Title: Topological phases in Kitaev Materials

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Collection: Quantum Matter: Emergence & Entanglement 3

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Abstract: We discuss recent progress in theory and experiment on emergent topological phases in Kitaev materials. Here the competition between different anisotropic spin-exchange interactions may lead to a number of exotic phases of matter. We investigate possible emergence of quantum spin liquid, topological magnons, and topological superconductivity in two and three dimensional systems. We make connections to existing and future experiments.
Quantum Spin Liquids

Quantum Paramagnet \[ \langle S \rangle = 0 \]

Correlated insulator with no broken translational symmetry

Resonating Valence Bond state (RVB);
Superposition of Valence Bond coverings

\[ \Psi = \sum_{vb} A_{vb} |vb\rangle \]

\[ |RVB\rangle = \sum_{vb} A_{vb} |vb\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \]

Valence Bond

P.W. Anderson
Rokhsar-Kivelson
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.

Electrons possess magnetic behavior through the quantum mechanical property of spin. The magnetic properties of materials then arise from the collective interaction of electrons on atoms within the crystal. Below a transition temperature, the electron spins of normal magnets “freeze” into an ordered array of magnetic dipoles. Whether the ordering is ferromagnetic (all the dipoles point in the same direction) or antiferromagnetic (the dipoles on adjacent sites point in opposite directions) is determined by the sign and strength of the interaction between the electrons. Early theoretical work has indicated a departure from these ordered states, suggesting that quantum mechanical fluctuations of the spin could be so strong that ordering would be suppressed and the spin ensemble would remain in a liquid-like state, even down to the lowest temperatures. Experimental evidence, which has until recently remained elusive, is emerging in favor of this long-predicted state of quantum matter.

To understand the controversy surrounding this exotic quantum spin liquid state, it is instructive to go back to the description of antiferromagnetism. Soon after the invention of quantum mechanics, Heisenberg pointed out that electron spins on neighboring atoms can have short-range interaction due to quantum mechanical exchange. Louis Néel

Ordered spins. (Left) Néel’s picture of antiferromagnet ordering with an alternate spin-up-spin-down pattern across the lattice. (Right) Quantum fluctuations lead to mutual spin flips, which Landau argued would disorder Néel’s state.

Until ~15 years ago, candidate materials were limited.

Good theoretical models existed (numerically solvable to high accuracy)
Candidate Materials (selected, as of April 2019)

$\kappa-(\text{BEDT-TTF})_2\text{Cu}_2(\text{CN})_3$
$\text{EtMe}_3\text{Sb}[\text{Pd(dmit)}_2]_2$
$\kappa-(\text{BEDT-TTF})_2\text{Ag}_2(\text{CN})_3$
$\kappa-\text{H}_3(\text{Cat-EDT-TTF})_2$

$\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$  herbertsmithite
$\text{Cu}_3\text{Zn(OH)}_6\text{FBr}$  $\text{Cu}_4(\text{OH})_6\text{FBr}$  barlowite
$\text{Cu}_3\text{Zn(OH)}_6\text{FCl}$  $\text{Cu}_4(\text{OH})_6\text{FCl}$  claringbullite

$\text{PbCuTe}_2\text{O}_6$  hyper-kagome
$\text{Na}_4\text{Ir}_3\text{O}_8$

$\text{Yb}_2\text{Ti}_2\text{O}_7$  pyrochlore
$\text{Pr}_2\text{Zr}_2\text{O}_7$

$\text{YbMgGaO}_4$  triangular

Kitaev Materials  honeycomb  hyper-honeycomb
Candidate Materials (selected, as of April 2019)

$\kappa-(BEDT-TTF)_2Cu_2(CN)_3$

$EtMe_3Sb[Pd(dmit)_2]_2$

$\kappa-(BEDT-TTF)_2Ag_2(CN)_3$

$\kappa-H_3(Cat-EDT-TTF)_2$

$ZnCu_3(OH)_6Cl_2$  herbertsmithite

$Cu_3Zn(OH)_6FBr$  barlowite

$Cu_3Zn(OH)_6FCl$  claringbullite

$PbCuTe_2O_6$  hyper-kagome

$Na_4Ir_3O_8$  hyper-kagome

$Yb_2Ti_2O_7$  pyrochlore

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\[ \text{ZnCu}_3(\text{OH})_6\text{Cl}_2 \quad \text{herbertsmithite} \]

