

Classification of 3D Kitaev spin liquids

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(soon Gothenburg)



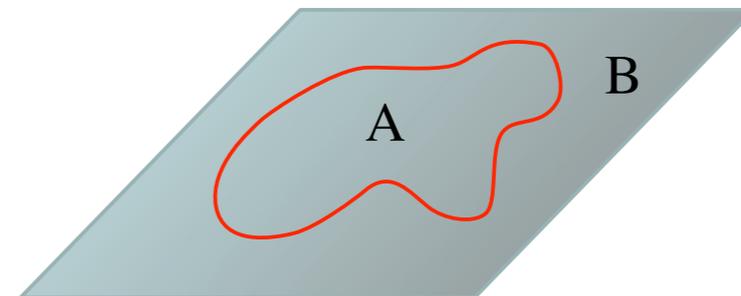
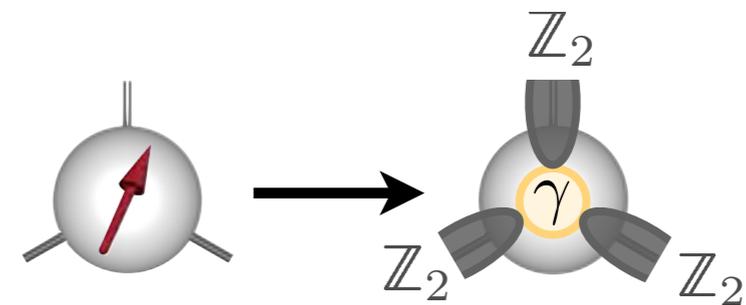
Quantum Spin Liquids

What is a Quantum Spin Liquid?

- ▶ no magnetic order
- ▶ no (spontaneous) symmetry-breaking
- ▶ strongly fluctuating spins down to zero temperature
- ▶ spin fractionalization
- ▶ long-range (topological) entanglement

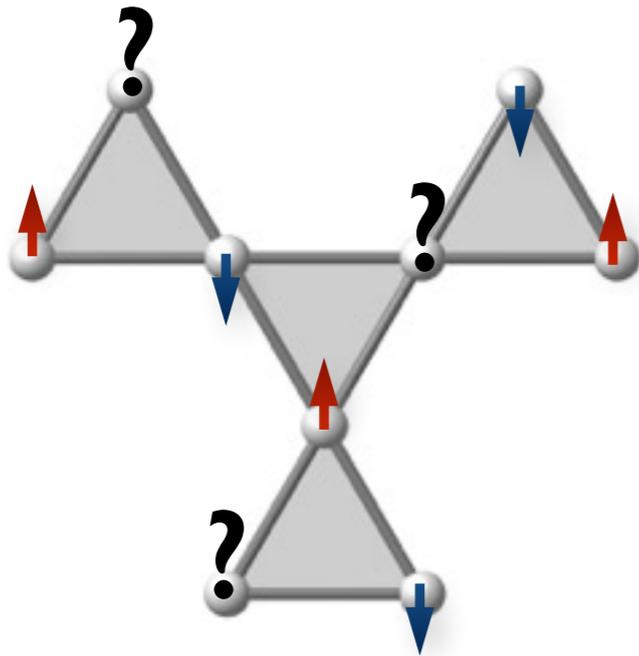


Francis Pratt / ISIS /STFC



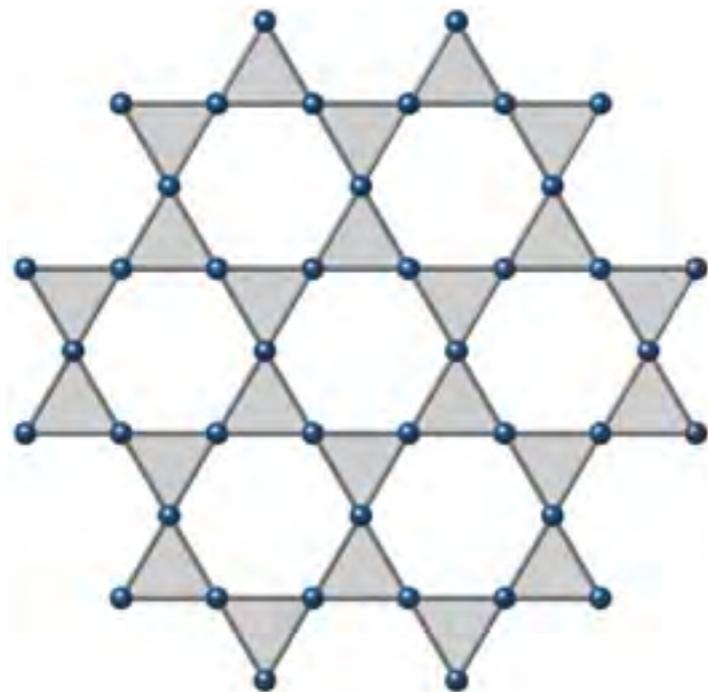
Towards quantum spin liquids – frustration

geometric frustration



Towards quantum spin liquids – frustration

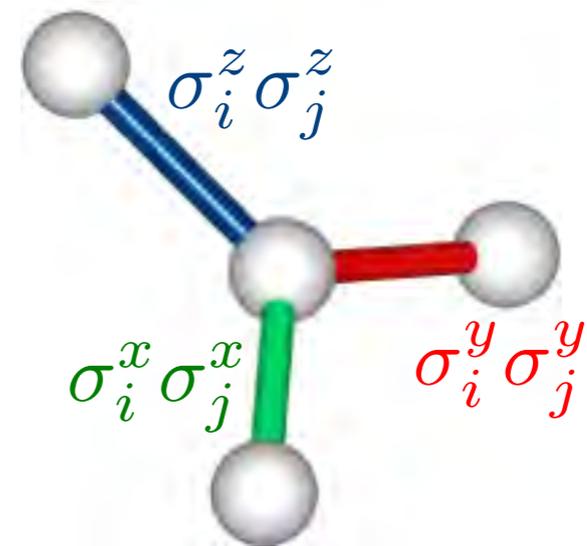
geometric frustration



Herbertsmithite
 $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$

Han et al., Nature (2012)

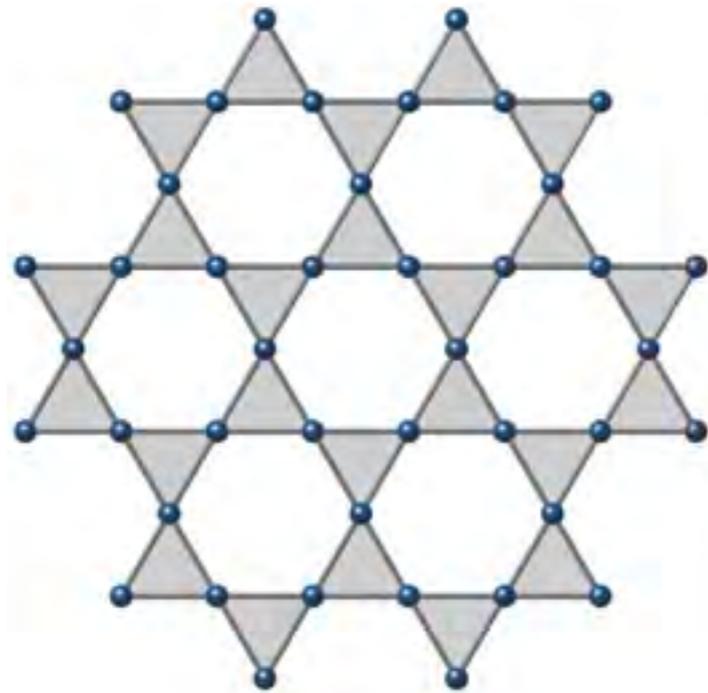
exchange frustration



Kitaev honeycomb model

Towards quantum spin liquids – frustration

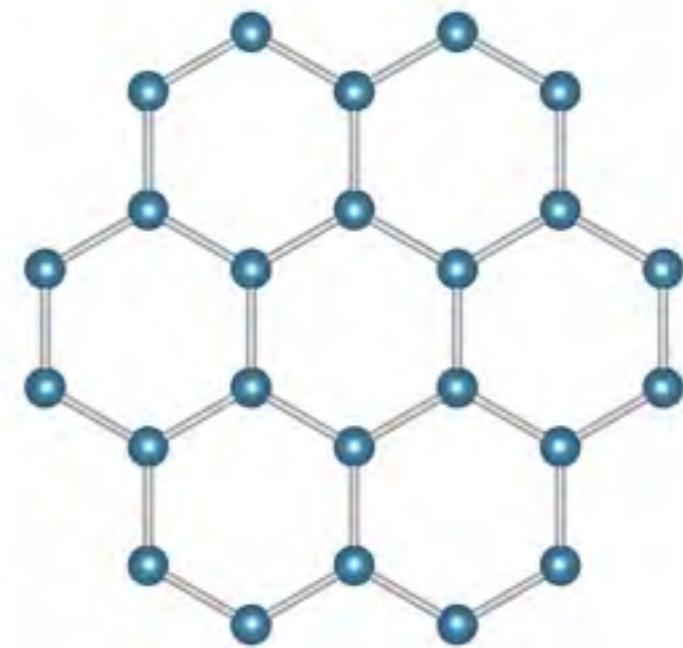
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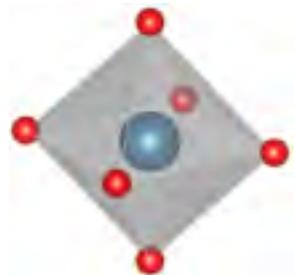
honeycomb lattice
 $\alpha\text{-Li}_2\text{IrO}_3$

