Title: Common features in spin-orbit excitations of Kitaev materials

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Collection: Quantum Matter Workshop

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Abstract: "Magnetic materials with 4d or 5d transition metals have drawn much attention for their unique magnetic properties arising from J_eff=1/2 magnetic states. Among them, a honeycomb lattice material with unusual bond-dependent interactions called Kitaev interactions is of particular interest due to the potential for realizing the Kitaev quantum spin liquid state. Although much progress has been made in understanding magnetic and spin-orbit excitations in Kitaev materials, such as Na2IrO3 and alpha-RuCl3, using resonant inelastic X-ray scattering (RIXS), there are still many unanswered questions regarding the nature of electronic excitations in these materials. Of particular interest is the sharp peak observed around 0.4 eV in the RIXS spectrum of Na2IrO3, the exact nature of which remains controversial. In this context, it is interesting to note that a similar lower energy "excitonic" peak was observed in our recent RIXS investigation of alpha-RuCl3. Given that the electronic parameters in alpha-RuCl3 are probably very different from those in Na2IrO3 (alpha-RuCl3 has a large bandgap of ~1eV, well above any SO excitation energy scale), the observed similarity is surprising. The RIXS spectra from these two compounds as well as other Kitaev materials will be compared and the origin of common spectral features will be discussed.
"

Quantum Matter Workshop, Perimeter Institute
Nov. 16, 2022

Common features in Spin-Orbit Excitations of Kitaev Materials

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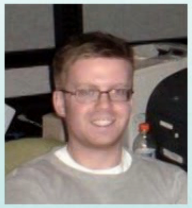

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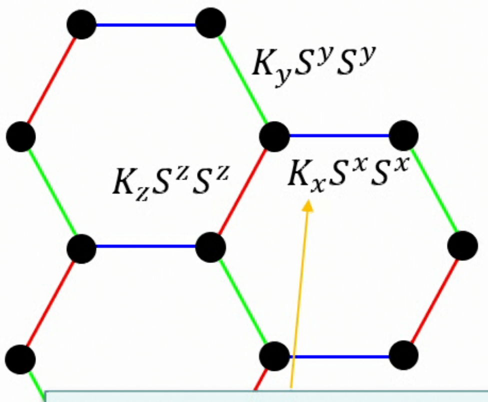
Outline

- Introduction
  - Kitaev Quantum Spin Liquid
  - Jackeli and Khaliullin mechanism for Kitaev materials
  - RIXS (Resonant Inelastic X-ray Scattering)
    - Previous studies on Na_2IrO_3
  - α-$RuCl_3$
    - Quantum Thermal Hall effect controversy (?)
- RIXS results
  - Comparison and common features
- Conclusions

Kitaev model – exchange frustration

Alexei Kitaev, Ann. Phys. 2006

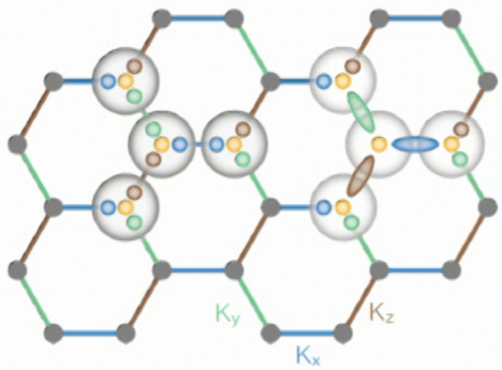


Kitaev interaction
– bond dependent Ising interaction

$$\mathcal{H}^{Kitaev} = -\sum_{i,\gamma} K_\gamma S_i^\gamma S_{i+\vec{e}_\gamma}^\gamma$$

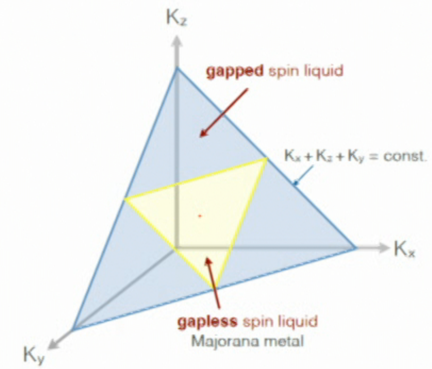
Nussinov and van den Brink Rev. Mod. Phys. 2015
Hermanns et al. Annu. Rev. Condens. Matter Phys. 2018
Takagi et al. Nat. Rev. Phys. 2019

- Exactly solvable model



- Low-energy degree of freedom
  - Majorana fermion
- Ground states
  - QSL

- There are many QSL ground states depending on the anisotropy and magnetic field

