Iridates

The New Frontier

Mike Norman

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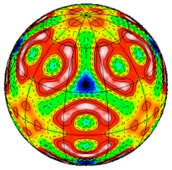


KIAS, Dec. 19, 2009

Spin Liquids are insulators that have large Curie-Weiss temperatures, but do not order or show spin glass behavior. Particularly relevant are those with S=1/2.

PHYSICS

An End to the Drought of Quantum Spin Liquids

Patrick A. Lee

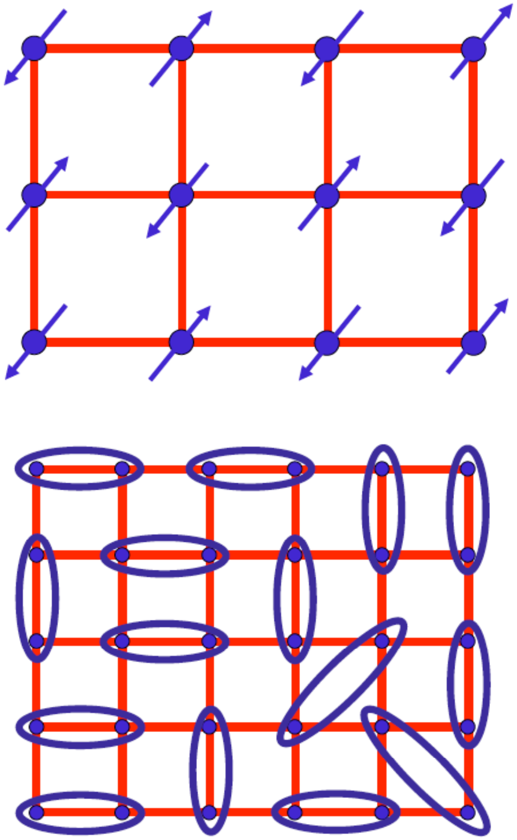
After decades of searching, several promising examples of a new quantum state of matter have now emerged.

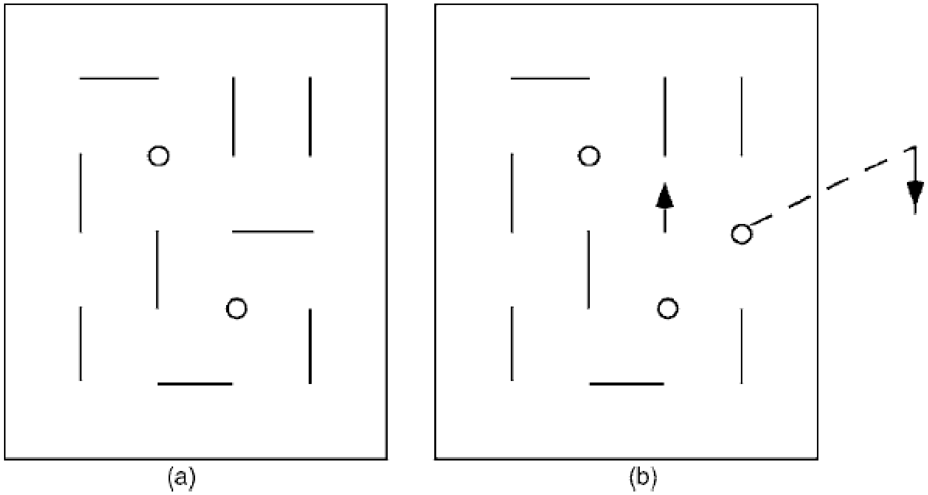
Science 321, 1306 (2008)

- κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$ (triangular)
- $ZnCu_3(OH)_6Cl_2$ (kagome)
- $Na_4Ir_3O_8$ (hyper-kagome)

(See also article in Physics Today by Barbara Goss Levi, page 16, February 2007)

RVB - a liquid of spin singlets

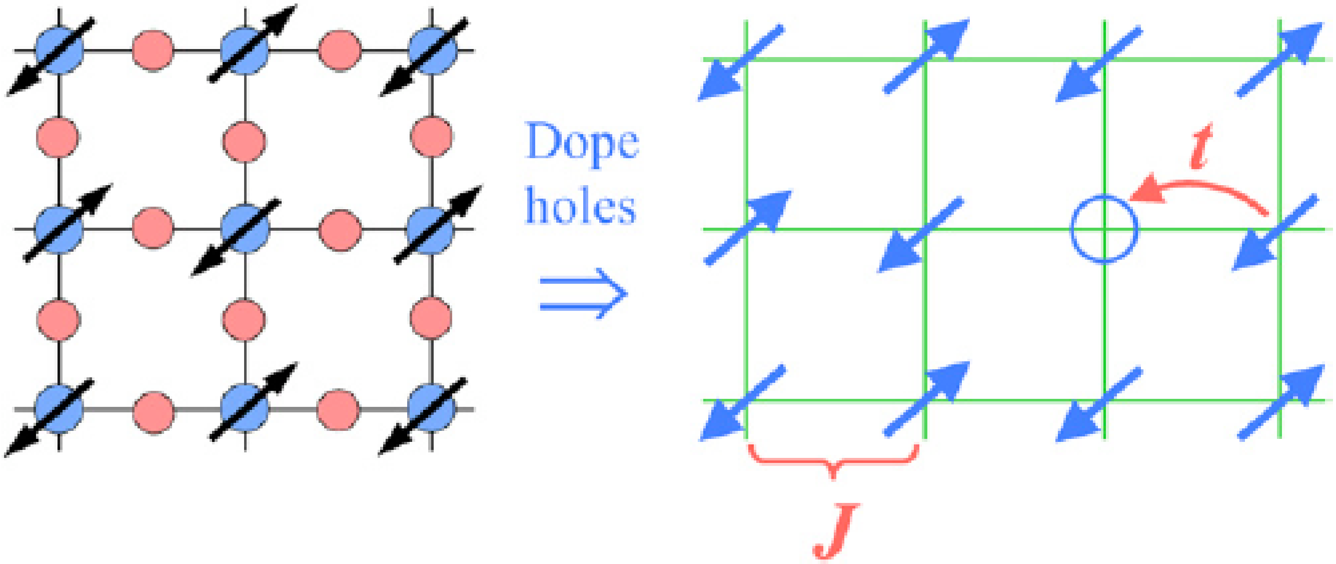




(a) (b)

In the uniform RVB state, the S=1/2 excitations (spinons) possess a zero energy Fermi surface (Anderson, 1987)

Square Lattice (Anderson, 1987)



$J\, S{\cdot}S$ where $J = 2\, t^2/U$

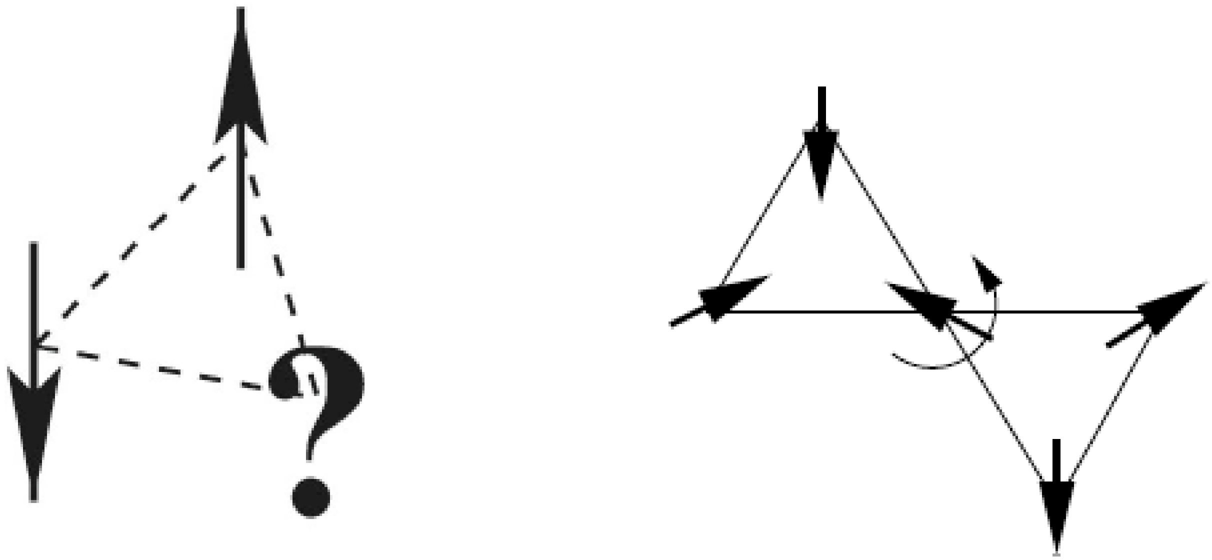
for $S=1/2$

Neel - $J/4$ per bond - $S_z S_z$

Singlet - $3J/4$ per bond - $S(S+1)$

Lee, Rep. Prog. Phys. 71, 012501 (2008)

Frustration on the Triangular Lattice (Anderson, 1973)



$$\boxed{\chi^{-1} = T - \Theta_{CW}}$$

κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$

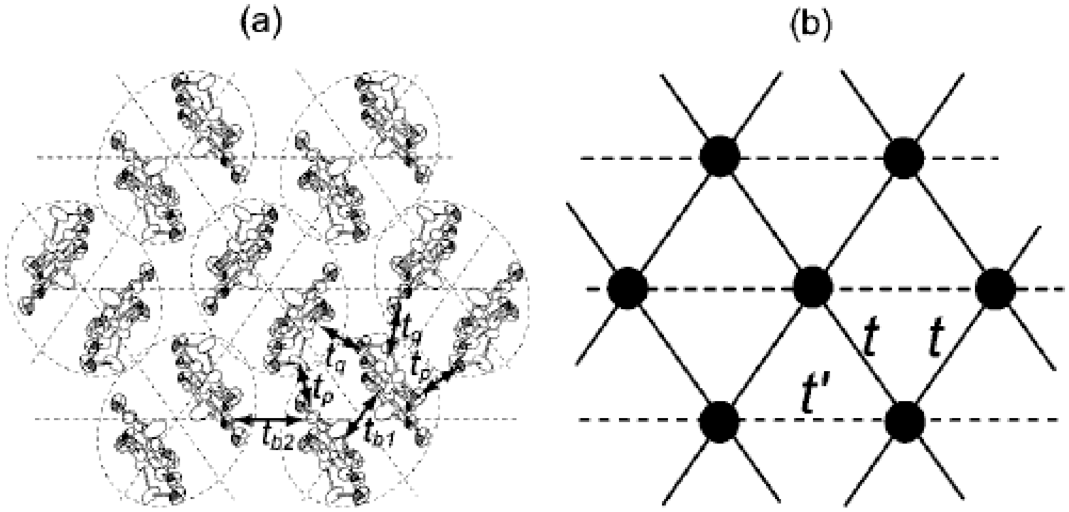
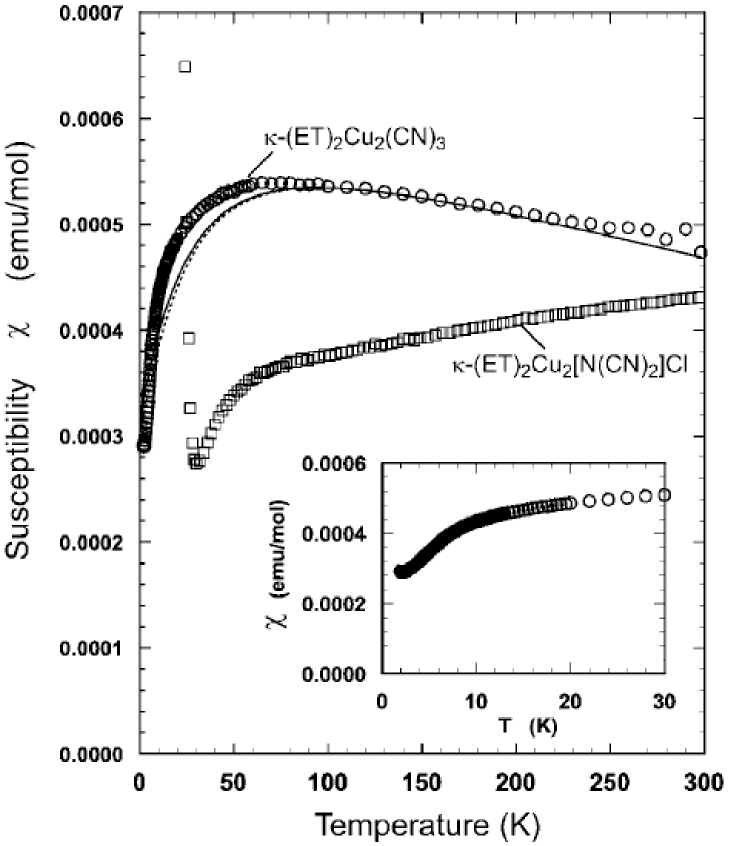
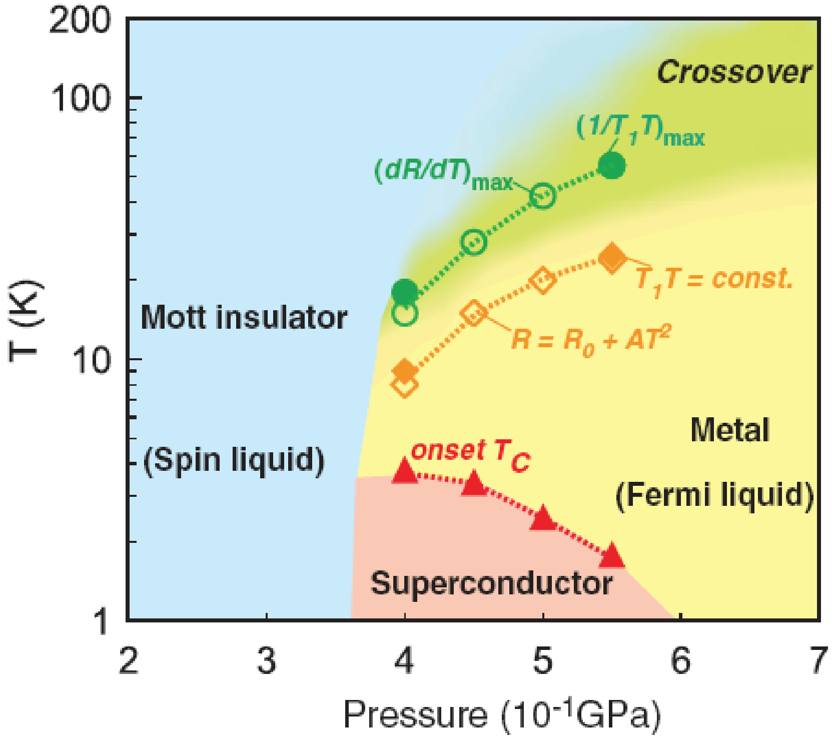


FIG. 1. (a) Crystal structure of an ET layer of κ-(ET)$_2$Cu$_2$(CN)$_3$ viewed along the long axes of ET molecules