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\[ \text{Na}_4\text{Ir}_3\text{O}_8 \quad \text{hyper-kagome} \]

\[ \text{Yb}_2\text{Ti}_2\text{O}_7 \]

\[ \text{Pr}_2\text{Zr}_2\text{O}_7 \quad \text{pyrochlore} \]

\[ \text{YbMgGaO}_4 \quad \text{triangular} \]

\[ \text{Kitaev Materials} \quad \text{honeycomb} \quad \text{hyper-honeycomb} \]

Geometric

Organic Materials

Triangular Lattice

Kagome

Hyper-kagome

Spin-orbit
Exact Question to the Answer (Kitaev)

\[ \mathcal{H}_K = - \sum_{\alpha \text{-links}} S^\alpha_i S^\alpha_j \quad b_i^x b_i^y b_i^z c_i = 1 \]

\[ S^\alpha_i = \frac{1}{2} i b_i^\alpha c_i \quad \{b_i^x, b_i^y, b_i^z, c\} \quad \text{Four Majorana Fermions} \]
Exact Question to the Answer (Kitaev)

\[ \mathcal{H}_K = - \sum_{\alpha \text{-links}} S_i^\alpha S_j^\alpha \quad b_i^x b_i^y b_i^z c_i = 1 \]

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Four Majorana Fermions
Exact Question to the Answer (Kitaev)

\[ H_K = - \sum_{\alpha - \text{links}} S_i^\alpha S_j^\alpha \quad b_i^x b_i^y b_i^z c_i = 1 \]

\[ S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \quad \{b_i^x, b_i^y, b_i^z, c\} \quad \text{Four Majorana Fermions} \]

\[ H_K = - \frac{i}{4} \sum_{\alpha - \text{links}} u_{ij}^\alpha c_i c_j \]

\[ u_{ij}^\alpha = i b_i^\alpha b_j^\alpha \]
Exact Question to the Answer (Kitaev)

\[ \mathcal{H}_K = - \sum_{\alpha \text{-links}} S_i^\alpha S_j^\alpha \quad b_i^x b_i^y b_i^z c_i = 1 \]

\[ S_i^\alpha = \frac{1}{2} i b_i^\alpha c_i \quad \{b_i^x, b_i^y, b_i^z, c\} \]

Four Majorana Fermions

Ground state is in the zero-flux sector

\[ W_p = +1 \]

\[ \mathcal{H}_K = -\frac{i}{4} \sum_{\alpha \text{-links}} u_{ij}^\alpha c_i c_j \]

\[ u_{ij}^\alpha = i b_i^\alpha b_j^\alpha \]

Majorana Fermions with Dirac Dispersion

\[ W_p = 2^6 S_1^x S_2^y S_3^z S_4^x S_5^y S_6^z \]
Kitaev Spin Liquid is almost a Superconductor

Making connection to "Superconductor"

\[
\begin{align*}
  f_{i \uparrow} &= \frac{1}{\sqrt{2}} (c_i + i b_i^z) \\
  f_{i \downarrow} &= \frac{i}{\sqrt{2}} (b_i^x + i b_i^y)
\end{align*}
\]

\[
S_i^a = \frac{1}{2} f_{i \alpha}^\dagger \sigma^a_{\alpha \beta} f_{i \beta}
\]

with \[ \sum_{\alpha} f_{i \alpha}^\dagger f_{i \alpha} = 1 \]
Kitaev Spin Liquid is almost a Superconductor

Making connection to "Superconductor"

\[
\begin{align*}
f_{i\uparrow} &= \frac{1}{\sqrt{2}}(c_i + ib_i^z) \\
f_{i\downarrow} &= \frac{i}{\sqrt{2}}(b_i^x + ib_i^y)
\end{align*}
\]

\[
S_i^a = \frac{1}{2} f_{i\alpha}^\dagger \sigma^a_{\alpha\beta} f_{i\beta}
\]

with \[
\sum_\alpha f_{i\alpha}^\dagger f_{i\alpha} = 1
\]

\[
H = \sum_{\langle ij \rangle \in a} \left\{ f_{i\alpha}^\dagger [T^a]_{\alpha\beta} f_{j\beta} + f_{i\alpha} [\Delta^a]_{\alpha\beta} f_{j\beta} \right\}
\] exactly one particle per site (insulator)
Kitaev Spin Liquid is almost a Superconductor