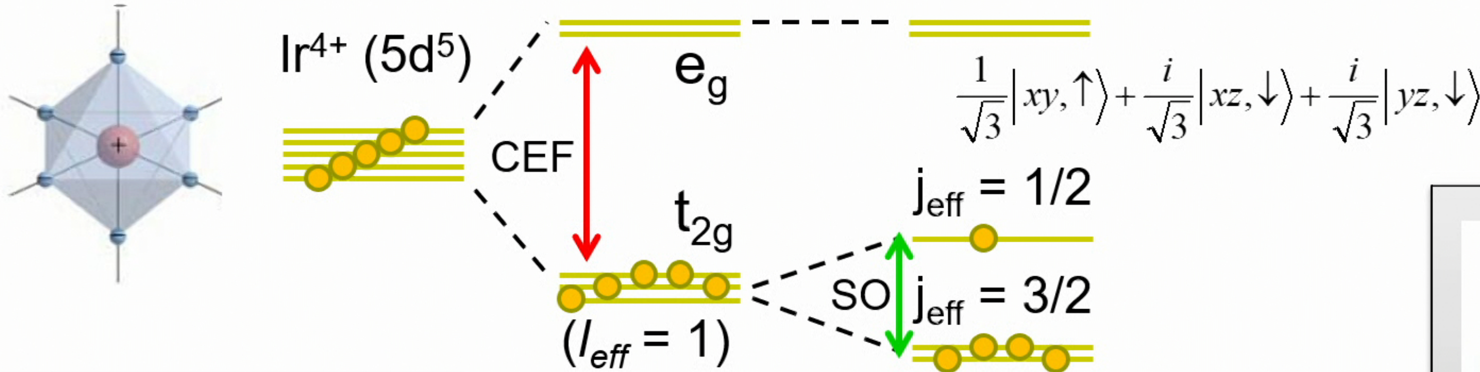


- Interests due to non-abelian anyons useful for topological quantum computing

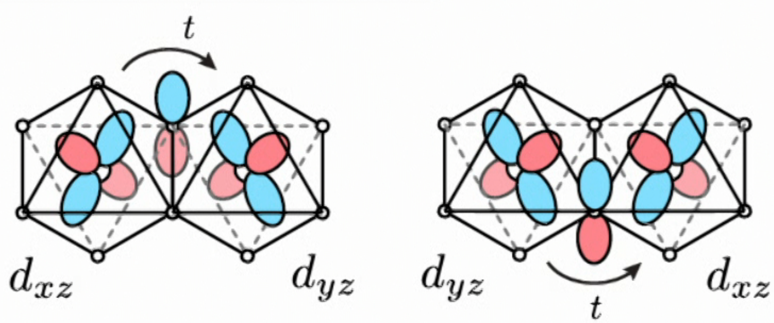
S. Trebst, Phys. Rep. 2022
S. Kim et al. APL Materials 2022

Jackeli-Khaliullin mechanism

Jackeli and Khaliullin PRL 2009



Edge-sharing octahedra

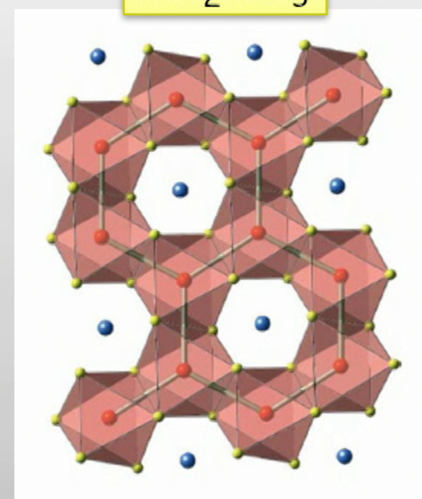


Winter et al. J. Phys. Cond. Matt. 2017 (review)

Lowest order super-exchange contributions interfere destructively.

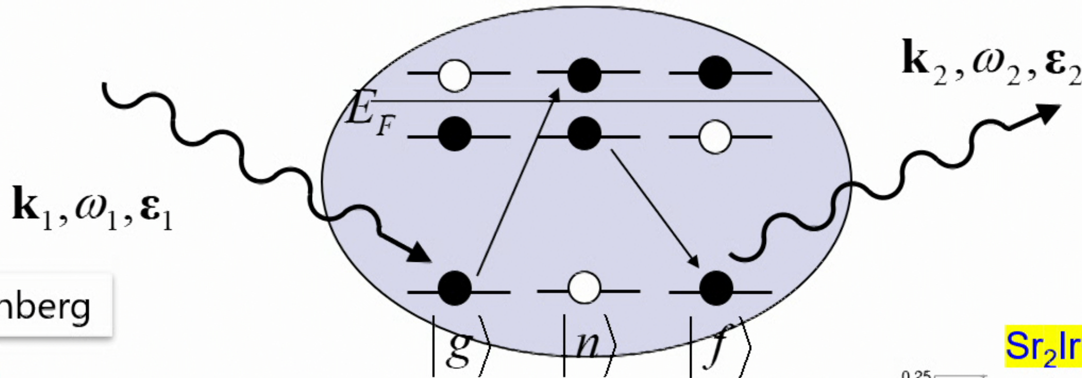
Dominant higher order contribution ➔ Kitaev interaction

Na_2IrO_3



Yogesh Singh and P. Gegenwart PRB 2010

Resonant Inelastic X-ray Scattering



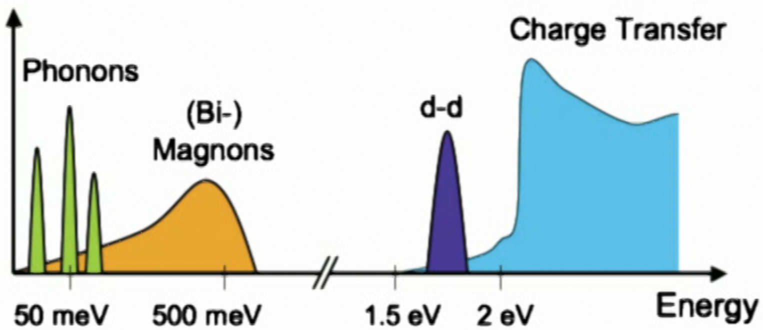
$$\mathbf{Q} \equiv \mathbf{k}_1 - \mathbf{k}_2$$