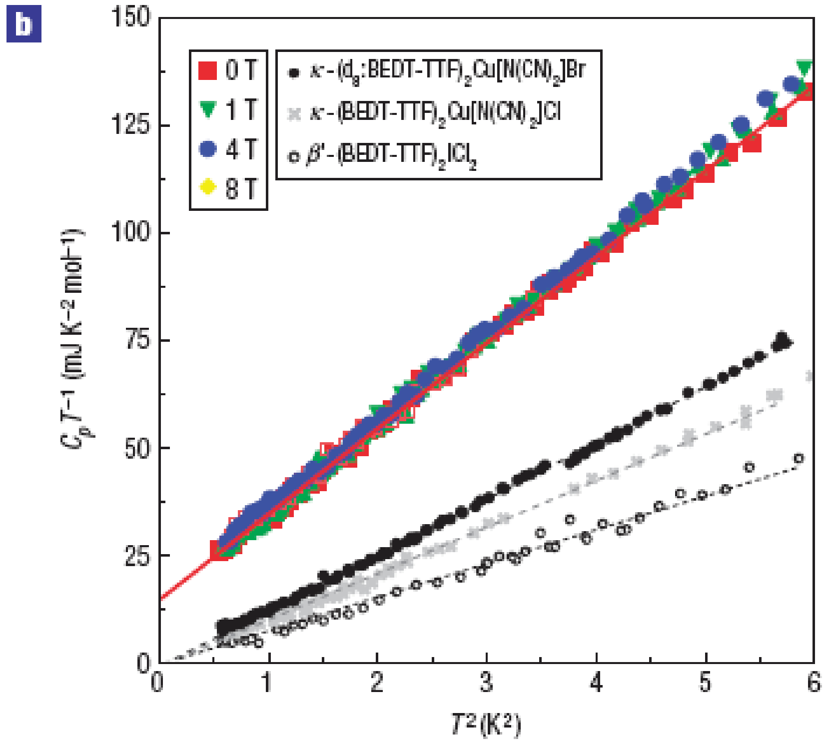
Geiser *et al.*, Inorg. Chem. 30, 2586 (1991)



Shimizu *et al.*, PRL 91, 107001 (2003)

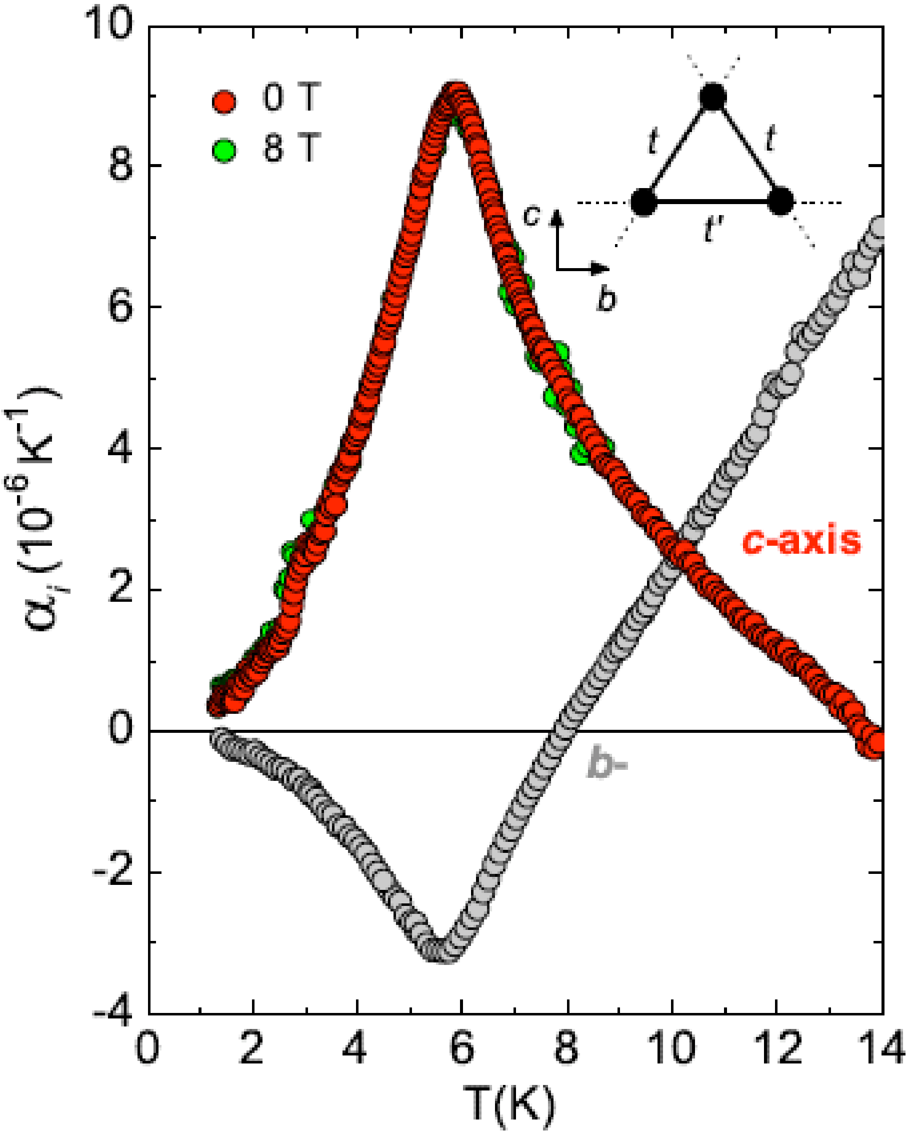


Kurosaki *et al.*, PRL 95, 177001 (2005)



Yamashita *et al.*, Nat. Phys. 4, 459 (2008)

Ordering at 6 K?



Manna *et al.*, arXiv:0909.0718

The Universe is a String-Net Liquid

Herbertsmithite

Zeeya Merali, New Scientist (15 March 2007)

Herbertsmithite $ZnCu_3(OH)_6Cl_2$

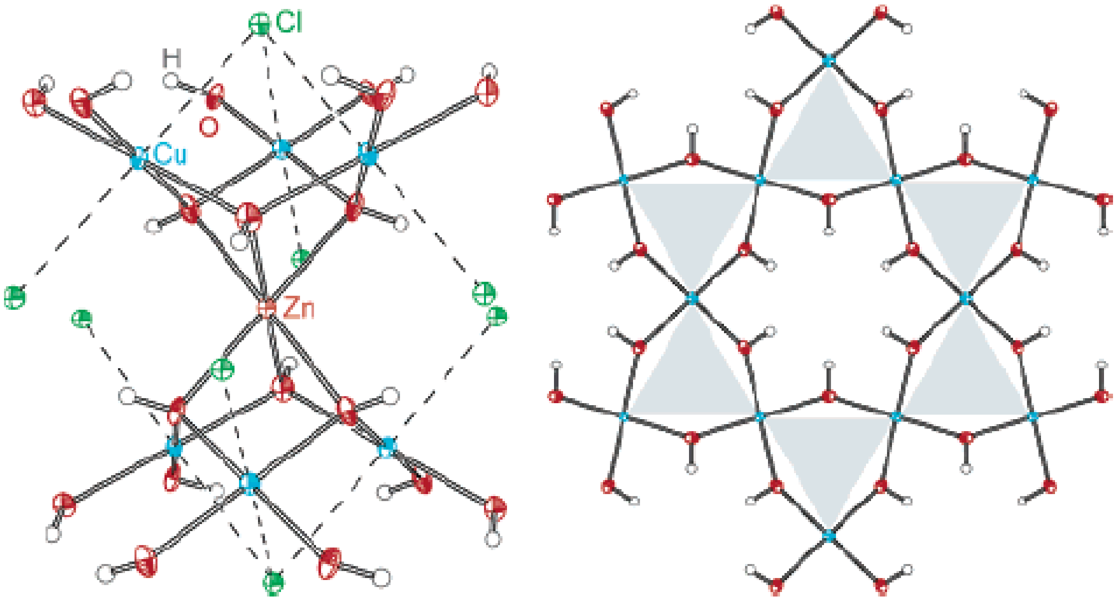
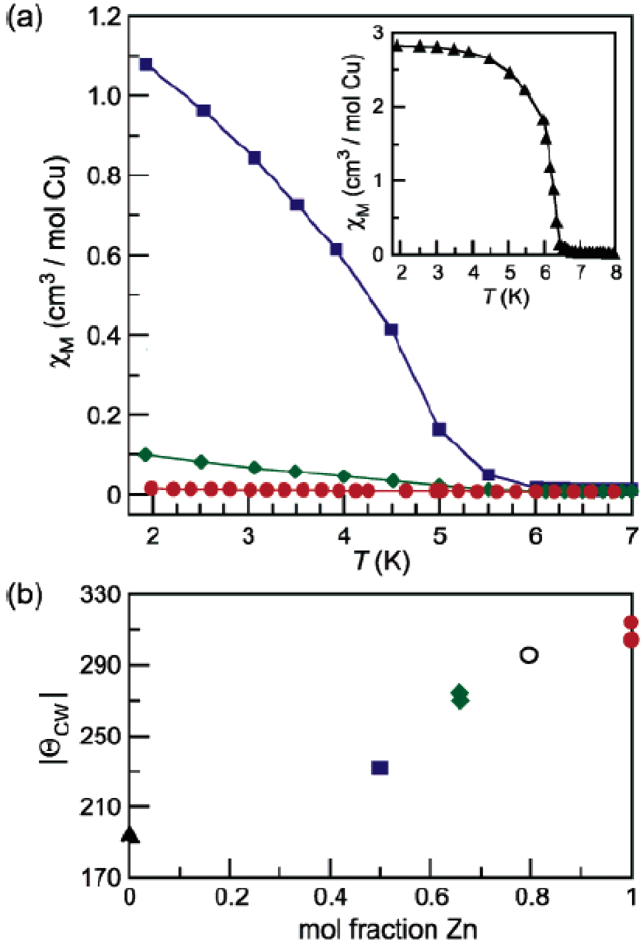
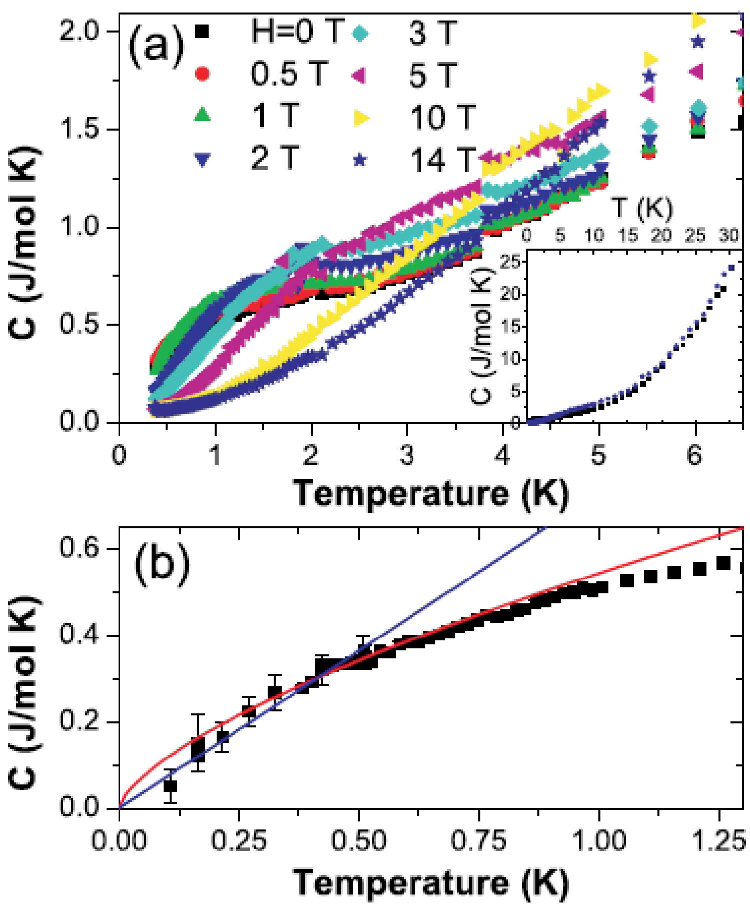


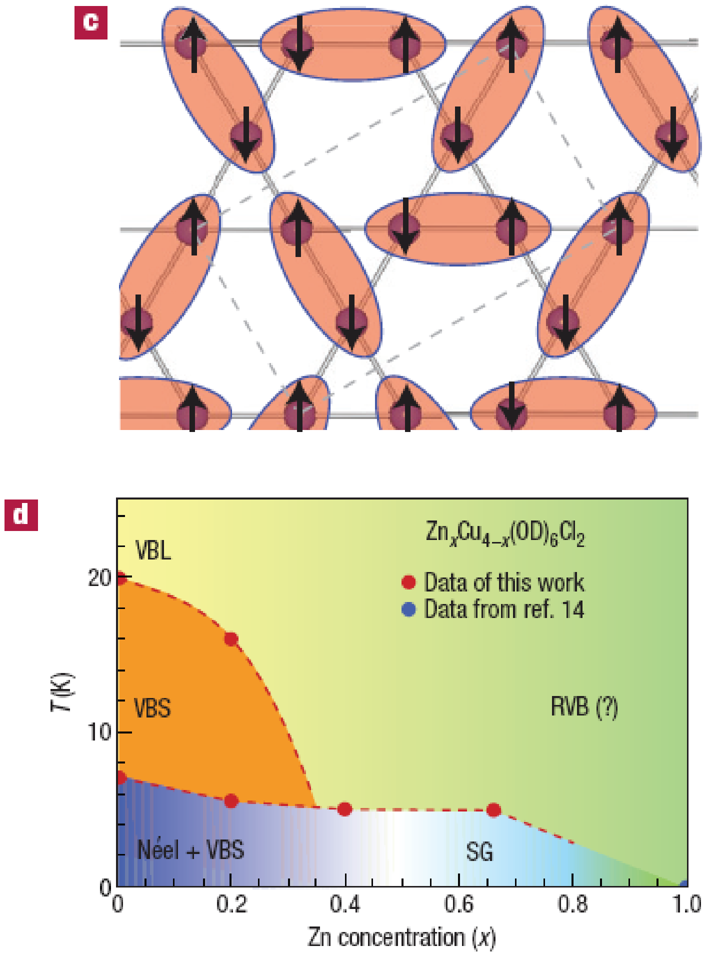
Figure 1. Crystal structure of Zn−paratacamite (**1**), $Zn_{0.33}Cu_{3.67}(OH)_6Cl_2$.



