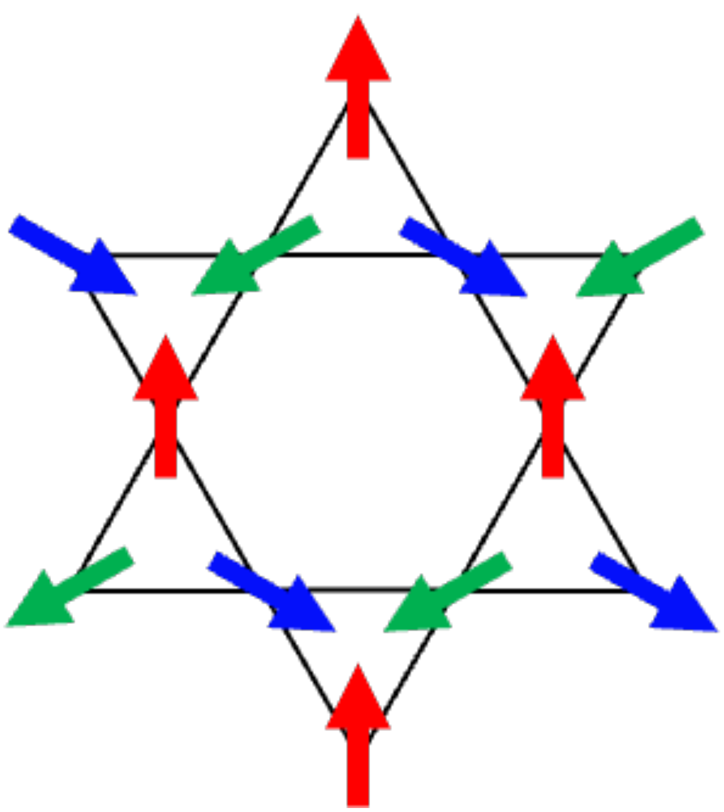


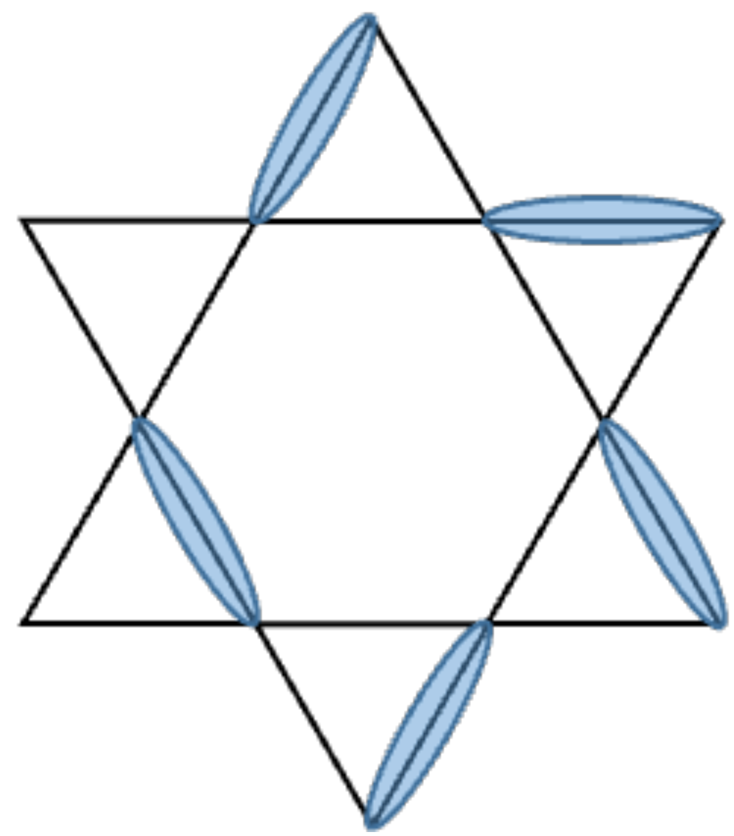
2D Heisenberg S=1/2 Kagome AF



$$\mathcal{H} = J\boldsymbol{S}_i.\boldsymbol{S}_j,\ J > 0$$







$$E_{classical} = zJ\mathbf{S_i}\cdot\mathbf{S_j}/2$$

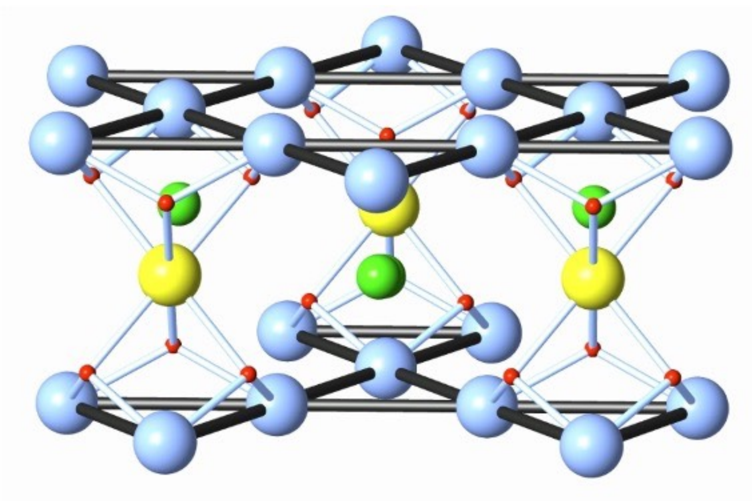
$$E_{Quantum} = -3J/8$$

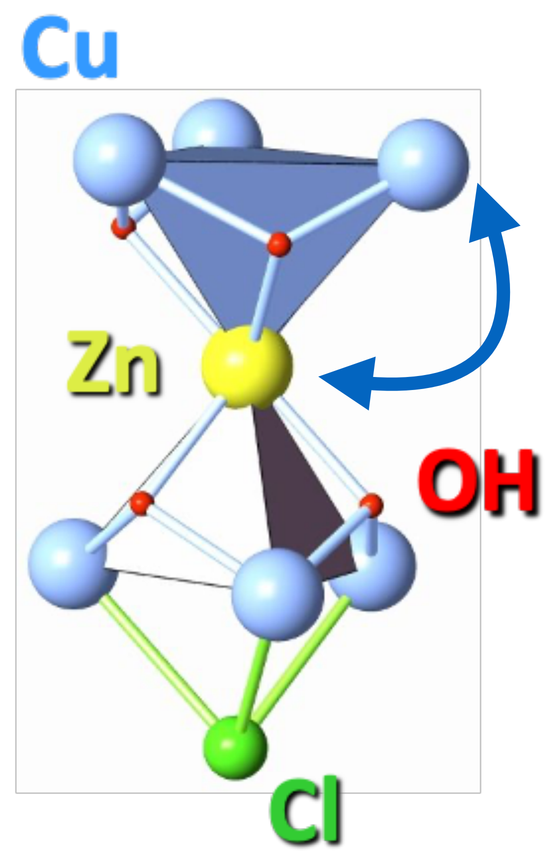
2D Heisenberg S=1/2 Kagome AF

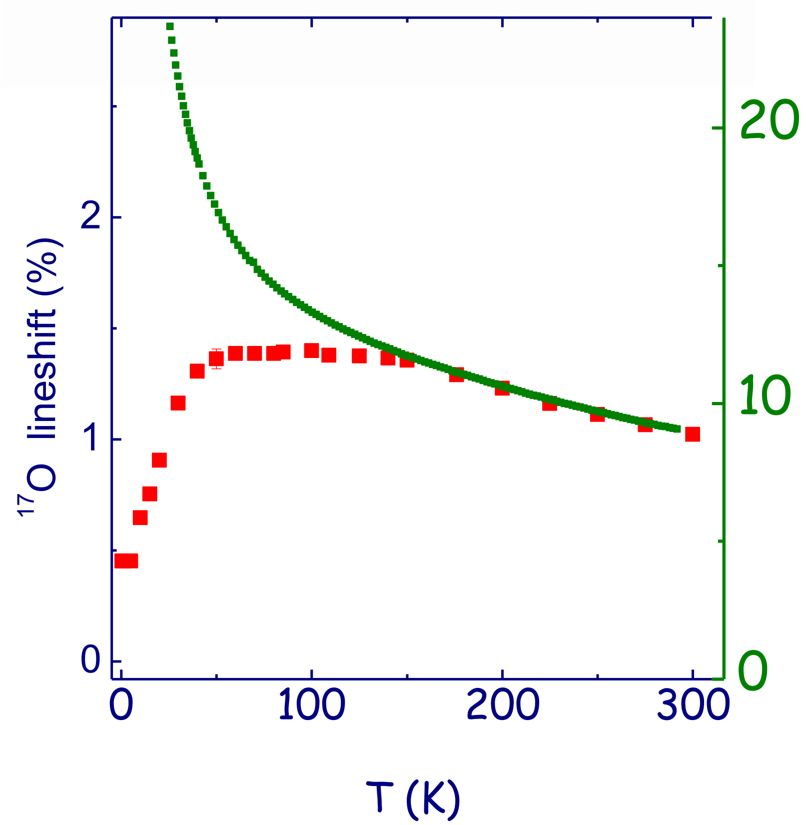
J|A|C|S COMMUNICATIONS
Published on Web 09/09/2005

A Structurally Perfect $S = {}^{1}/_{2}$ Kagomé Antiferromagnet

Matthew P. Shores, Emily A. Nytko, Bart M. Bartlett, and Daniel G. Nocera*







Olariu et al, PRL 100, 087202 (2008)

PHYSICAL REVIEW B **88**, 075106 (2013)

First-principles determination of Heisenberg Hamiltonian parameters for the spin-$\frac{1}{2}$ kagome antiferromagnet $ZnCu_3(OH)_6Cl_2$

Harald O. Jeschke,* Francesc Salvat-Pujol, and Roser Valentí

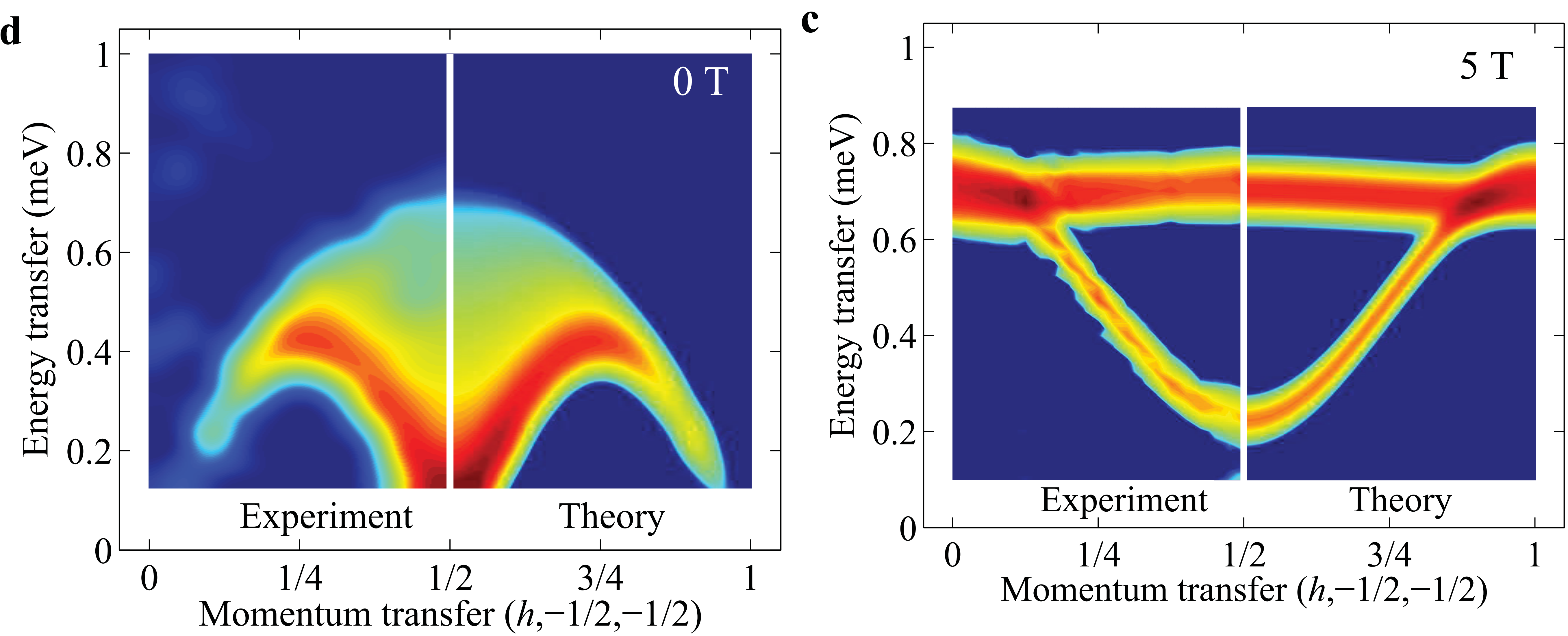
TABLE II. Exchange coupling constants for $ZnCu_3(OH)_6Cl_2$ (herbertsmithite) determined from total energies of nine different spin configurations. Energies were calculated with GGA + U functional at $U = 6$ eV, $J = 1$ eV and with atomic-limit double-counting correction.

Name	d_{Cu-Cu}	Type	J_i (K) $U = 6$ eV
		Kagome layer couplings	
J_1	3.4171	Kagome nn	182.4
J_3	5.91859	Kagome 2nd nn	3.4
J_5	6.8342	Kagome 3rd nn	−0.4
		Interlayer couplings	
J_2	5.07638	Interlayer 1st nn	5.3
J_4	6.11933	Interlayer 2nd nn	−1.5
J_6	7.00876	Interlayer 3rd nn	−6.4
J_7	8.51328	Interlayer 4th nn	3.0
J_9	9.17347	Interlayer 6th nn	2.5

Best Understood Spin Liquid:
S=1/2 Heisenberg AF chain

Deconfined spinons as elementary excitations in zero field
Spin waves in field-polarized state