Making connection to “Superconductor”

\[
f_{i\uparrow} = \frac{1}{\sqrt{2}} (c_i + ib_i^z)
\]

\[
f_{i\downarrow} = \frac{i}{\sqrt{2}} (b_i^x + ib_i^y)
\]

\[
S_i^a = \frac{1}{2} f_{i\alpha}^\dagger \sigma_{\alpha\beta}^a f_{i\beta}
\]

with \( \sum_\alpha f_{i\alpha}^\dagger f_{i\alpha} = 1 \)

\[
H = \sum_{\langle ij \rangle \in a} \{ f_{i\alpha}^\dagger [T^a]_{\alpha\beta} \delta f_{j\beta} + f_{i\alpha} [\Delta^a]_{\alpha\beta} \delta f_{j\beta} \}
\]

exactly one particle per site (insulator)

Class BDI
Spin-Triplet
Superconductor
\( \langle n_i \rangle = 1 \)

Hubbard U \( \Rightarrow \infty \)

Kitaev Spin Liquid
\( n_i = 1 \)
Kitaev Materials
Kitaev Interaction

\[ H = \sum_{\langle i,j \rangle \in \gamma} -K S_i^\gamma S_j^\gamma \]

G. Jackeli and G. Khaliullin, PRL 102, 256403 (2009)

Ir\(^{4+}\) 5\(d^5\)  \hspace{1cm} Ru\(^{3+}\) 4\(d^5\)

Crystal Field  \hspace{1cm} Spin-Orbit Coupling

Strong Spin-Orbit Coupling leads to Spin-Orbit entangled pseudo-spin basis (Kramers Doublet)

edge sharing octahedra
How realistic is the Kitaev model?

\[ H = \sum_{\langle i,j \rangle \in \gamma} K S_i^\gamma S_j^\gamma \]

if only the super-exchange via oxygens are considered

G. Jackeli and G. Khaliullin (2009)
How realistic is the Kitaev model?

\[ H = \sum_{(i,j) \in \alpha \beta(y)} \left( J \vec{S}_i \cdot \vec{S}_j + K S^\gamma_i S^\gamma_j + \Gamma \left( S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) \right) \]

but direct exchange is also important due to large extent of 4d/5d orbitals

How realistic is the Kitaev model?

\[ H = \sum_{(i,j) \in \alpha\beta(y)} \left[ J \vec{S}_i \cdot \vec{S}_j + K S_i^\gamma S_j^\gamma + \Gamma \left( S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha \right) \right] \]

- \( K S_i^x S_j^x + \Gamma [S_i^y S_j^z + S_i^z S_j^y] \) \( x\)-bond
- \( K S_i^y S_j^y + \Gamma [S_i^z S_j^x + S_i^x S_j^z] \) \( y\)-bond
- \( K S_i^z S_j^z + \Gamma [S_i^x S_j^y + S_i^y S_j^x] \) \( z\)-bond

How essential/important are these additional interactions?

Realization of Kitaev Quantum Spin Liquid

2D
Honeycomb
α- Na$_2$IrO$_3$
α- Li$_2$IrO$_3$
α- H$_3$LiIr$_2$O$_6$
α- RuCl$_3$

β- Li$_2$IrO$_3$
3D Hyper-Honeycomb
γ- Li$_2$IrO$_3$
3D Stripy-Honeycomb
Realization of Kitaev Quantum Spin Liquid?

\[ T_N \]
- zig-zag, 14K
- incomm. spiral, 15K
- no magnetic order (NMR)
- zig-zag, 7K

**2D Honeycomb**
- \( \alpha - \text{Na}_2\text{IrO}_3 \)
- \( \alpha - \text{Li}_2\text{IrO}_3 \)
- \( \alpha - \text{H}_3\text{LiIr}_2\text{O}_6 \)
- \( \alpha - \text{RuCl}_3 \)

**\( \beta - \text{Li}_2\text{IrO}_3 \)**
- 3D Hyper-Honeycomb

**\( \gamma - \text{Li}_2\text{IrO}_3 \)**
- 3D Stripy-Honeycomb

incomm. spiral, 38K
incomm. spiral, 38K
Realization of Kitaev Quantum Spin Liquid?