Shores *et al.*, JACS 127, 13462 (2005)

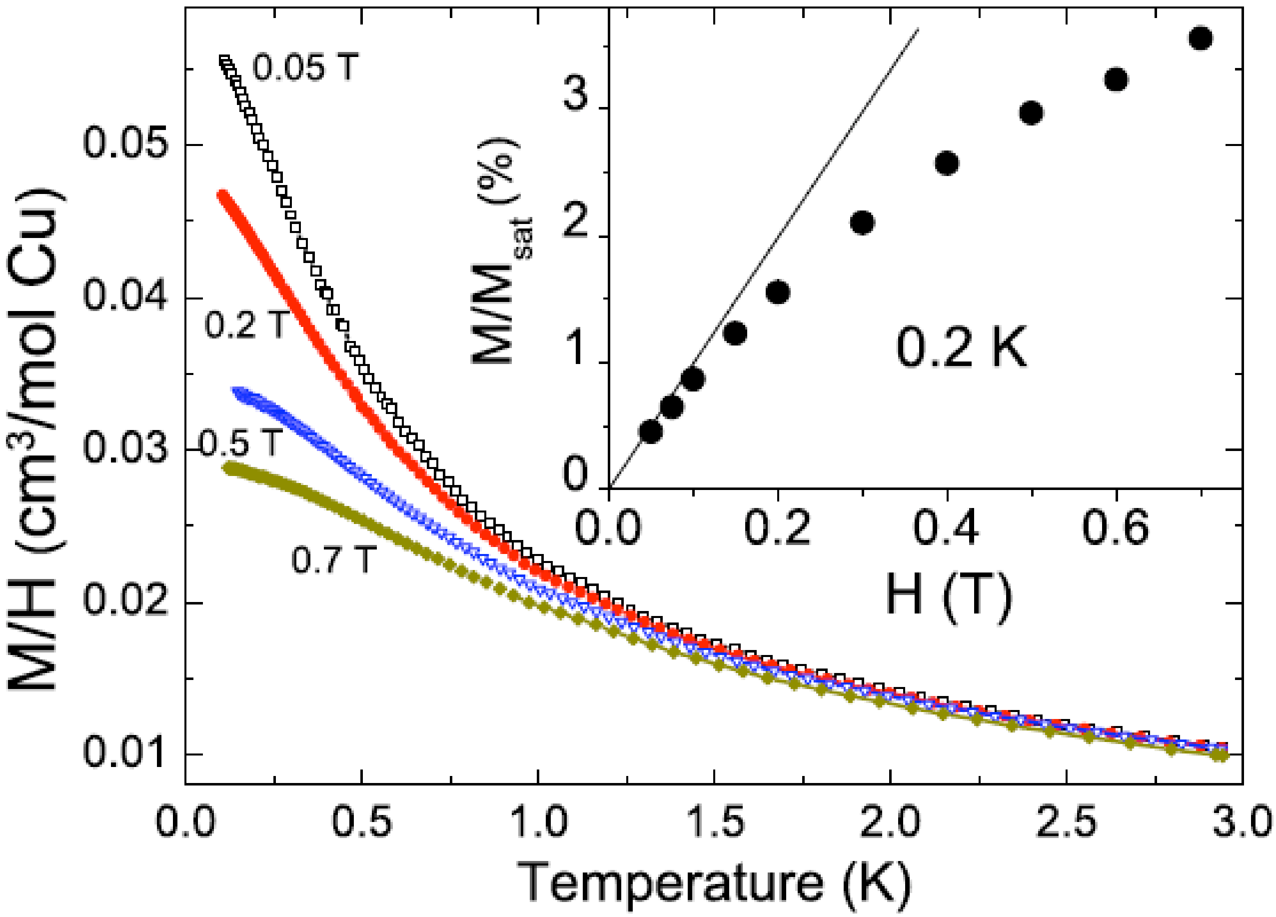


Helton *et al.*, PRL 98, 107204 (2007)



Lee *et al.*, Nat. Matls. 6, 853 (2007)

But, there is a large defect concentration (Cu - Zn)



Bert *et al.*, PRB 76, 132411 (2007)

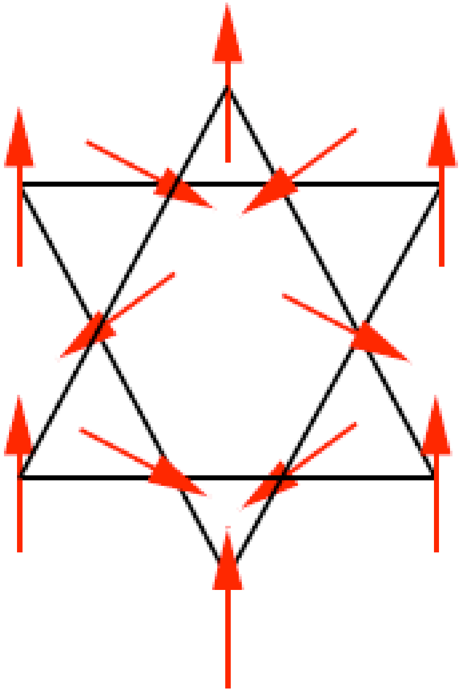
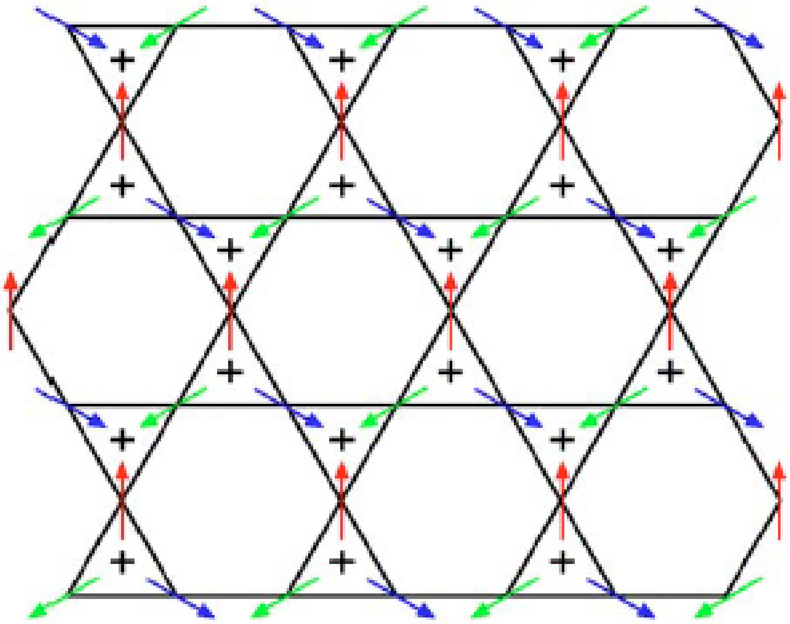
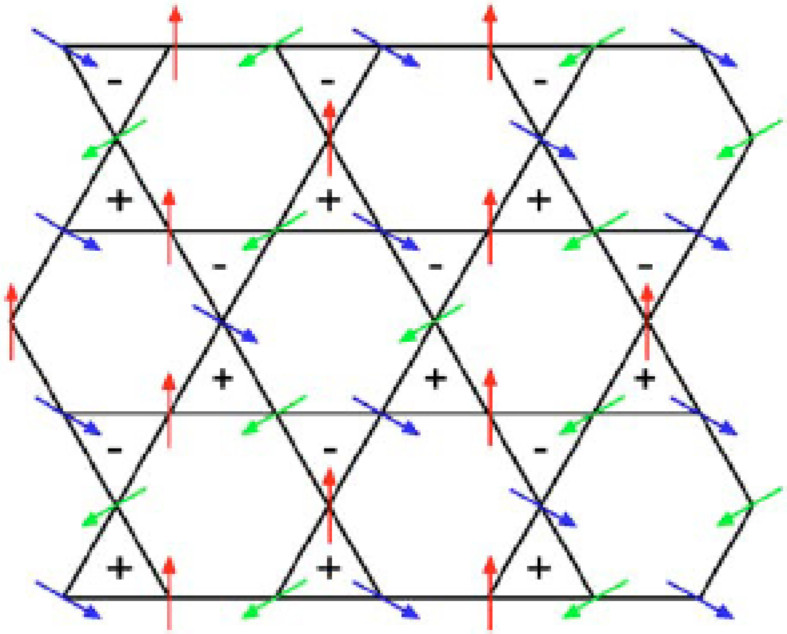


Fig. 1.5. Illustration of how ground state degrees of freedom arise for the Heisenberg model on the kagome lattice: spins on the central hexagon may be rotated together through any angle about the axis defined by the outer spins, without leaving the ground state.

Chalker, arXiv:0901.3492

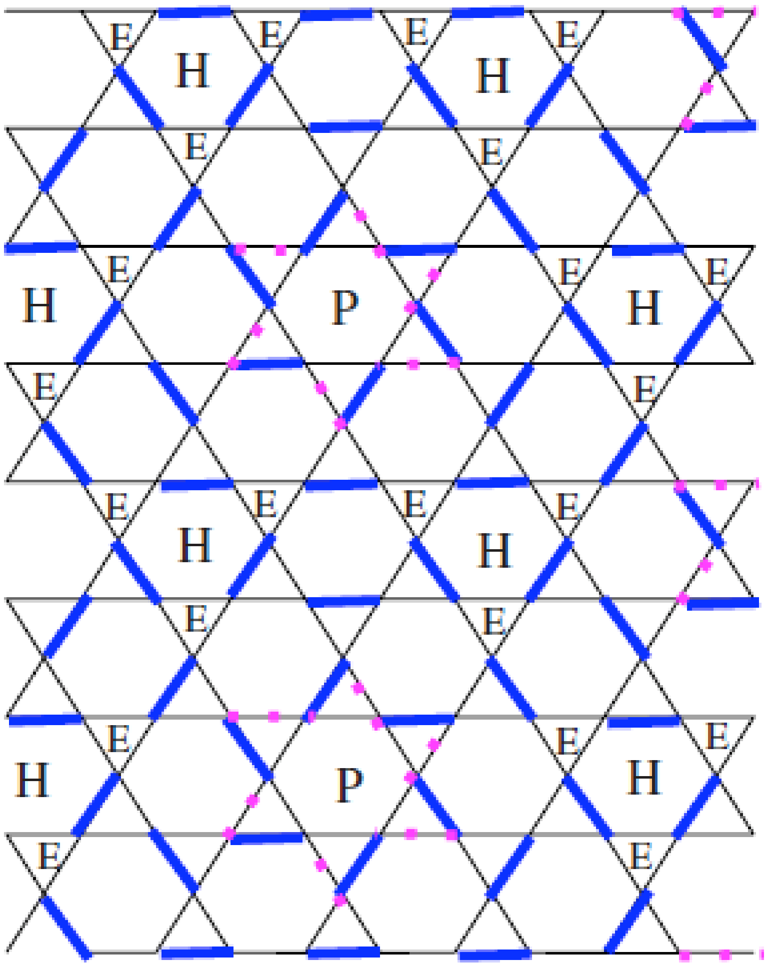
Classical Kagome Ground States


$q=0$


$\sqrt{3}\times\sqrt{3}$

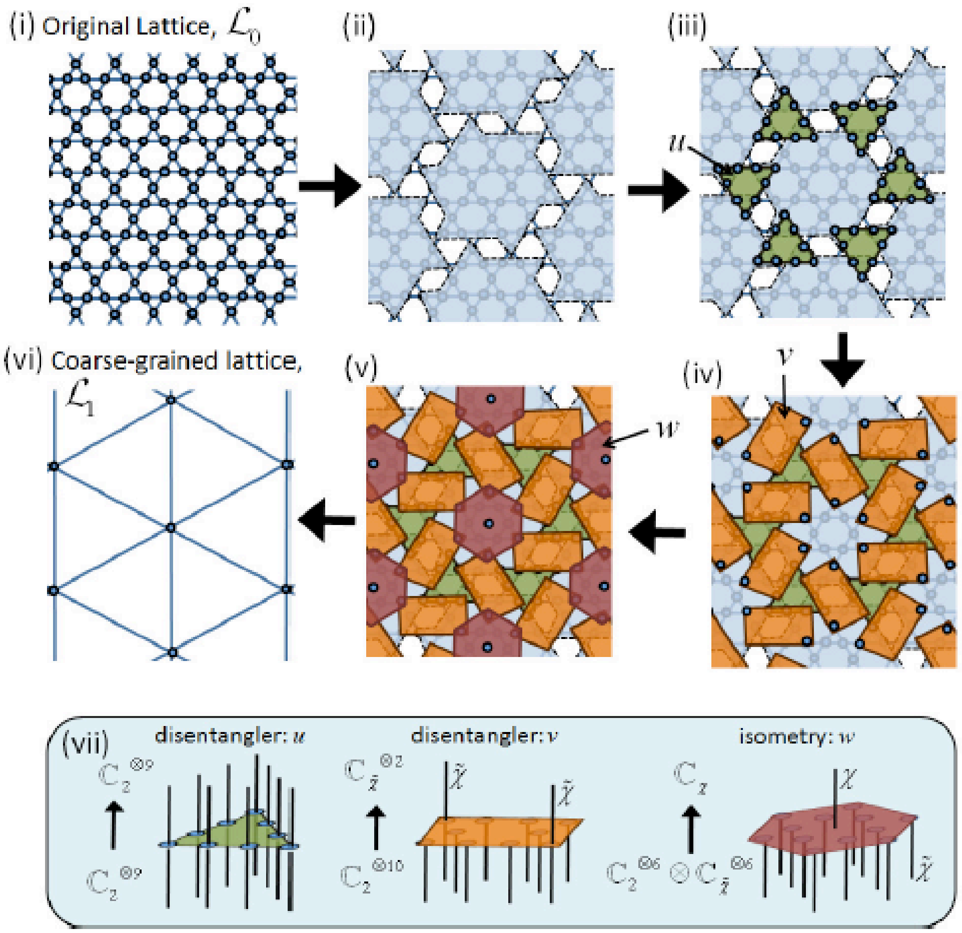
Ryu *et al.*, PRB 75, 184406 (2007)

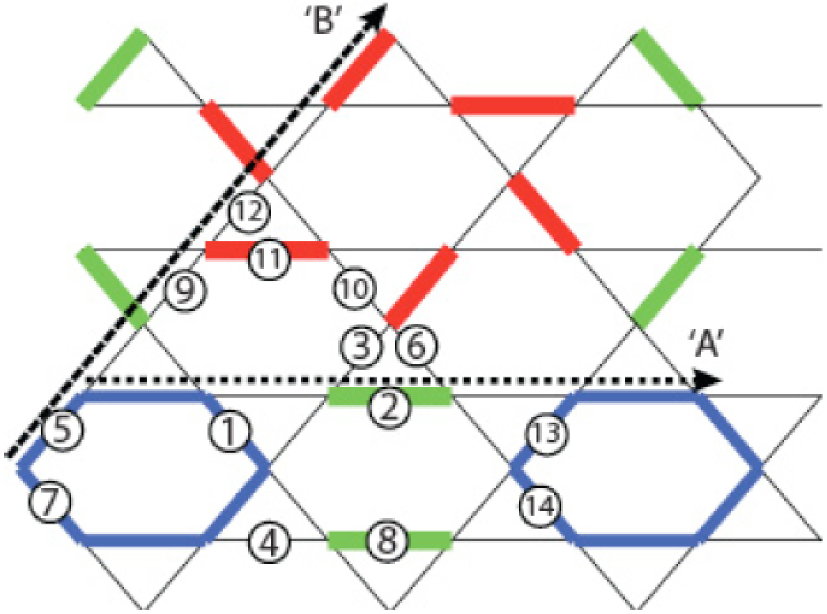
Valence Bond Ground State for Kagome?