$$\omega \equiv \omega_1 - \omega_2$$

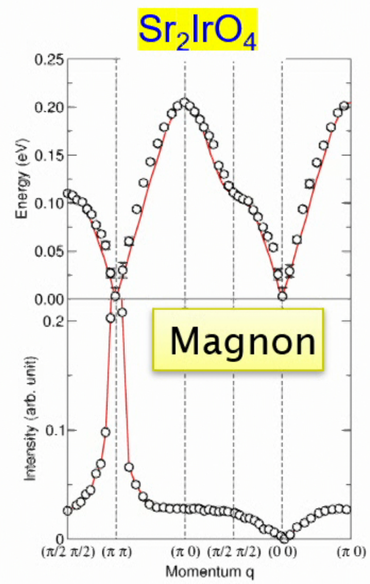
Kramers-Heisenberg

$$I(\omega, \mathbf{k}, \mathbf{k}', \boldsymbol{\epsilon}, \boldsymbol{\epsilon}')$$

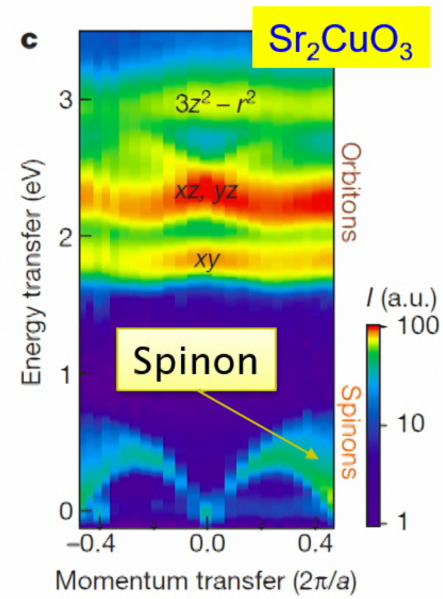
$$= r_e^2 m^2 \omega_{\mathbf{k}'}^3 \omega_{\mathbf{k}} \sum_{\mathrm{f}} \left| \sum_n \frac{\langle f|\mathcal{D}'^\dagger|n\rangle\langle n|\mathcal{D}|g\rangle}{E_g + \hbar\omega_{\mathbf{k}} - E_n + i\Gamma_n} \right|^2 \delta(E_g - E_f + \hbar\omega),$$