Singh et al., PRL (2008)

Exchange Frustration in Iridates

G. Khaliullin, Prog.Theor. Phys. Suppl. **160**, 155 (2005)

G. Jackeli and G. Khaliullin, PRL **102**, 017205 (2009)



IrO_6

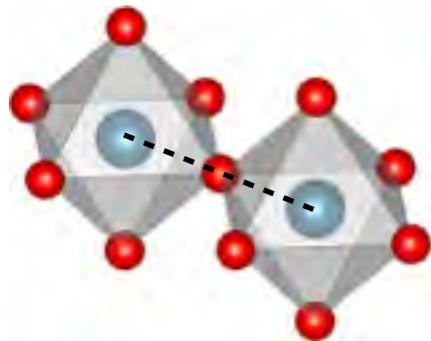
- Interplay of
- octahedral crystal field
 - spin-orbit coupling
 - e^-e^- correlations



Mott insulator with spin-orbit-entangled spin-1/2 on Ir atom

Heisenberg exchange

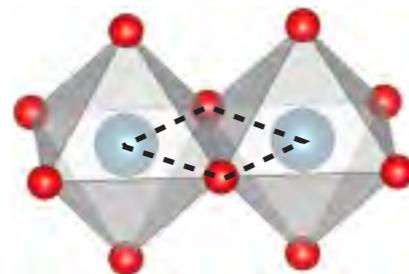
corner-sharing



Sr_2IrO_4

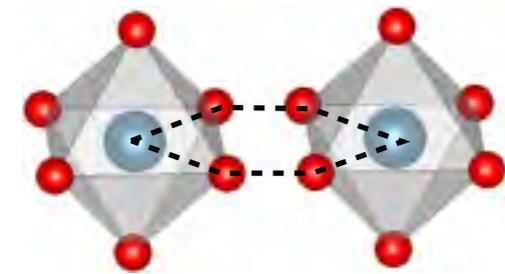
dominant Kitaev exchange

edge-sharing



Na_2IrO_3 / Li_2IrO_3

parallel edge-sharing



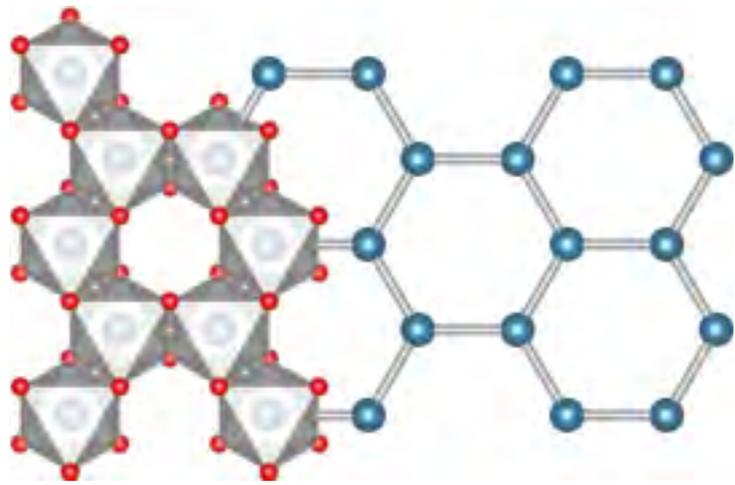
$\text{Ba}_3\text{IrTi}_2\text{O}_9$

Becker et al. PRB B **91**, 155135 (2015)

A family of Li_2IrO_3 compounds

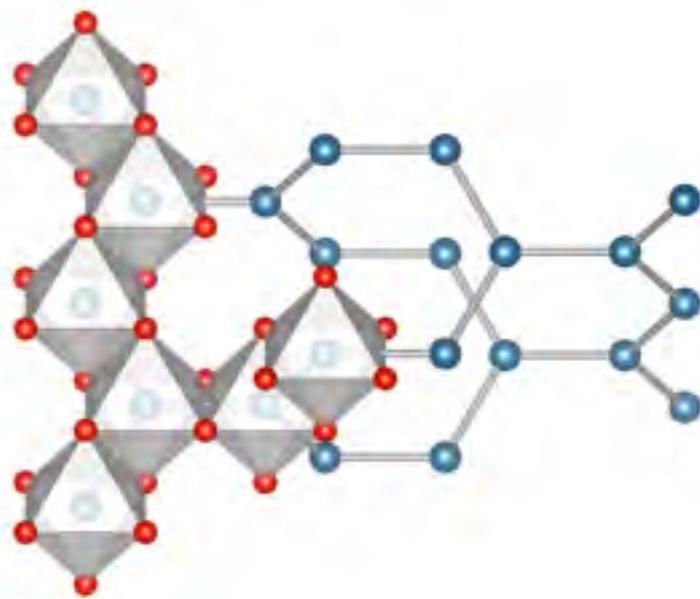
crystals

$\alpha\text{-Li}_2\text{IrO}_3$



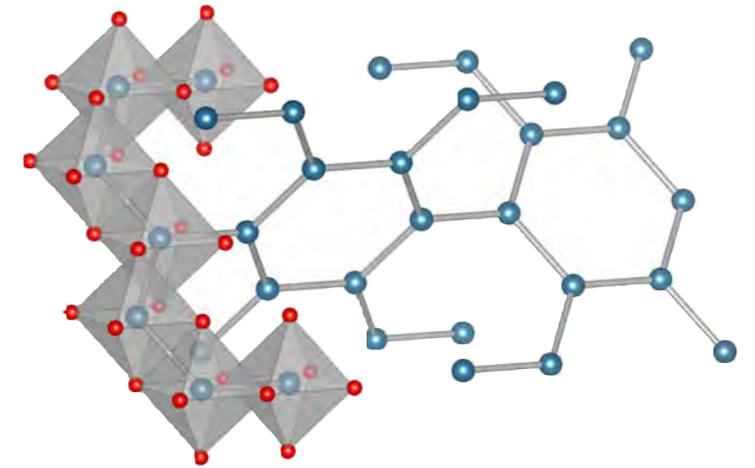
Singh et al., PRL (2008)

$\beta\text{-Li}_2\text{IrO}_3$



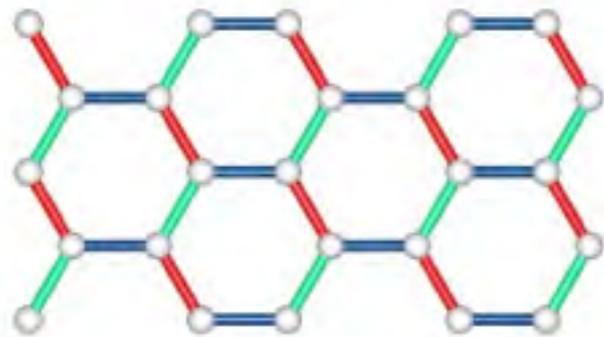
Takayama et al., PRL (2015)

$\gamma\text{-Li}_2\text{IrO}_3$

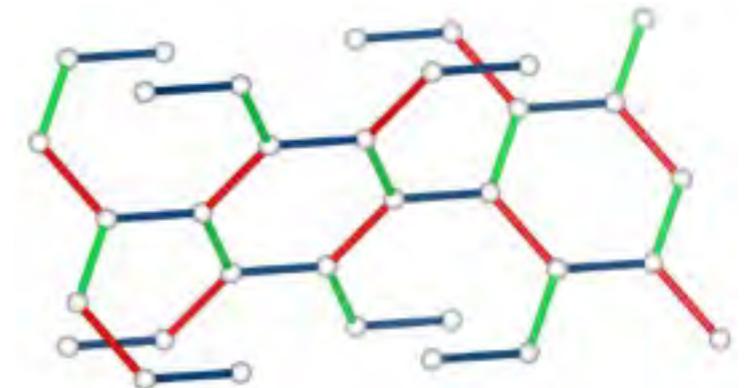
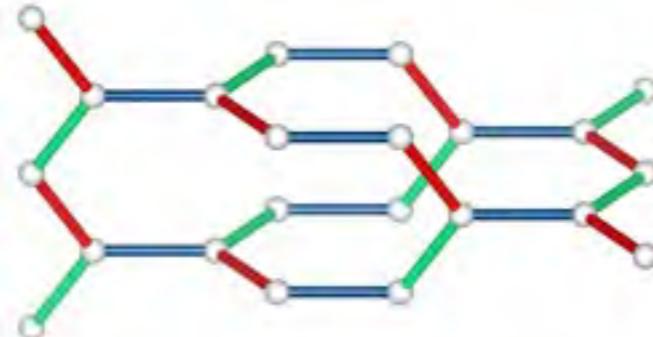


Modic et al., Nat. Comm. (2014)