Singh & Huse, PRB 76, 180407 (2007)

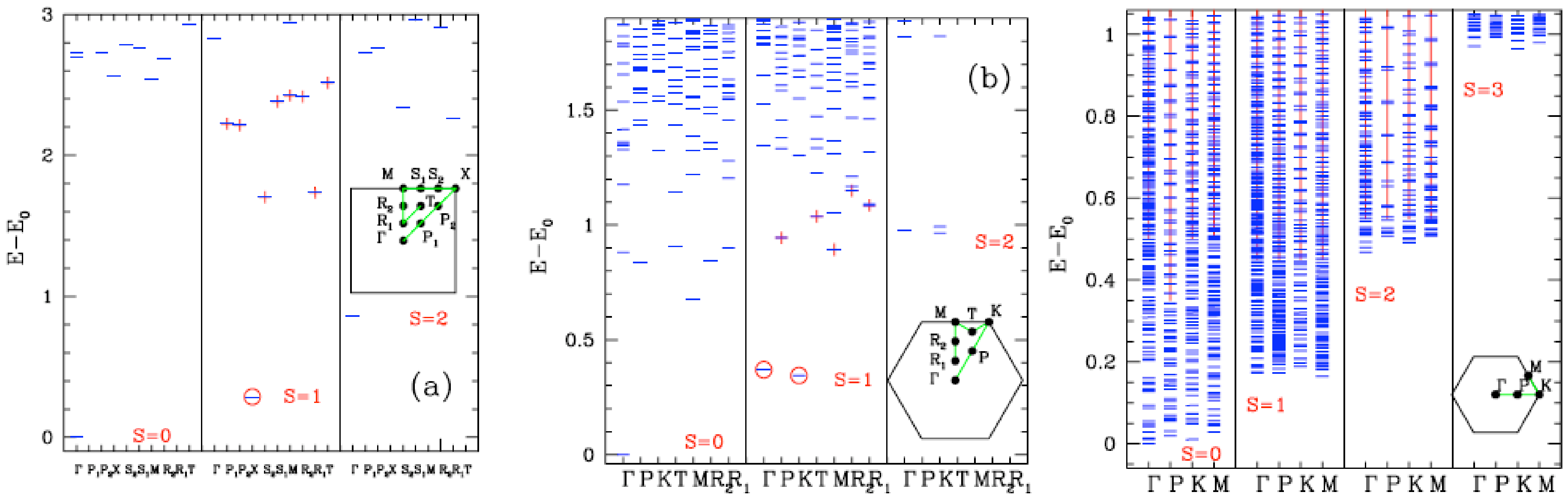
Multi-scale entanglement renormalization ansatz (MERA)





Evenbly & Vidal, arXiv:0904.3383

Exact Diagonalization (36 sites)



square

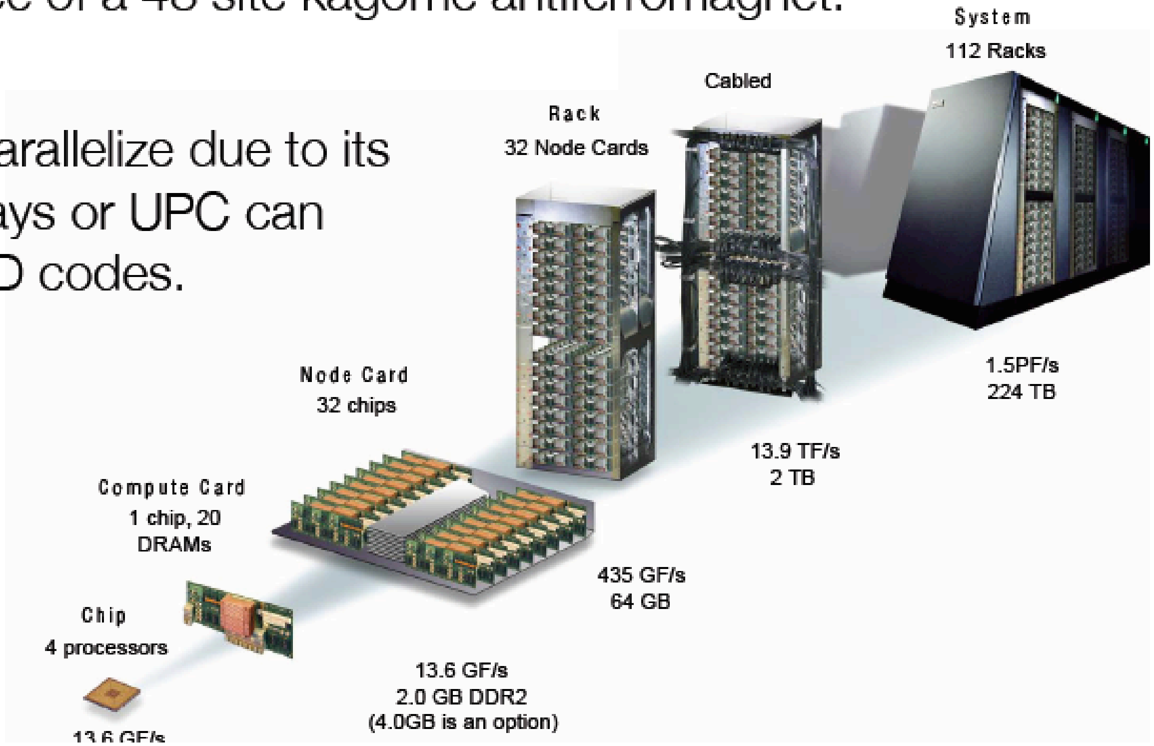
triangular

Kagome

Sindzingre & Lhuillier, EPL 88, 27009 (2009)

Parallelization:
How to harness the petaflop computers ?

- Cutting edge petaflop systems have a huge number of core, but only a moderate amount of node-local memory.
- Next generation ED codes need to be developed in order to attack e.g. the 80 billion Hilbert space of a 48 site kagome antiferromagnet.
- Problem remains difficult to parallelize due to its all-to-all structure. Global Arrays or UPC can help developing distributed ED codes.



Andreas Lauchli, QS2009 Workshop

$Na_4Ir_3O_8$

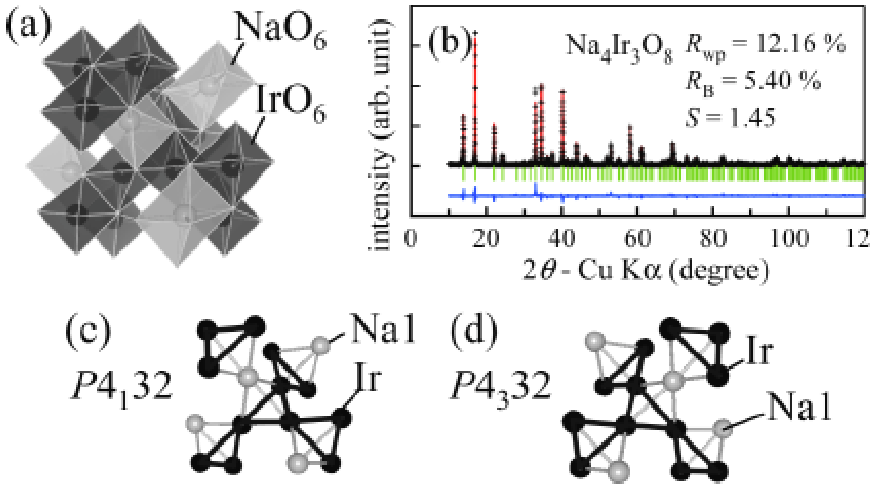
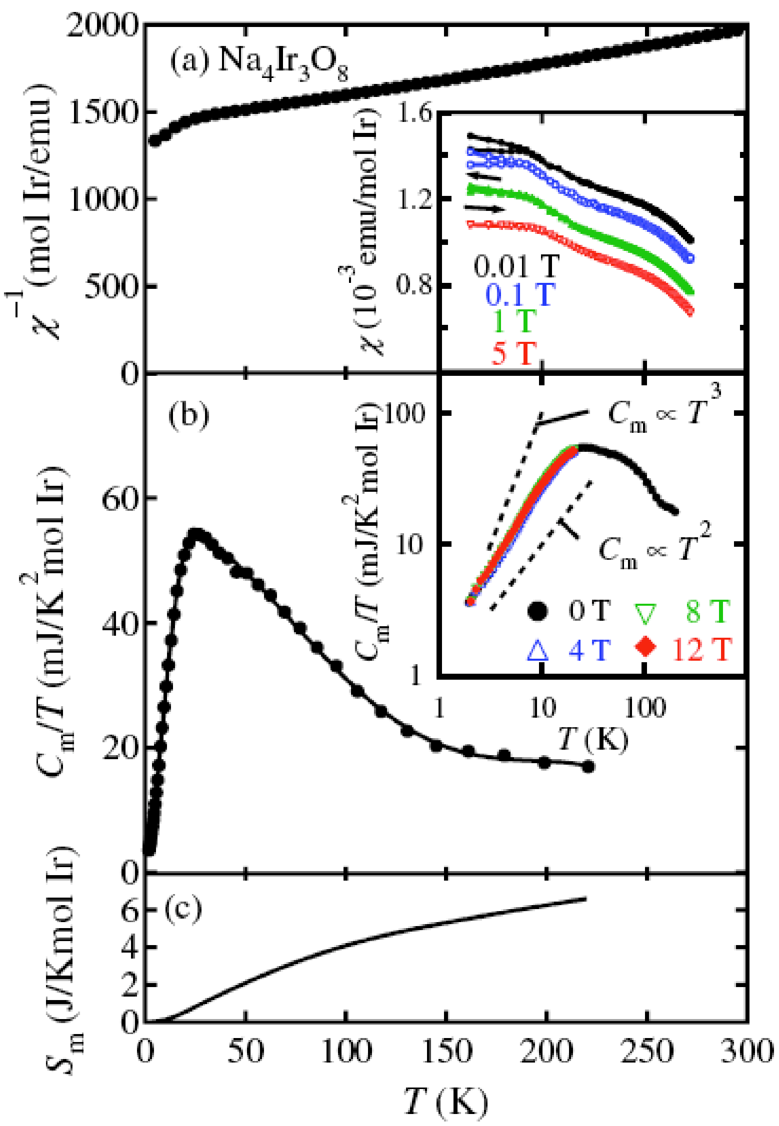


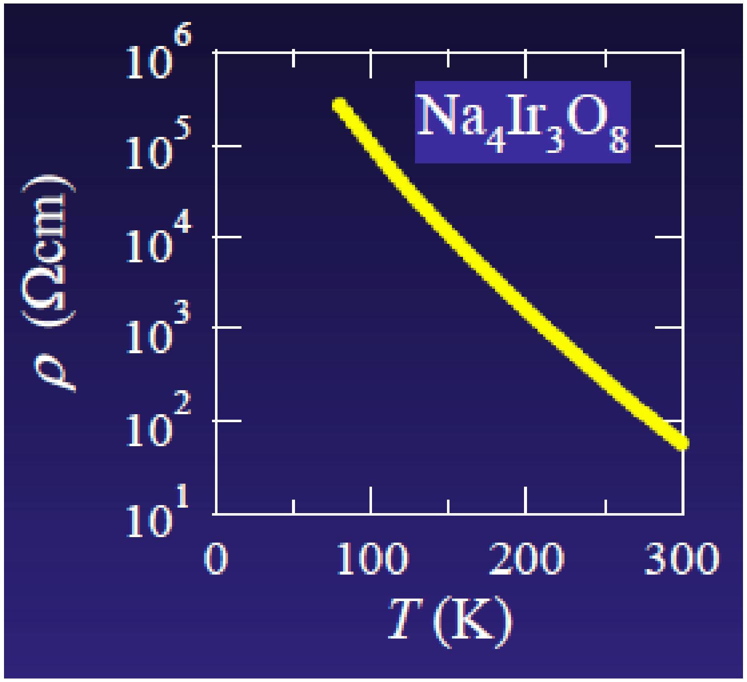
FIG. 1 (color online). (a) Crystal structure of $Na_4Ir_3O_8$

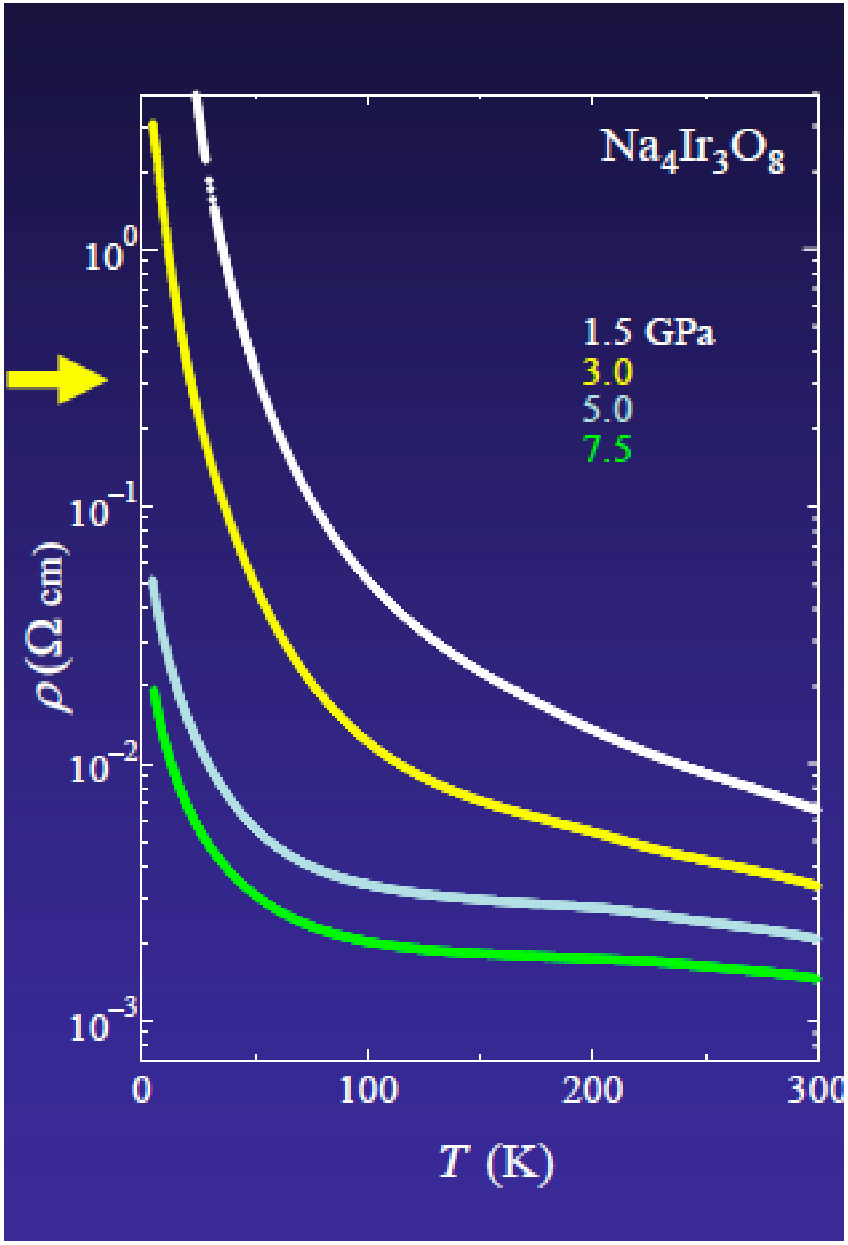


Θ_{CW} ~ -650 K, μ_{eff} ~ 2 μ_B

Okamoto *et al.*, PRL 99, 137207 (2007)