Ament et al. Review of Modern Physics 2011

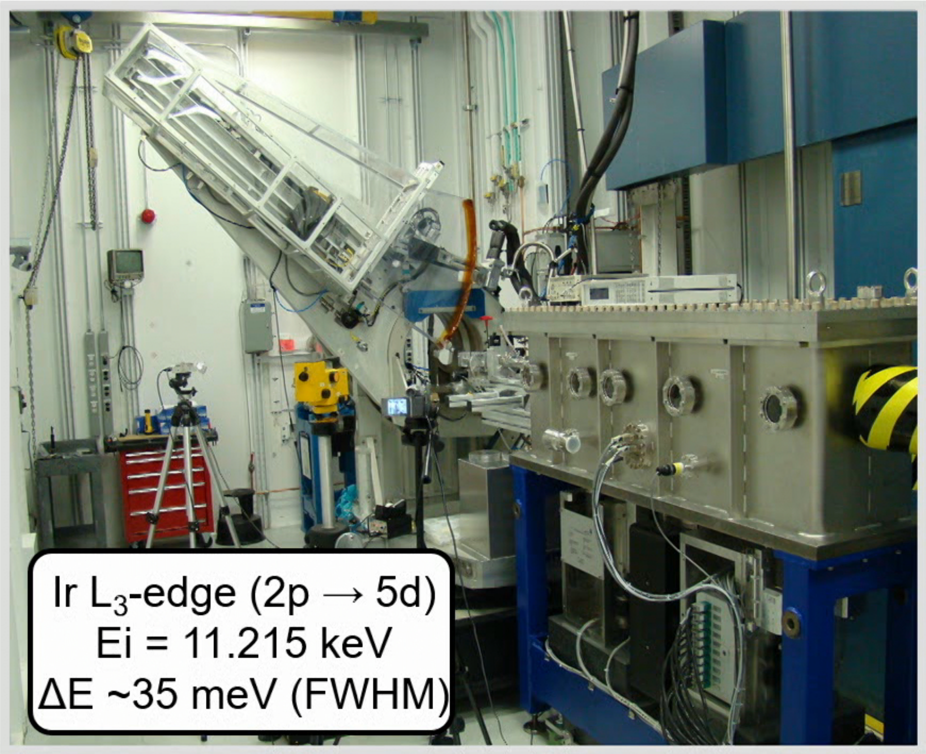


Jungho Kim et al. PRL 2012

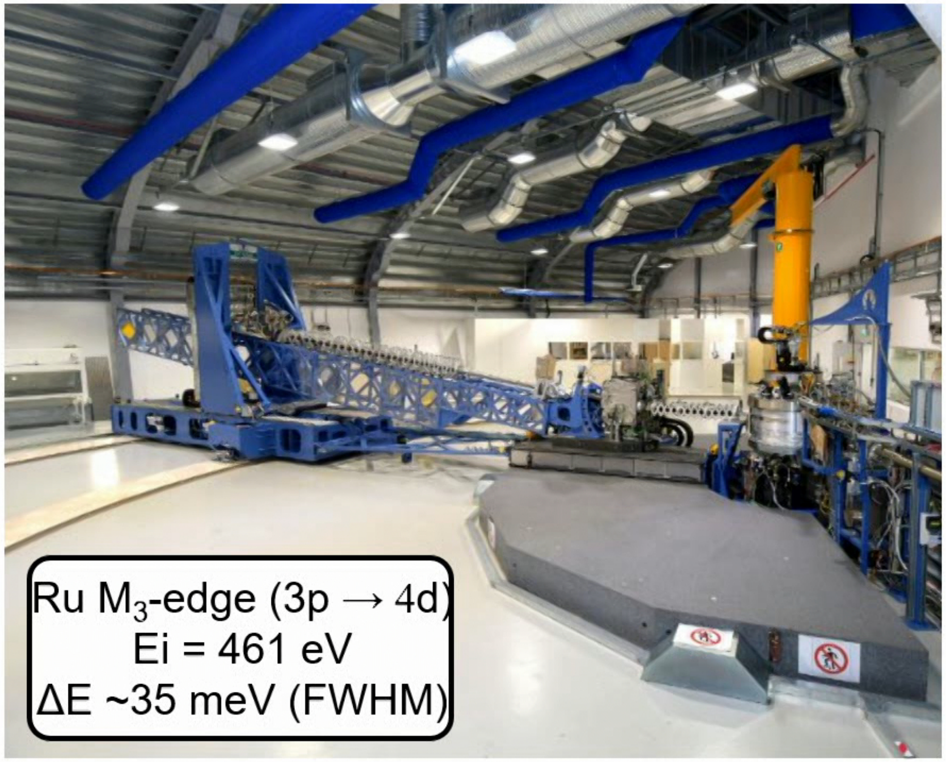


Schlappa et al., Nature 2012

Instrumentation

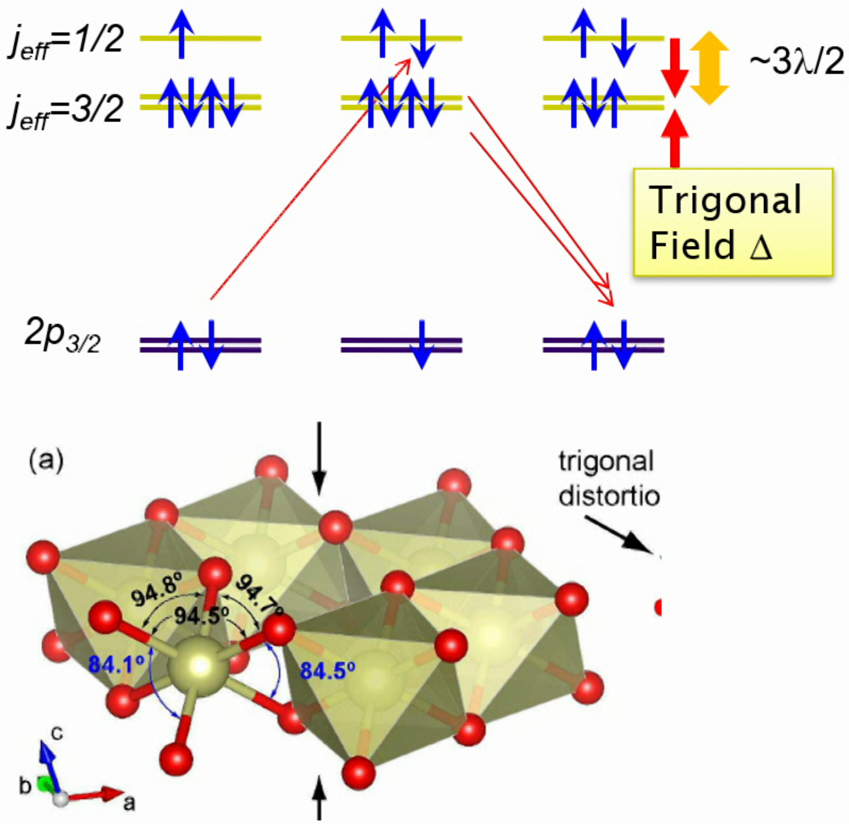


Advanced Photon Source MERIX (27ID)
Argonne National Laboratory