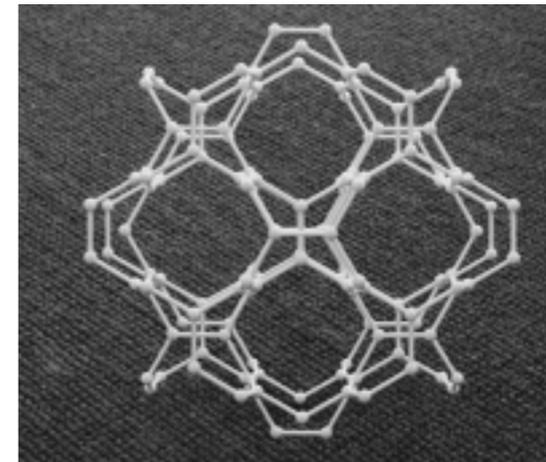
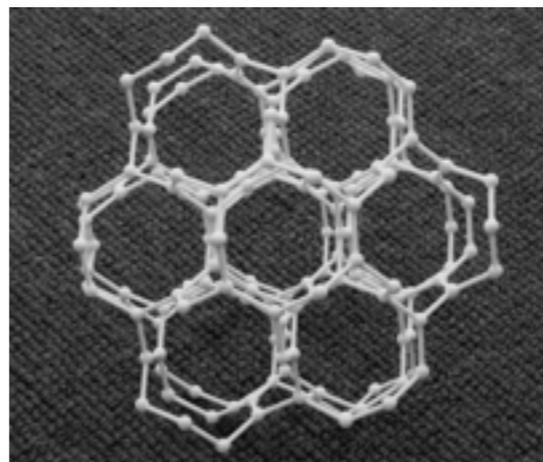
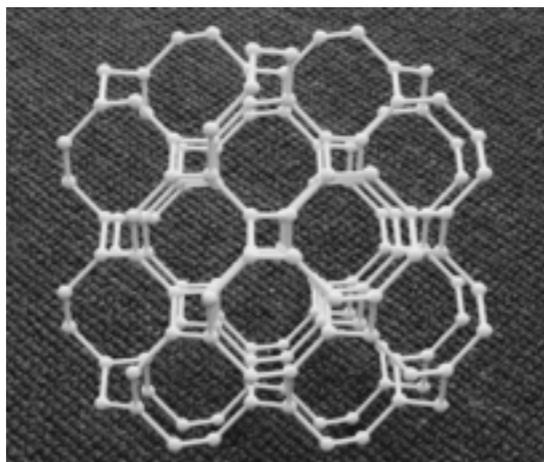
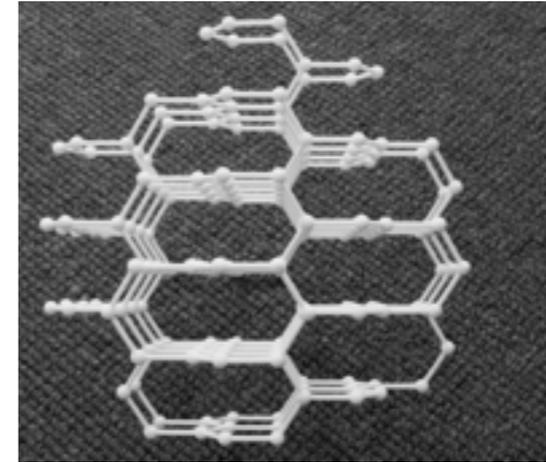
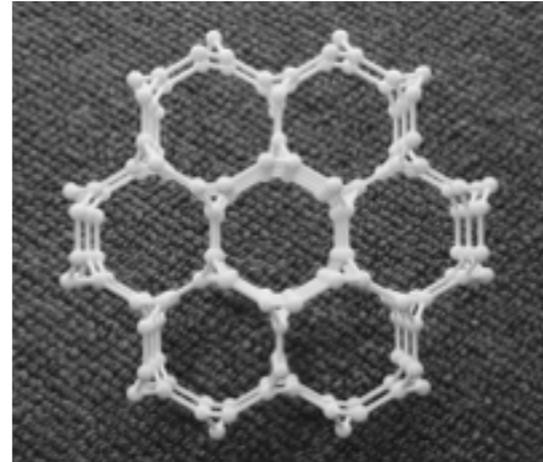
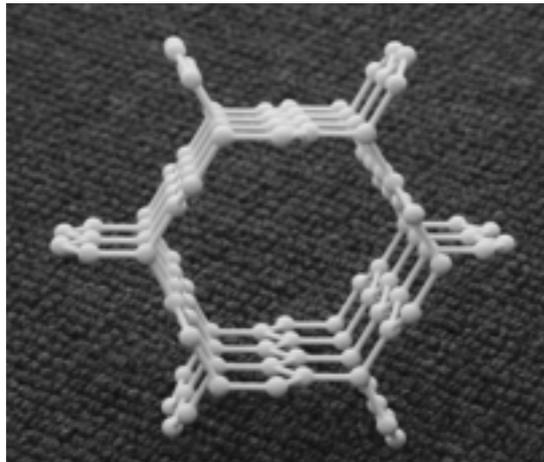
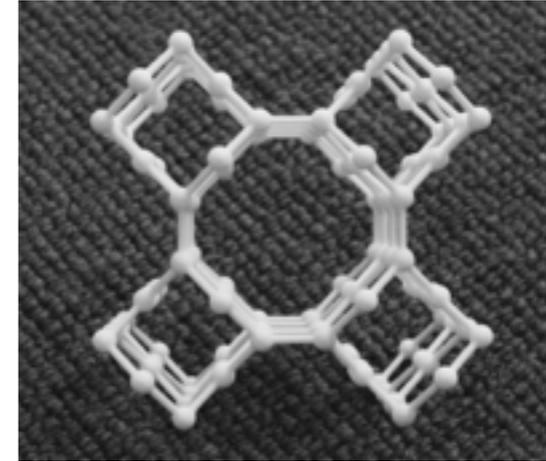
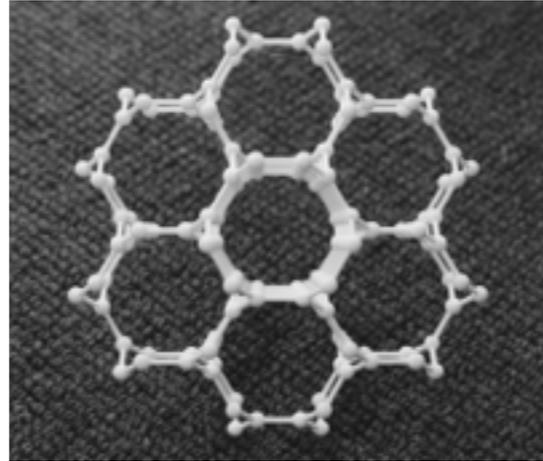
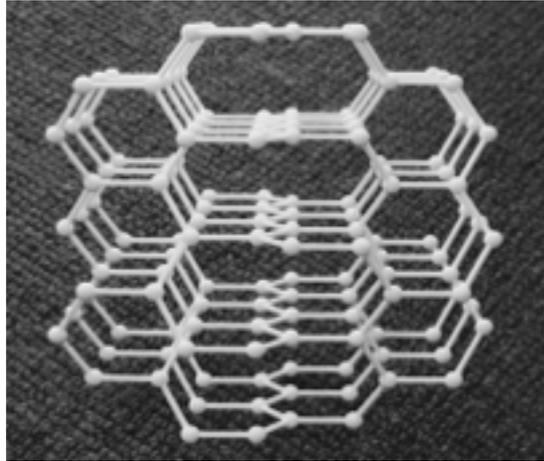
Kitaev models



Na_2IrO_3 : Gegenwart group (2010)
 RuCl_3 : Nagler group (2015)

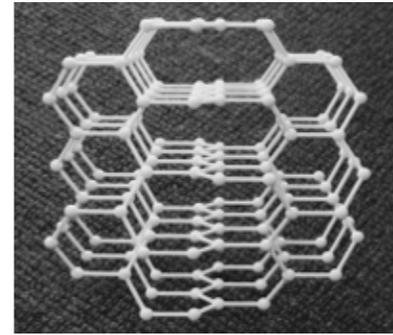
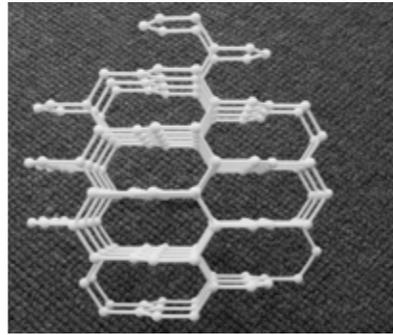
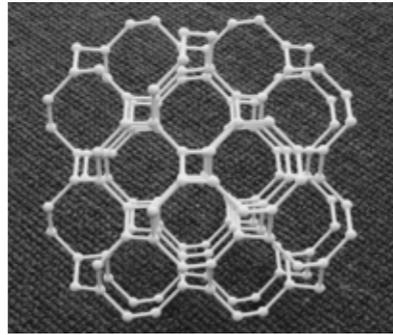


Tricoordinated lattices in 3D

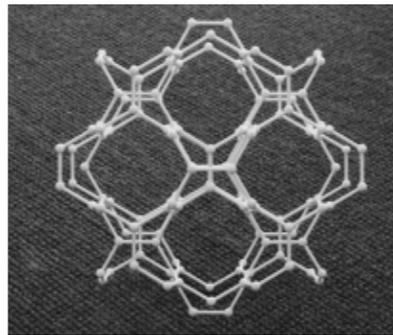
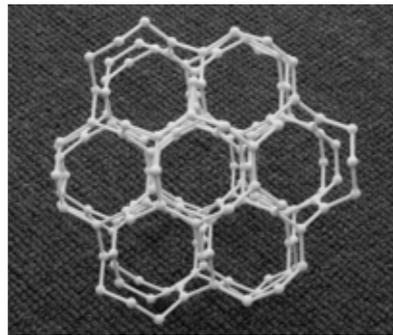


