KITAEV MATERIAL

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For Prof. Jak Chakhalian’s Solid State Physics
What is Kitaev Material?

“spin-orbit assisted Mott insulators”

- What makes it Mott Insulator?
- What gives it high magnetic frustration? (Spin Liquids?)
- What is unusual about it?

Spin-Orbit Coupling

Z+, large radius (large band width)
SOC+, suppress band width

- Large band width—
  U don’t split the band

- Small band width—
  U might split the gap
  Mott Gap

arXiv:1704.06007 [cond-mat.str-el]  
Electronic correlation

Two exchange paths

Interference of wave function

bond-directional coupling (Kitaev couplings)

\[ -\frac{8t^2 J_H}{3U^2} S_1^\gamma S_2^\gamma \]

I: corner-sharing

II: edge-sharing

“parallel edge”-sharing

Ising-like coupling

Exchange frustration

\[ H = - \sum_{\gamma-\text{bonds}} J \mathbf{S}_i \mathbf{S}_j + K \mathbf{S}_i^\gamma \mathbf{S}_j^\gamma + \Gamma \left( S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) \]

strong exchange frustration:
these interactions cannot be simultaneously minimized

ground-state entropy

Frustration * 2 ~ Quantum Spin Liquid!

Why is Kitaev materials special?

Ferromagnetic

Magnetic anisotropy

(Majorana Fermions)
Possible Kitaev materials:

Hexagonal: Na$_2$IrO$_3$

Triangle: Ba$_3$Ir(2-x)Ti$_x$O$_9$

3D: Theoretical prediction

Fig. 14: Illustration of the elementary tricoordinated lattices by photographs of 3D printed models. Further information on these lattices is provided in Table 1.
Example:

Na₂IrO₃
a family of spin-orbit assisted $j=1/2$ Mott insulators
bond-directional exchange induces frustration
unconventional forms of magnetism