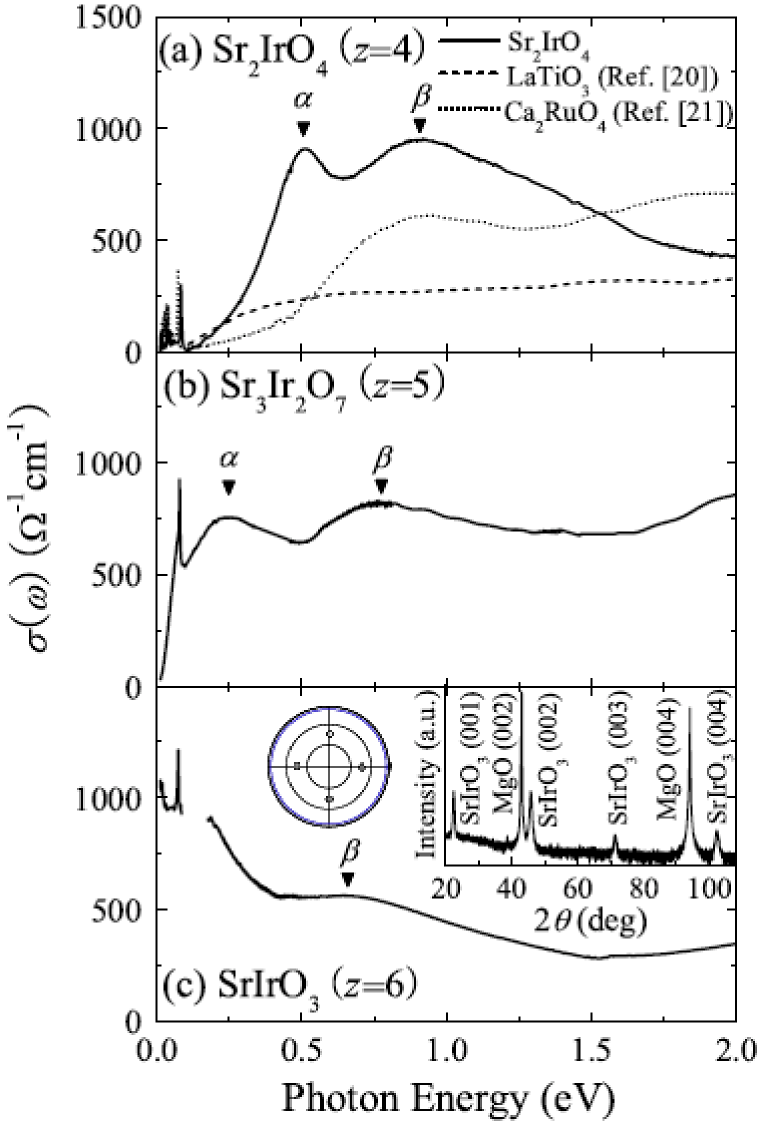
Mott Insulator?





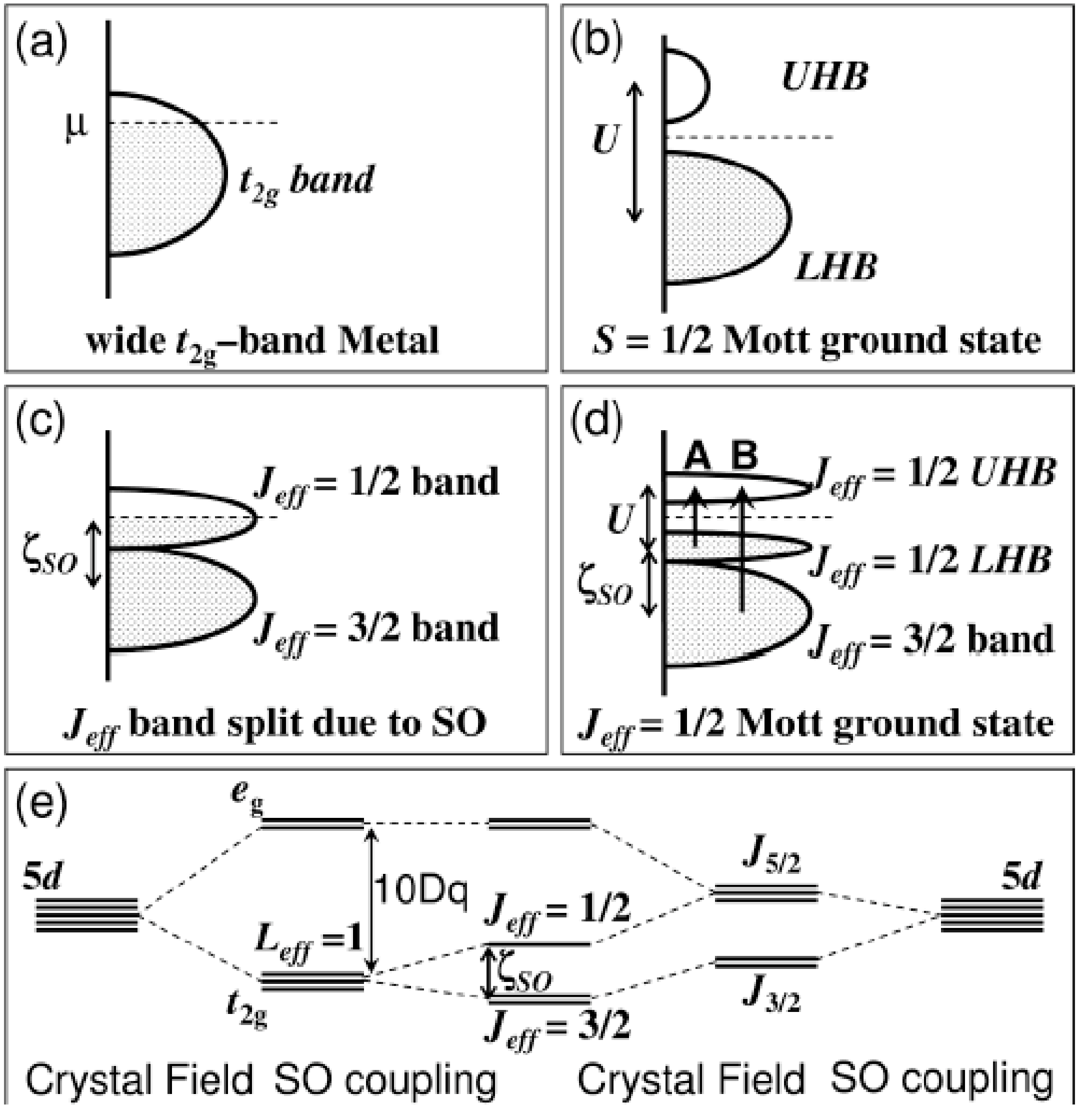
H. Takagi, unpublished

Sr_2IrO_4 (La_2CuO_4 analogue) appears to be a Mott insulator



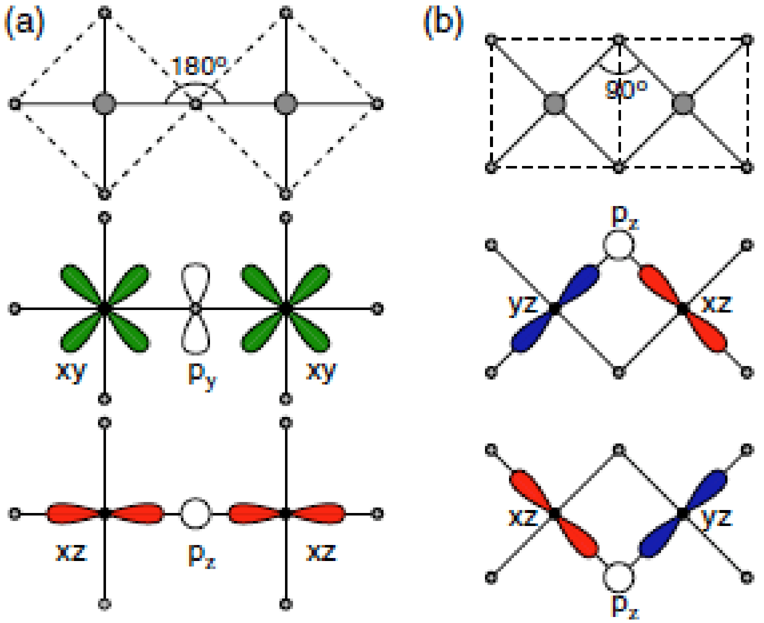
Moon *et al*., PRL 101, 206402 (2008)

Spin-orbit plus d^5 configuration leads to a half filled doublet

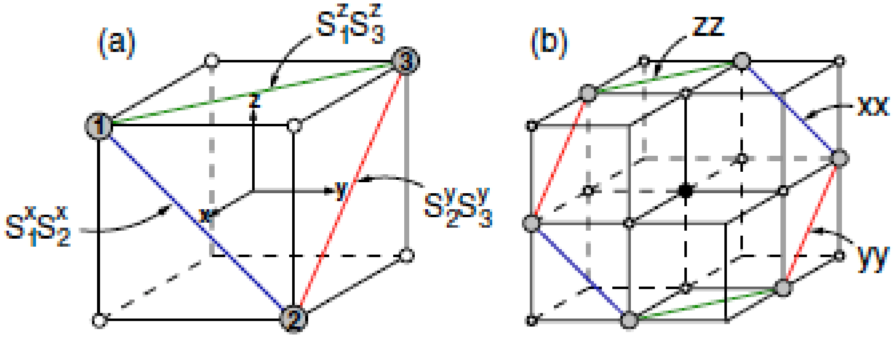


Kim *et al.*, PRL 101, 076402 (2009)

Realization of the Kitaev Model?

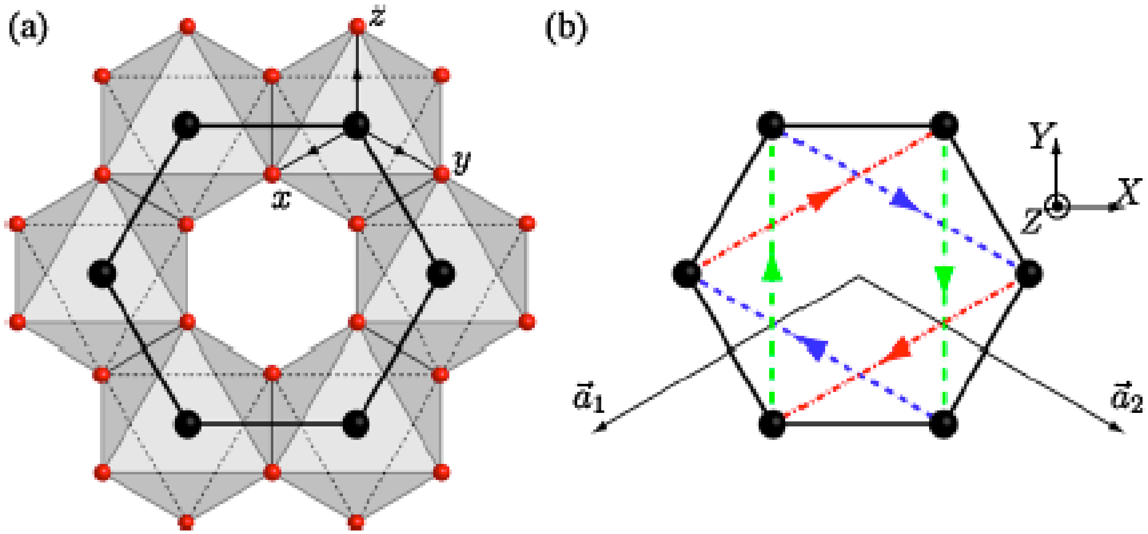


$$\boxed{\mathcal{H}_{ij}^{(\gamma)} = -J S_i^{\gamma} S_j^{\gamma}}$$



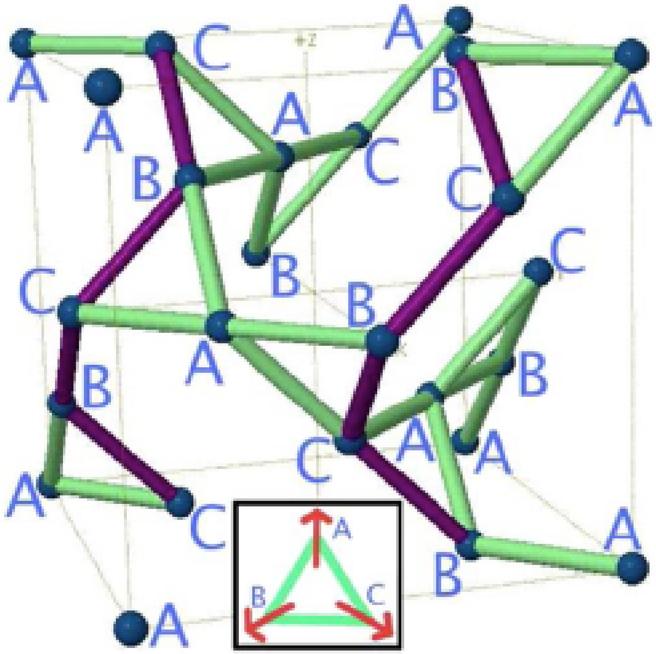
Jackeli & Khaliullin, PRL 102, 017205 (2009)

Quantum Spin Hall Effect in Na_2IrO_3?