- **2D Honeycomb**
  - α- Na₂IrO₃
  - α- Li₂IrO₃
  - α- H₃LiIr₂O₆
  - α- RuCl₃

- **Incomm. Spiral**
  - Incomm. Spiral, 15K
  - Incomm. Spiral, 38K

- **Zig-Zag**
  - Zig-Zag, 14K
  - Zig-Zag, 7K

- **No Magnetic Order (NMR)**

- **Hydrogen Intercalation**
  - H.in > 8T
  - S. Nagler, Y.-J. Kim, R. Coldea, ...

- **Pressure**
  - P > 2.5 GPa
    - H. Takagi, D. Haskel
  - P > 1.5 GPa
    - J. Analytis, D. Haskel
Three-dimensional Hyper-honeycomb Iridates

$\beta$-Li$_2$IrO$_3$
Three dimensional “Hyper-Honeycomb” lattice

$\beta$- Li$_2$IrO$_3$

H. Takagi (PRL, 2014)

Close to ideal structure

Magnetic order

$T_c = 38K$

Strong Magnetic Anisotropy
Three dimensional “Hyper-Honeycomb” lattice

$\beta$- Li$_2$IrO$_3$

H. Takagi (PRL, 2014)

Close to ideal structure

Magnetic order

$T_c = 38K$

Strong Magnetic Anisotropy

Kitaev Model exactly solvable

Nodal Line

Majorana Fermions

S. Mandal and N. Surendran (2009)

Classical Analysis

\[ H = \sum_{(ij) \in \alpha(\beta \gamma)} JS_i \cdot S_j + KS_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta) \]

\[ K < 0 \quad J > 0 \quad \Gamma < 0 \]

\[ |K| > |\Gamma| \gg J \]

Non-coplanar counter-propagating incommensurate spiral order


Radu Coldea (PRL, PRB, 2014)
Classical Analysis

\[
H = \sum_{(i,j) \in \alpha(\beta\gamma)} J S_i \cdot S_j + K S_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta)
\]

\[
J = \cos \phi \sin \theta \\
K = \sin \phi \sin \theta \\
\Gamma = \cos \theta
\]

EXPERIMENT

High Pressure Experiment (H. Takagi, D. Haskel)

Magnetic order disappear near 2-2.5 GPa

What’s the paramagnetic state at P > 2-2.5GPa?

Structure change at P > 4GPa
Effect of External Pressure (Theory, Ab Initio)

\[ H = \sum_{(i,j) \in \alpha(\beta\gamma)} JS_i \cdot S_j + K S_i^\alpha S_j^\alpha + \Gamma^\alpha (S_i^\beta S_j^\gamma + S_i^\gamma S_j^\beta) \]

AF-Kitaev

\[ K \text{ dominant Low-P} \]
\[ \Gamma \text{ dominant High-P} \]

Highly Frustrated
New Spin Liquid?


Classification
B. Huang, W. Choi, YBK, Y.-M. Lu (2018)
\( \alpha - \text{RuCl}_3 \) (Y. J. Kim, S. Nagler, R. Coldea ...)

Spinon Continuum?

\[
\begin{align*}
\text{Intensity (arb. units)} \\
\text{E (meV)}
\end{align*}
\]

\( T = 5 \text{ K} \)

\( T = 10 \text{ K} \)

Spinon-Antispinon pair excitations

Well-defined dispersion --

Threshold energy for pair excitations

A. Banerjee, S. Nagler et al. (2016)
Field-induced Paramagnet: Spin Liquid?

C. Balz, S. Nagler et al.

arXiv:1903.00056
\[ T \]

\[ \alpha\text{-RuCl}_3 ? \]

\[ \text{spin liquid} \]

\[ \text{Zig-zag} \]

\[ \sim 8T \]

\[ H_{\text{inplane}} \]

\[ \text{Chiral spin liquid?} \]

\[ \text{Polarized paramagnet?} \]

C. Hickey, S. Trebst (2018)
L. Zou, Y.-C. He (2018)
H.-C. Jiang, C.-Y. Wang, B. Huang, Y.-M. Lu (2018)
(AF-Kitaev, 111 magnetic field)
Field-induced Paramagnet: Spin Liquid?
Field-induced Paramagnet: Spin Liquid?