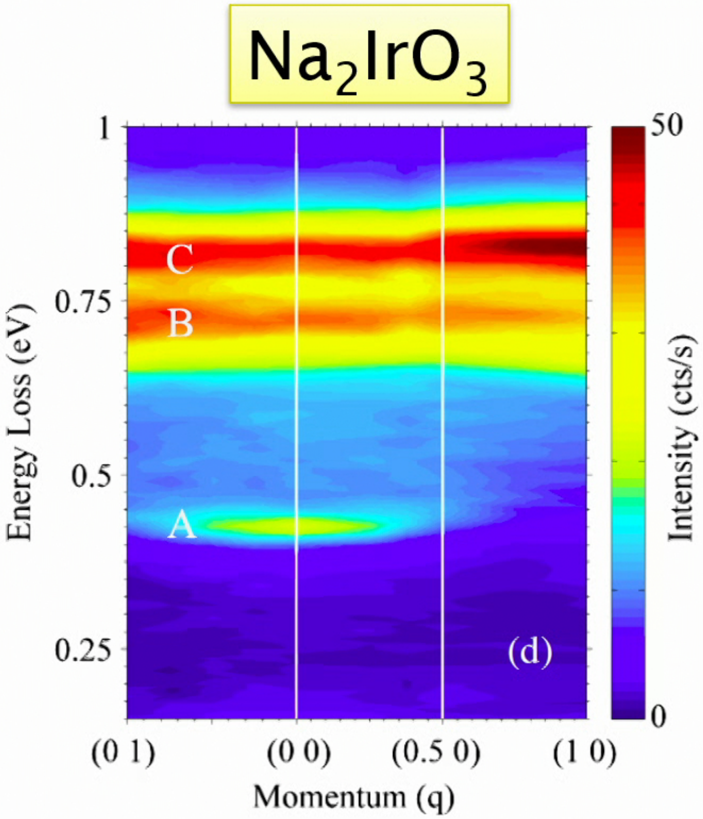


Diamond Light Source I21
Oxford, UK

Measuring SOC with RIXS

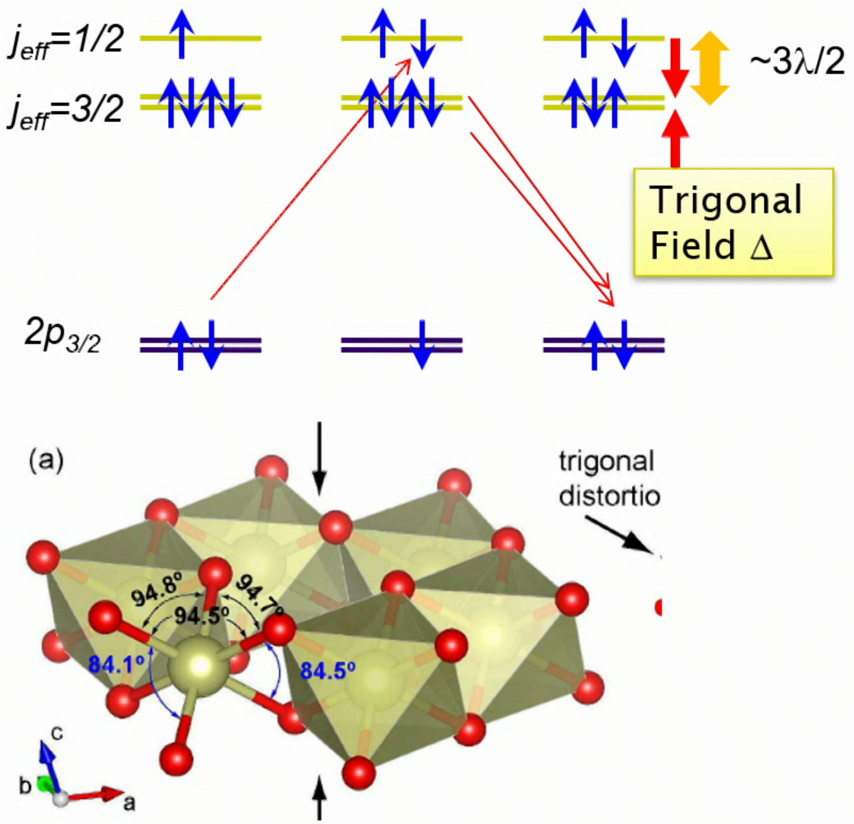


Y. Singh and P. Gegenwart, PRB 82, 064412 (2010).
F. Ye et al., PRB 85 180403 (2012)

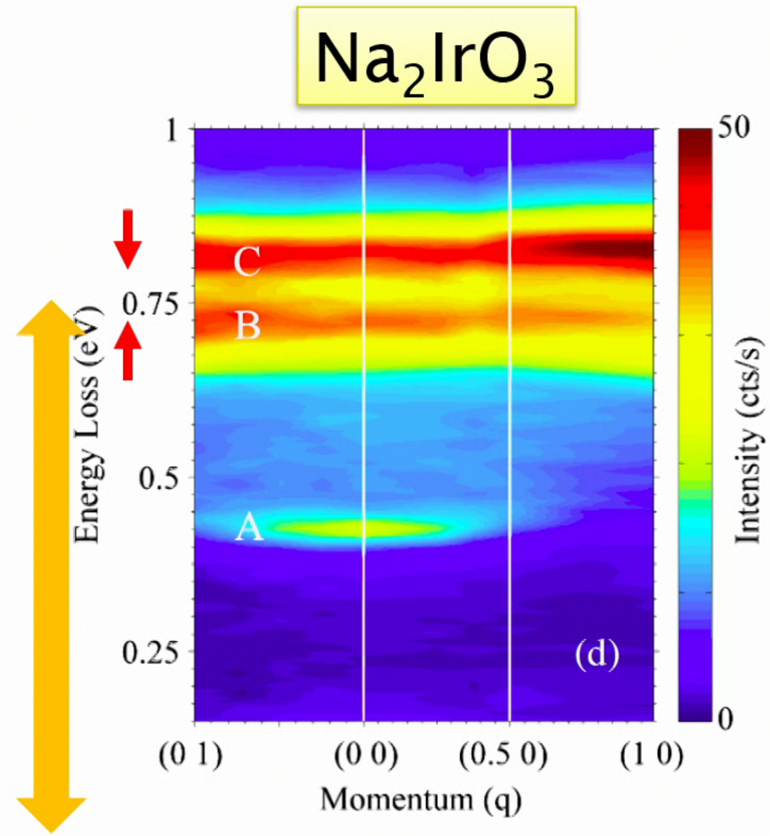


Gretarsson et al. PRL 110, 076402 (2013)