Shitade *et al.*, PRL 102, 256403 (2009)

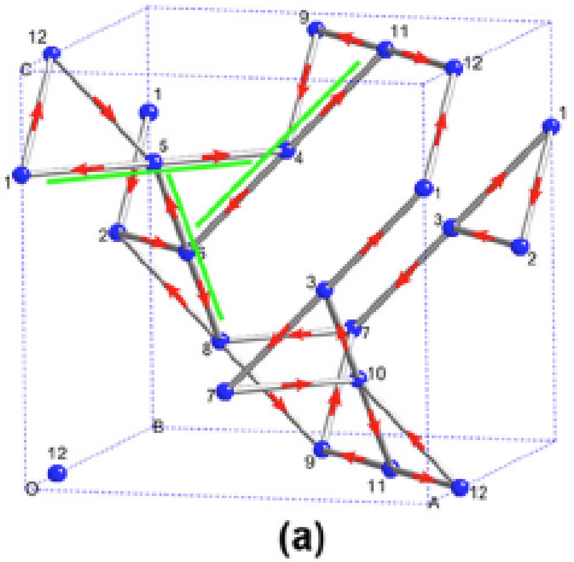
$Na_4Ir_3O_8$ - Ir ions form a network of corner sharing triangles



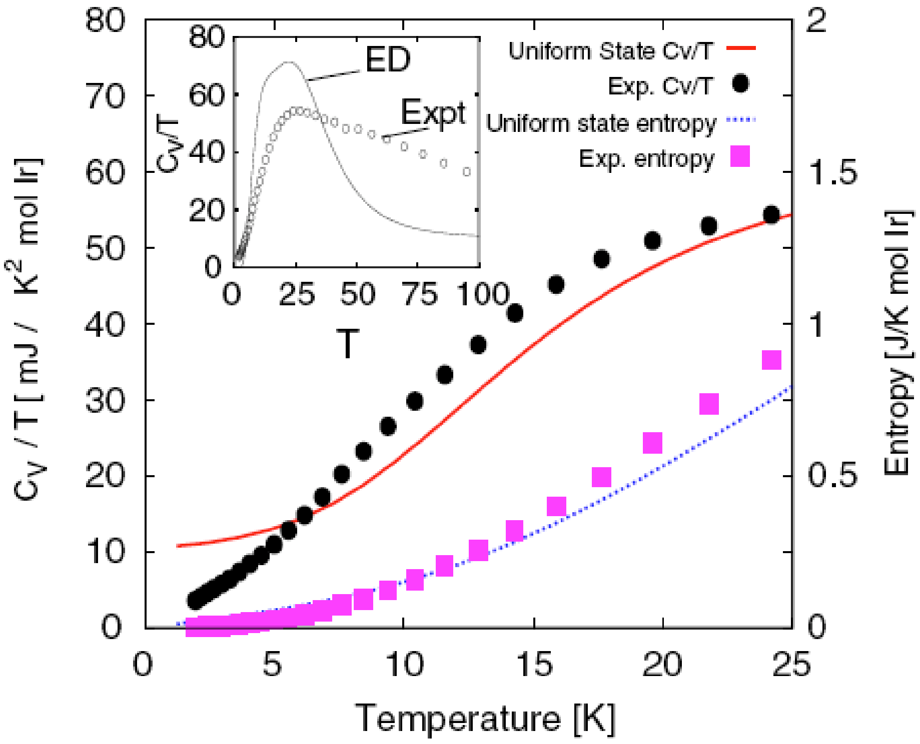
Semiclassical - J S·S

Lawler *et al.*, PRL 100, 227201 (2008)

10 site loops



Zhou *et al.*, PRL 101, 197201 (2008)



Lawler *et al.*, PRL 101, 197202 (2008)

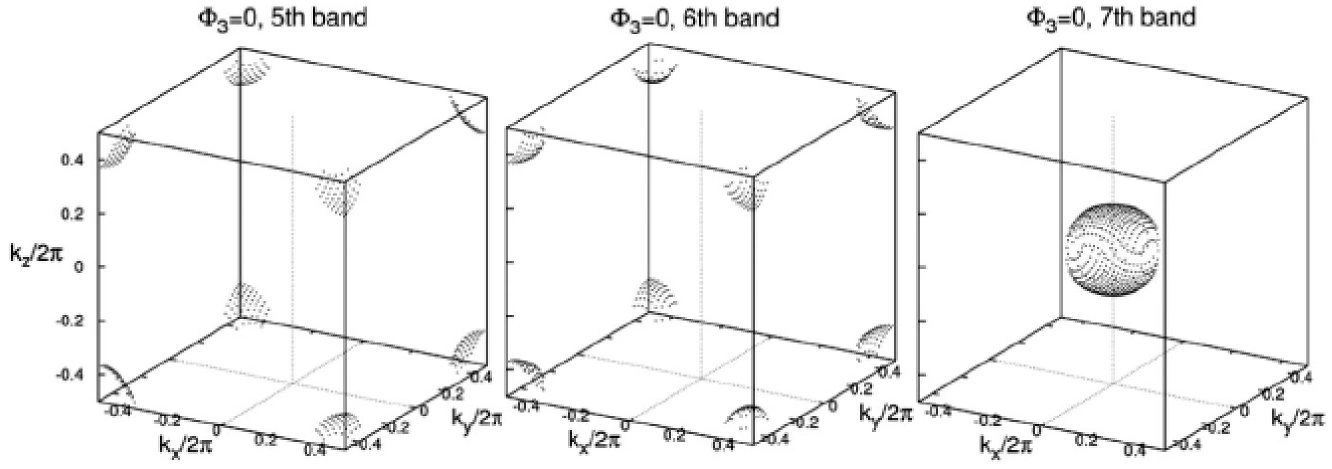


FIG. 2. Fermi surfaces of the zero flux state at half-filling.

Pairing Instability of Spinon Fermi surface?

Line Nodes ($C \sim T^2$)

1. Δ_{singlet}

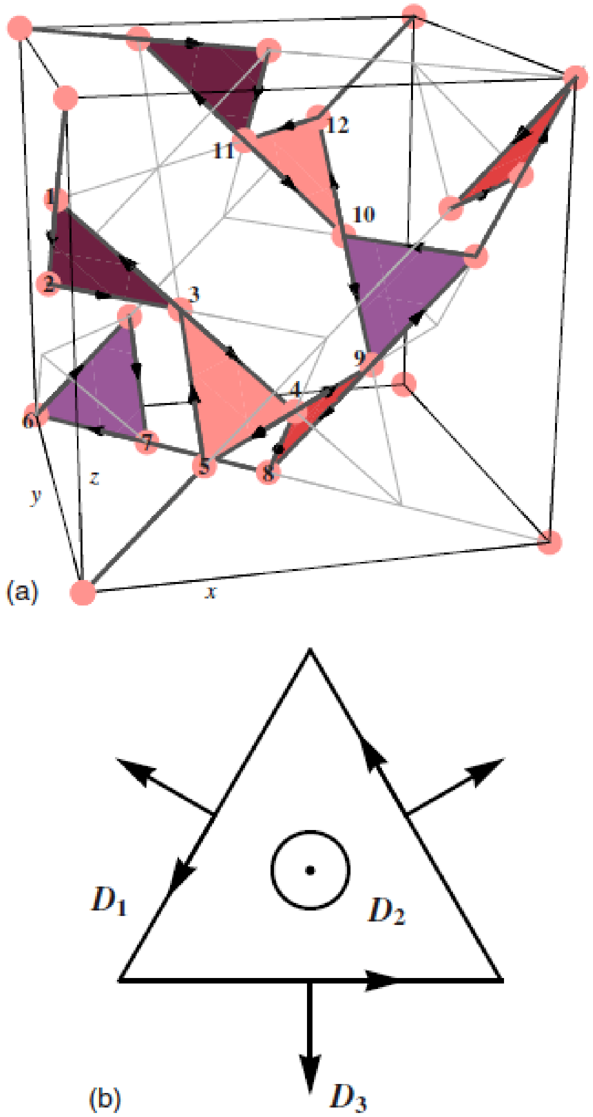
2. $\Delta = \Delta_{\text{singlet}} + \Delta_{\text{triplet}}$
   line nodes if Δ_{triplet} is large enough

   Zhou *et al*., PRL 101, 197201 (2008)

3. Δ_{triplet}
   line nodes on zone face

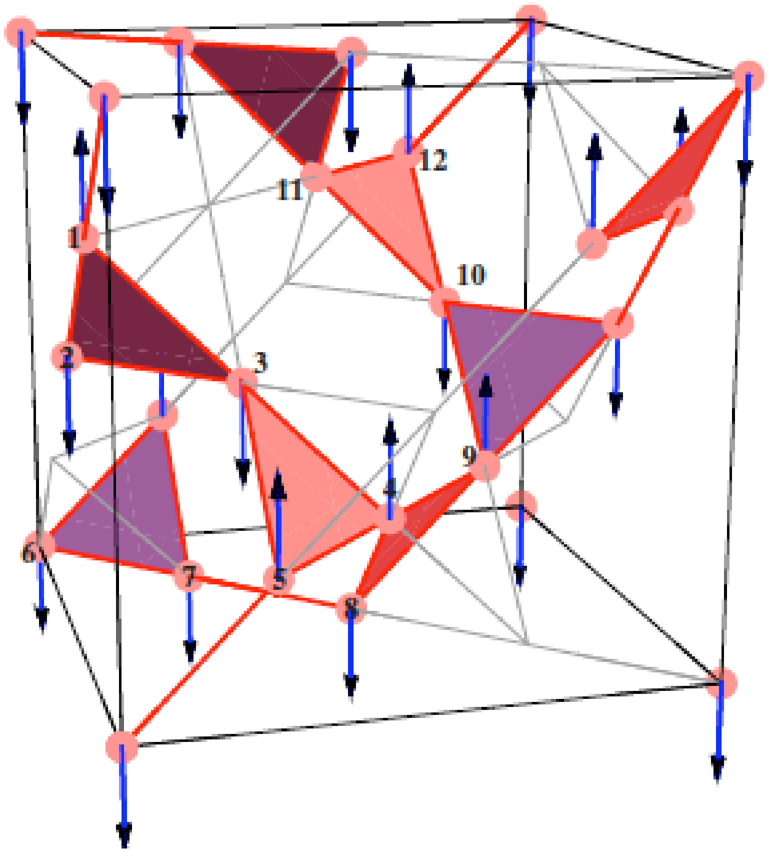
   Micklitz & Norman, PRB 80, 100506 (2009)

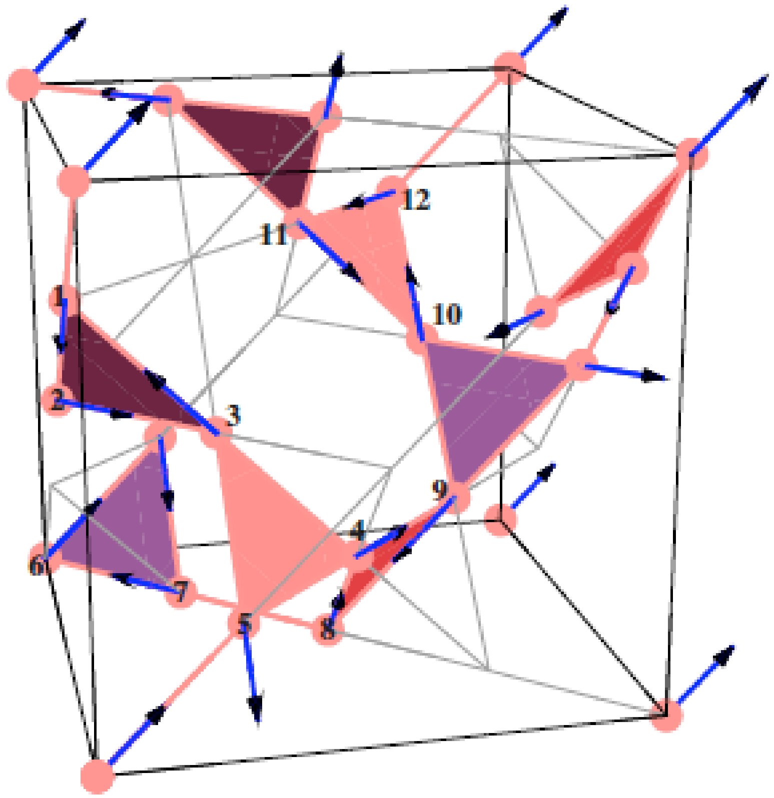
$Na_4Ir_3O_8$ - anisotropy important due to spin-orbit coupling



Chen & Balents, PRB 78, 094403 (2008)

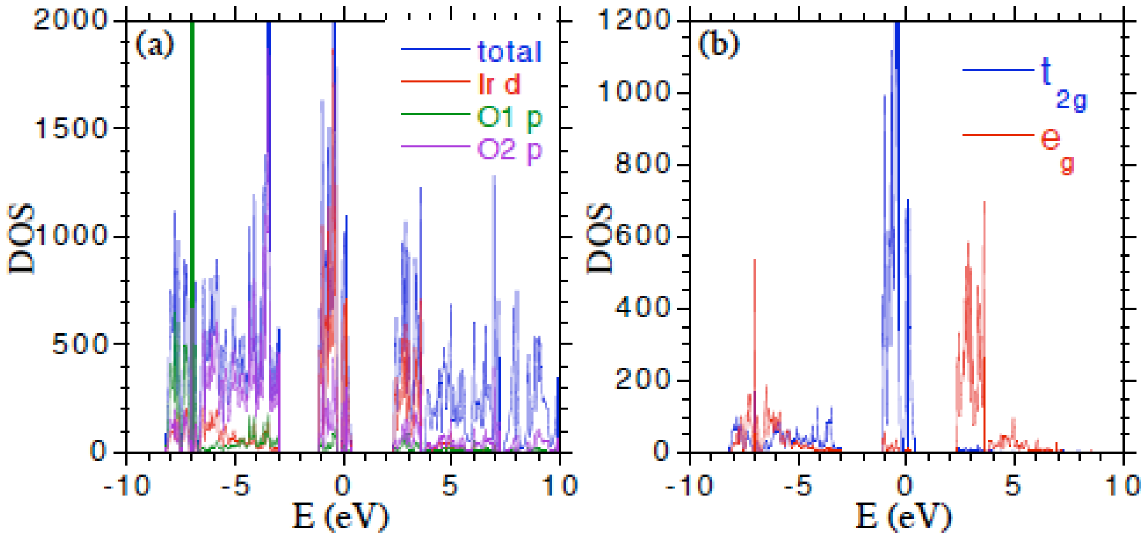
Possible ground states in the presence of anisotropy



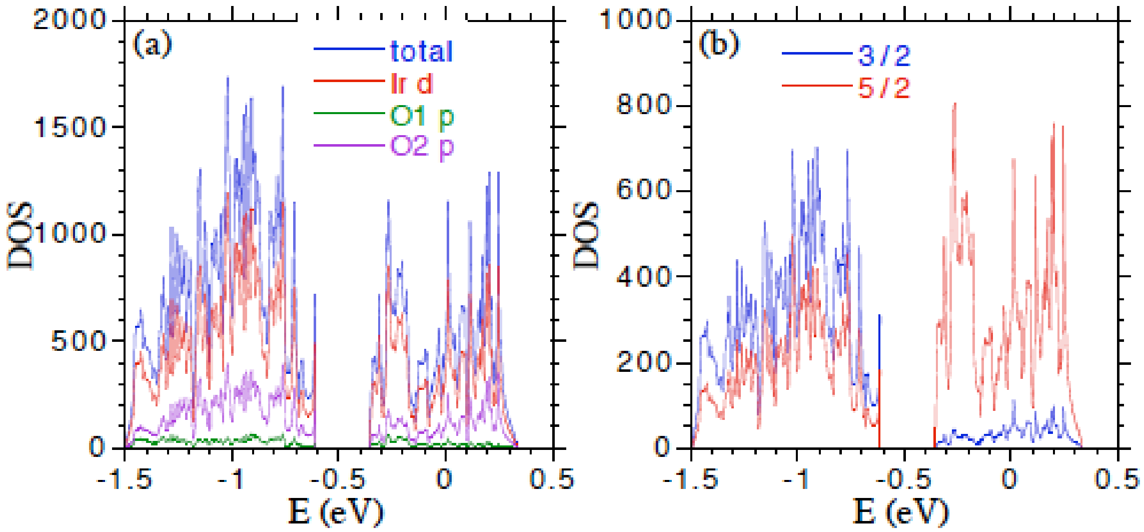


Chen & Balents, PRB 78, 094403 (2008)