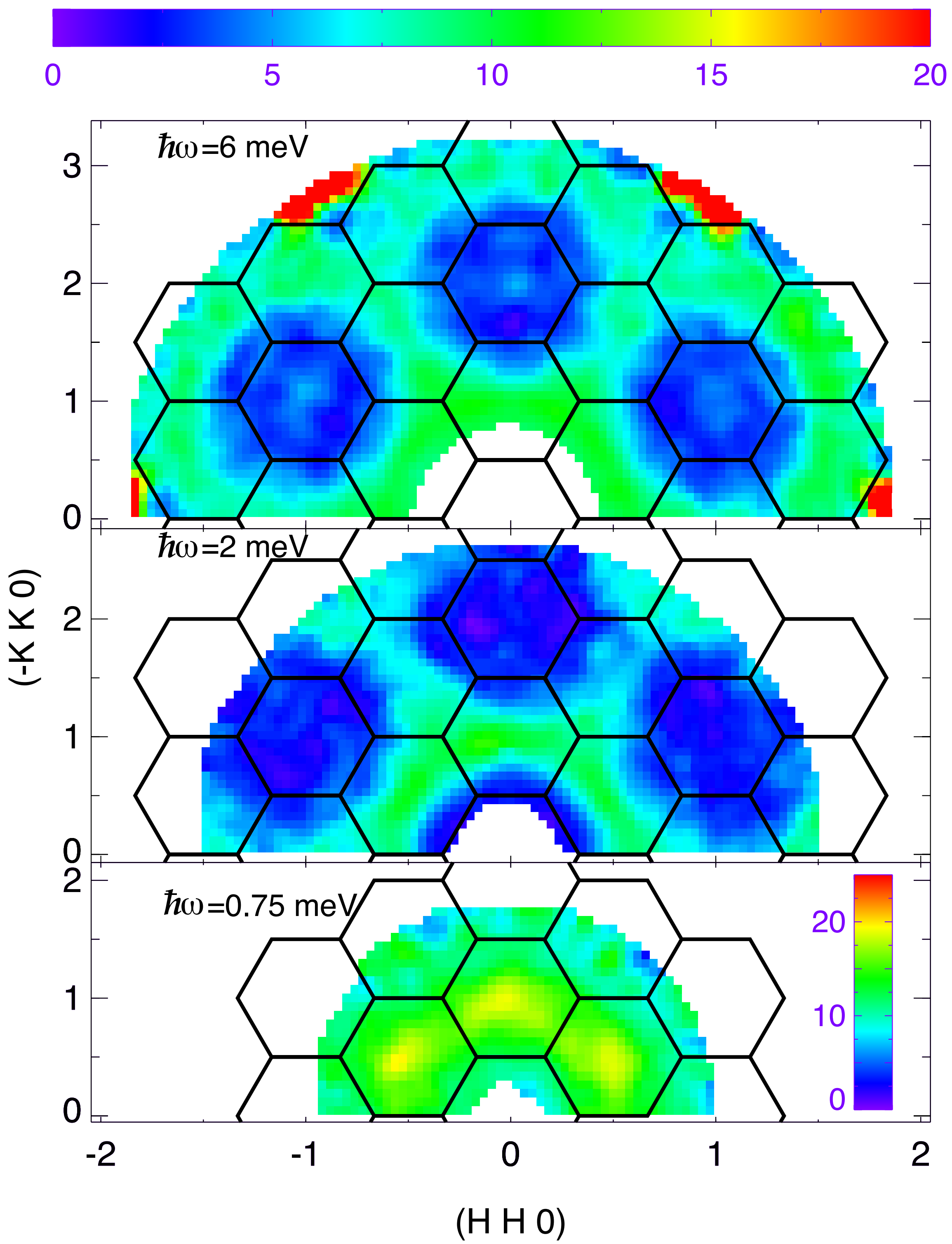
$CuSO_4 \cdot 5D_2O$

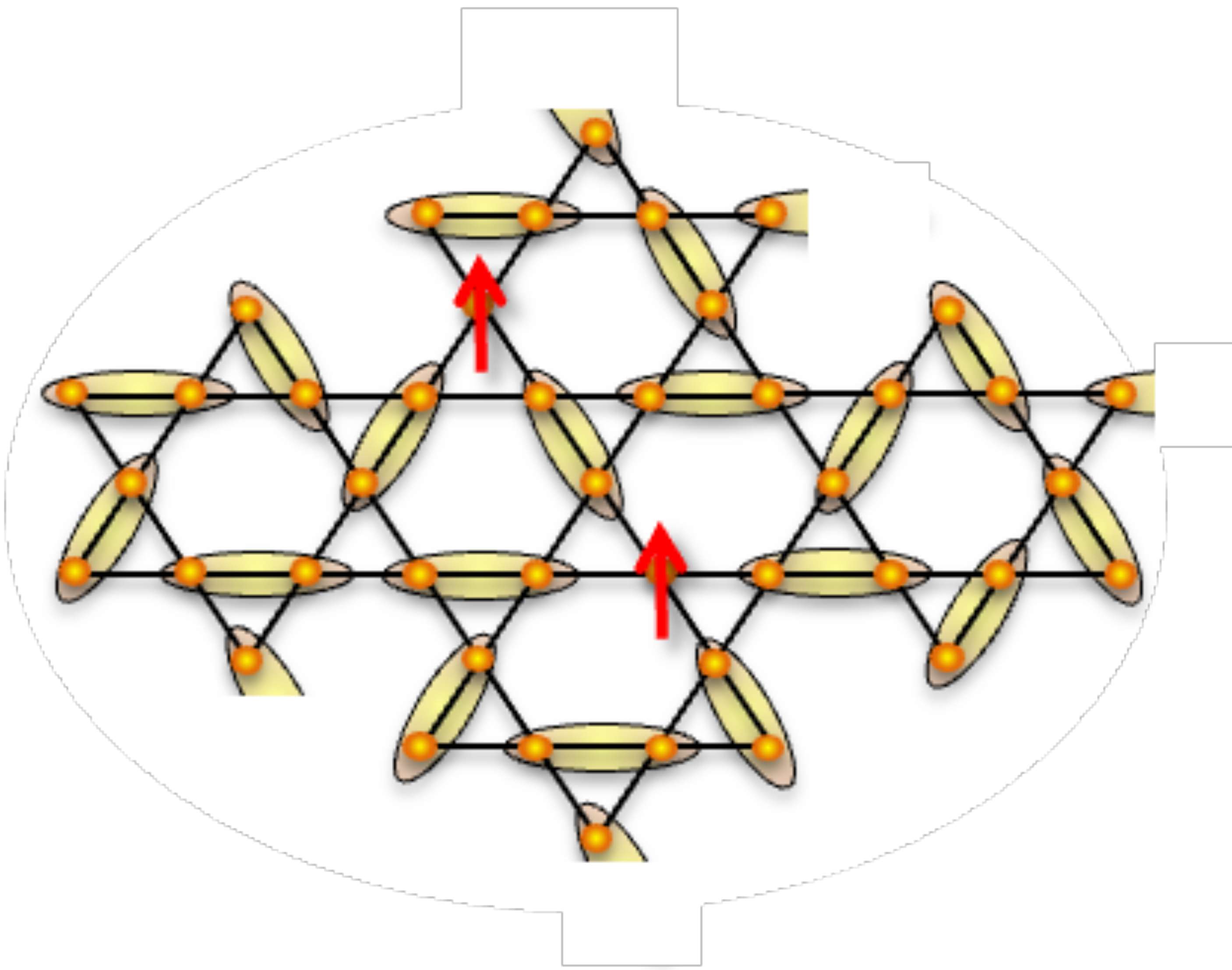


M. Mourigal et al, Nature Physics, 9, 435, 2013

2D Heisenberg S=1/2 Kagome AF

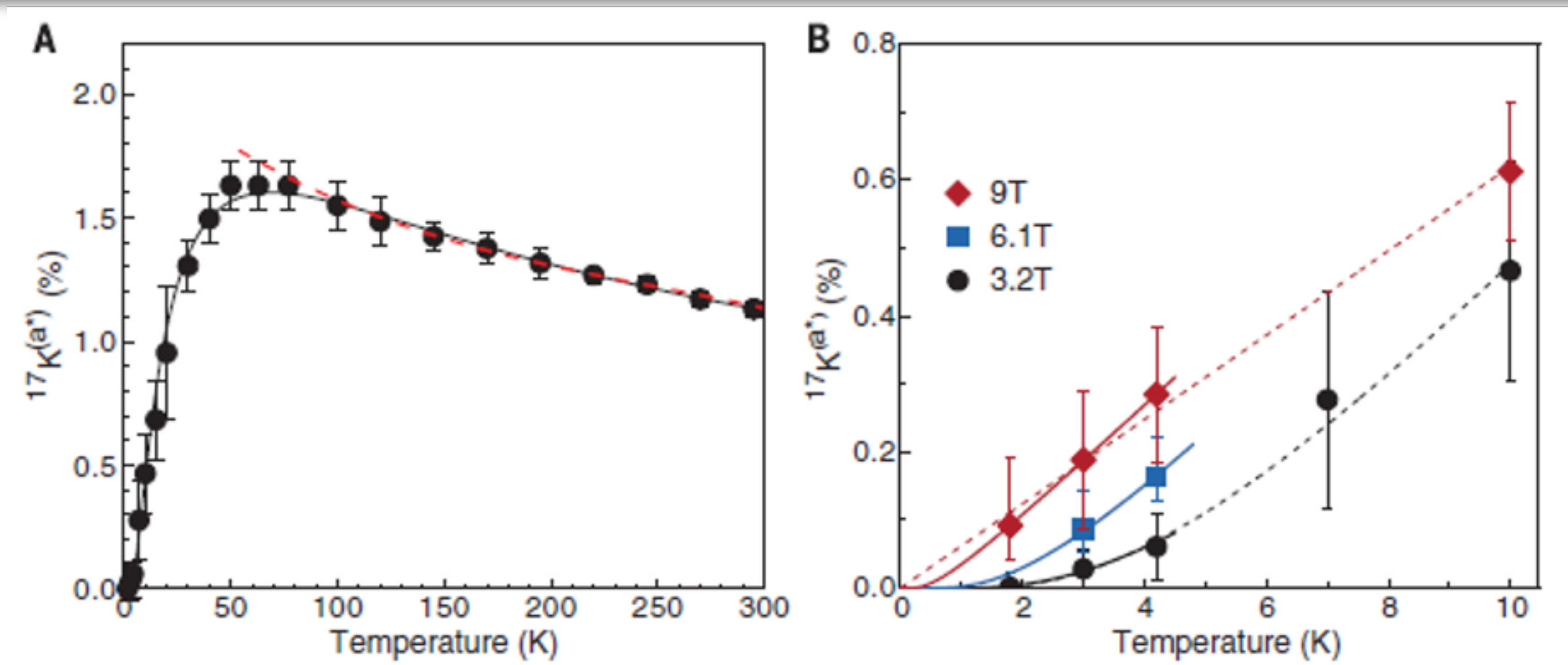
(a) $ZnCu_3(OH)_6Cl_2$





T.-H. Han et al.,
Nature 492, 406-410 (2012).

2D S=1/2 Kagome Antiferromagnet: Gapped or Ungapped in Herbertsmithite?



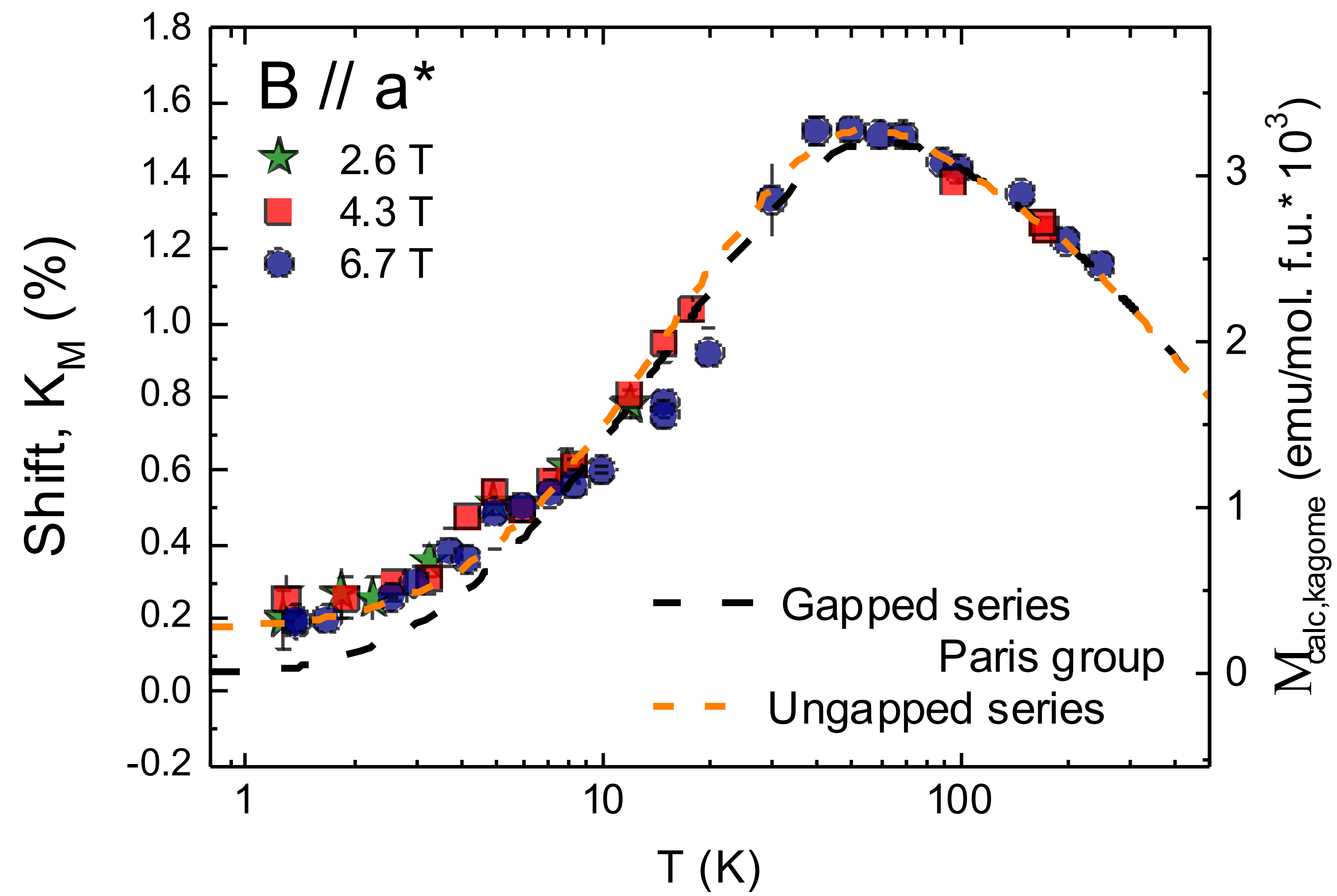
Fu et al,
Science 350, 655 (2016)

Gap ~ 9 K
(and closes with H)

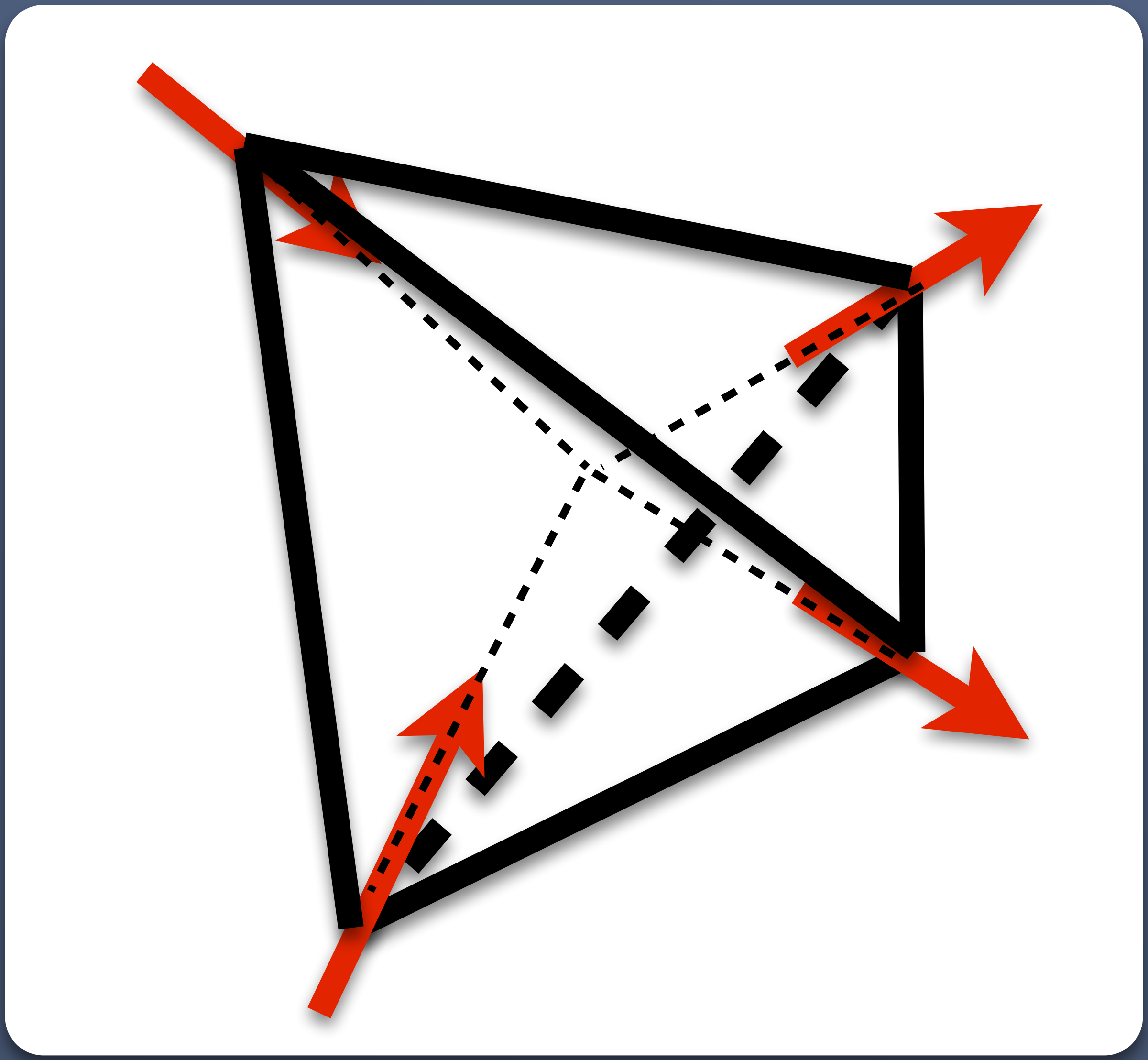
P. Khuntia et al.,
Nature Physics 16, 469 (2020)

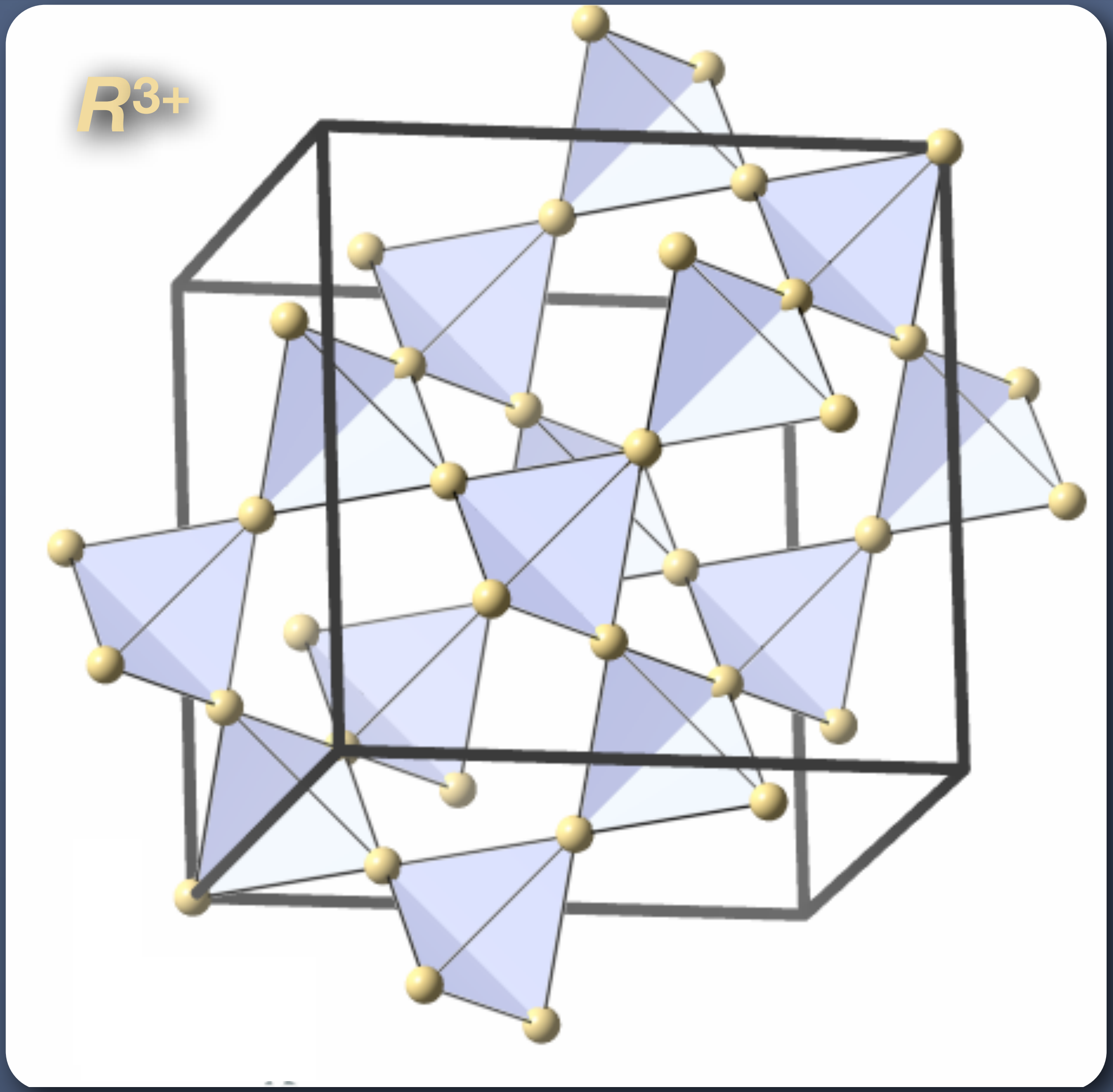
Barthélemy et al.,
Phys. Rev. X (2022)

Gap consistent with 0 K



Physics of Frustration in 3D on Tetrahedra





Cubic Pyrochlore Lattice

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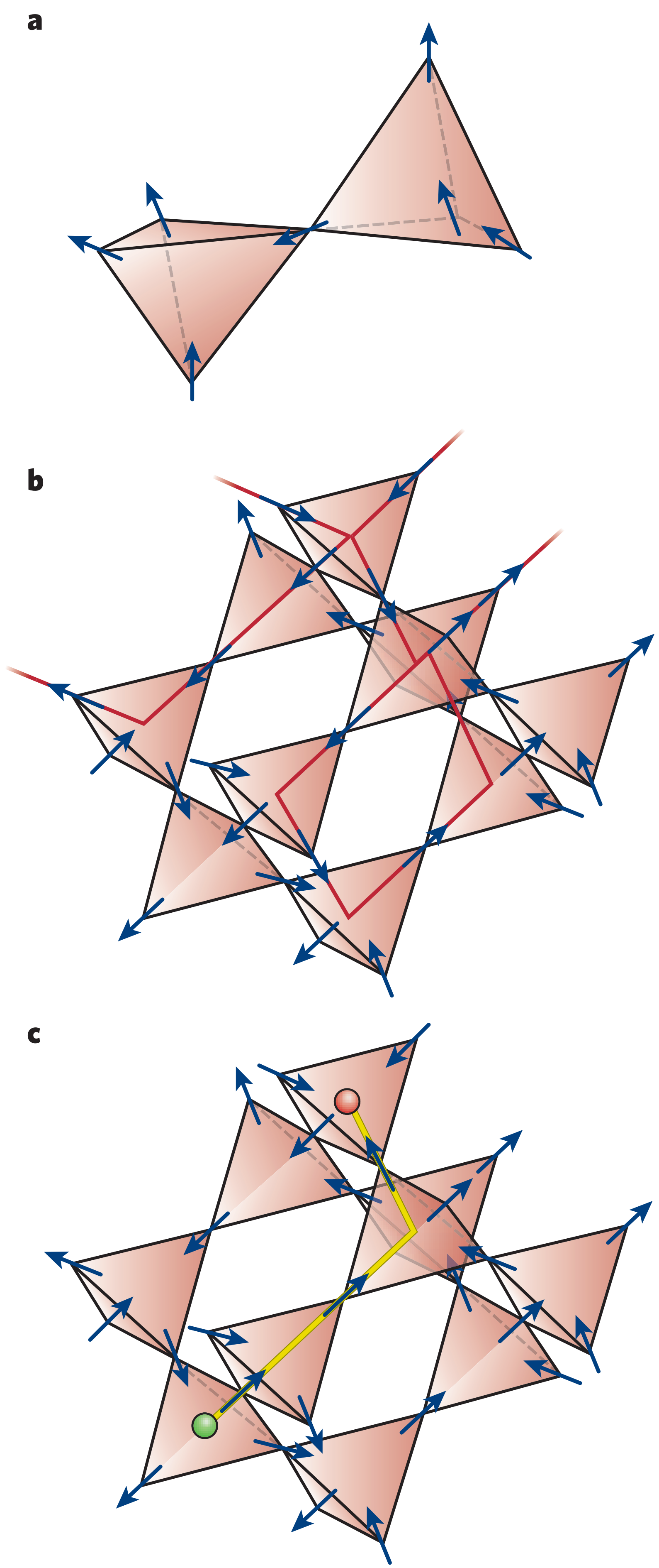
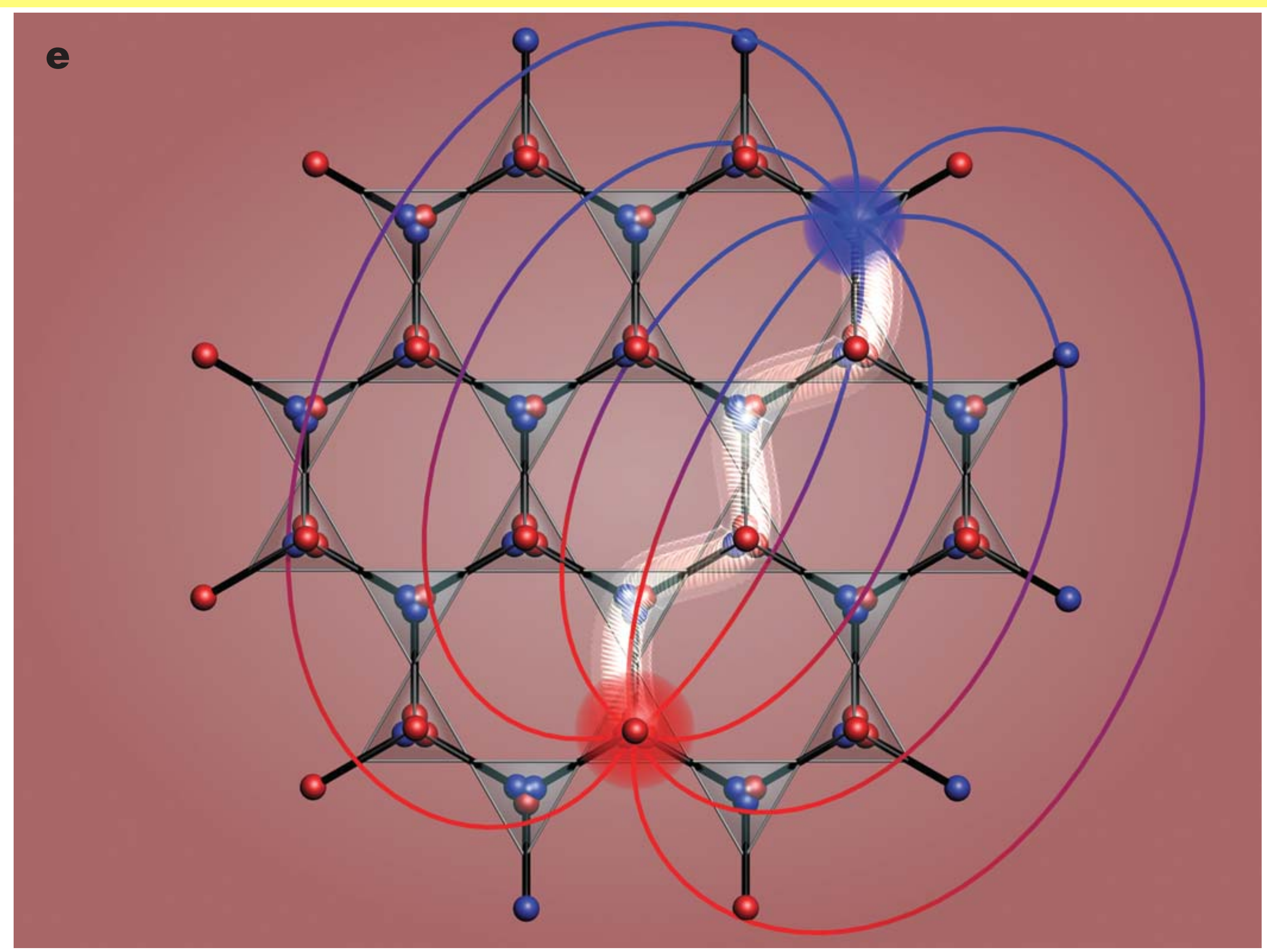
M.J. Harris, S.T. Bramwell, D.F. McMorrow, T. Zeiske, and K.W. Godfrey, PRL 79 2554 (1997)