Measuring SOC with RIXS

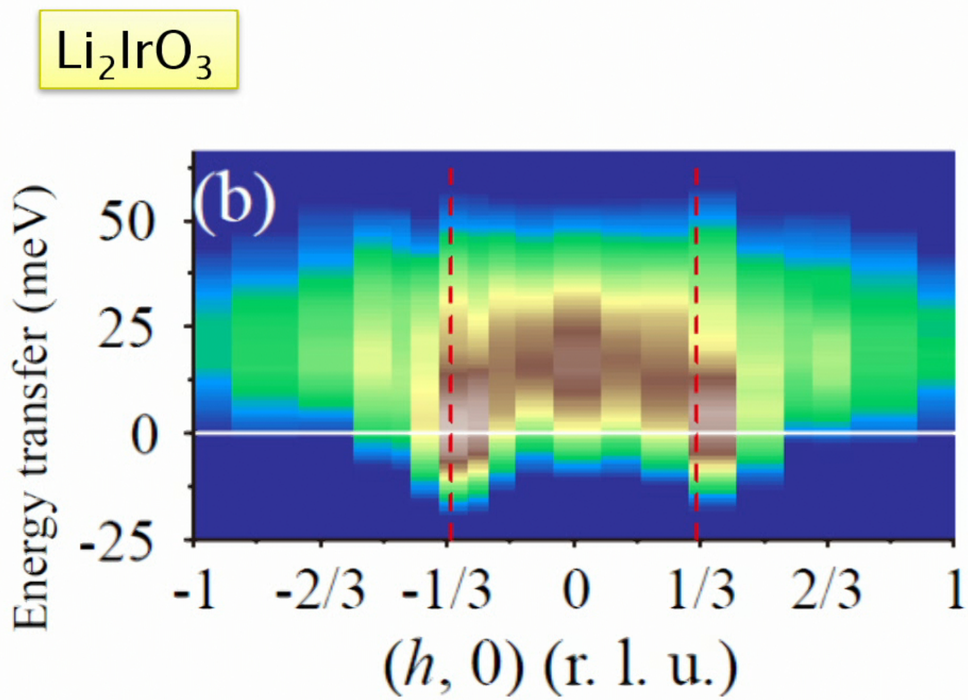


Y. Singh and P. Gegenwart, PRB 82, 064412 (2010).
F. Ye et al., PRB 85 180403 (2012)

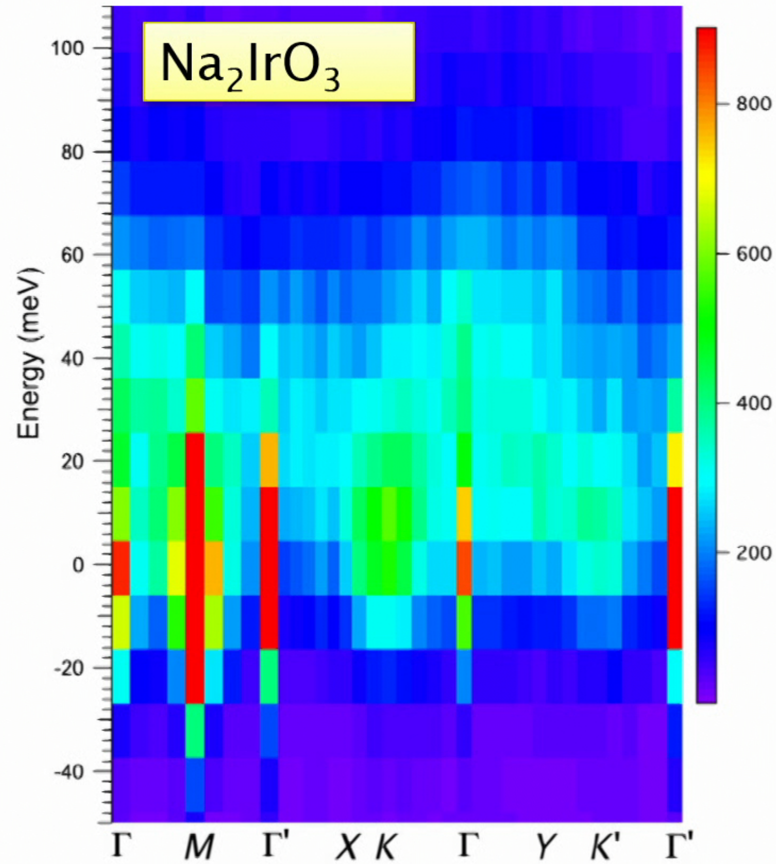


Gretarsson et al. PRL 110, 076402 (2013)