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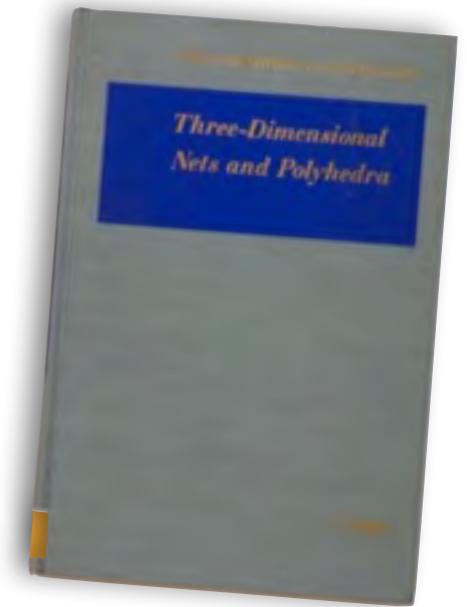
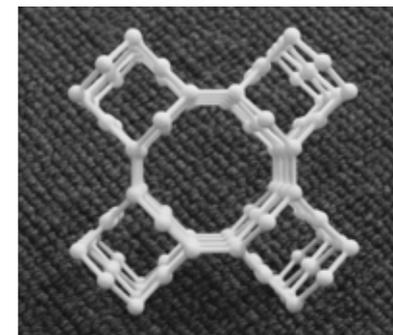
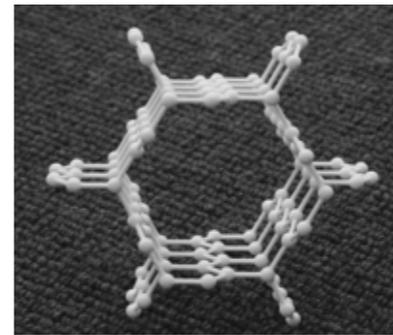
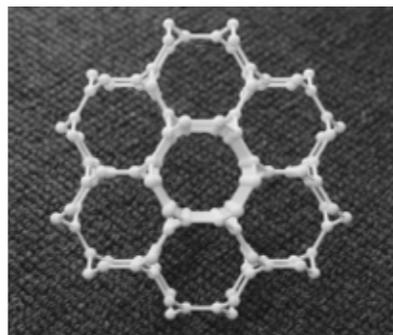
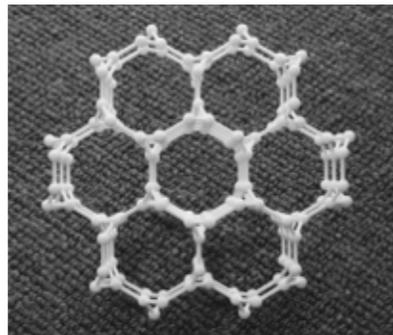
(10,3)



(9,3)



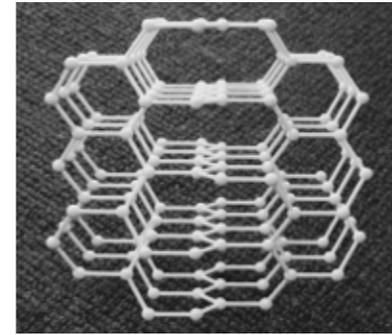
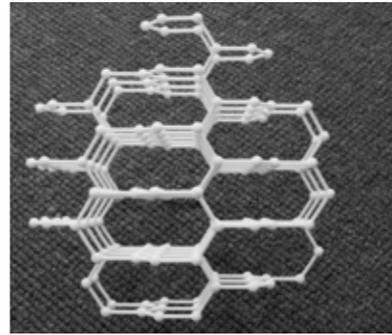
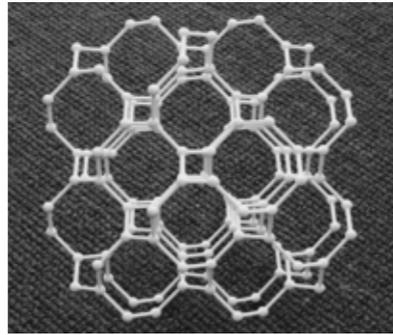
(8,3)



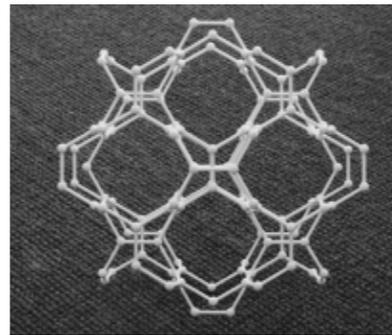
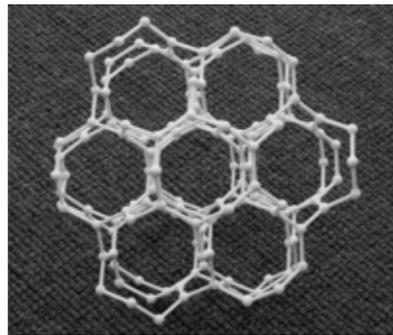
A.F.Wells, 1977

Tricoordinated lattices in 3D

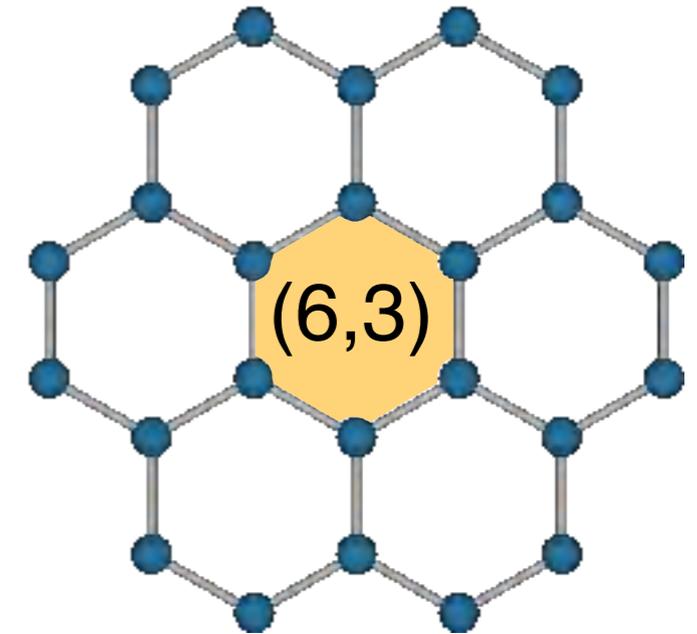
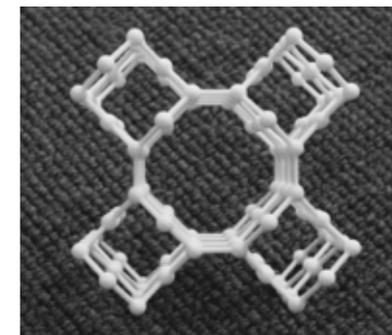
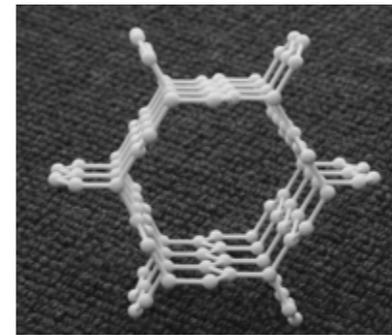
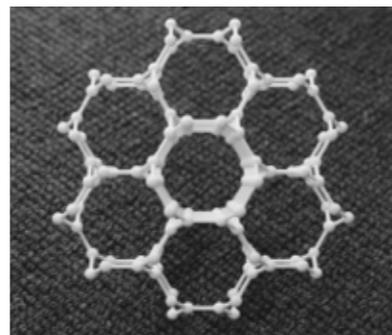
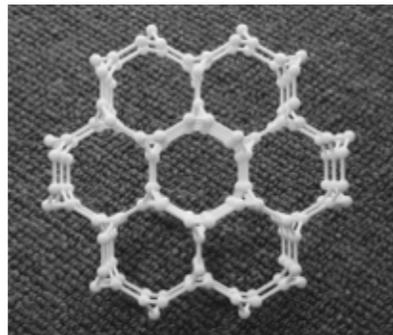
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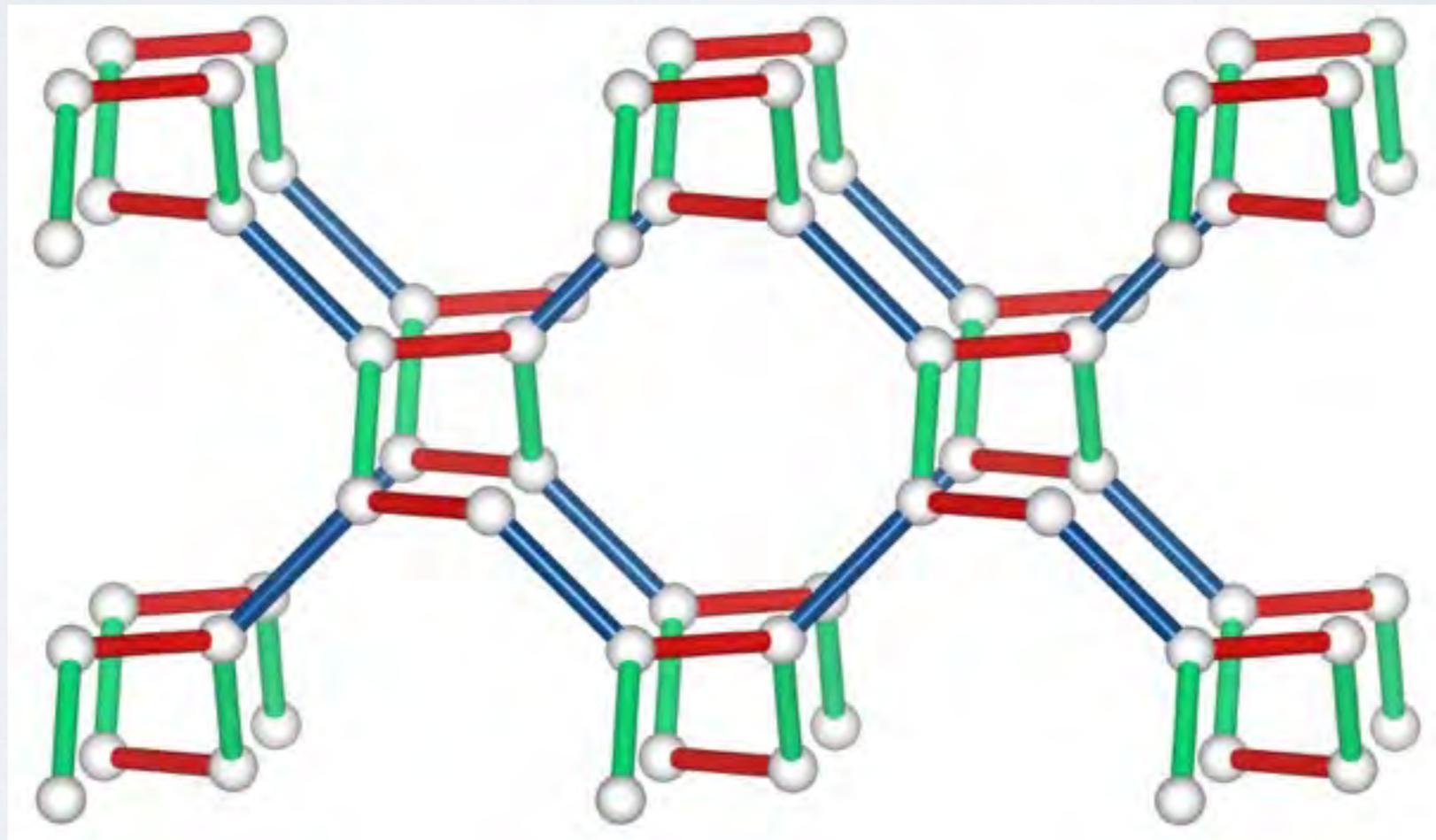
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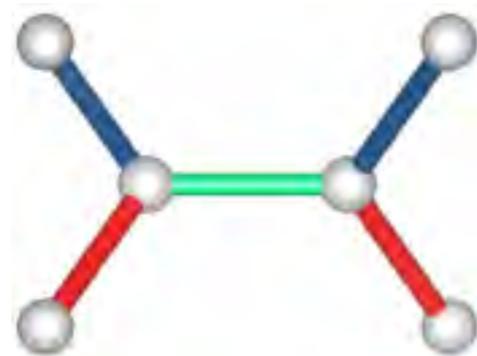