Spin Ice

- **Classical macroscopic degeneracy**
- **Supports monopole excitations**
- **Rare example of deconfined excitations in 3D**



C. Castelnovo, R. Moessner, and S.L. Sondi, Nature, 451, 43 (2007)
L. Balents, Nature, 464, 199 (2010)

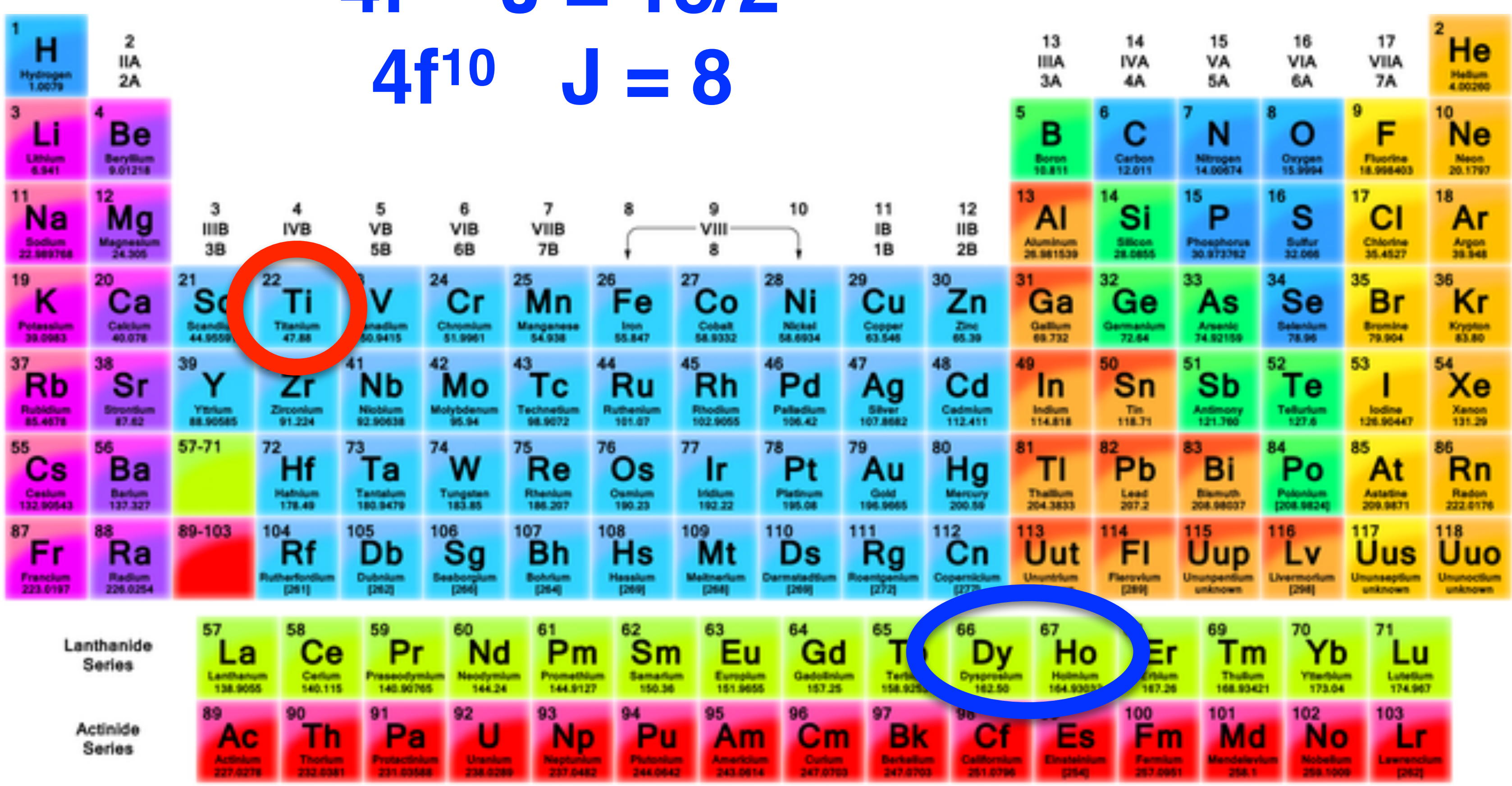
Pyrochlores have the quintessential lattice for the phenomena of magnetic frustration in 3D.

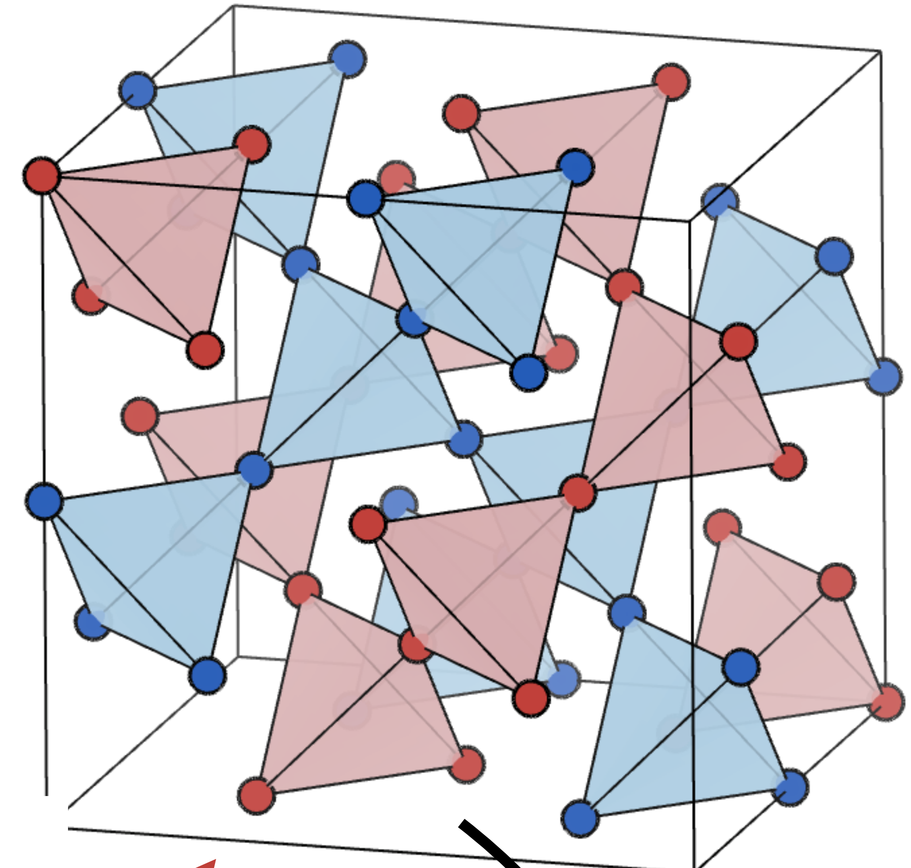
$(Dy^{3+})_2(Ti^{4+})_2O_7$

$(Ho^{3+})_2(Ti^{4+})_2O_7$

$4f^9$ $J = 15/2$

$4f^{10}$ $J = 8$





…

….

"disorder-free" spin glass

classical spin ice

quantum spin ice

metal-insulator transitions

spin liquid

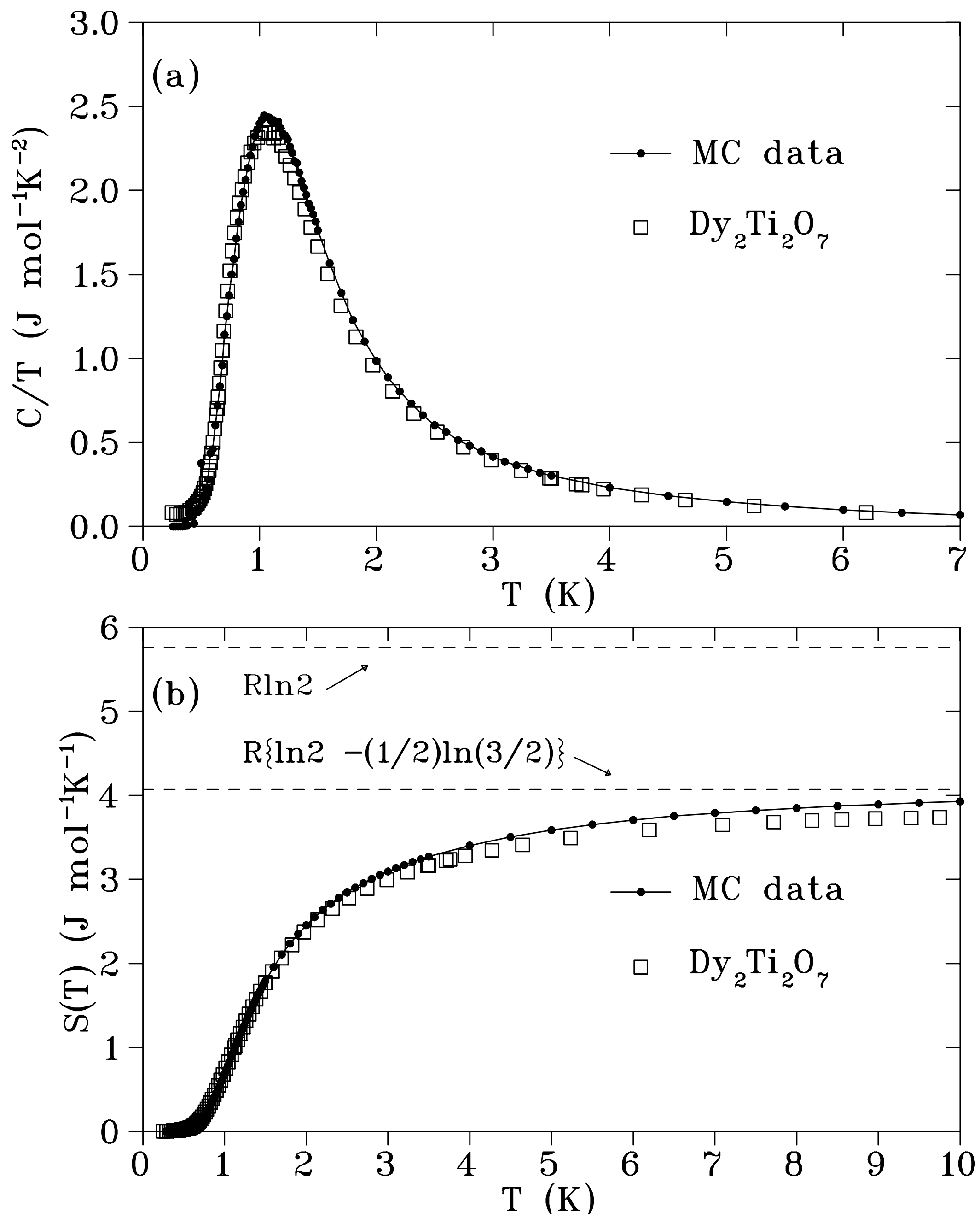
order-by-disorder

moment fragmentation

Gardner, Gingras, and Greedan, Rev. Mod. Phys **82**, 53 (2010)

Hallas, Gaudet, and Gaulin, ARCMP, **9**, 105 (2018)

Missing Pauling entropy is a defining characteristic of classical spin ice



Minimal dipolar spin ice Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i^{z_i} \cdot \mathbf{S}_j^{z_j} + D r_{nn}^3 \sum_{i>j} \frac{\mathbf{S}_i^{z_i} \cdot \mathbf{S}_j^{z_j}}{|\mathbf{r}_{ij}|^3} - \frac{3(\mathbf{S}_i^{z_i} \cdot \mathbf{r}_{ij})(\mathbf{S}_j^{z_j} \cdot \mathbf{r}_{ij})}{|\mathbf{r}_{ij}|^5}$$

R = 8.314 J K^{-1} $mole^{-1}$
2 states/Dy^{3+} ion
S = R ln (2)

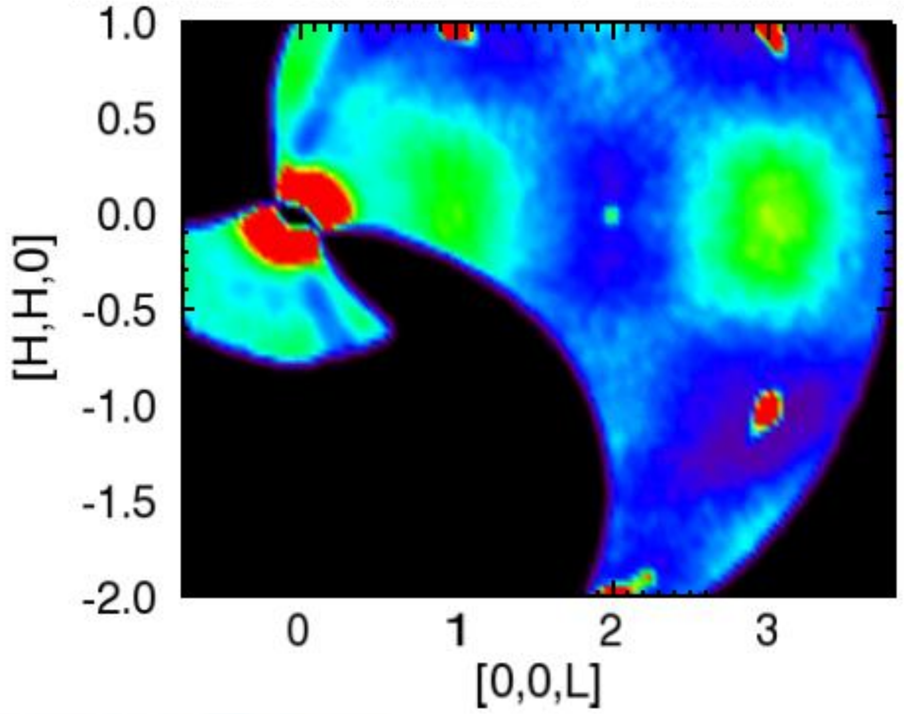
$$S(T) = \int^{T} Cp/T \, dT$$

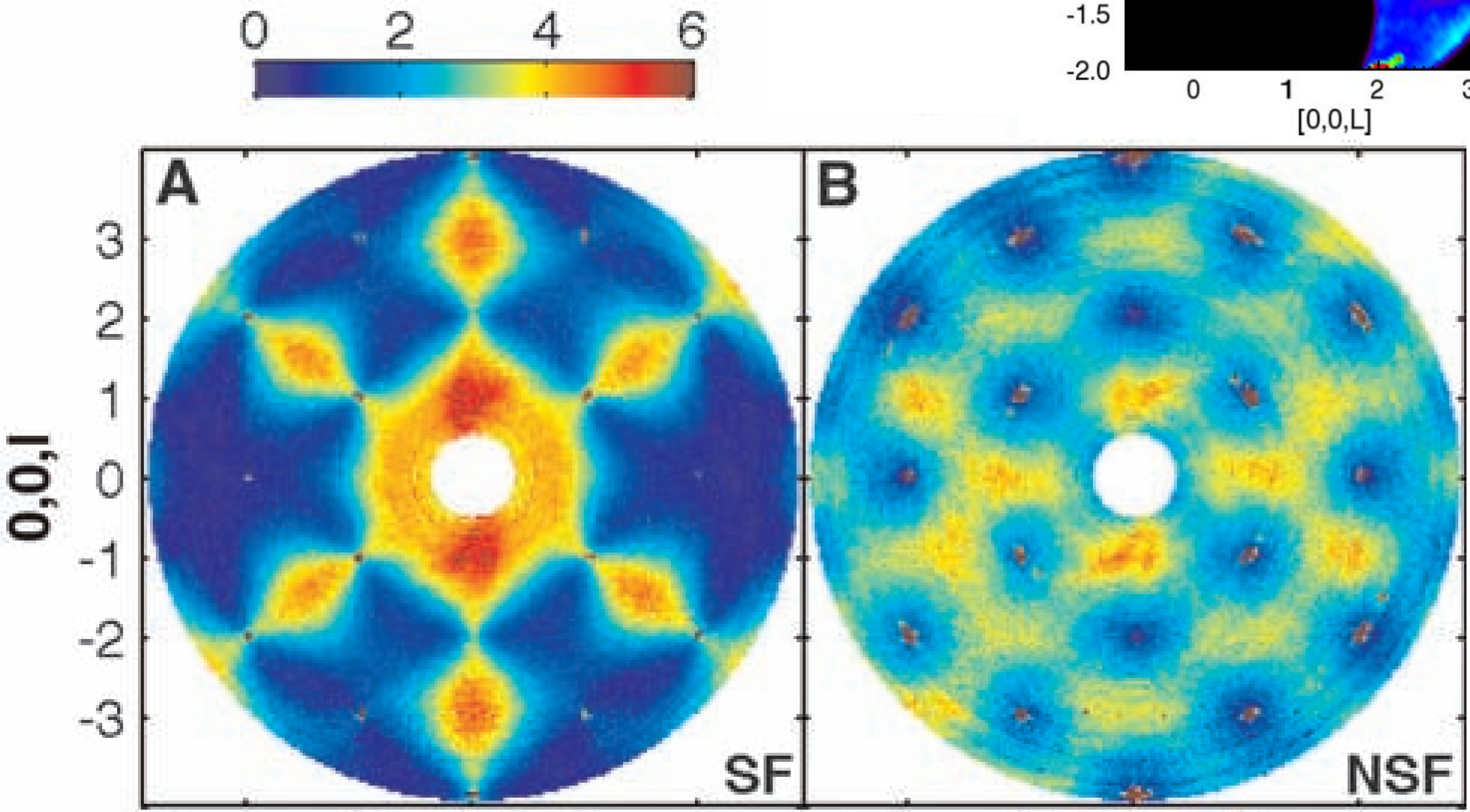
lower bound

A. P. Ramirez, A. Hayashi, R. J. Cava, R. Siddharthan, Nature 399, 333 (1999)
B. C. den Hertog, M. J. P. Gingras, Phys. Rev. Lett. 84, 3430 (2000)

Spin Ice Ground State in $Ho_2Ti_2O_7$

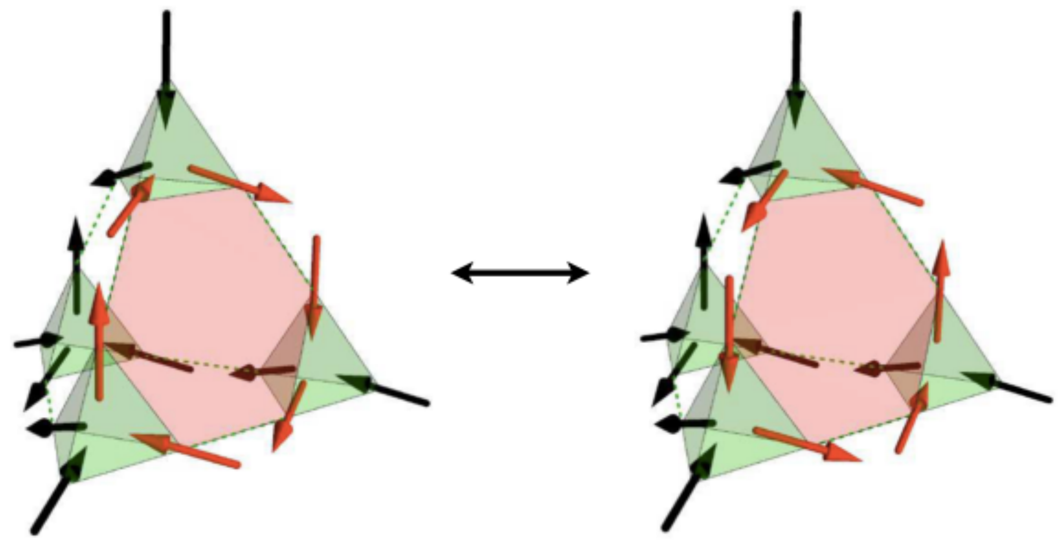
J. P. Clancy, et al.,
Phys. Rev. B 79, 014408 (2009)