LDA



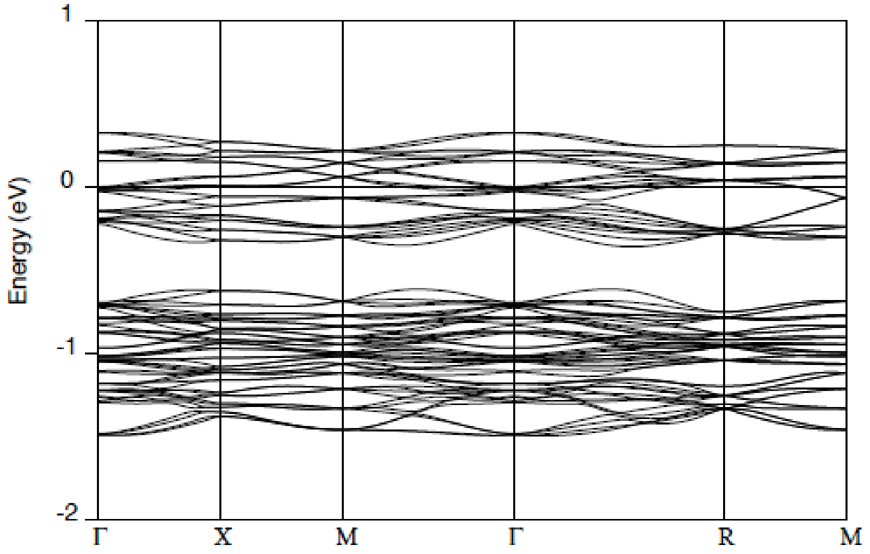
No spin-orbit



Spin-orbit

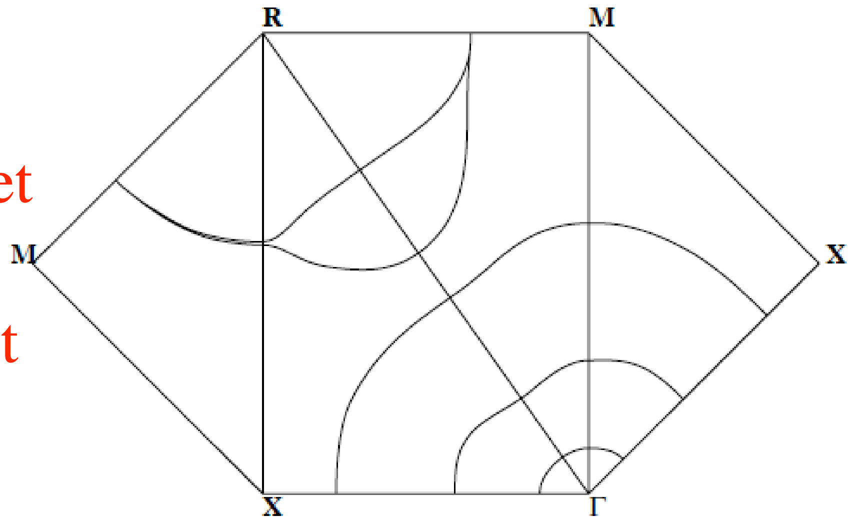
Norman & Micklitz, arXiv:0911.1373

LDA (spin-orbit)

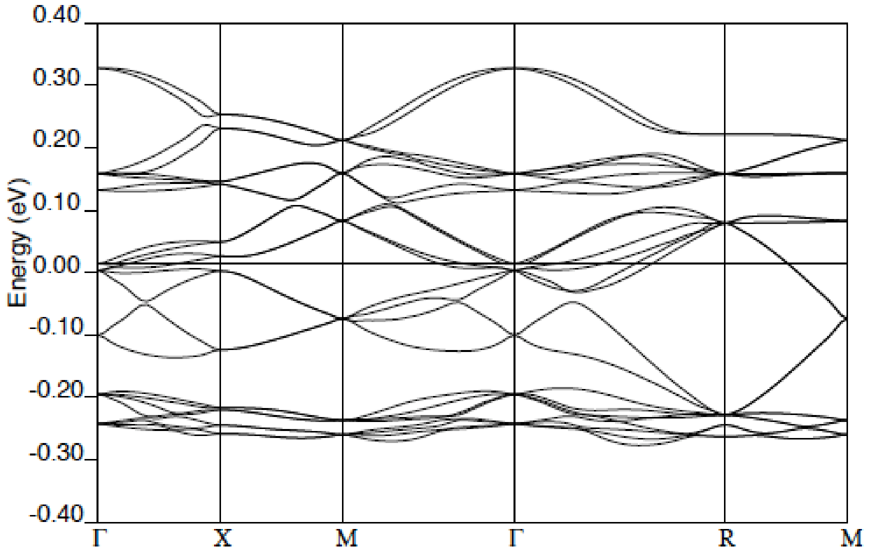


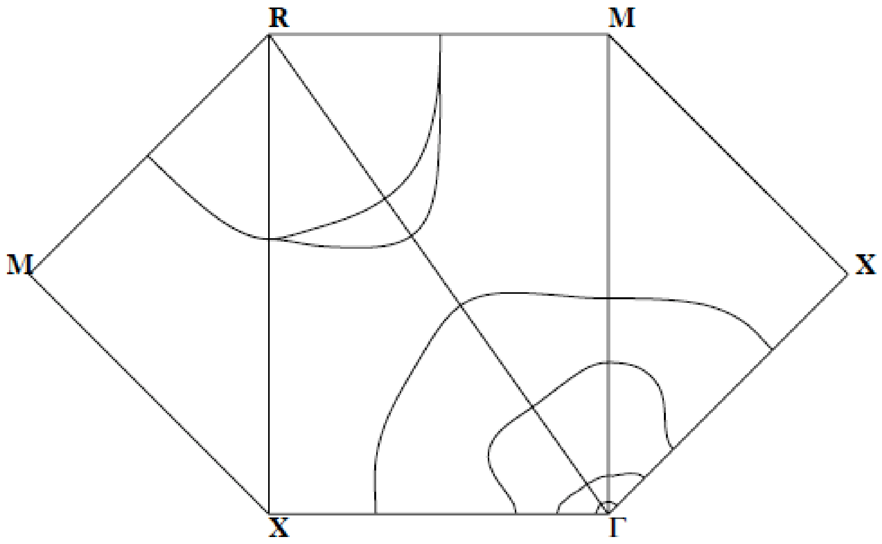
doublet

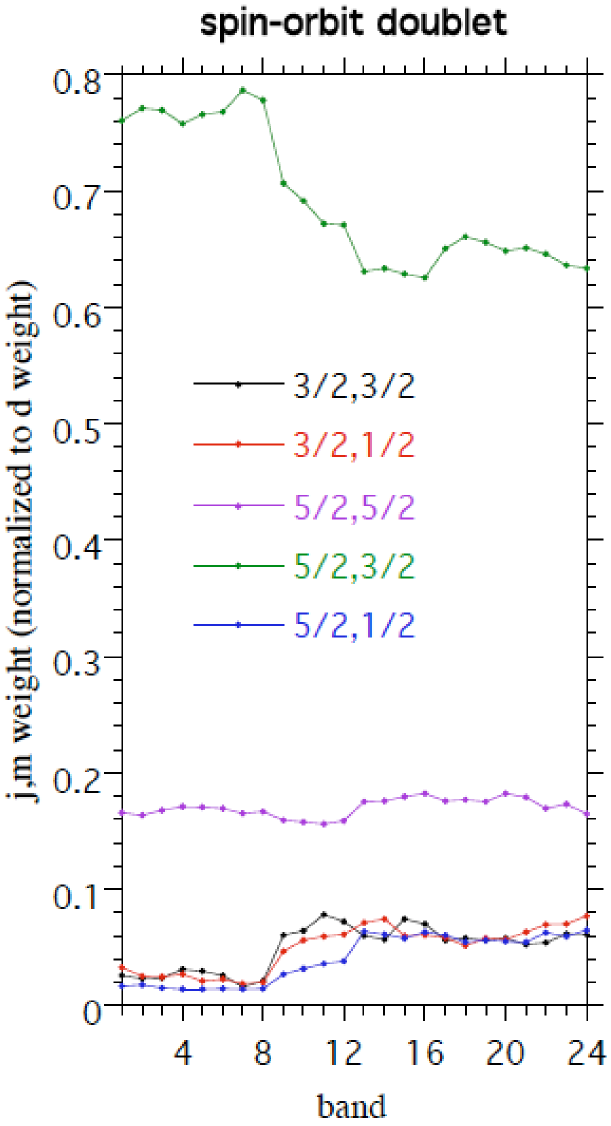
quartet



Tight Binding Fit







Effective cubic model - 83% |5/2,±3/2> + 17% |5/2,±1/2>

Direct Ir-Ir Exchange is Isotropic!

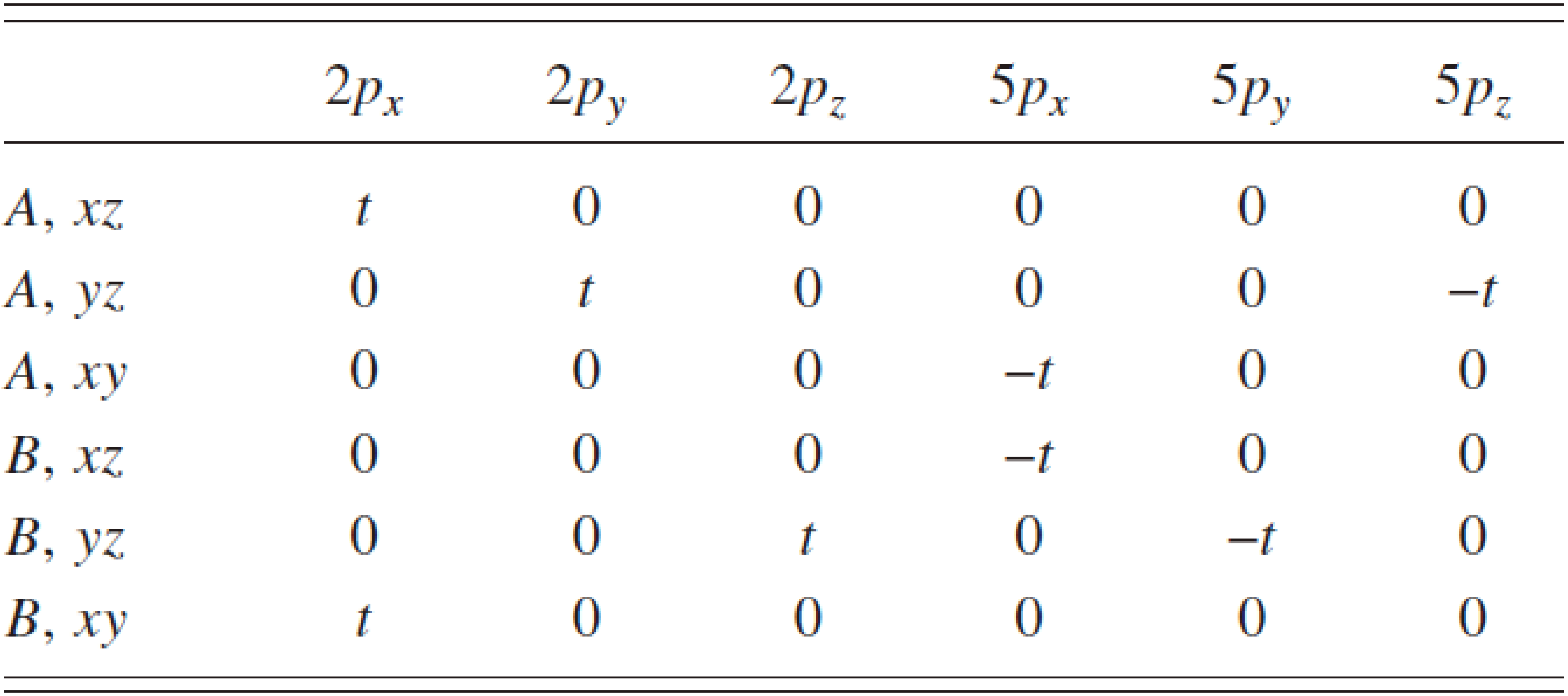
$J = 2\, t^2/U$

where

$$t = \frac{1}{4}t^{\sigma}_{dd} + \frac{1}{3}t^{\pi}_{dd} + \frac{5}{12}t^{\delta}_{dd}$$

But superexchange is present which should gives rise to anisotropic exchange plus Dzyaloshinskii-Moriya

$$a_{i3\uparrow} = \frac{1}{\sqrt{3}}((-i)d_{i,xz\downarrow} + d_{i,yz\downarrow} + d_{i,xy\uparrow})$$

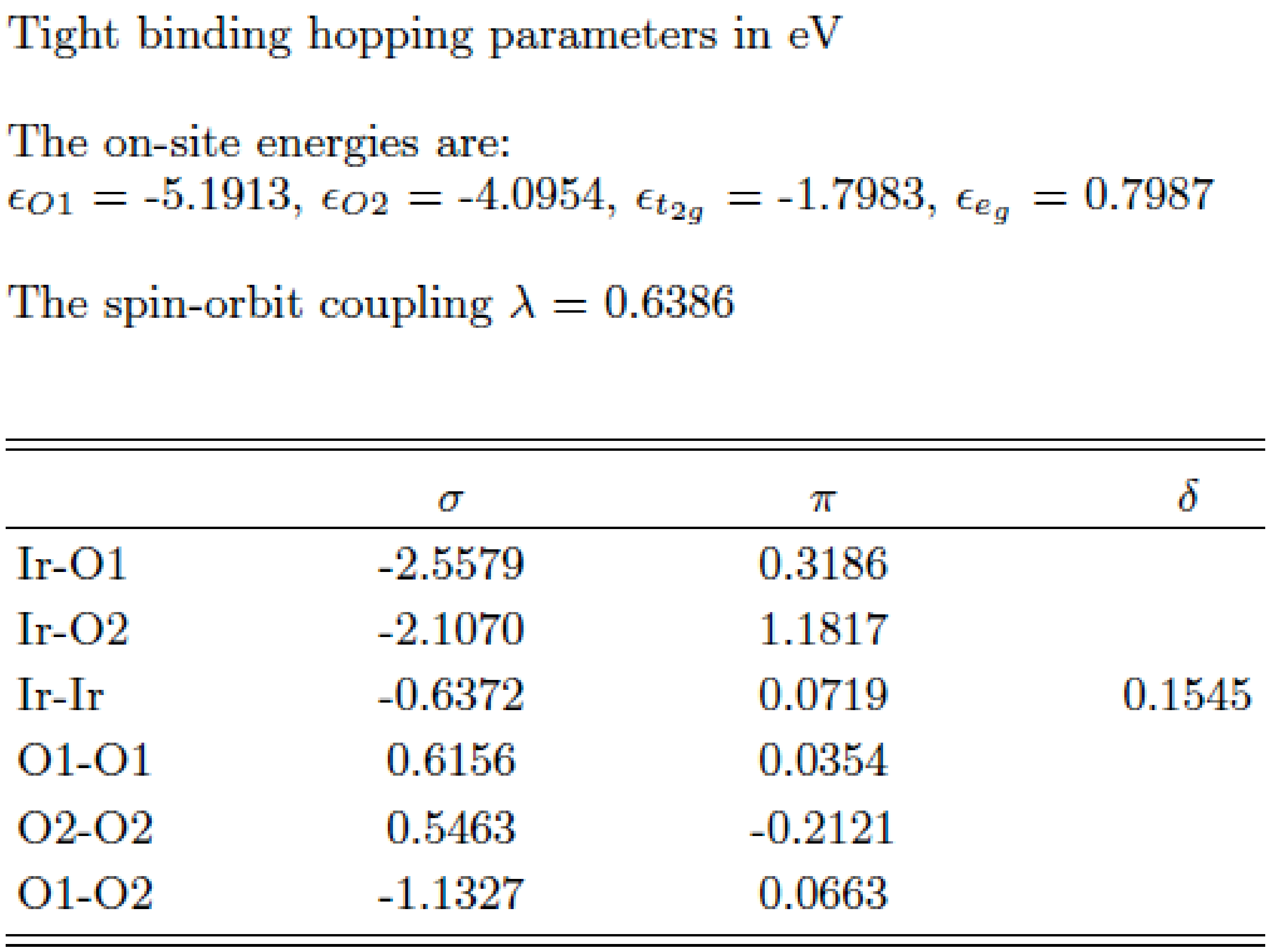


	$2p_x$	$2p_y$	$2p_z$	$5p_x$	$5p_y$	$5p_z$
A, xz	t	0	0	0	0	0
A, yz	0	t	0	0	0	$-t$
A, xy	0	0	0	$-t$	0	0
B, xz	0	0	0	$-t$	0	0
B, yz	0	0	t	0	$-t$	0
B, xy	t	0	0	0	0	0

$$\mathcal{H}_{AB} = -JS_A^x S_B^x + JS_A^y S_B^y + JS_A^z S_B^z,$$

Chen & Balents, PRB 78, 094403 (2008)