Magnetic Excitations with RIXS



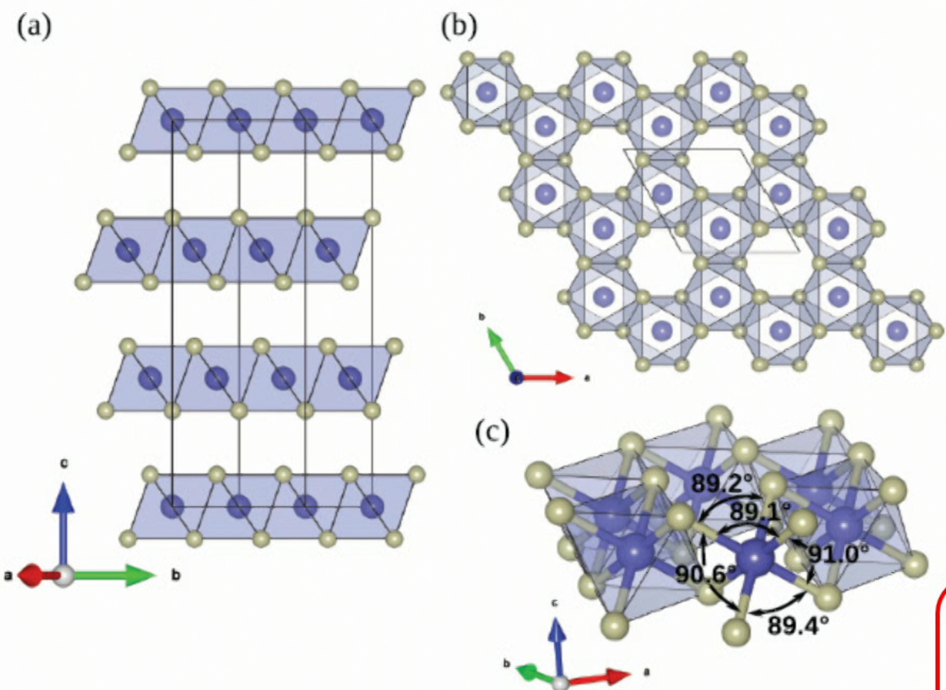
S. H. Chun, YJK et al. PRB 103, L020410 (2021)



Jungho Kim et al. PRX 10, 021034 (2020)

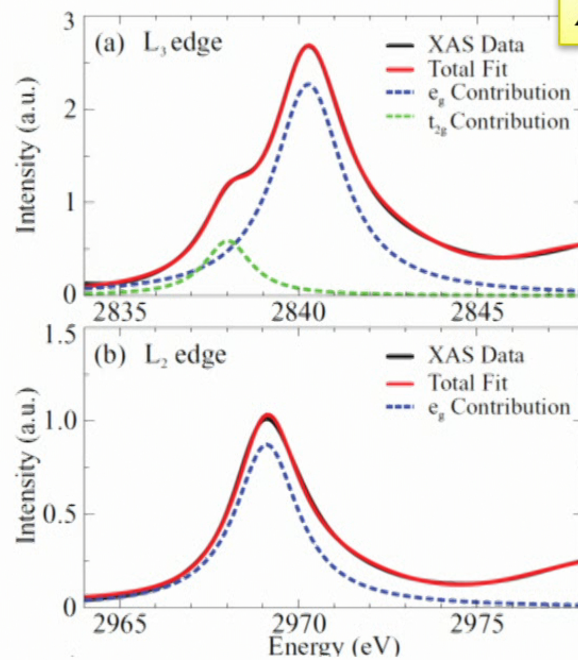
α-$RuCl_3$ as a candidate Kitaev material

Q: Is Jackeli-Khaliullin mechanism still good for Ru with smaller SOC (about 1/3 of SOC of Ir4+)?



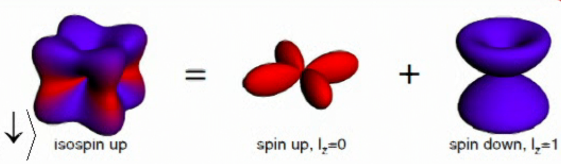
K. W. Plumb et al. Phys. Rev. B 90, 041112 (2014).

XAS



J_{eff} = ½ state

$$\frac{1}{\sqrt{3}}\left|xy,\uparrow\right\rangle+\frac{i}{\sqrt{3}}\left|xz,\downarrow\right\rangle+\frac{1}{\sqrt{3}}\left|yz,\downarrow\right\rangle$$