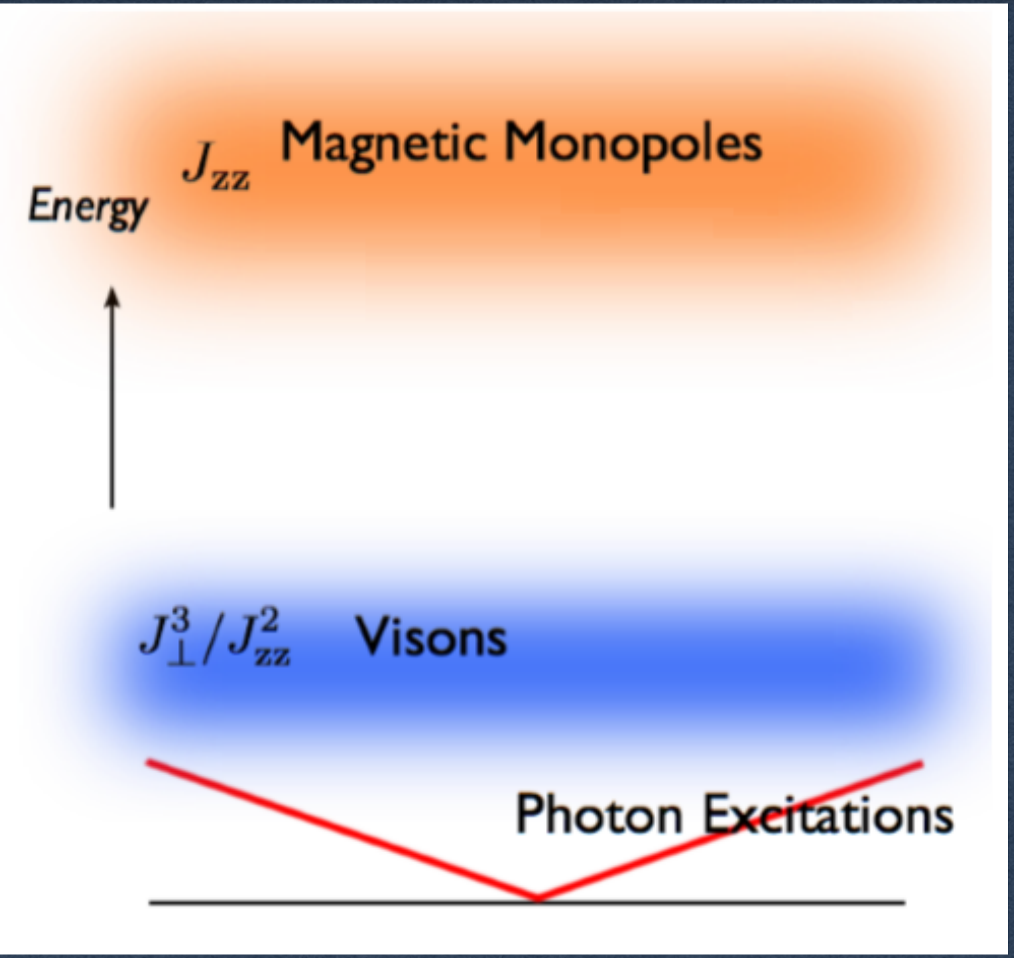


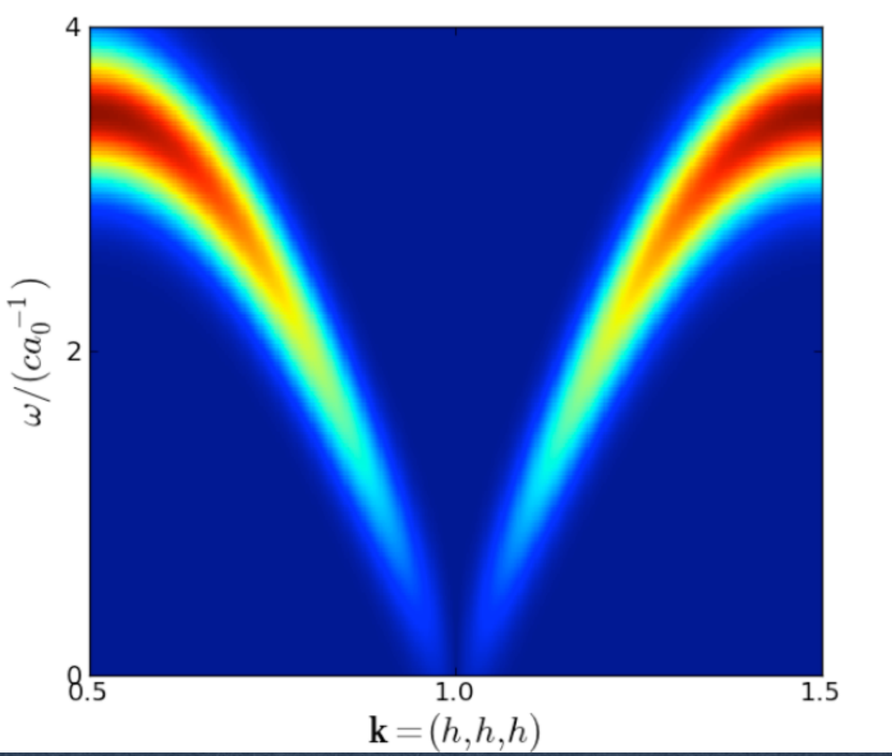
T. Fennell et al., Science, 326 (5951): 415-417 (2009)

Quantum Spin Ice: A U(1) Quantum Spin Liquid



$$\mathcal{H}_{\mathrm{U(1)}} = \frac{\mathcal{U}}{2} \sum_{\langle \mathbf{rr'} \rangle} [(\nabla_{\bigcirc} \times \mathcal{A})_{\mathbf{rr'}}]^2 + \frac{\mathcal{K}}{2} \sum_{\langle \mathbf{ss'} \rangle} \mathcal{E}^2_{\mathbf{ss'}}$$





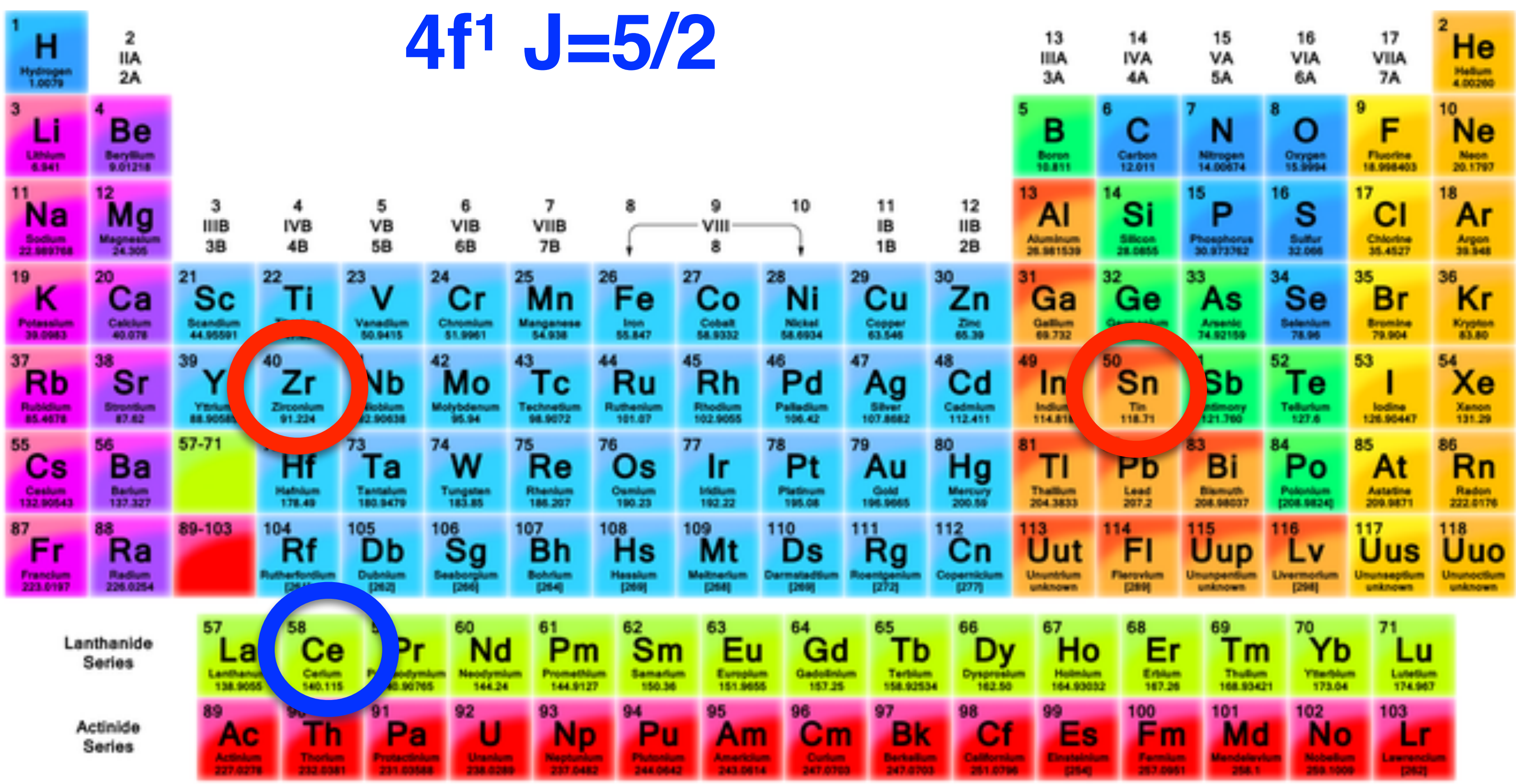
- **QSI possesses an emergent QED**
- **Can tunnel between ice rules states**
- **Introduces *fluctuations* in the gauge field**

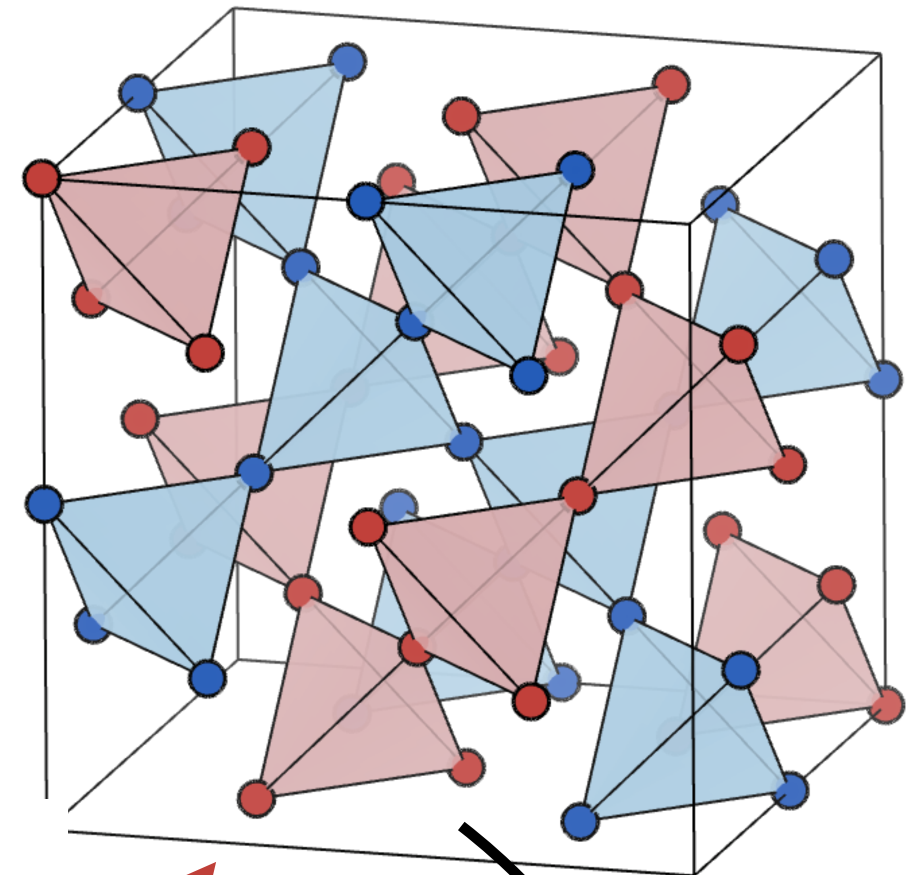
Hermele et al, PRB 69, 064404 (2004)
Banerjee et al, PRL, 100, 047208 (2008)
Shannon et al, PRL 100, 047201 (2012)
Benton et al, PRB 86, 075154 (2012)
Gingras and McClarty, RPP,77, 056501 (2014).

Pyrochlores have the quintessential lattice for the phenomena of magnetic frustration in 3D.

$(Ce^{3+})_2(Zr^{4+})_2O_7$
$(Ce^{3+})_2(Sn^{4+})_2O_7$

$4f^1$ J=5/2

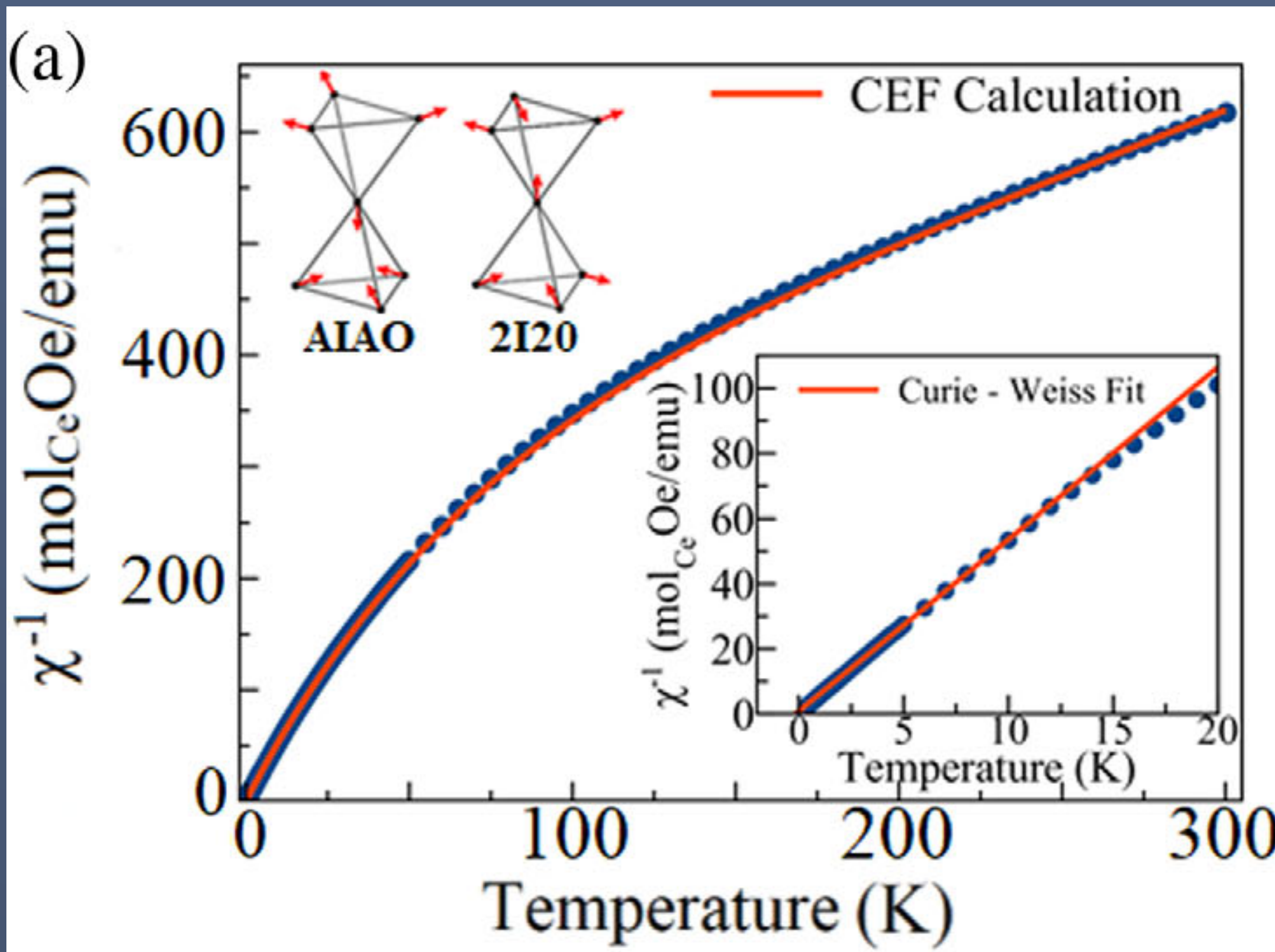




...
....
"disorder-free" spin glass
classical spin ice
quantum spin ice
metal-insulator transitions
spin liquid
order-by-disorder
moment fragmentation

Gardner, Gingras, and Greedan, Rev. Mod. Phys **82**, 53 (2010)
Hallas, Gaudet, and Gaulin, ARCMP, **9**, 105 (2018)

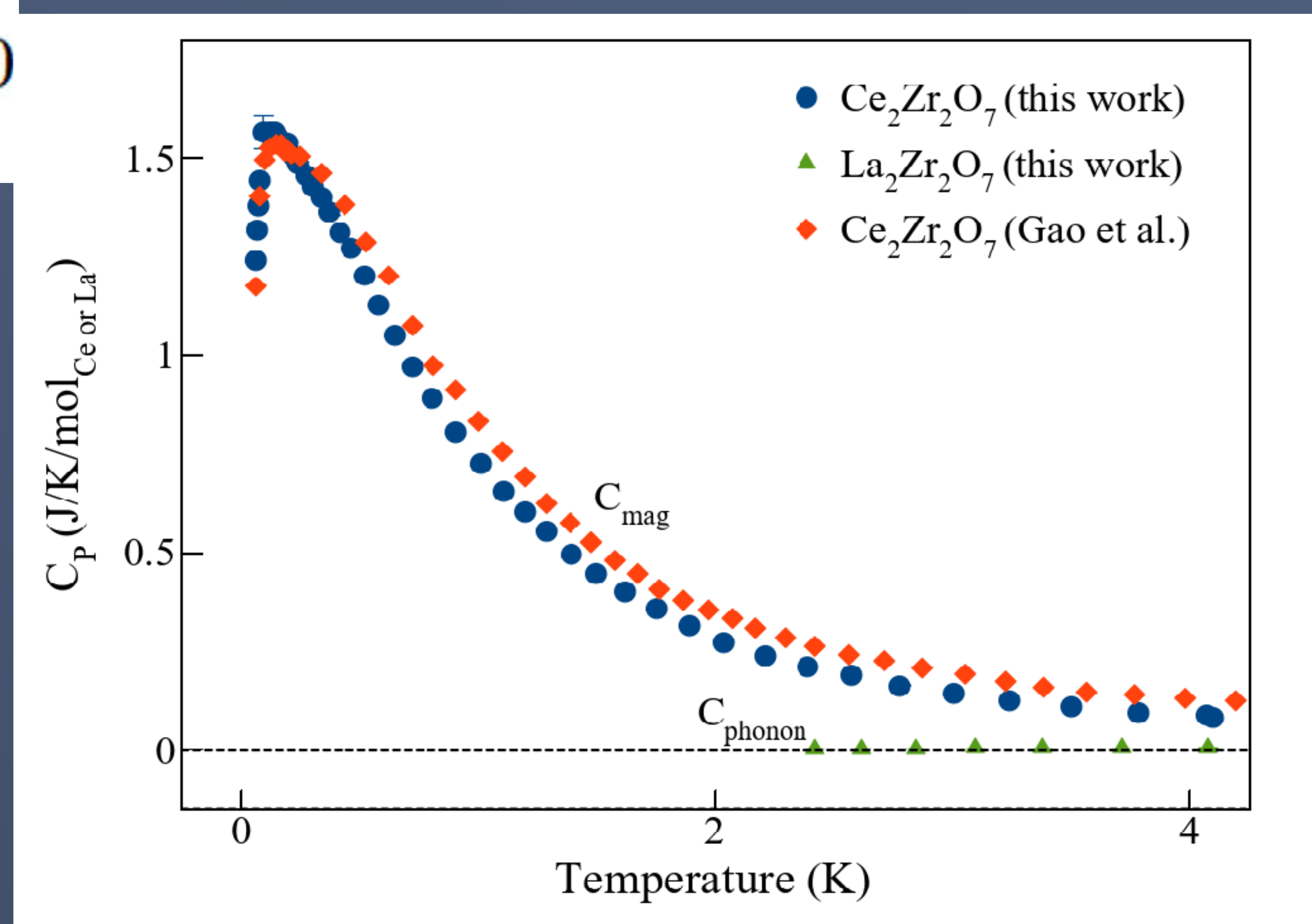
$Ce_2Zr_2O_7$: No obvious phase transition for T > 0.06 K



$$\chi_{CEF} = \frac{N_A g_J^2 \mu_B^2 X}{k_B Z} \sum_\alpha \left(\sum_n \frac{|\langle n|J_\alpha|n\rangle|^2 e^{-E_n/T}}{T} + \sum_n \sum_{m \neq n} \frac{|\langle m|J_\alpha|n\rangle|^2 (e^{-E_n/T} - e^{-E_m/T})}{E_m - E_n} \right)$$

$$\Theta_{CW} \sim -0.4\ K$$

$$\mu_p = 1.3(1) \mu_B$$



J. Gaudet et al, PRL 122, 187201 (2019)
B. Gao et al, Nat. Physics, 15, 1052 (2019)

Rare Earth-based Insulators often display A separation of Energy Scales: SOC >> CEF >> Exchange