Tight Binding Fit (18 parameters)



Tight binding hopping parameters in eV

The on-site energies are:
ϵ_{O1} = -5.1913, ϵ_{O2} = -4.0954, $\epsilon_{t_{2g}}$ = -1.7983, ϵ_{e_g} = 0.7987

The spin-orbit coupling $\lambda = 0.6386$

	σ	π	δ
Ir-O1	-2.5579	0.3186	
Ir-O2	-2.1070	1.1817	
Ir-Ir	-0.6372	0.0719	0.1545
O1-O1	0.6156	0.0354	
O2-O2	0.5463	-0.2121	
O1-O2	-1.1327	0.0663	

Norman & Micklitz, arXiv:0911.1373

Anisotropic Exchange

Exchange integrals in meV (U=0.5 eV, U_p=0)

$$H_{ex} = (J_d + J_s)\mathbf{S}_n \cdot \mathbf{S}_m + \mathbf{D}^{nm} \cdot (\mathbf{S}_n \times \mathbf{S}_m) + \mathbf{S}_n \cdot \mathbf{\Gamma}^{nm} \cdot \mathbf{S}_m$$

Ir site m is along (0,1,-1) relative to Ir site n

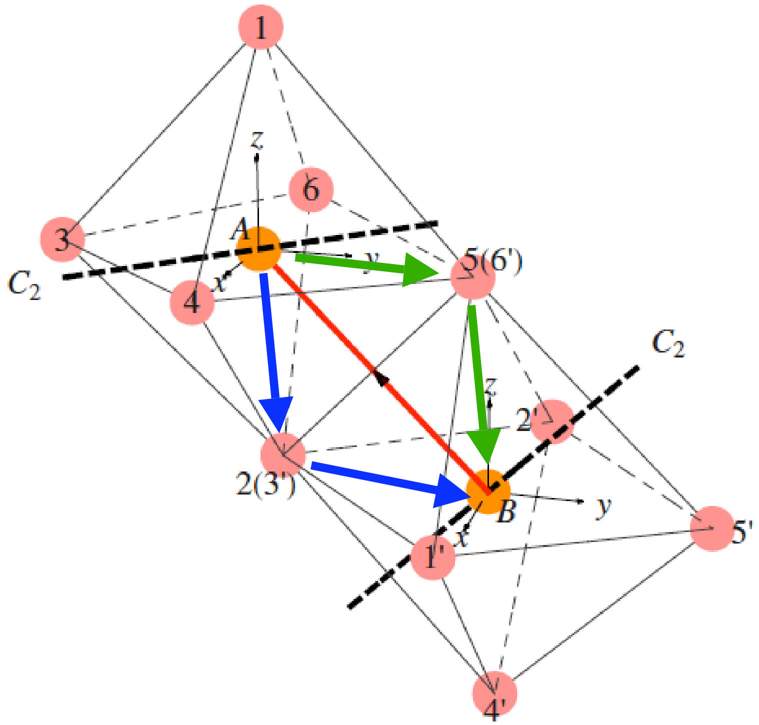
$J_d = 20.1$ meV, $J_s = 12.9$ meV

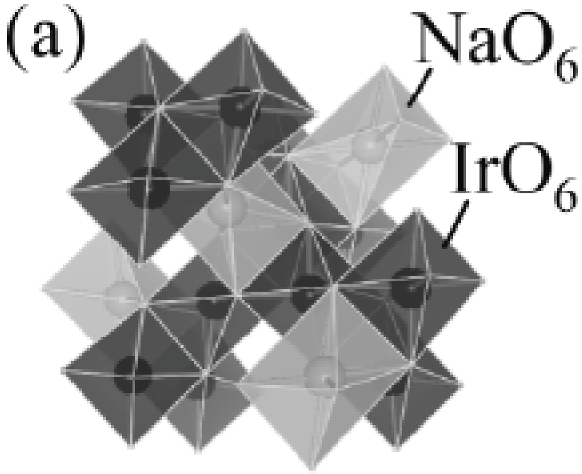
$J_{ii} = J_d + J_s + \Gamma_{ii}$

i (jk)	x (xy)	y (xz)	z (yz)
D_i	47.3	1.3	-4.7
Γ_{ii}	36.1	-36.8	-36.2
Γ_{jk}	2.1	-8.3	-0.2
J_{ii}	69.2	-3.7	-3.1

How to Get Rid of the Superexchange

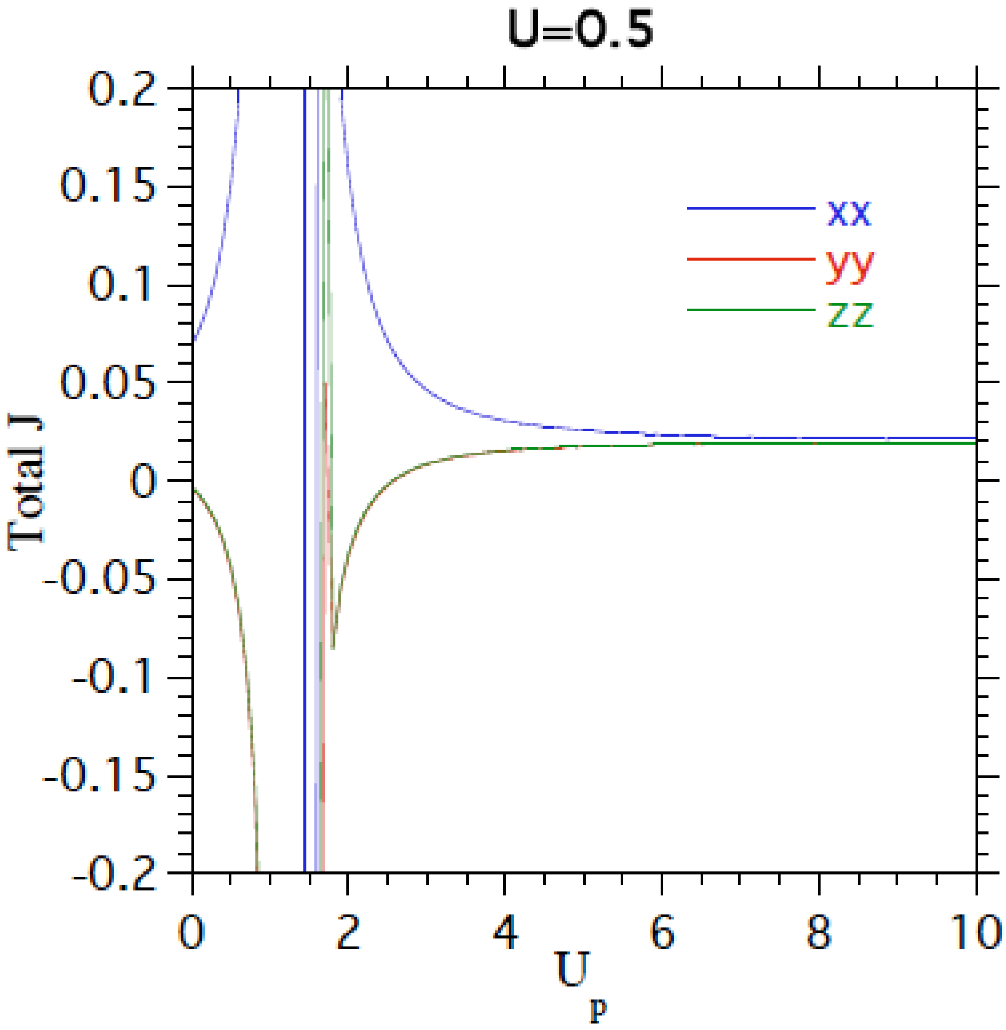
Dephasing due to partial Na site occupation?





How to Get Rid of the Superexchange

Large U_p?



How to Detect a Spinon Fermi Surface

Norman & Micklitz, PRL 102, 067204 (2009)

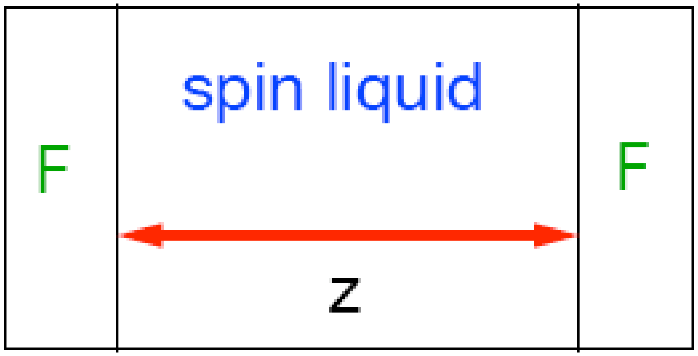


FIG. 1: (Color online) The proposed experiment involves two ferromagnetic layers (F) with a spin liquid spacer of variable thickness, z. Depending on the sign of the oscillatory coupling, the two ferromagnets will be aligned or anti-aligned.

Parkin *et al.*, PRL 64, 2304 (1990)

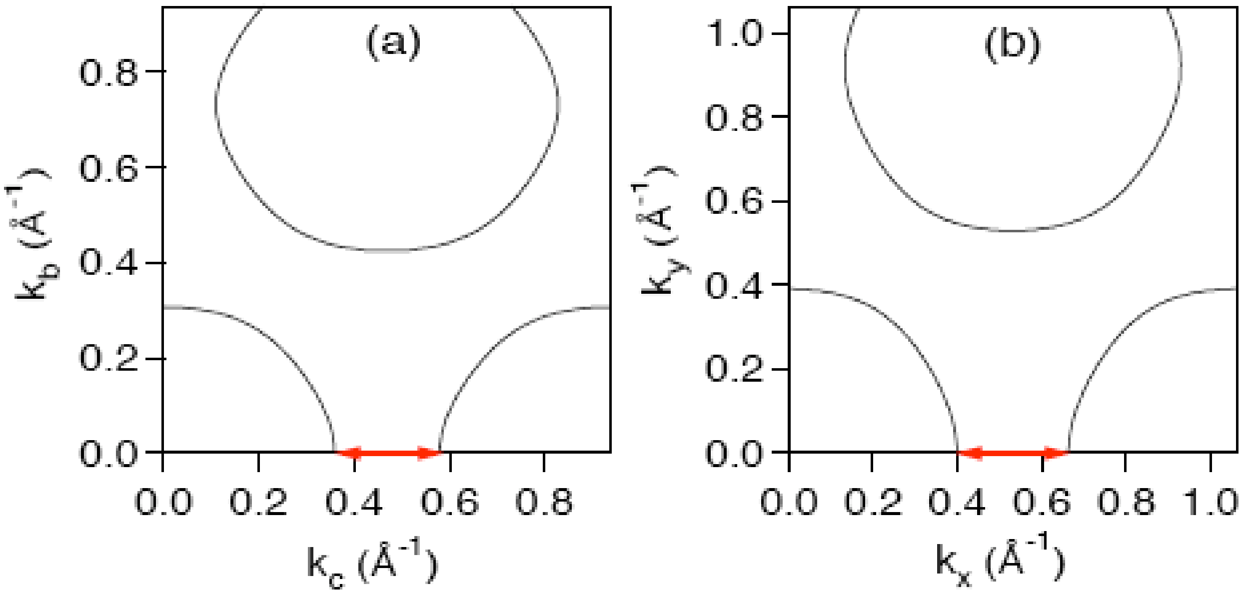


FIG. 2: (Color online) Spinon Fermi surface for (a) κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ (b=8.59Å, c=13.40Å) and (b) ZnCu$_3$(OH)$_6$Cl$_2$ (a=6.84Å). Spanning vectors are indicated by arrows.

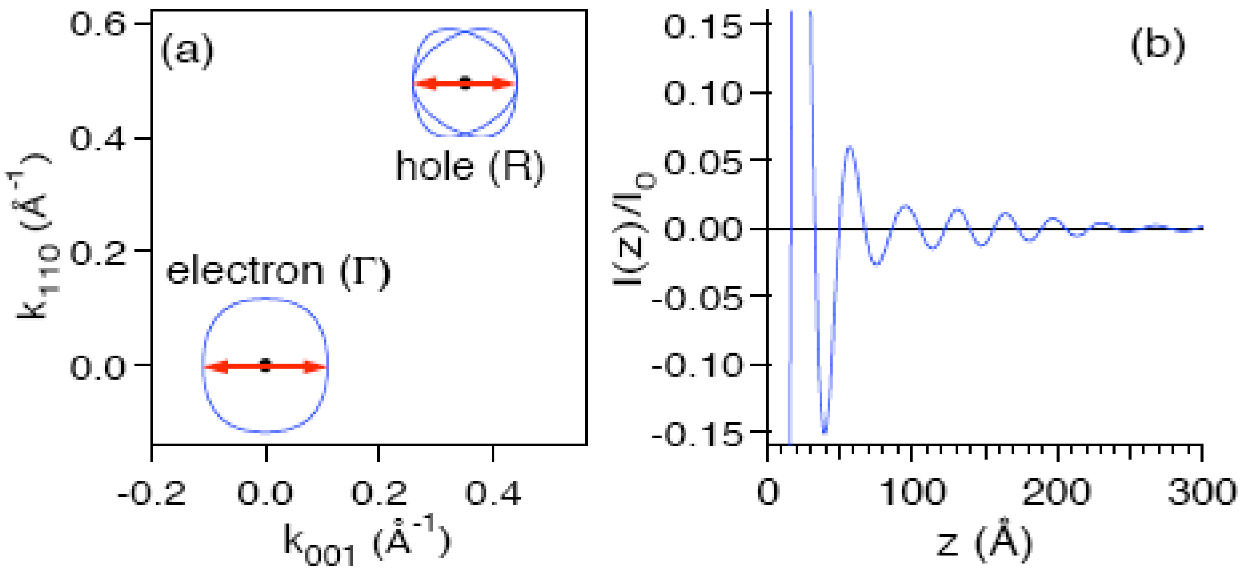


FIG. 3: (Color online) (a) Spinon Fermi surface for $Na_4Ir_3O_8$ (a=8.985Å). Spanning vectors are indicated by arrows. (b) Calculated oscillatory response from Eq. 7.

$$\boxed{I(z) = I_0(\frac{d}{z})^2 \sum_n \frac{m_n^*}{m} \sin(2k_{Fn}z)}$$

Bruno & Chappert, PRB 46, 261 (1992)

Cuprates are Mott insulators characterized by
a half filled band

So are iridates!

Can iridates be doped, and if so, will they
become high temperature superconductors?