3D Kitaev models



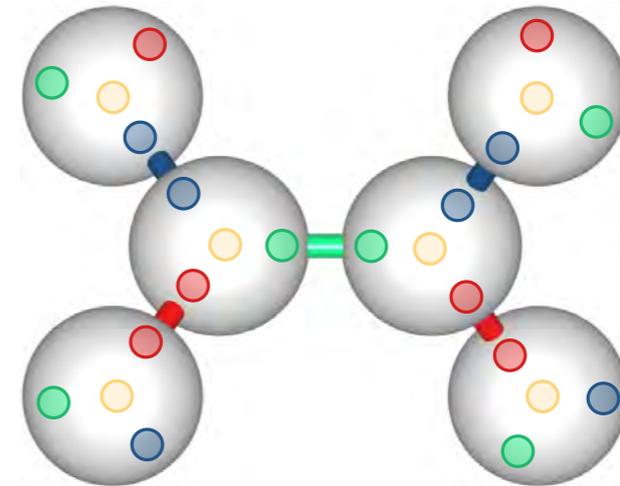
Spin fractionalization and Majorana fermions

A. Kitaev, Annals of Physics (2006)



$$H = - \sum_{\gamma\text{-bond}} J_{\gamma} \sigma_j^{\gamma} \sigma_k^{\gamma}$$

splitting spins
 $\sigma^{\alpha} = i a^{\alpha} c$



● a^x
● a^y
● a^z
● c

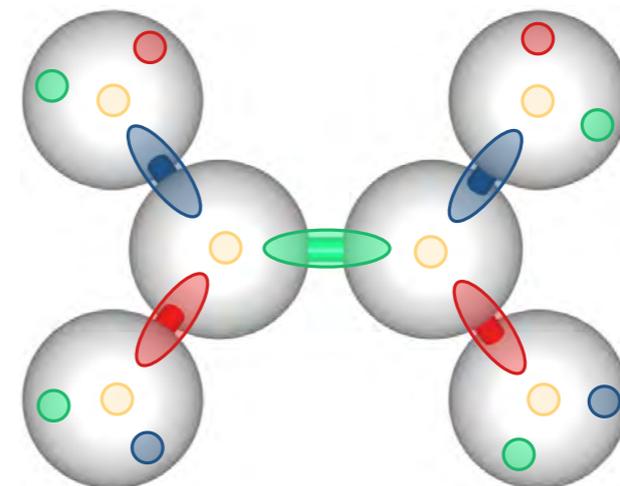
- represent spins by four **Majorana fermions**
- emergent **\mathbf{Z}_2 gauge field** on bonds

$$H = i \sum_{\gamma\text{-bond}} J_{\gamma} \hat{u}_{jk} c_j c_k$$

- gauge field is **static** and **gapped**
- Majorana fermions “**spinons**” are **free**

$$H = i \sum_{\gamma\text{-bond}} \tilde{J}_{\gamma} c_j c_k$$

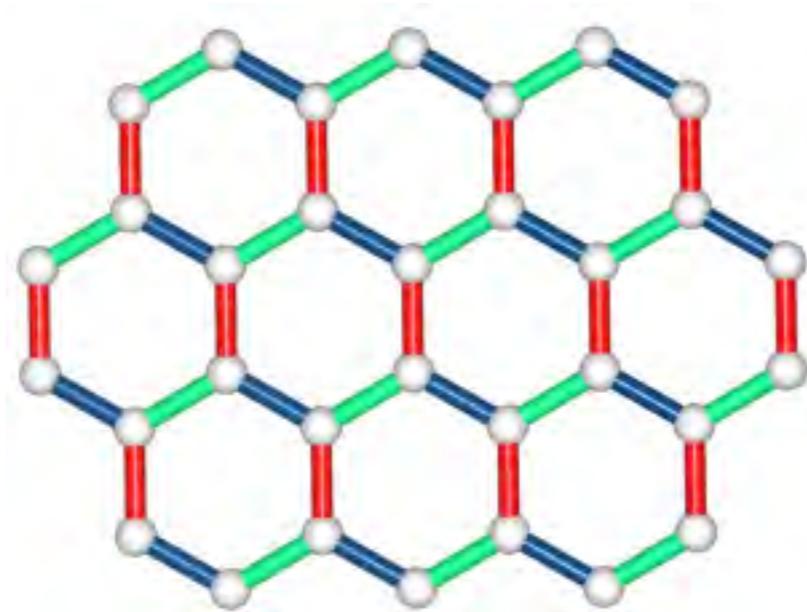
joining Majoranas
 $\hat{u}_{jk} = i a_j^{\alpha} a_k^{\alpha}$



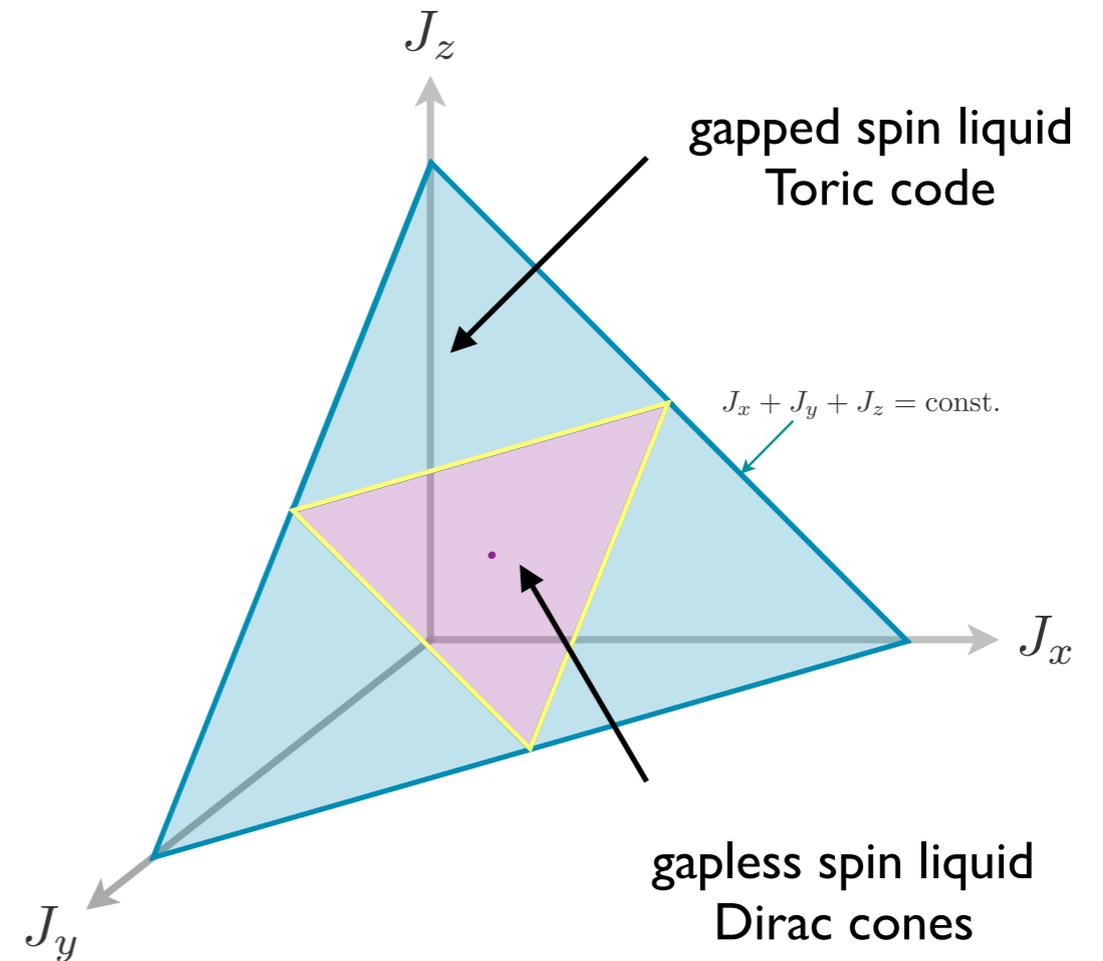
● $i a^x a^x$
● $i a^y a^y$
● $i a^z a^z$
● c