Quantized Thermal Hall Conductivity

Y. Kasahara, ... Y. Matsuda et al. (2017, 2018)
Field-induced Paramagnet: Spin Liquid?

\[
\kappa_{xy}^{2D}/T = q(\pi/6)(k_B^2/\hbar)
\]
\[
q = 1/2
\]

Quantized Thermal Hall Conductivity

Y. Kasahara, ... Y. Matsuda et al. (2017, 2018)
Chiral spin liquid in magnetic field


$$\mathcal{H}_Z = -2 \sum_{i,\alpha} S_i^\alpha h^\alpha,$$

$$\mathcal{H}^{(3)} \sim -\frac{8h^x h^y h^z}{K^2} \sum_{i,j,k} S_i^x S_j^y S_k^z,$$

Majorana mass gap  $\Delta_0 \sim 4h^x h^y h^z / K^2$

Majorana chiral edge mode

$$\kappa_{xy}^{2D} / T = q(\pi/6)(k_B^2 / \hbar)  \quad q = 1/2$$

half-quantization
in thermal Hall conductivity
Too good to be true?

1) Very small Hall angle

$$\frac{K_{xy}}{K_{xx}} \sim 10^{-3}$$

Much larger bulk thermal conduction

Presumably due to phonons

Bulk and edge not well separated?
Too good to be true?

1) Very small Hall angle

\[
\frac{K_{xy}}{K_{xx}} \sim 10^{-3}
\]

Much larger bulk thermal conduction
Presumably due to phonons
Bulk and edge not well separated?

Y. Vinkler-Aviv, A. Rosch (2018)

Majorana mode and phonons can exchange energy at the edge

Coupling between Majorana and phonons help to make the Hall effect observable

Quantization is good w.r.t. phonon temperature
Too good to be true?

2) Other significant interactions

\[ H = \sum_{\langle \langle ij \rangle \rangle} J_{ij}^{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle i j \rangle, \gamma} K^\gamma S_i^\gamma S_j^\gamma + \sum_{\langle i j \rangle, \gamma} \sum_{\alpha, \beta \neq \gamma} \Gamma^\gamma [S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha] \]

Ab Initio Modeling

<table>
<thead>
<tr>
<th>Bond</th>
<th>( J_n )</th>
<th>( K_n )</th>
<th>( \xi_n )</th>
<th>( \Gamma_n )</th>
<th>( \Gamma'_n )</th>
<th>( \zeta_n )</th>
</tr>
</thead>
<tbody>
<tr>
<td>X₁, Y₁</td>
<td>-1.4</td>
<td>-7.5</td>
<td>+0.2</td>
<td>+5.9</td>
<td>-0.8</td>
<td>+0.2</td>
</tr>
<tr>
<td>Z₁</td>
<td>-2.2</td>
<td>-5.0</td>
<td>-</td>
<td>+8.0</td>
<td>-1.0</td>
<td>-</td>
</tr>
<tr>
<td>X₂, Y₂</td>
<td>-0.1</td>
<td>-0.6</td>
<td>+0.1</td>
<td>+0.6</td>
<td>+0.6</td>
<td>+0.1</td>
</tr>
<tr>
<td>Z₂</td>
<td>+0.1</td>
<td>-0.9</td>
<td>-</td>
<td>+0.6</td>
<td>+0.3</td>
<td>-</td>
</tr>
<tr>
<td>X₃, Y₃</td>
<td>+3.0</td>
<td>-0.1</td>
<td>0.0</td>
<td>-0.1</td>
<td>-0.1</td>
<td>-0.1</td>
</tr>
<tr>
<td>Z₃</td>
<td>+2.4</td>
<td>+0.3</td>
<td>-</td>
<td>-0.1</td>
<td>-0.1</td>
<td>-</td>
</tr>
</tbody>
</table>

Nearest-Neighbour \( K < 0 \)

Nearest-Neighbour \( \Gamma > 0 \)