SOC

100s of meV

$4f^1$ J = 7/2

~ 250 meV

$4f^1$ J =5/2

$Ce_2Zr_2O_7$

CEF

10s of meV

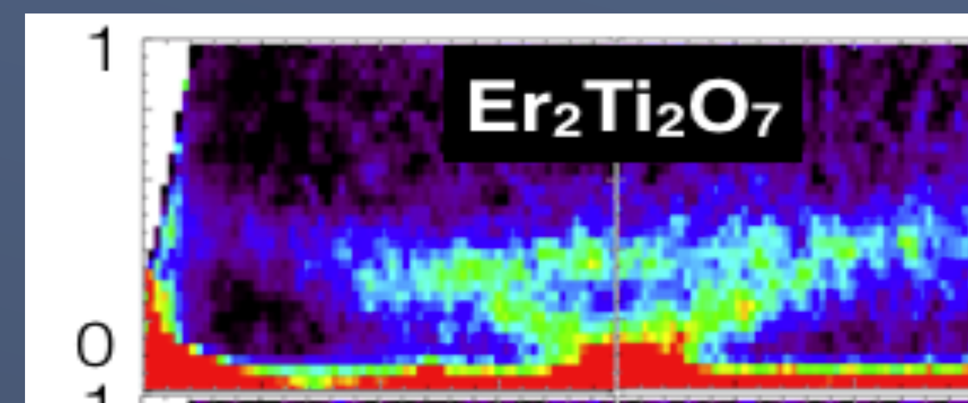
110 meV

55 meV

~ 600 K

Exchange interactions

~ 1meV or less



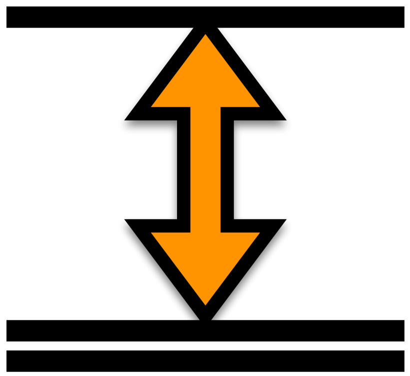
spin waves,

phase transitions

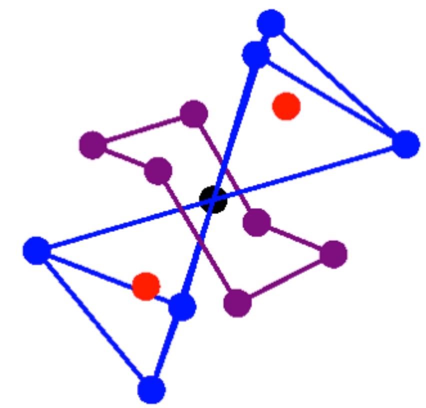
etc

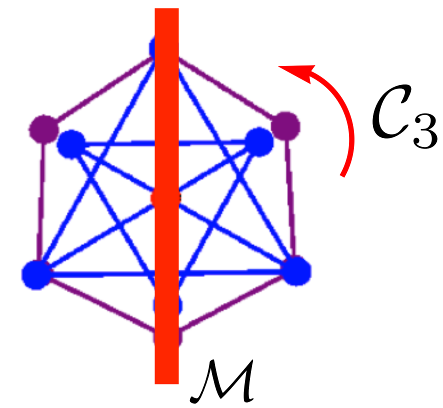
Different Types of CEF Ground State Doublets

Define pseudospin-1/2 operator acting within states of CEF doublet



S_i^x, S_i^y, S_i^z

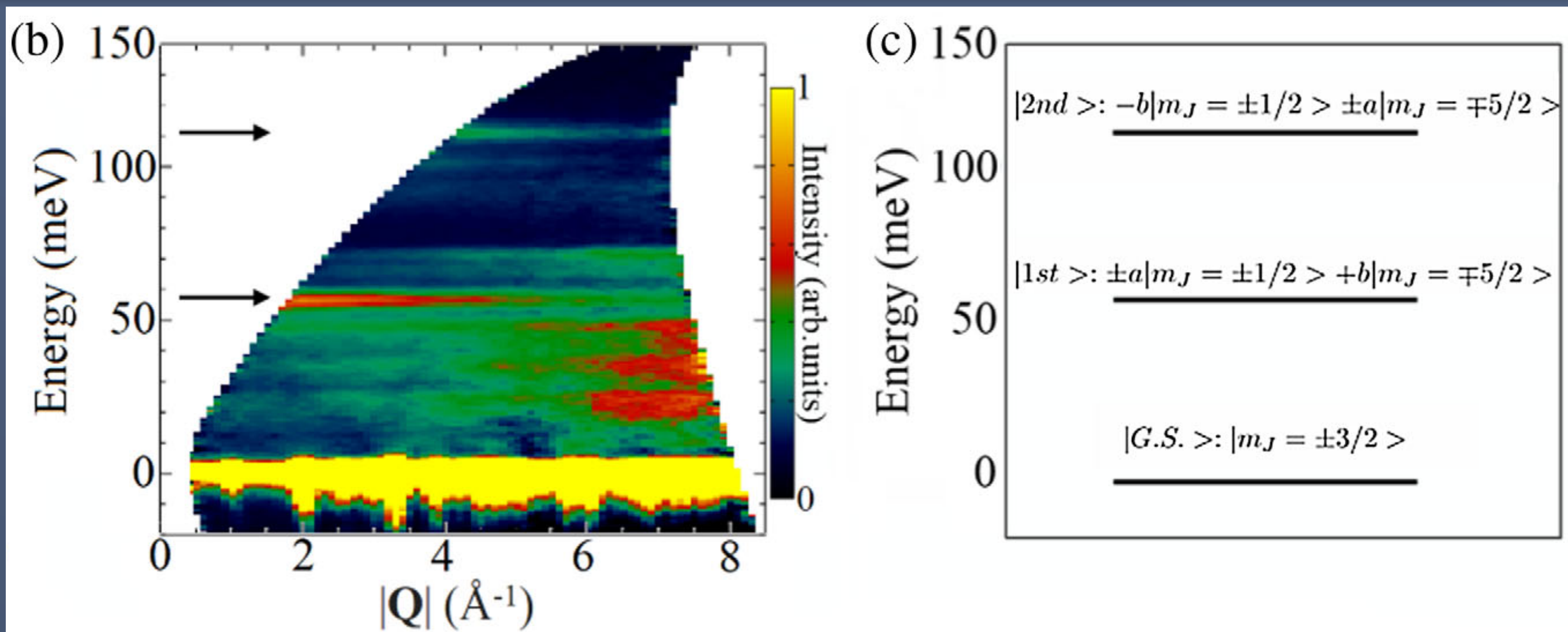




Behavior of this operator under time reversal and local D_{3d} symmetry divides $R_2M_2O_7$ pyrochlores into three groups

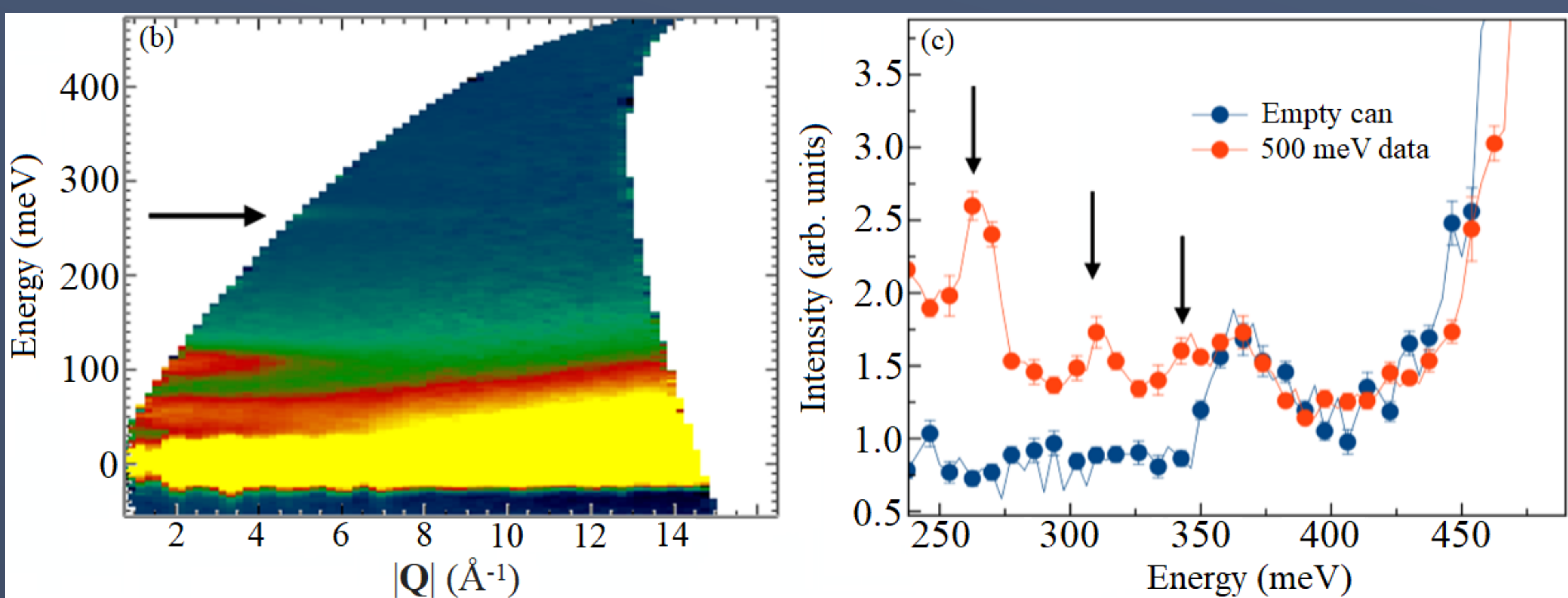
	# of f electrons	Symmetry of ground state doublet
Dy, Yb, Er	Odd: Kramer's (dipolar)	S^z, S^x, S^y transform like dipoles
Ce, Sm, Nd	Odd: Kramer's (dipole-octupole)	S^z, S^x transform like dipoles S^y transforms like an octupole
Ho, Tb, Pr	Even: non-Kramers	S^z transforms like dipoles S^x, S^y tranform like quadrupoles

High Energy Physics: CEF excitations and Dipole-Octupole Ground State in $Ce_2Zr_2O_7$



Moment in the GS doublet is small

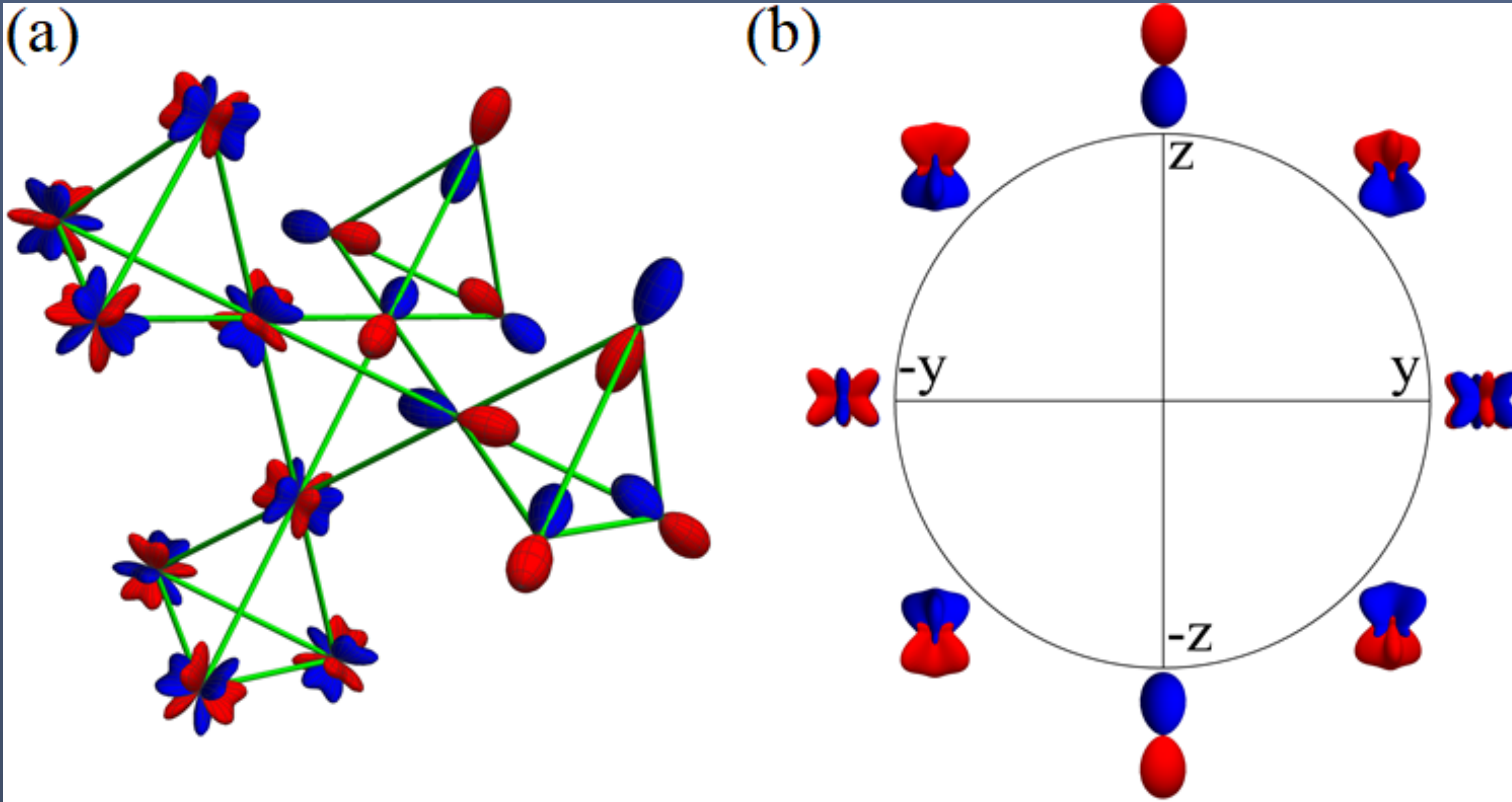
$$\mu_{GS} = 1.286\,\mu_B$$



J=7/2 excited state multiplet is ~ 200 meV above the J=5/2 GS, as expected

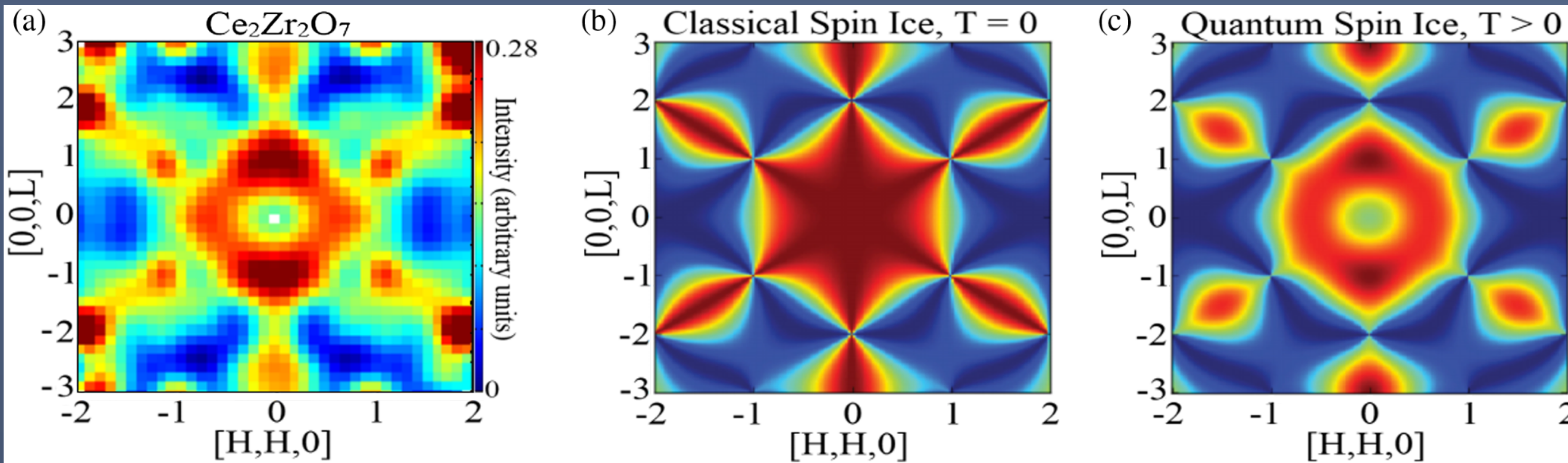
J. Gaudet et al, PRL 122, 187201 (2019)

Two components of S_{eff}=1/2 for Ce^{3+} in $Ce_2Zr_2O_7$ transform as Dipoles; One component transforms as an Octupole

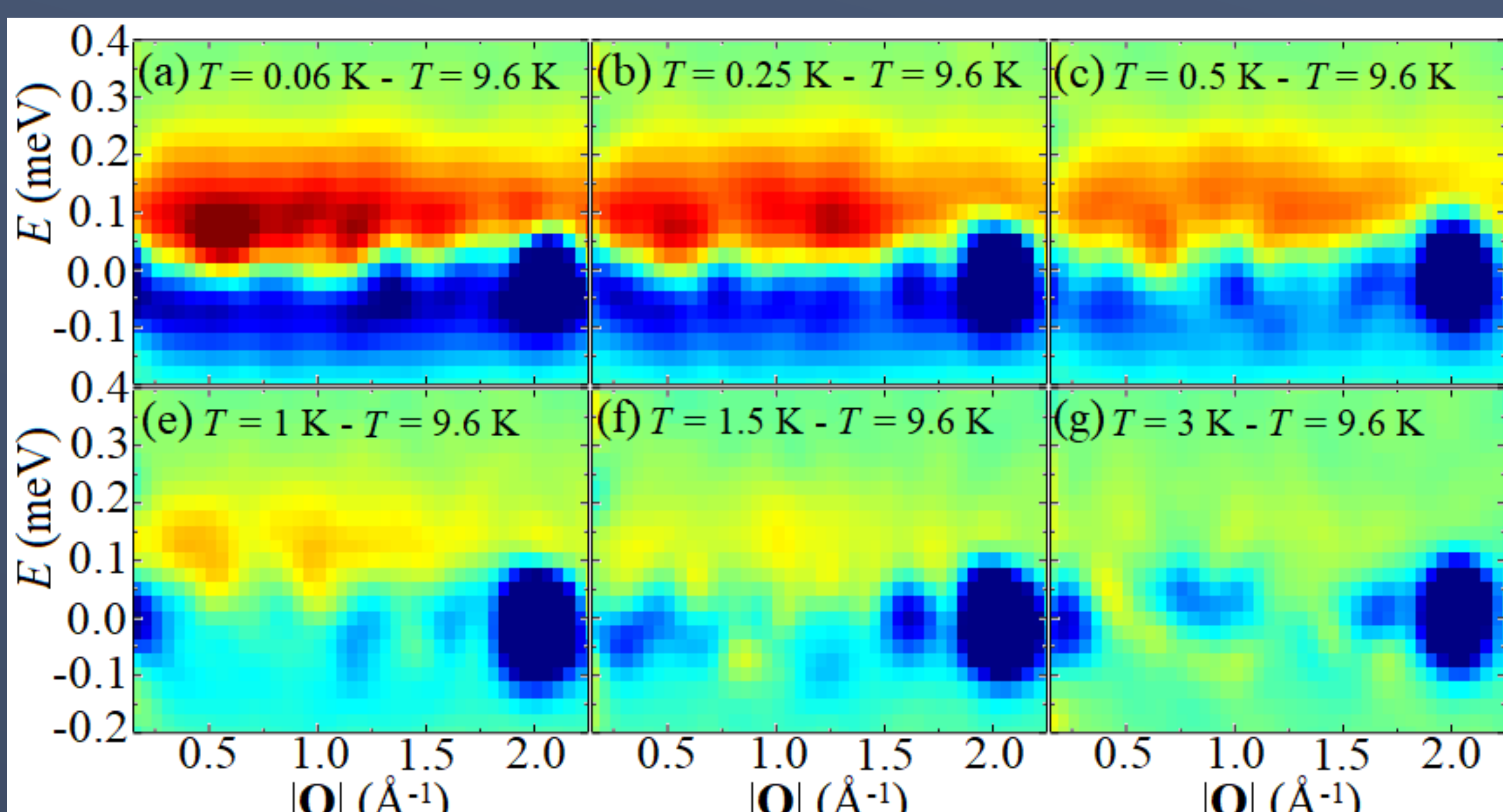


Smith et al, PRX 12, 021015 (2022)