Kitaev spin liquids in 2D

A. Kitaev, Annals of Physics (2006)

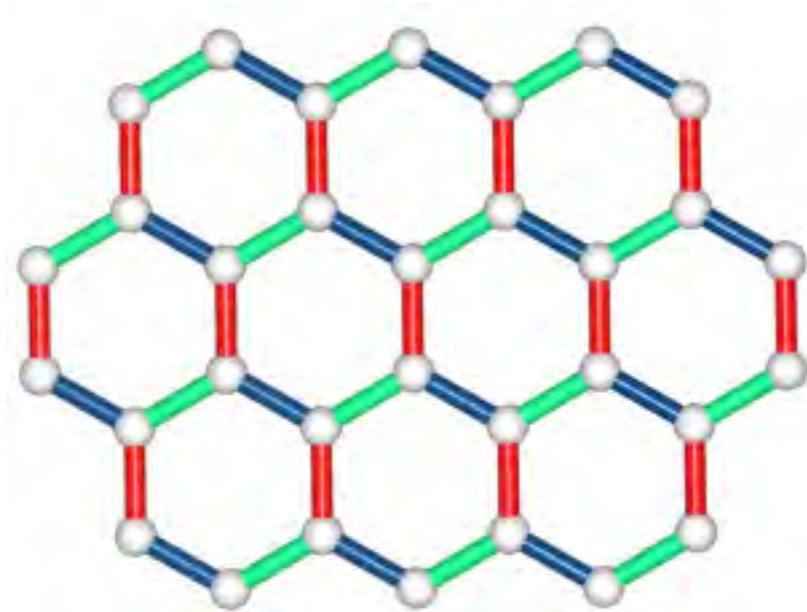


$$H = i \sum_{\gamma\text{-bond}} J_{\gamma} c_j c_k$$

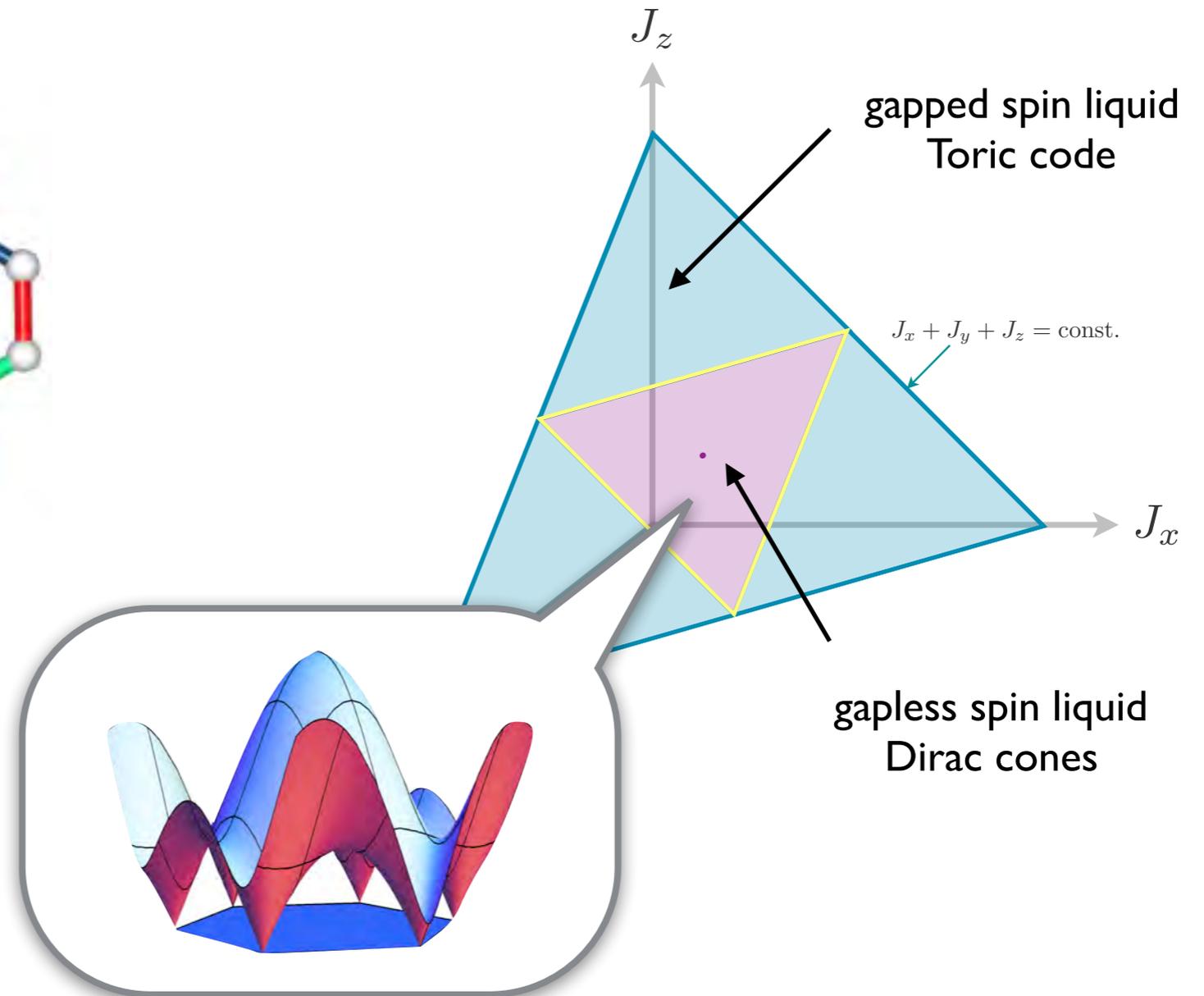


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A. Kitaev, Annals of Physics (2006)



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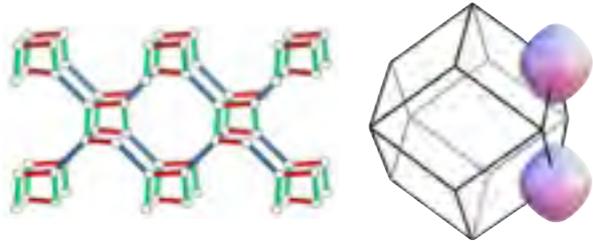
Kitaev spin liquids in 3D

K. O'Brien, M.H, S.Trebst, PRB 93, 085101 (2016)

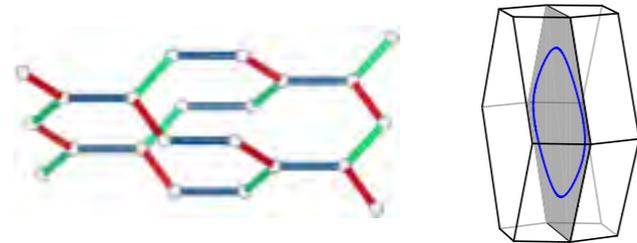
Finite range of stability for the QSL phase due to flux gap!