\(|K| \sim |\Gamma|\)

Third-Neighbour \( J_3 > 0 \)

Zig-Zag magnetic order

Winter, Li, Jeschke, Valenti (2016)
“Star Shape” continuum

A. Banerjee, S. Nagler et al. (2016)
"Star Shape" continuum

Dynamical Structure Factor
(K-Γ model, 24-site ED)

Kitaev model \( \frac{\Gamma}{|K|} \sim 0.6 \)

\( K < 0, \Gamma > 0 \)

M. Gohlke, G. Wachtel,
Y. Yamaji, F. Pollmann, YBK, (2017)

A. Banerjee, S. Nagler et al. (2016)
Large magnetic anisotropy

\[ H = \sum_{\langle jk \rangle, \alpha \beta (\gamma)} K S_j^\gamma S_k^\gamma + \Gamma (S_j^\alpha S_k^\beta + S_j^{\beta \gamma} S_k^{\alpha \gamma}) \]

1st order transition

\[ \sim 0.1 \quad \sim 0.5 \]

Pure (ferro-)Kitaev

Spin Liquid ?

Broken lattice rotational symmetry (DMRG)

\[ H = \sum_{\langle jk \rangle, \alpha \beta (\gamma)} KS_j^\gamma S_k^\gamma + \Gamma (S_j^\alpha S_k^\beta + S_j^\beta S_k^\alpha) \]

1st order transition

\[ \sim 0.1 \quad \sim 0.5 \]

Pure (ferro-)Kitaev

Spin Liquid ?

Broken lattice rotational symmetry (DMRG)

Addition of small $J_3$ leads to Zig-Zag order for $\Gamma/|K| > 0.1$

\[ H = \sum_{\langle jk \rangle, \alpha\beta(\gamma)} K S_j^\gamma S_k^\gamma + \Gamma (S_j^\alpha S_k^\beta + S_j^\beta S_k^\alpha) \]

1st order transition


\[ \Gamma / |K| \]

~0.1

Pure (ferro-)Kitaev

Spin Liquid?

\[ + \Gamma' (S_j^\alpha S_k^\gamma + S_j^\gamma S_k^\alpha + S_j^\beta S_k^\gamma + S_j^\gamma S_k^\beta) \quad \Gamma' = -0.03 \]

~0.07

Pure (ferro-)Kitaev

Zig-Zag 24-site ED

J. S. Gordon, A. Catuneabum E. S. Sorensen, H.-Y. Kee (2019)
\[ H = \sum_{\langle jk \rangle, \alpha \beta (\gamma)} K S_j^\gamma S_k^\gamma + \Gamma(S_j^\alpha S_k^\beta + S_j^\beta S_k^\alpha) + \Gamma'(S_j^\alpha S_k^\gamma + S_j^\gamma S_k^\alpha + S_j^\beta S_k^\gamma + S_j^\gamma S_k^\beta) \]

can arise due to trigonal distortion

Polarized paramagnet

Chiral spin liquid?

small $\Gamma'$ induces Zig-Zag order

In contrast, ... Ab initio Model

[111] field (perpendicular to 2D plane)

24-site Exact Diagonalization

There is an intermediate phase

But it is not connected to the Kitaev (chiral) spin liquid

It disappears as soon as the magnetic field is tilted away from [111] direction

A spin–orbital–entangled quantum liquid on a honeycomb lattice

K. Kitagawa¹*, T. Takayama²*, Y. Matsumoto², A. Kato¹, R. Takano¹, Y. Kishimoto³, S. Bette², R. Dinnebier², G. Jackeli²–⁴ & H. Takagi¹,²,⁴

\[ \alpha \text{-Li}_2\text{IrO}_3 \]

\[ \begin{align*}
    a &= 5.1633(2) \text{ Å} \\
    b &= 8.9294(3) \text{ Å} \\
    c &= 5.1219(2) \text{ Å}
\end{align*} \]

\[ \text{enlogated } a/b \]

\[ \begin{align*}
    a &= 5.3489(8) \text{ Å} \\
    b &= 9.2431(14) \text{ Å} \\
    c &= 4.8734(6) \text{ Å}
\end{align*} \]

**Reduced interlayer spacing**