Low energy neutron scattering from $Ce_2Zr_2O_7$



T=0.06 K - T=2 K **Classical spin ice** **Quantum spin ice**

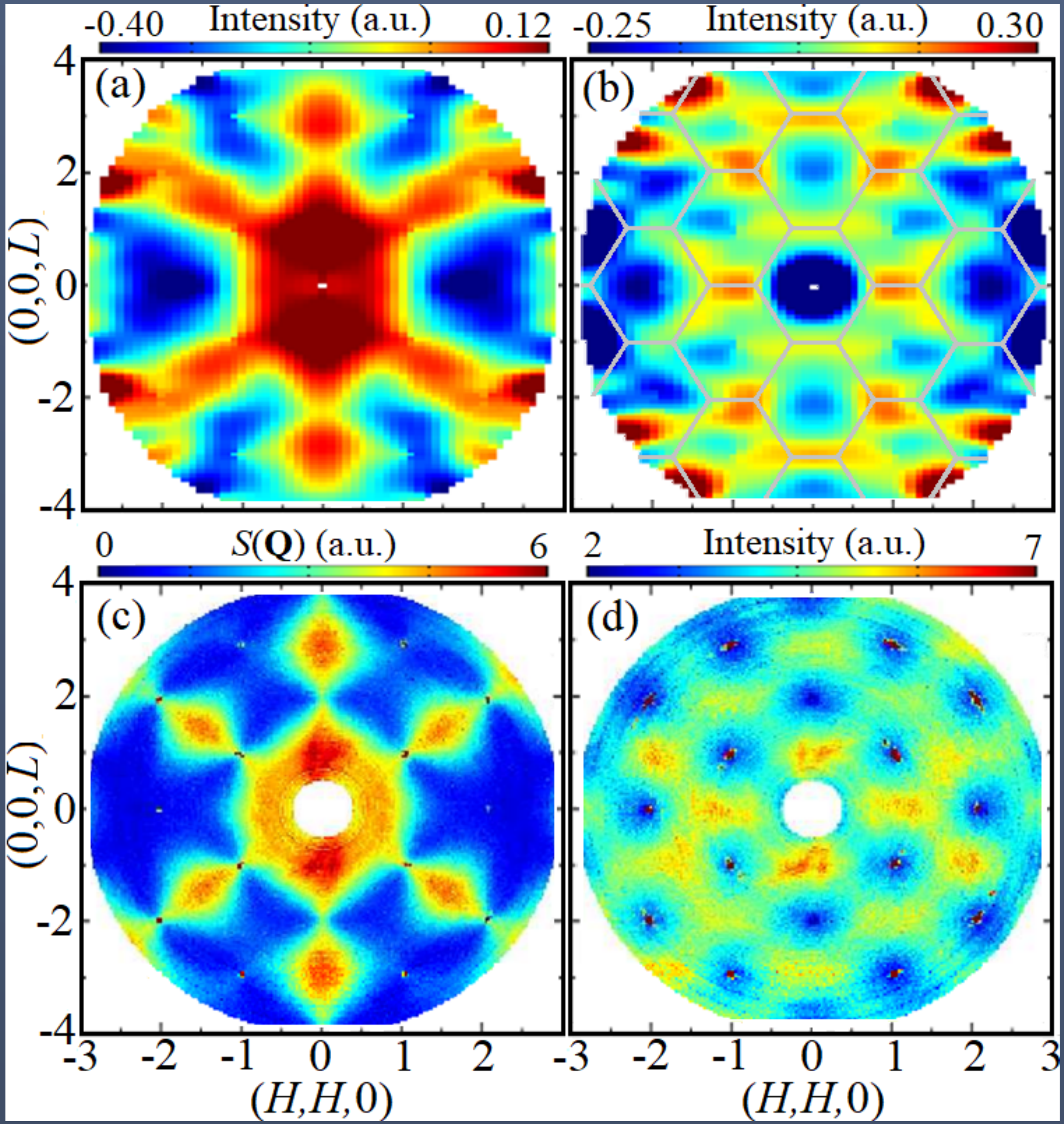


Inelastic scattering shows no static moment at any T > 0.06 K

J. Gaudet et al, PRL 122, 187201 (2019)

Polarized diffraction from single crystal $Ce_2Zr_2O_7$ resembles classical spin ice $Ho_2Ti_2O_7$

Spin Flip **Non-Spin Flip**



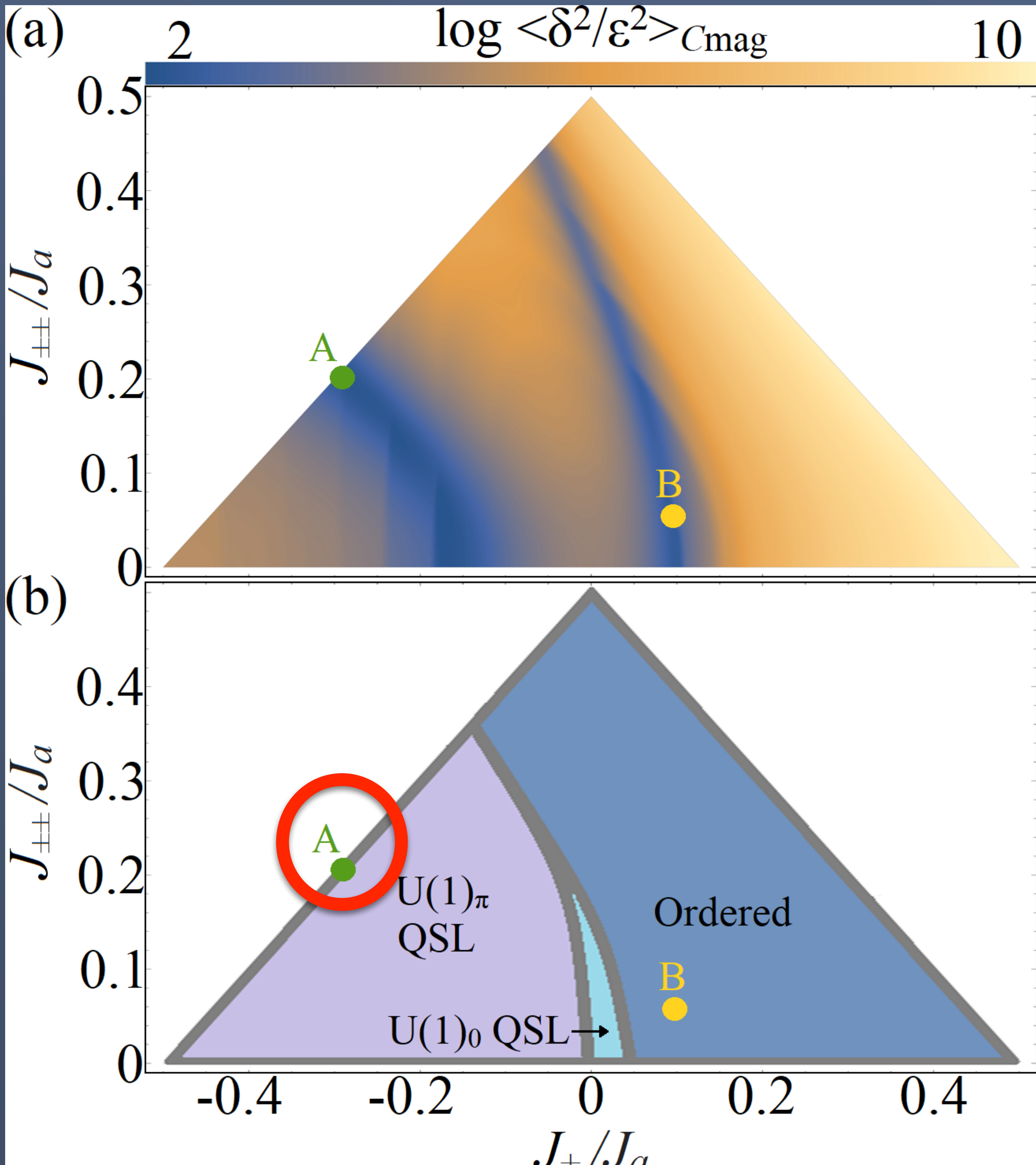
$Ce_2Zr_2O_7$

Quantum Spin Ice/Liquid
Smith et al,
PRX 12, 021015 (2022)

$Ho_2Ti_2O_7$

Classical Spin Ice
Fennel et al,
Science, 326, 415 (2009)

Heat Capacity and Neutron Scattering Place $Ce_2Zr_2O_7$ within its Generalized Hamiltonian Phase Diagram



- 4f¹ $Ce_2X_2O_7$ with X=Zr, Sn: No LRO, freezing for T>0.08 K
- Use NLC to Fit high T Cp and estimate Hamiltonian
- Strong evidence for U(1) π QSL ground state for $Ce_2Zr_2O_7$

Kitaev Physics on a 2D Honeycomb Lattice

Available online at www.sciencedirect.com
SCIENCE DIRECT
Annals of Physics 321 (2006) 2–111
ANNALS of PHYSICS
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Anyons in an exactly solved model and beyond

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Received 21 October 2005; accepted 25 October 2005

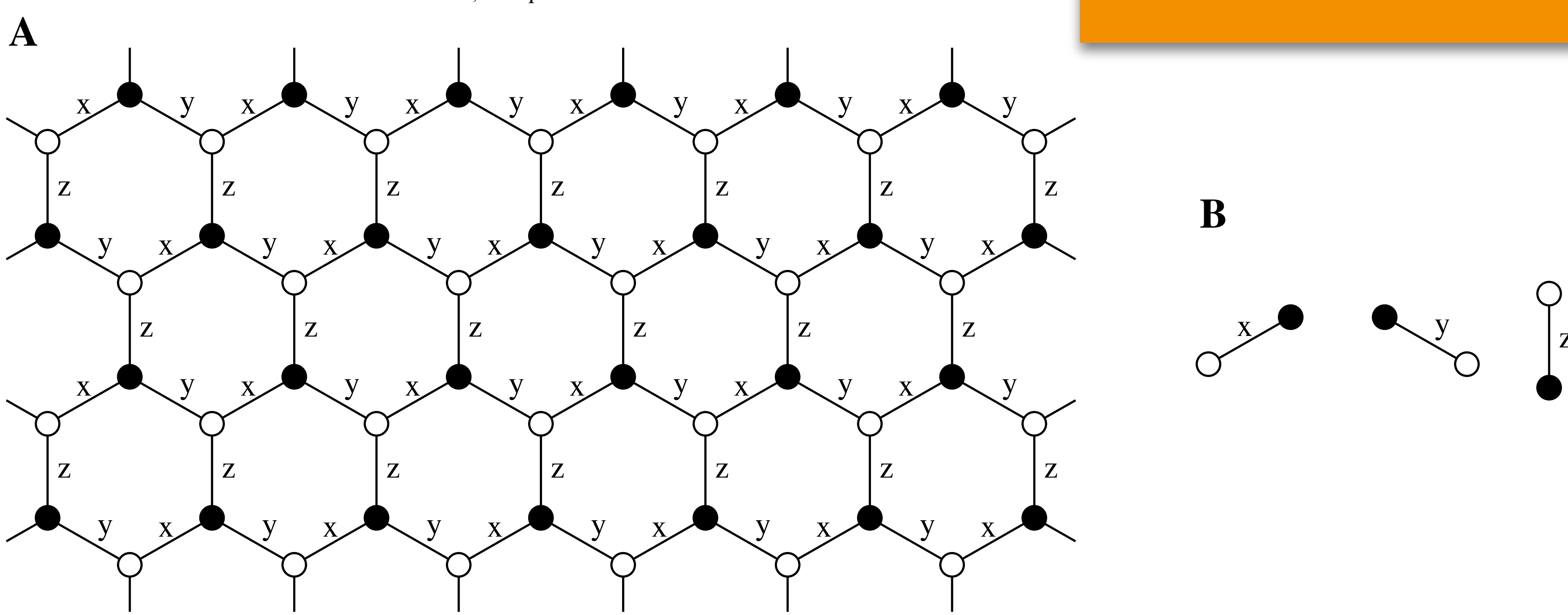
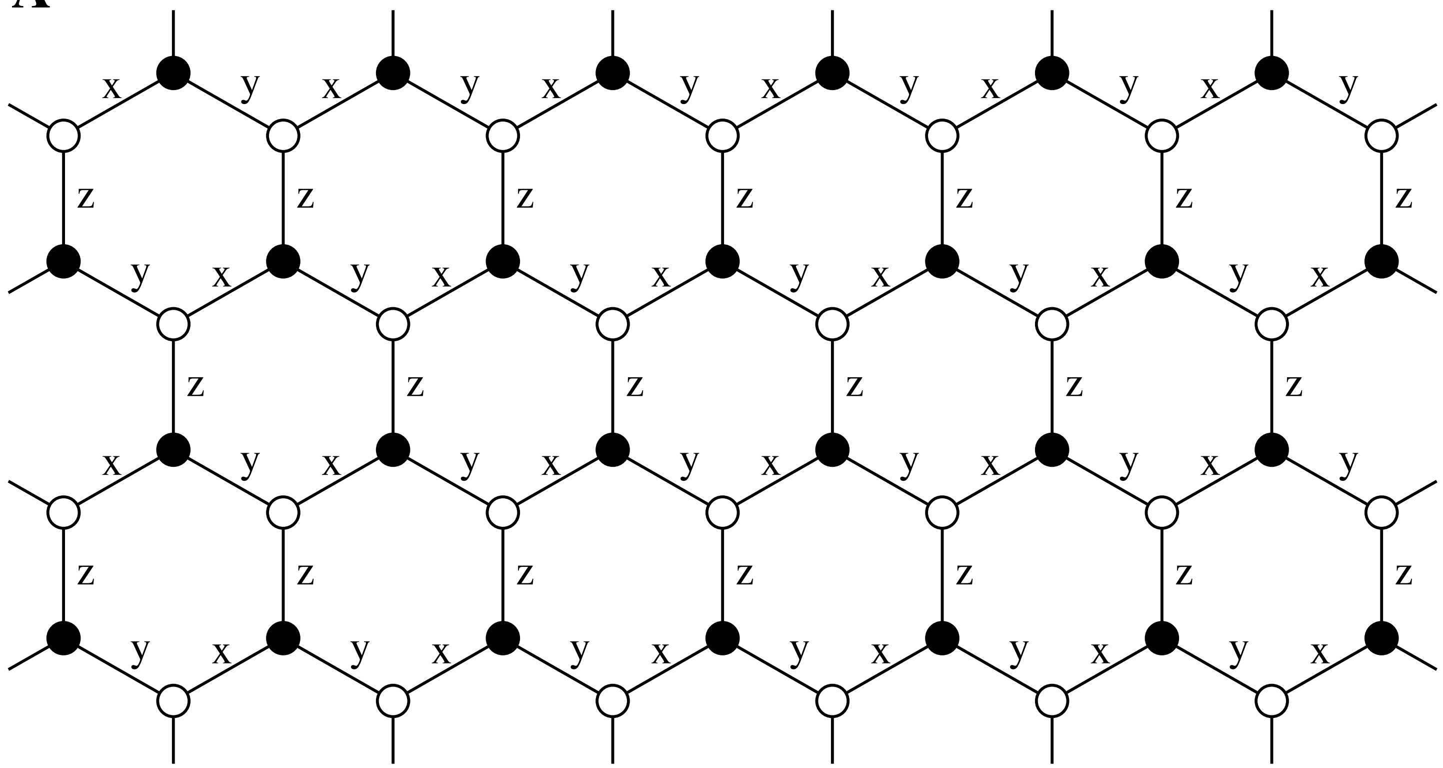


Fig. 3. Three types of links in the honeycomb lattice.

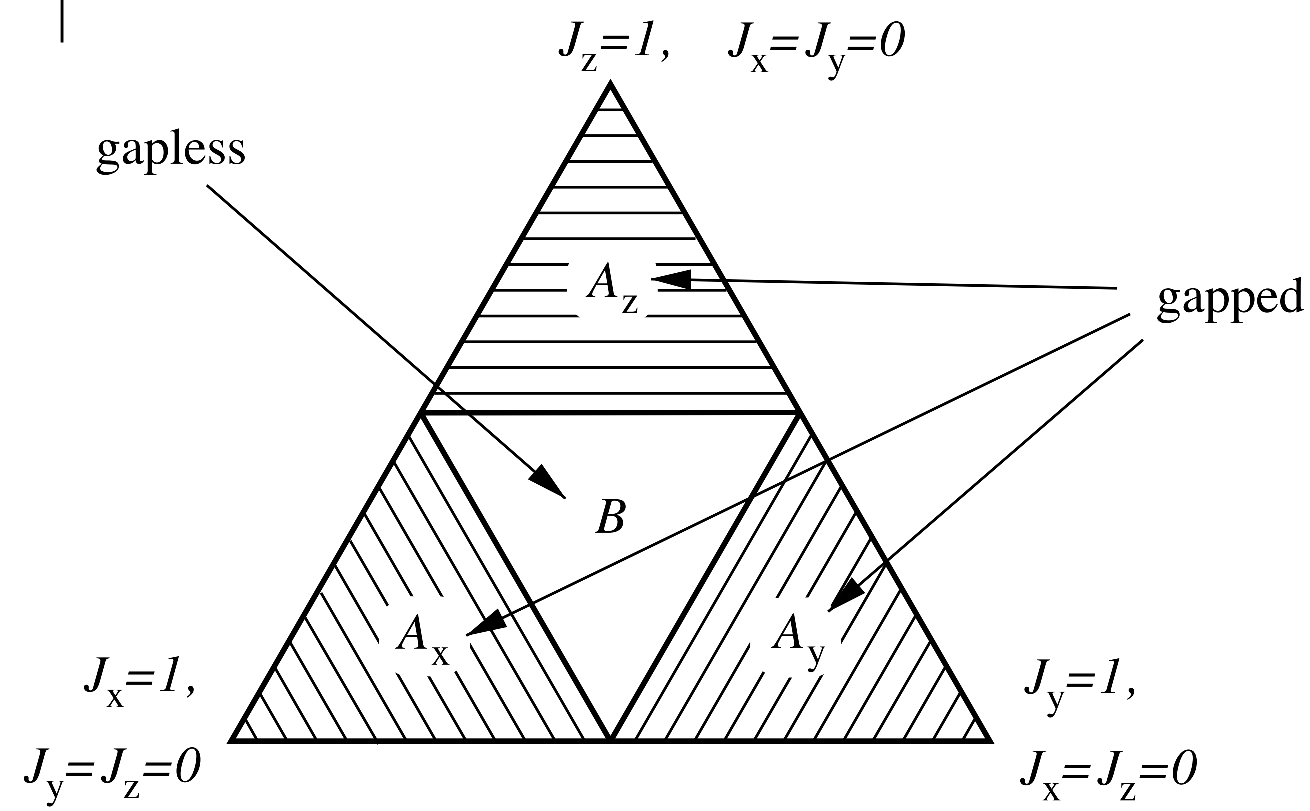
$$H = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z,$$

Kitaev Physics on a 2D Honeycomb Lattice

A



$$H = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z,$$



Kitaev Physics on a 2D Honeycomb Lattice

PRL **102,** 017205 (2009) PHYSICAL REVIEW LETTERS week ending 9 JANUARY 2009

Mott Insulators in the Strong Spin-Orbit Coupling Limit: From Heisenberg to a Quantum Compass and Kitaev Models