pure Kitaev

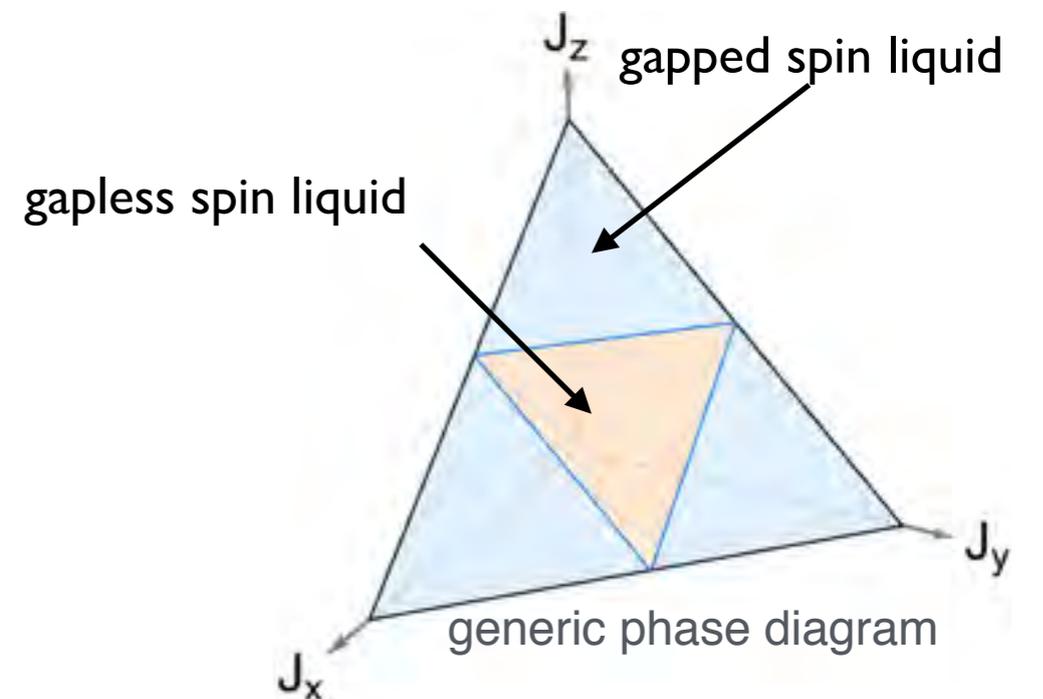
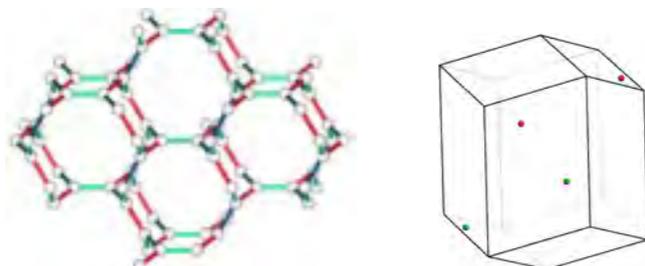
(10,3)a 'hyperoctagon'



(10,3)b 'hyperhoneycomb'



(8,3)b



projective symmetry

$$\mathcal{T} : \hat{h}(\mathbf{k}) = U_{\mathcal{T}} \hat{h}^*(-\mathbf{k}) U_{\mathcal{T}}^{-1}$$

$$\hat{h}(\mathbf{k}) = U_{\mathcal{T}} \hat{h}^*(-\mathbf{k} + \mathbf{k}_0) U_{\mathcal{T}}^{-1}$$

Beyond Kitaev Interactions

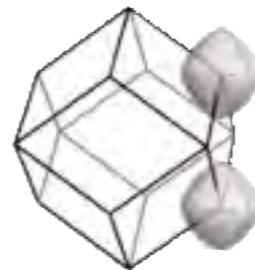
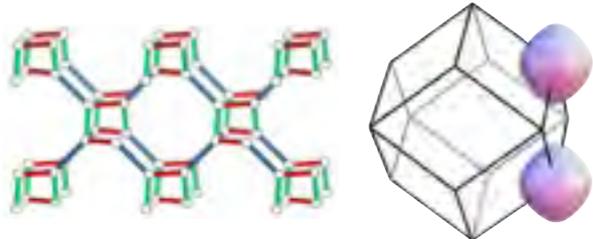
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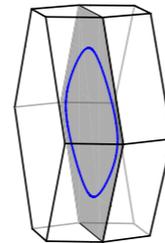
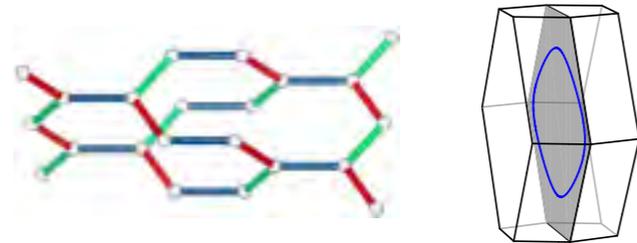
pure Kitaev

Heisenberg, Γ -term

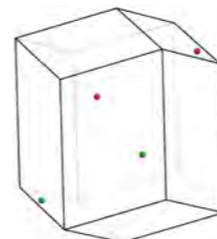
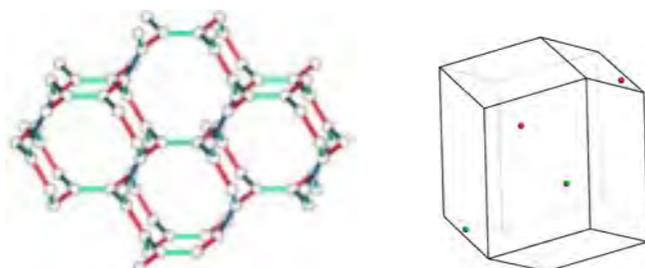
(10,3)a 'hyperoctagon'



(10,3)b 'hyperhoneycomb'



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Beyond Kitaev Interactions

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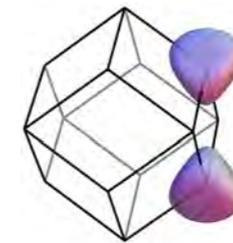
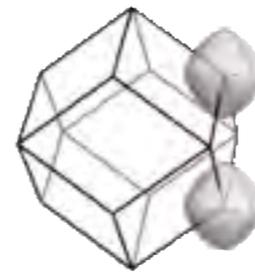
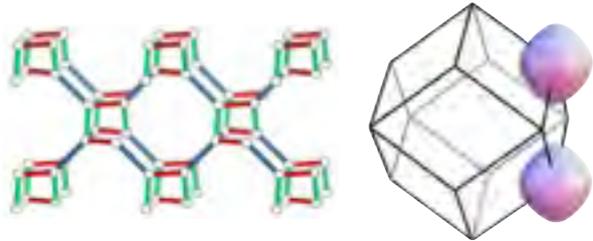
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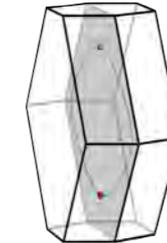
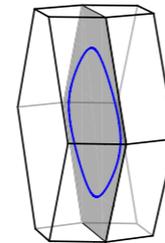
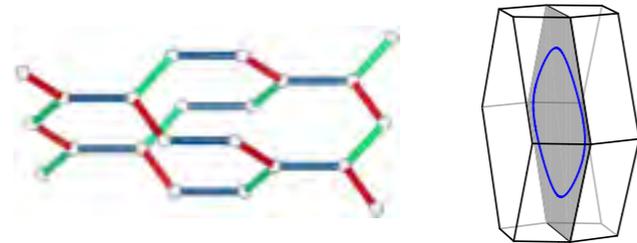
Heisenberg, Γ -term

magnetic field

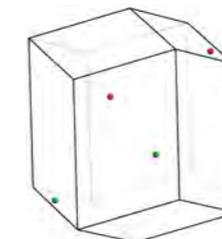
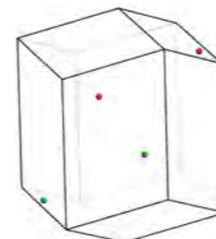
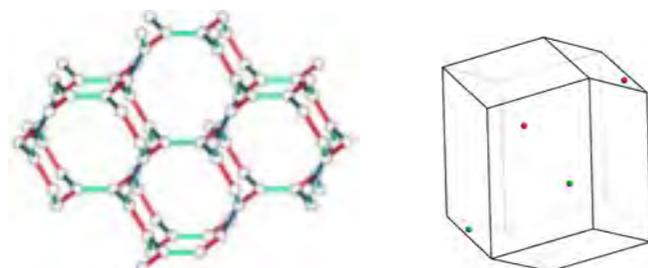
(10,3)a 'hyperoctagon'



(10,3)b 'hyperhoneycomb'



(8,3)b



Kitaev models in 3D

| Schäfli symbol | Majorana metal | TR breaking | Peierls instability |
|----------------|----------------|---------------|---------------------|
| (10,3)a | Fermi surface | Fermi surface | ✓ |
| (10,3)b | Fermi line | Weyl nodes | ✗ |
| (10,3)c | Fermi line | Fermi surface | ✗ |
| (9,3)a | Weyl nodes | Weyl nodes | ✗ |
| (8,3)a | Fermi surface | Fermi surface | ✓ |
| (8,3)b | Weyl nodes | Weyl nodes | (✓) |
| (8,3)c | Fermi line | Weyl nodes | ✗ |
| (8,3)n | gapped | Weyl nodes | ✗ |
| (6,3)a | Dirac points | gapped | ✗ |

Kitaev models in 3D

| Schäfli symbol | Majorana metal | TR breaking | Peierls instability |
|----------------|----------------|---------------|---------------------|
| (10,3)a | Fermi surface | Fermi surface | ✓ |
| (10,3)b | Fermi line | Weyl nodes | ✗ |
| (10,3)c | Fermi line | Fermi surface | ✗ |
| (9,3)a | Weyl nodes | Weyl nodes | ✗ |
| (8,3)a | Fermi surface | Fermi surface | ✓ |
| (8,3)b | Weyl nodes | Weyl nodes | (✓) |
| (8,3)c | Fermi line | Weyl nodes | ✗ |
| (8,3)n | gapped | Weyl nodes | ✗ |
| (6,3)a | Dirac points | gapped | ✗ |