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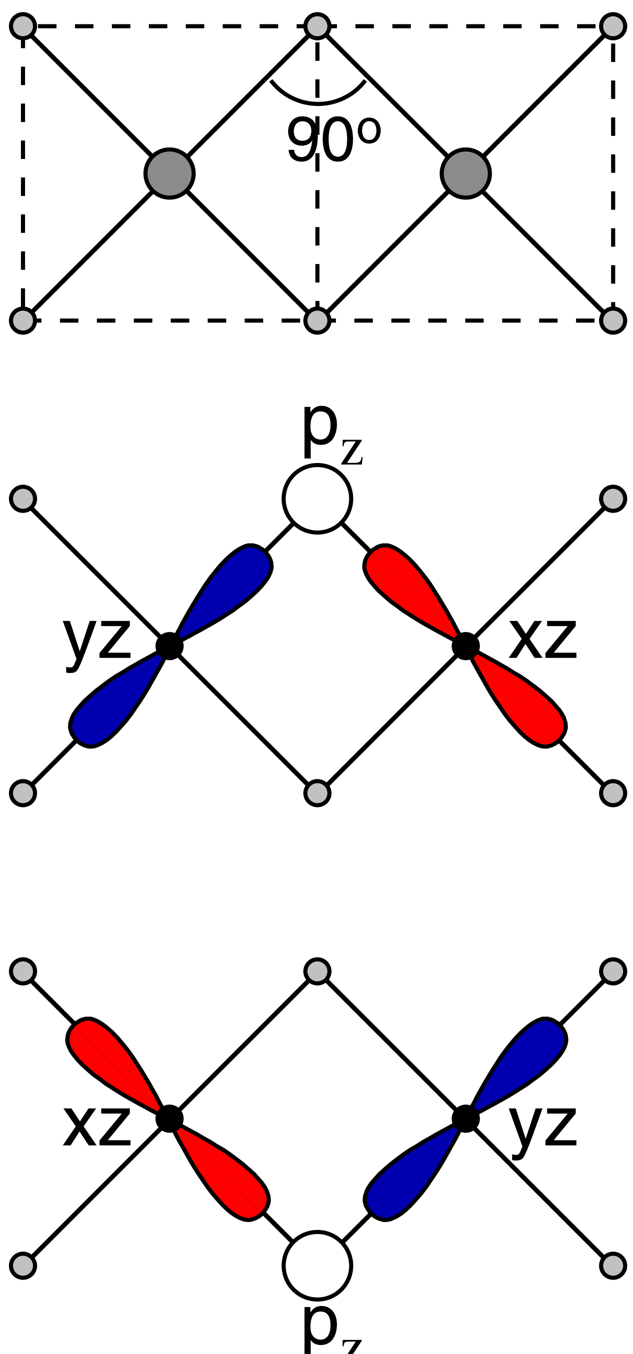
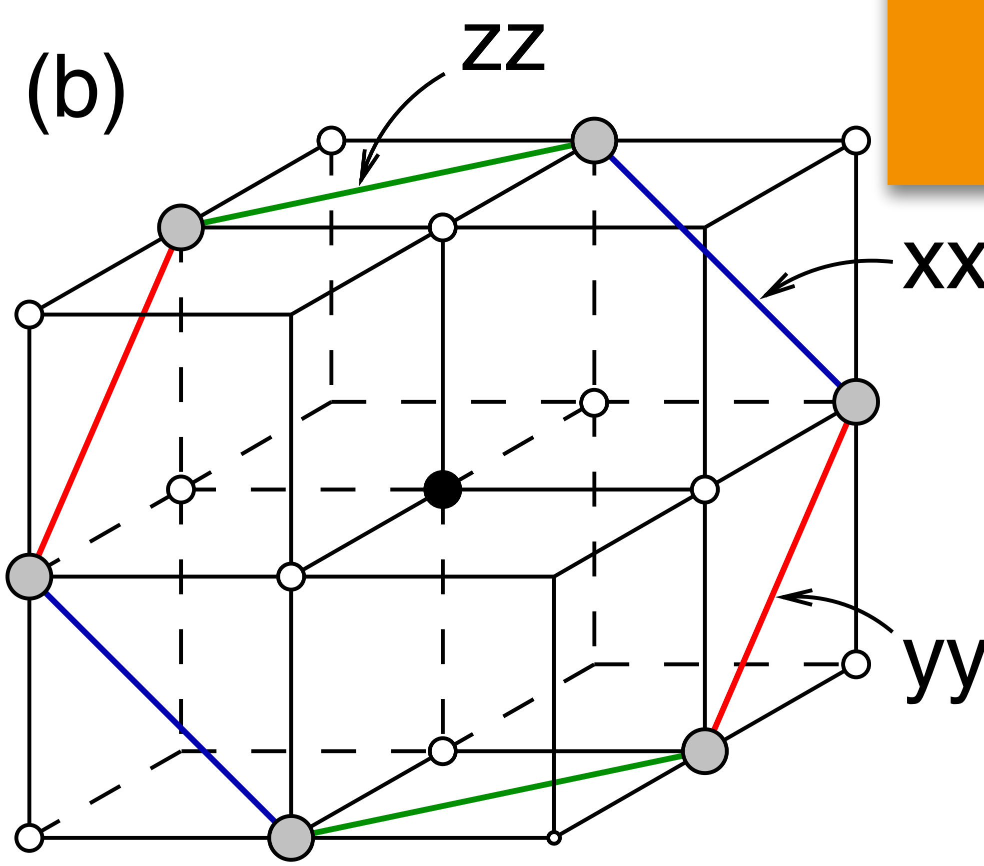
[1]*Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*

(Received 21 August 2008; published 6 January 2009)





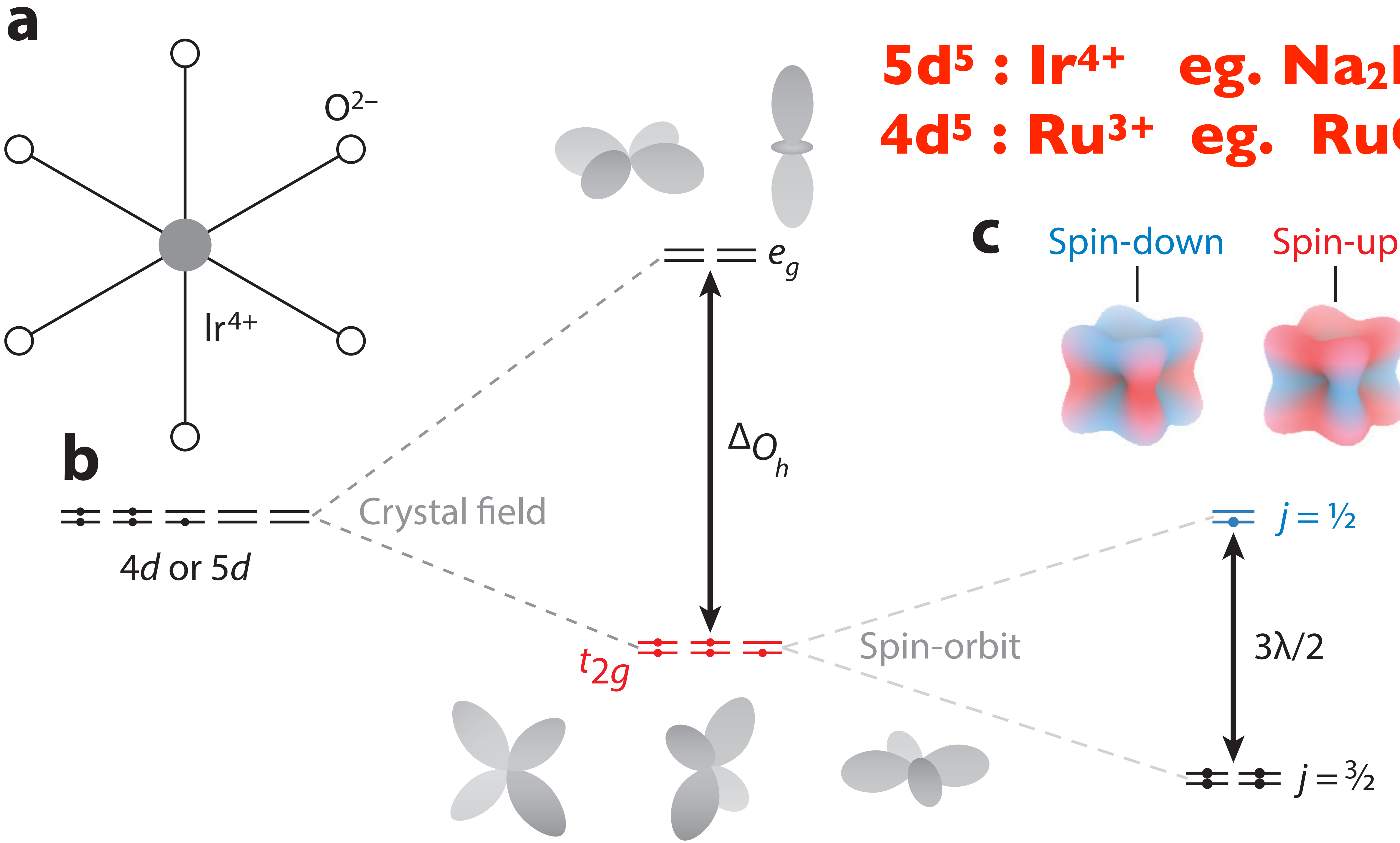
$$\mathcal{H}_{ij} = \mathbf{S}_i \cdot \mathbf{J}_{ij} \cdot \mathbf{S}_j$$

$$\mathcal{H}_{ij} = J_{ij}\,\mathbf{S}_i \cdot \mathbf{S}_j + K_{ij}\,S_i^{\gamma} S_j^{\gamma} + \Gamma_{ij}\left(S_i^{\alpha} S_j^{\beta} + S_i^{\beta} S_j^{\alpha}\right) + \Gamma'_{ij}\left(S_i^{\gamma} S_j^{\alpha} + S_i^{\gamma} S_j^{\beta} + S_i^{\alpha} S_j^{\gamma} + S_i^{\beta} S_j^{\gamma}\right)$$

Kitaev Physics on a 2D Honeycomb Lattice

5d^5 : Ir^{4+} eg. Na_2IrO_3

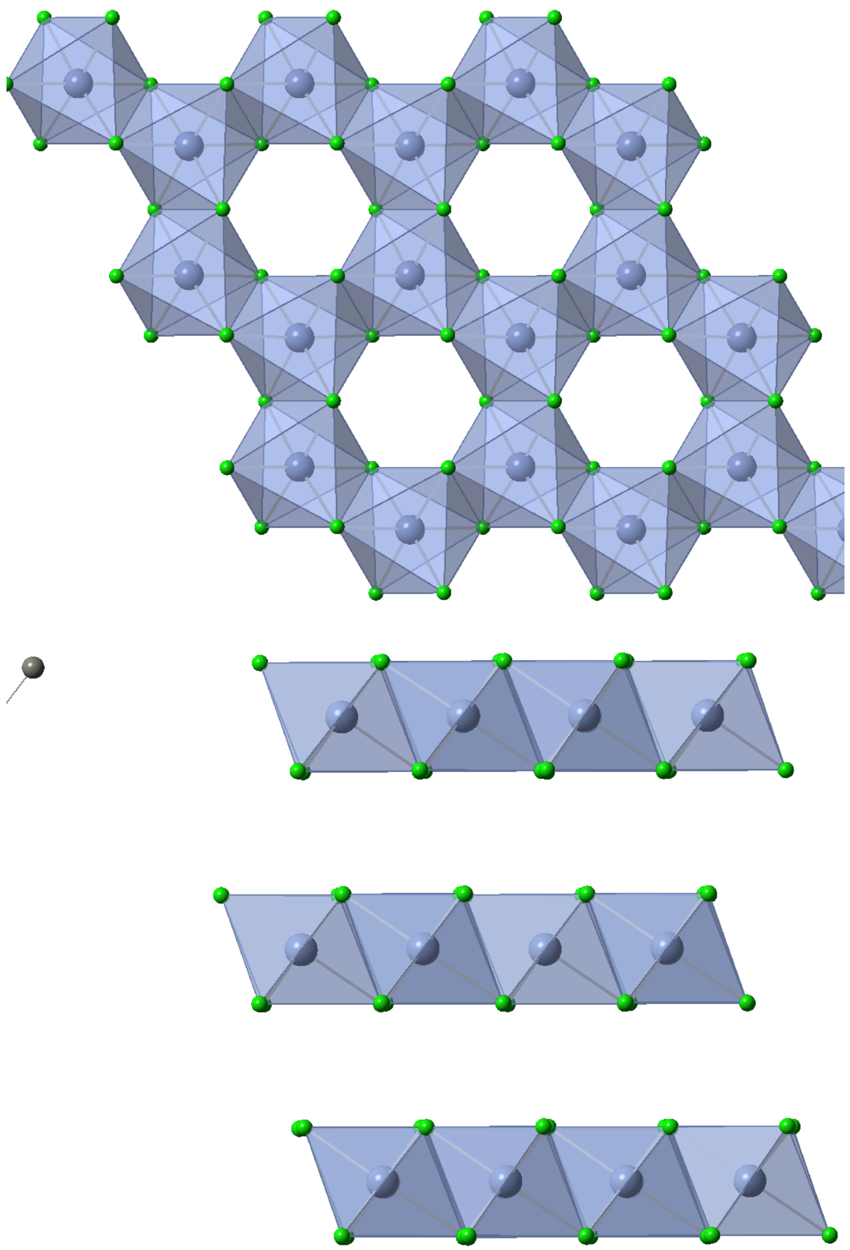
4d^5 : Ru^{3+} eg. $RuCl_3$

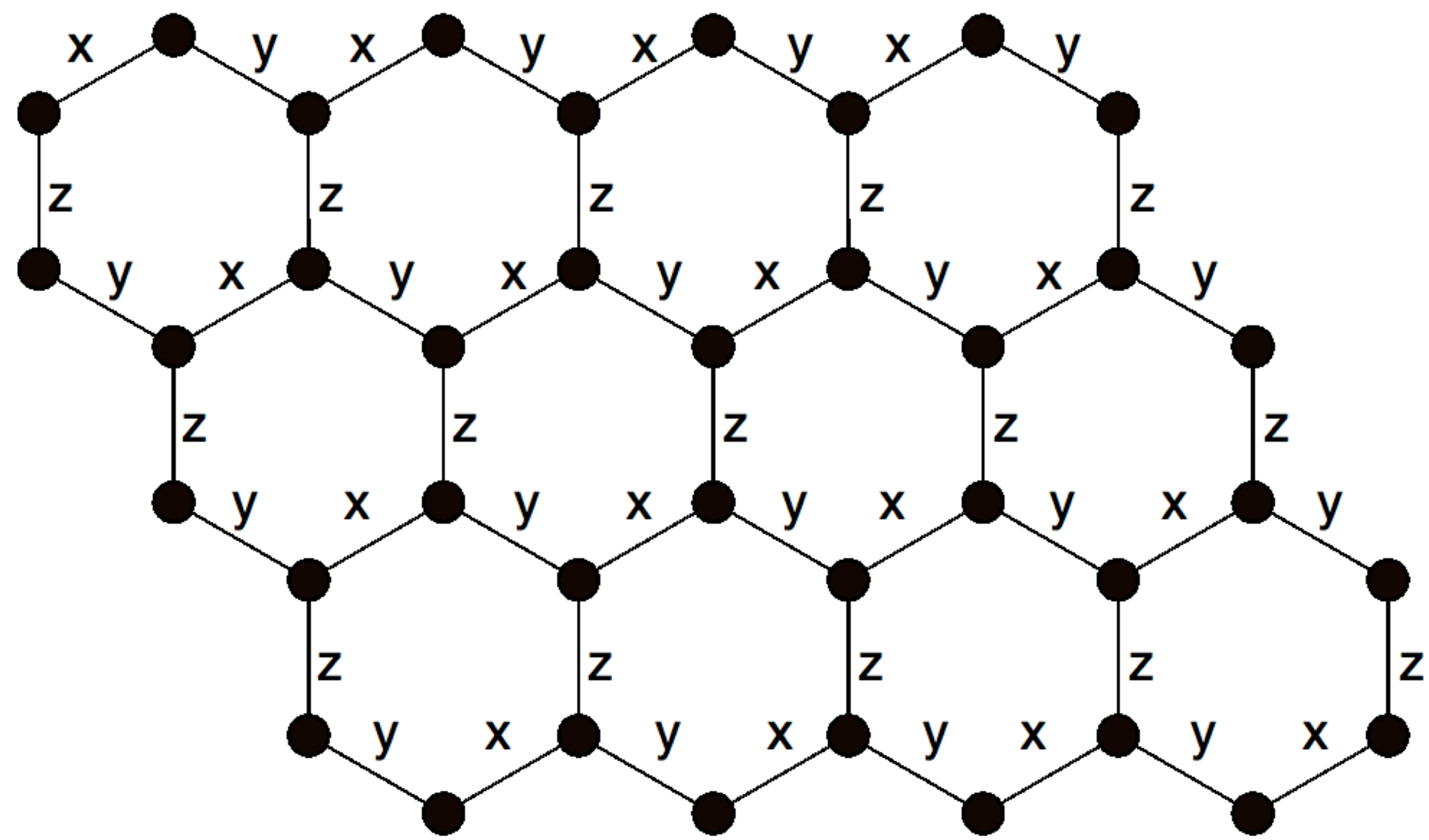


Rau et al., ARCMP 7, 195 (2016)

Kitaev Physics on a 2D Honeycomb Lattice: $RuCl_3$

(c) α-$RuCl_3$

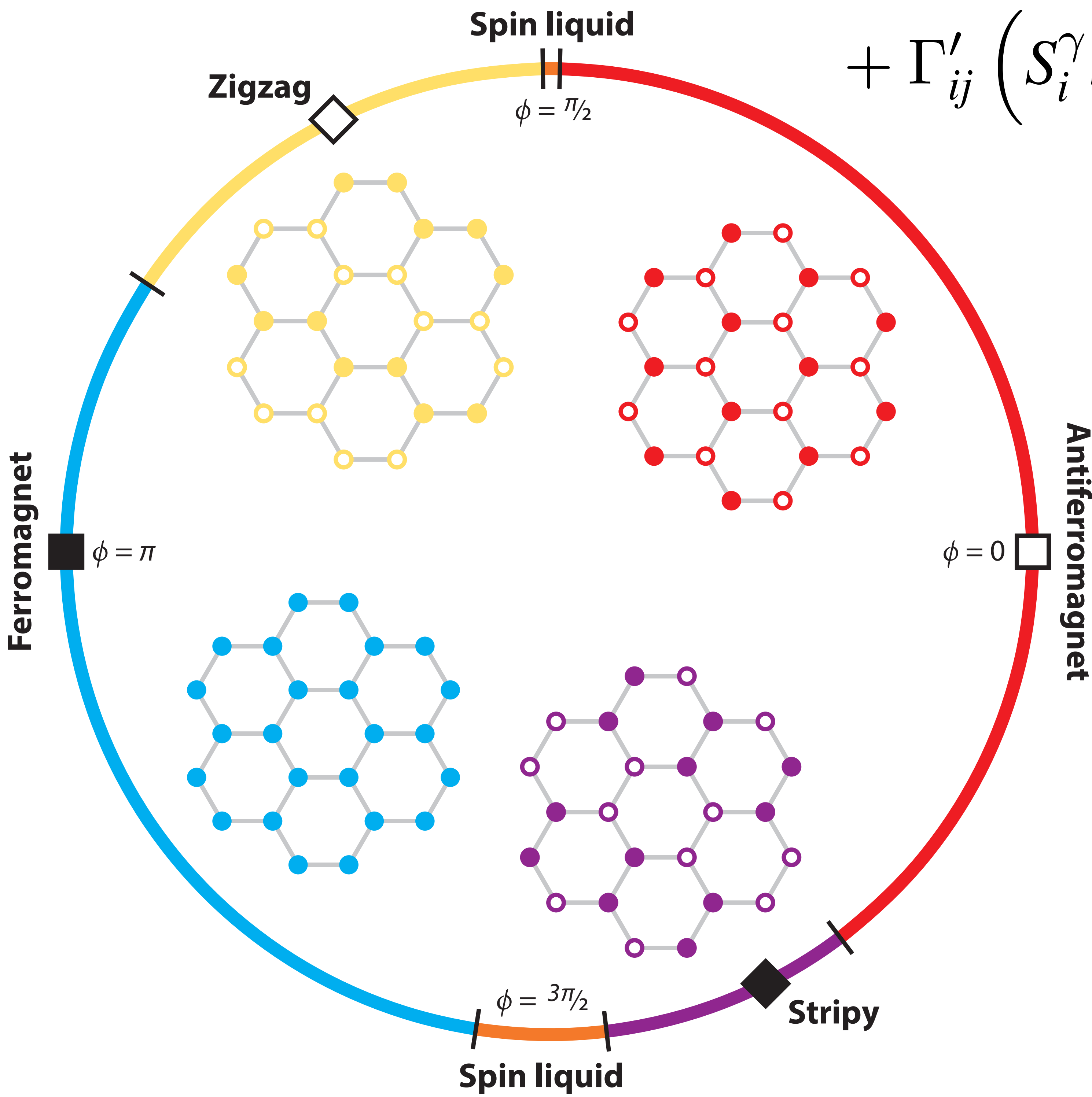




The honeycomb lattice is a bipartite lattice; geometric frustration is not relevant

Kitaev Physics on a 2D Honeycomb Lattice

$$\mathcal{H}_{ij} = J_{ij}\,\mathbf{S}_i \cdot \mathbf{S}_j + K_{ij}\,S_i^\gamma S_j^\gamma + \Gamma_{ij}\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)$$
$$+\,\Gamma'_{ij}\left(S_i^\gamma S_j^\alpha + S_i^\gamma S_j^\beta + S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma\right)$$



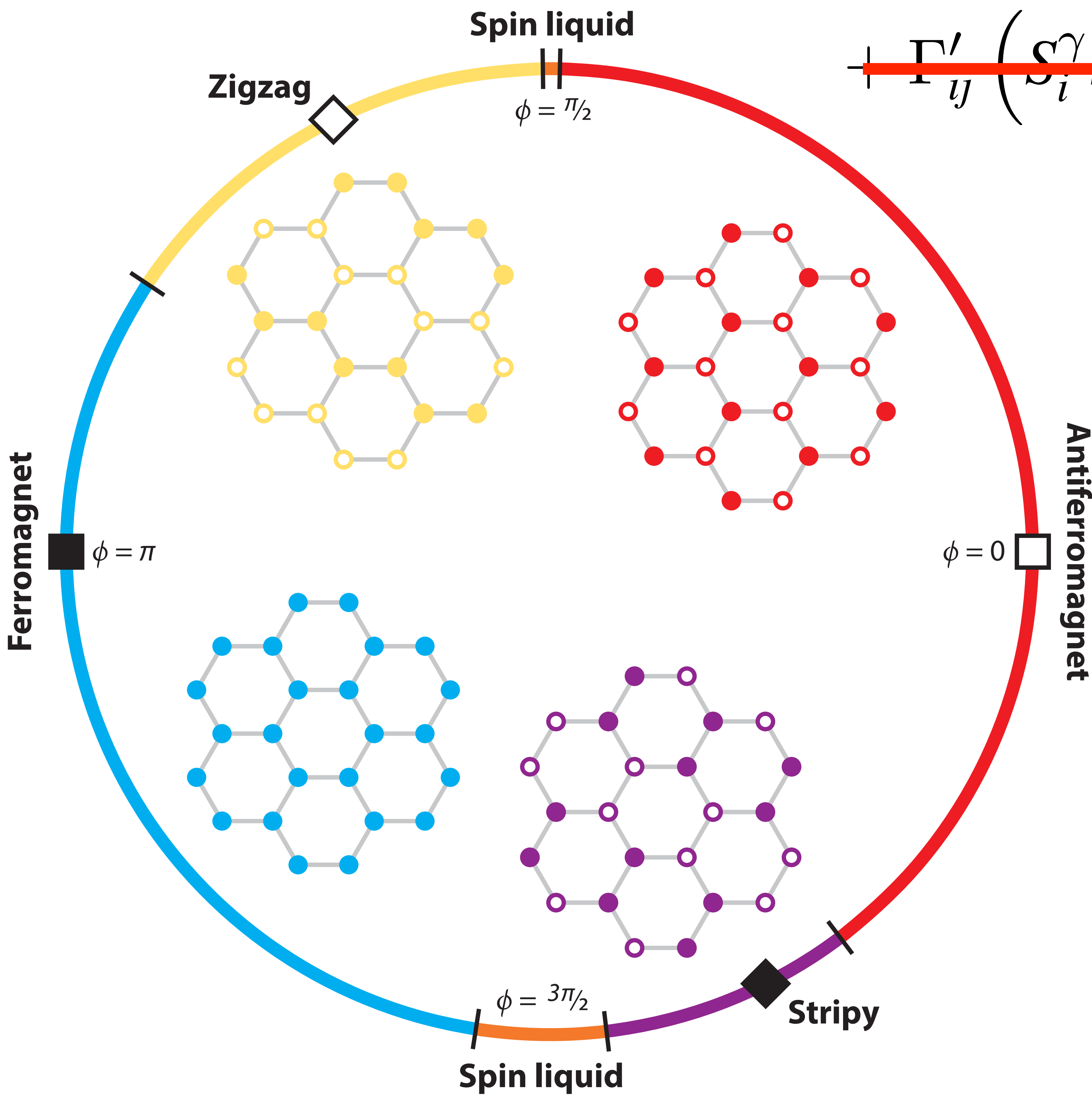
$$\mathcal{H}_{ij} = \mathbf{S}_i \cdot \mathbf{J}_{ij} \cdot \mathbf{S}_j$$