Kitaev models in 3D

| Schäfli symbol | Majorana metal | TR breaking | Peierls instability |
|----------------|----------------|---------------|---------------------|
| (10,3) | Fermi surface | Fermi surface | ✓ |
| (11,3) | Fermi line | Weyl nodes | ✗ |
| (12,3) | Fermi line | Fermi surface | ✗ |
| (9,3)a | Weyl nodes | Weyl nodes | ✗ |
| (8,3)a | Fermi surface | Fermi surface | ✓ |
| (8,3)b | Weyl nodes | Weyl nodes | (✓) |
| (8,3)c | Fermi line | Weyl nodes | ✗ |
| (8,3)n | gapped | Weyl nodes | ✗ |
| (8,3)h | Dirac points | gapped | ✗ |

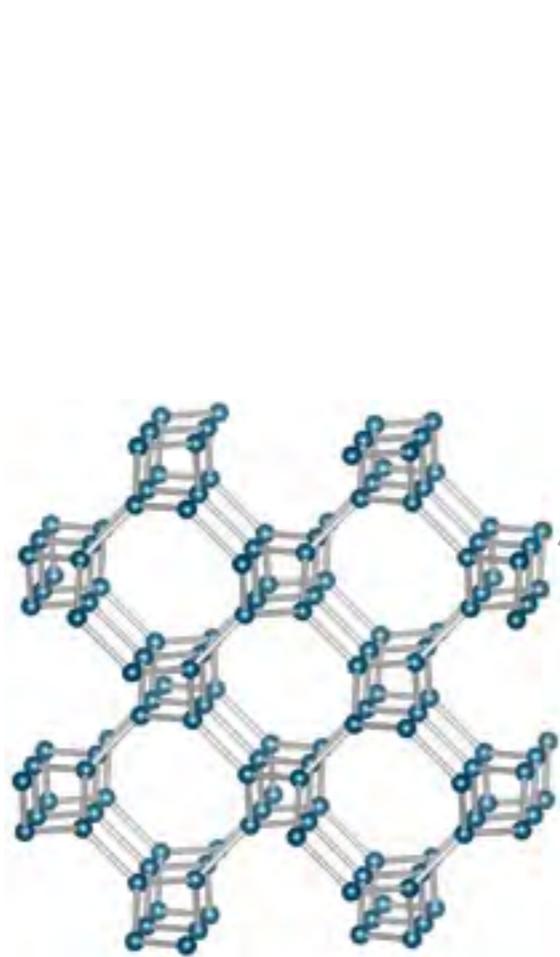
spontaneous breaking of time-reversal symmetry

Weyl spin liquid with inversion and time-reversal symmetry

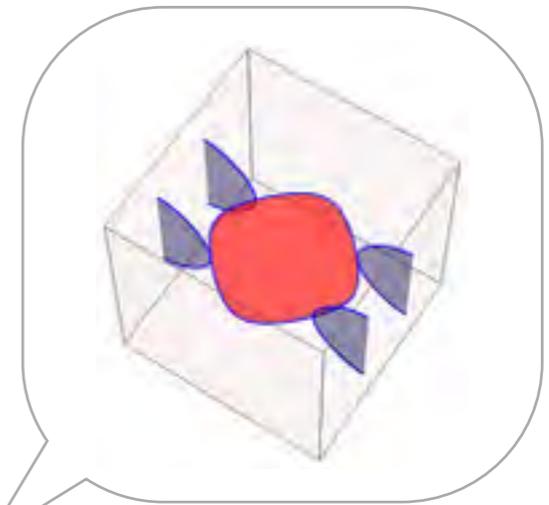
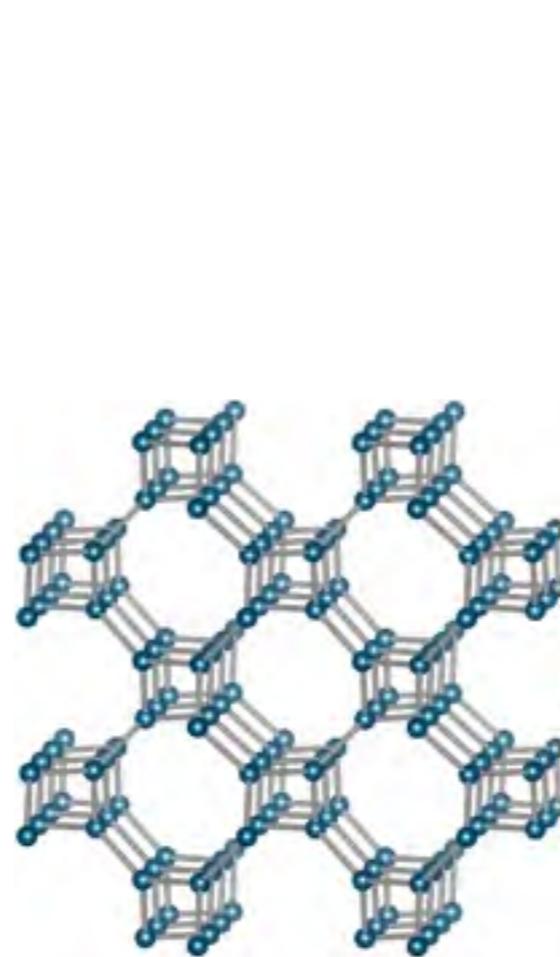
Crystalline Spin liquids

M. Yamada, V. Dwivedi, M. Hermanns, arXiv:1707.00898 (2017)

Kitaev spin liquids + non-symmorphic symmetries = richer band structures



Dirac points
four-fold screw



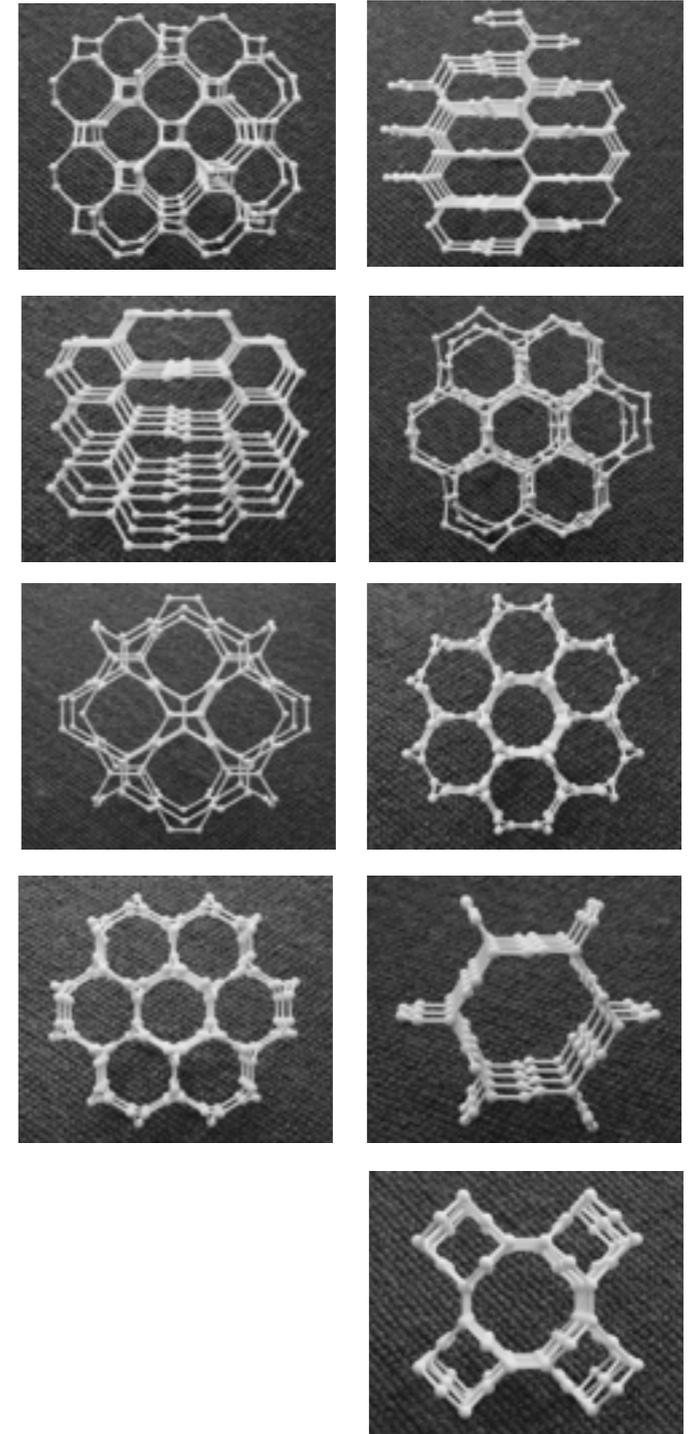
Nodal chain
glide

Conclusion

- 3D Kitaev models show rich behavior depending on the underlying lattice structure
- Z_2 spin liquid with
 - Majorana Fermi surface
 - Fermi line
 - nodal chains
 - Dirac nodes
 - Weyl nodes (Weyl spin liquid)

Experimental signatures

- specific heat
- neutron scattering
- Raman scattering
- thermal Hall effect (Weyl spin liquid)



Future Directions

The Kitaev spin liquid models provide a well-defined starting point to study

- finite-strength interactions
- effective Z_2 flux model
- 3D loop braiding statistics
- effect of disorder & dislocations
- ...

M.H., S. Trebst, PRB **89**, 235102 (2014)

M.H., K. O'Brien, S. Trebst, PRL **114**, 157202 (2015)

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M. Yamada, V. Dwivedi, M. Hermanns, arXiv:1707.00898 (2017)