Rau et al., ARCMP 7, 195 (2016)

Kitaev Physics on a 2D Honeycomb Lattice

$$\mathcal{H}_{ij} = J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j + K_{ij}\, S_i^\gamma S_j^\gamma + \Gamma_{ij}\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)$$

$$+ \Gamma'_{ij}\left(S_i^\gamma S_j^\alpha + S_i^\gamma S_j^\beta + S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma\right)$$



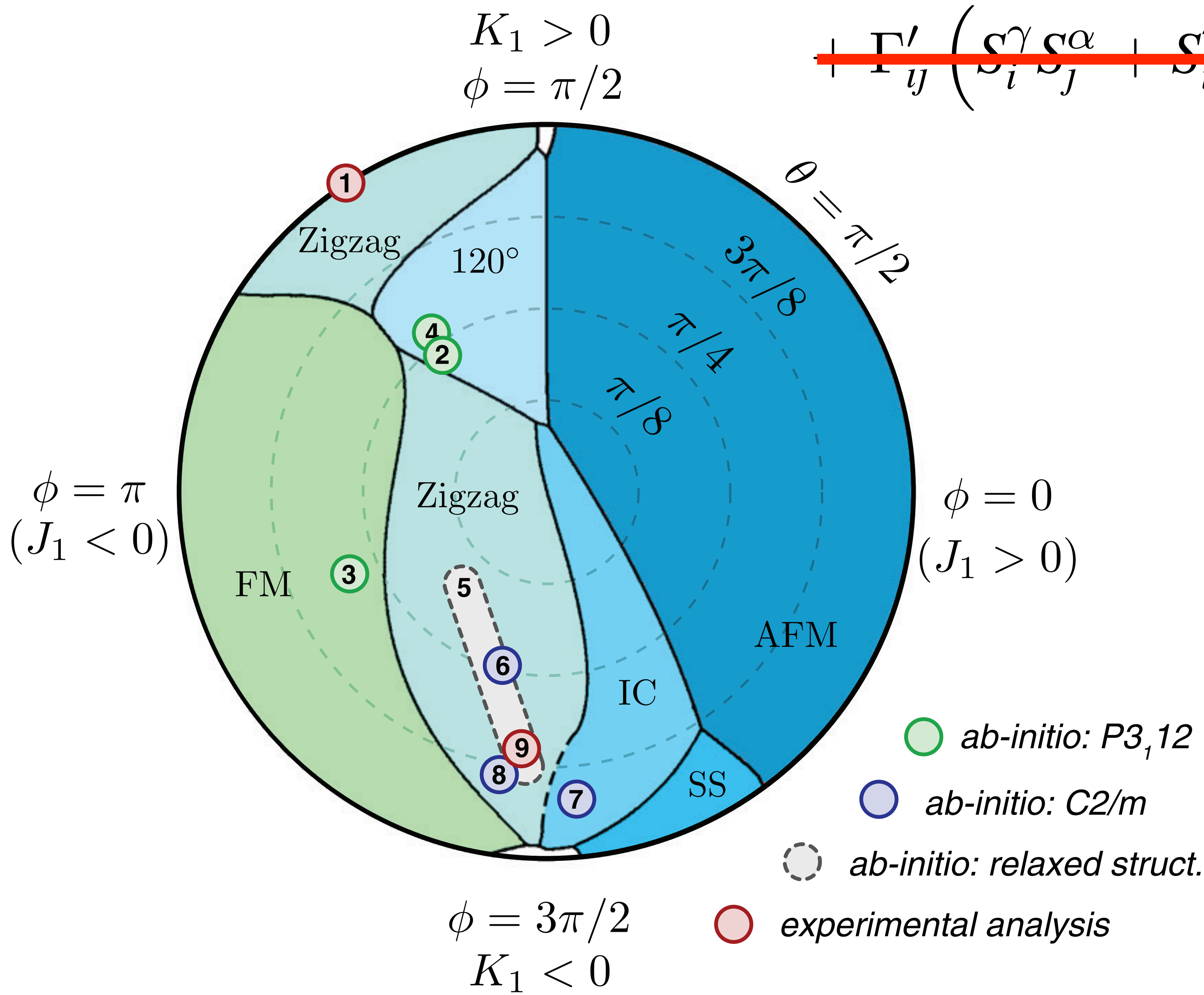
$$\mathcal{H}_{ij} = \mathbf{S}_i \cdot \mathbf{J}_{ij} \cdot \mathbf{S}_j$$

Rau et al., ARCMP 7, 195 (2016)

Kitaev Physics on a 2D Honeycomb Lattice

$$\mathcal{H}_{ij} = J_{ij}\,\mathbf{S}_i \cdot \mathbf{S}_j + K_{ij}\,S_i^\gamma S_j^\gamma + \Gamma_{ij}\left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha\right)$$

$$\cancel{+\Gamma'_{ij}\left(S_i^\gamma S_j^\alpha + S_i^\gamma S_j^\beta + S_i^\alpha S_j^\gamma + S_i^\beta S_j^\gamma\right)}$$



$$\mathcal{H}_{ij} = \mathbf{S}_i \cdot \mathbf{J}_{ij} \cdot \mathbf{S}_j$$

Winter S M et al., 2017
Nature Commun. 8 1152

Kitaev Physics on a 2D Honeycomb Lattice

Winter S M et al., Nature Commun. 8 1152 2017

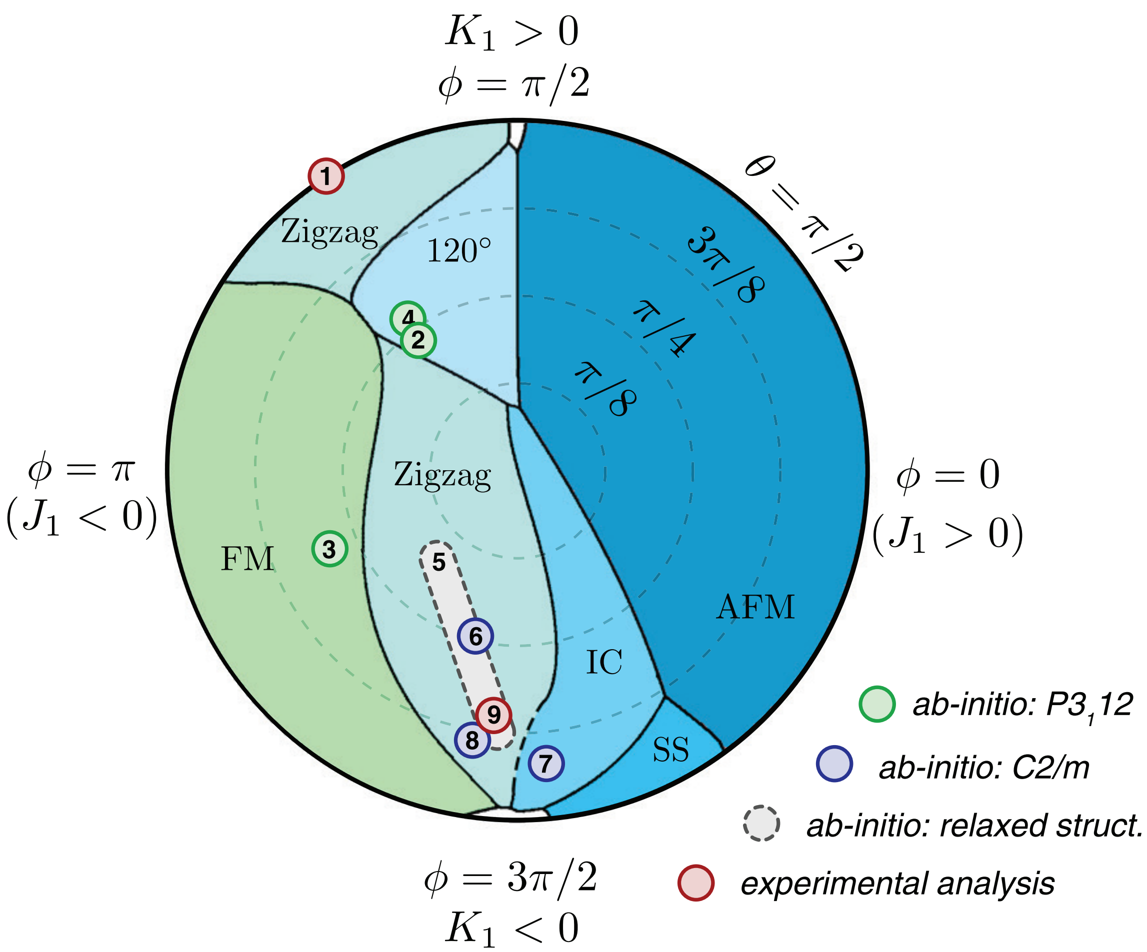


Table 2. Summary of magnetic parameters for honeycomb Na_2IrO_3, α-Li_2IrO_3, Li_2RhO_3, and α-$RuCl_3$. The latter material is discussed in section 2.3.2. See text for relevant references.

Property	Na_2IrO_3	α-Li_2IrO_3	Li_2RhO_3	α-$RuCl_3$
μ_{eff} (μ_B)	1.79	1.83	2.03	2.0 to 2.7
Θ_{iso} (K)	~ -120	-33 to -100	~ -50	$\sim +40$
Θ_{ab} (K)	-176	$\Theta_{ab} > \Theta_c$	—	$+38$ to $+68$
Θ_c (K)	-40	—	—	-100 to -150
T_N (K)	$13-18$	~ 15	(6)	7 to 14
Order	Zigzag	Spiral	Glassy	Zigzag
k-vector	$(0, 1, \frac{1}{2})$	$(0.32, 0, 0)$	—	$(0, 1, \frac{1}{2})$

Winter S M et al., J.Phys.: Condens. Matter 29 493002 (2017)

Kitaev Physics on a 2D Honeycomb Lattice: $RuCl_3$

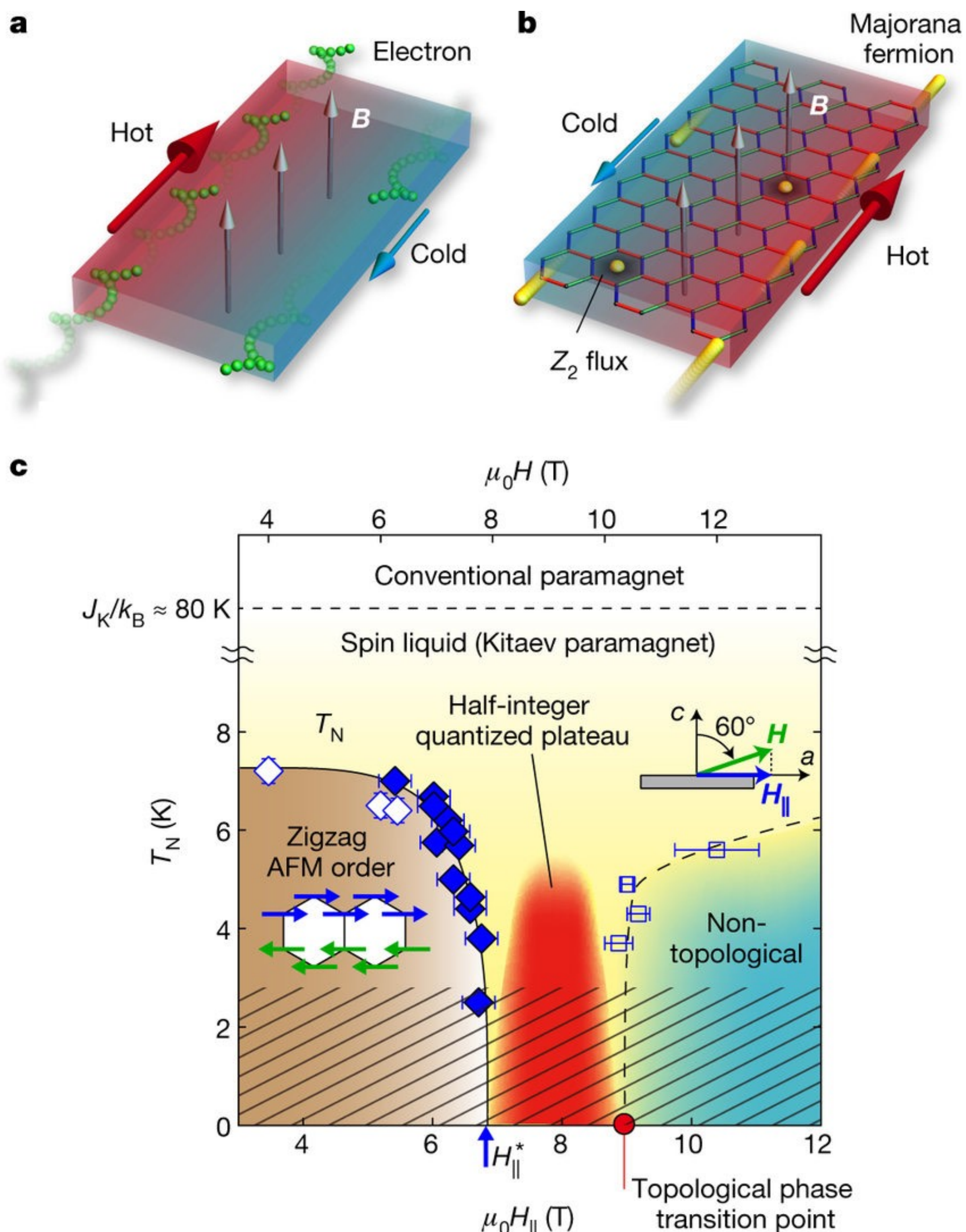
$$\mathcal{H}_{ij} = J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j + K_{ij}\, S_i^\gamma S_j^\gamma + \Gamma_{ij} \left(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right)$$

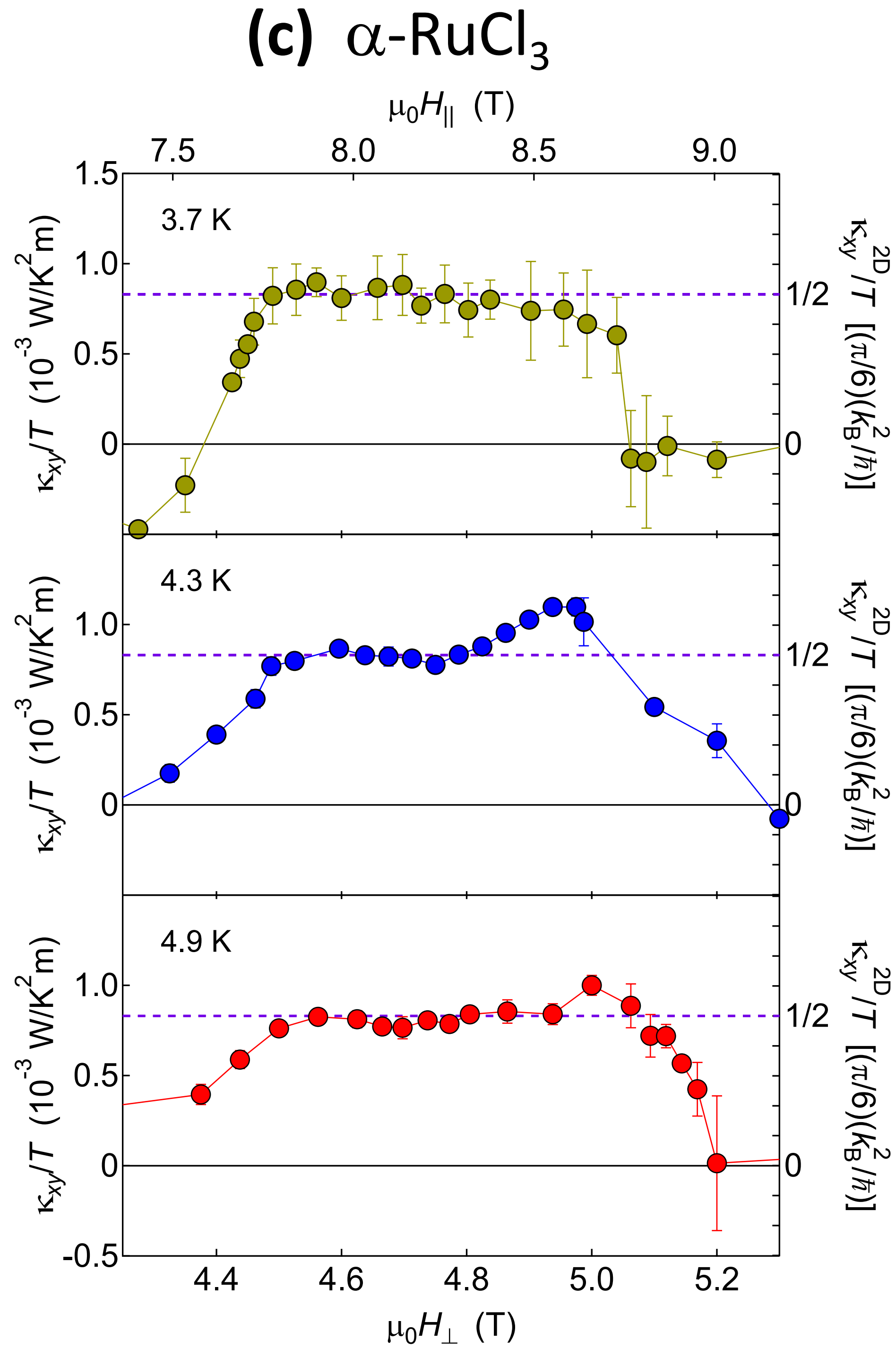
Table 5. Bond-averaged values of the largest magnetic interactions (in units of meV) within the plane for α-$RuCl_3$ obtained from various methods. For [149], the two numbers represent the range of values found in various relaxed structures. 'Pert. Theo.' refers to second order perturbation theory, 'QC' = quantum chemistry methods, 'ED' = exact diagonalization, 'DFT' = density functional theory total energy, 'Exp. An.' = experimental analysis. See also figure 19.

Method	Structure	J_1	K_1	Γ_1	J_3
Exp. An. [166]	—	−4.6	+7.0	—	—
Pert. Theo. [149]	$P3_112$	−3.5	+4.6	+6.4	—
QC (2-site) [41]	$P3_112$	−1.2	-0.5	+1.0	—
ED (6-site) [45]	$P3_112$	−5.5	+7.6	+8.4	+2.3
Pert. Theo. [149]	Relaxed	−2.8/ − 0.7	−9.1/ − 3.0	+3.7/+ 7.3	—
ED (6-site) [45]	$C2/m$	−1.7	−6.7	+6.6	+2.7
QC (2-site) [41]	$C2/m$	+0.7	−5.1	+1.2	—
DFT [180]	$C2/m$	−1.8	−10.6	+3.8	+1.3
Exp. An. [181]	—	−0.5	−5.0	+2.5	+0.5

Winter S M et al.,
J.Phys.: Condens. Matter 29 493002 (2017)

Kitaev Physics on a 2D Honeycomb Lattice: $RuCl_3$





Kasahara et al, 559, Nature, 227 (2018)

Search for Spin Liquid Candidate Ground States in Real Materials

- Different routes to spin liquid ground states: geometry and competing interactions.

- Materials issues are present and somewhat uncontrolled in all candidate materials.

- Of the 4 examples discussed, 2 are relatively simple: Herbertsmithite (2D Kagome AF) is relatively simple due to its spin-only S=1/2. The character of its gap (gapped or gapless) remains an outstanding issue. Classical spin ice pyrochlores are relatively simple as they can be successfully modelled classically.

- Both 3D pyrochlore candidates and 2D Kitaev candidates require moderate to strong SOC, and anisotropic exchange as a consequence.