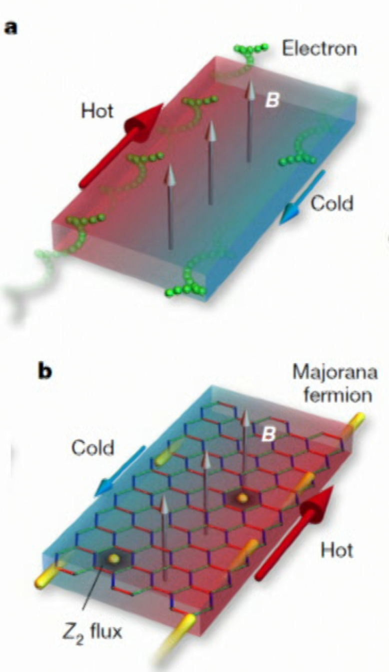


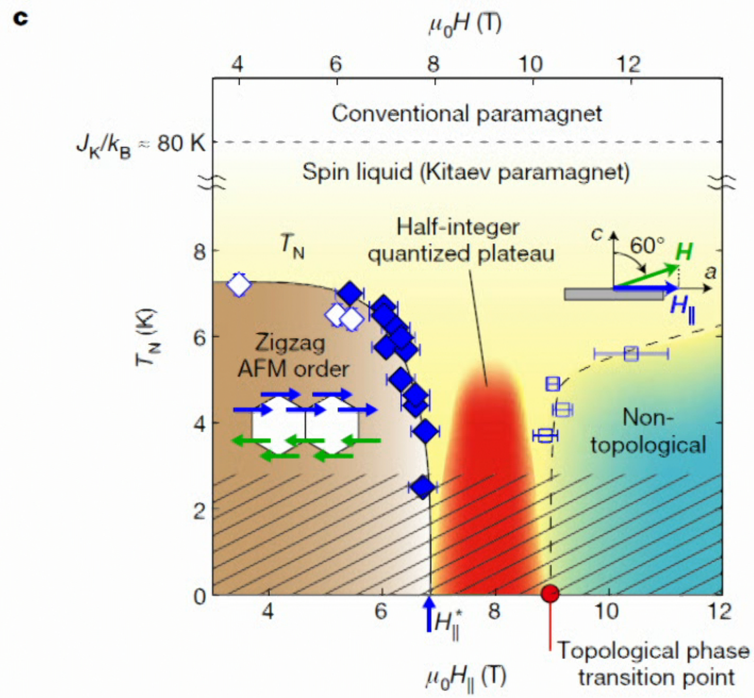
Quantized Thermal Hall effect

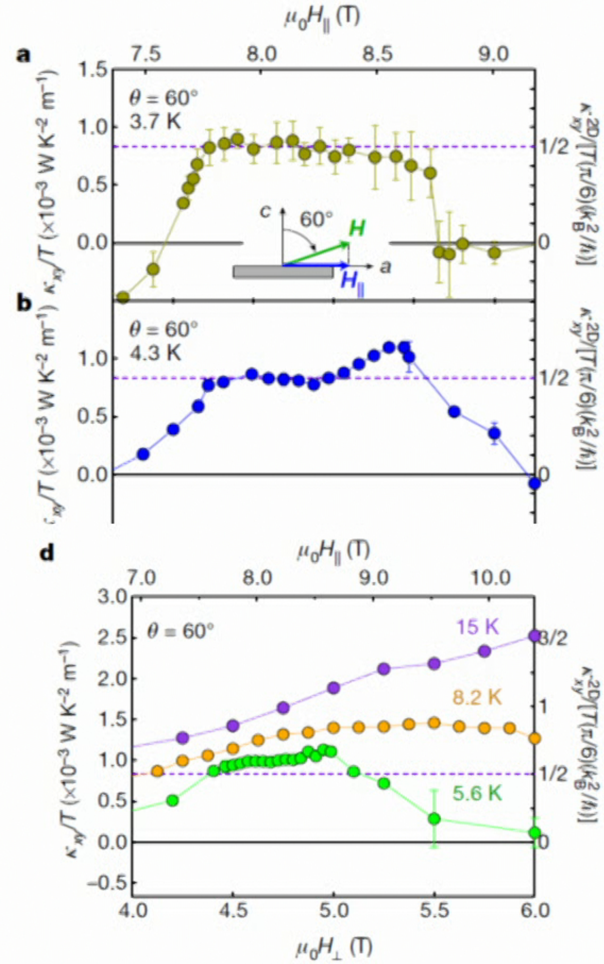
Nature 559, 227 (2018)

Majorana quantization and half-integer thermal quantum Hall effect in a Kitaev spin liquid

Y. Kasahara[1], T. Ohnishi[1], Y. Mizukami[2], O. Tanaka[2], Sixiao Ma[1], K. Sugii[3], N. Kurita[4], H. Tanaka[4], J. Nasu[4], Y. Motome[5], T. Shibauchi[2] & Y. Matsuda[1]*

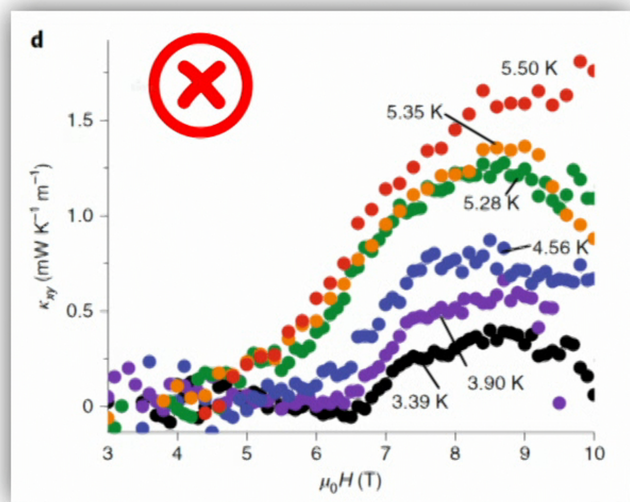




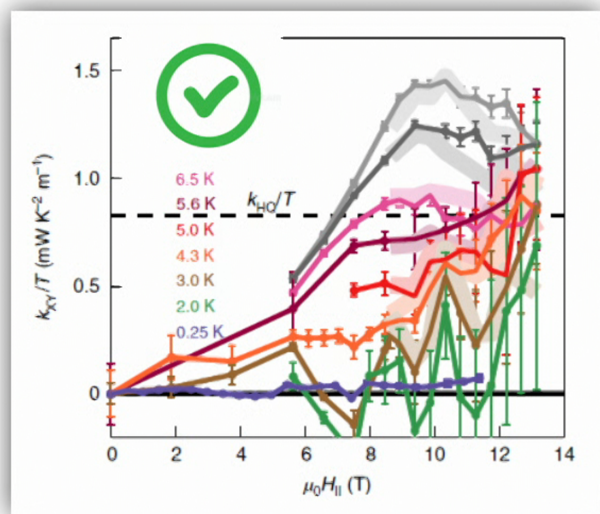


Controversial

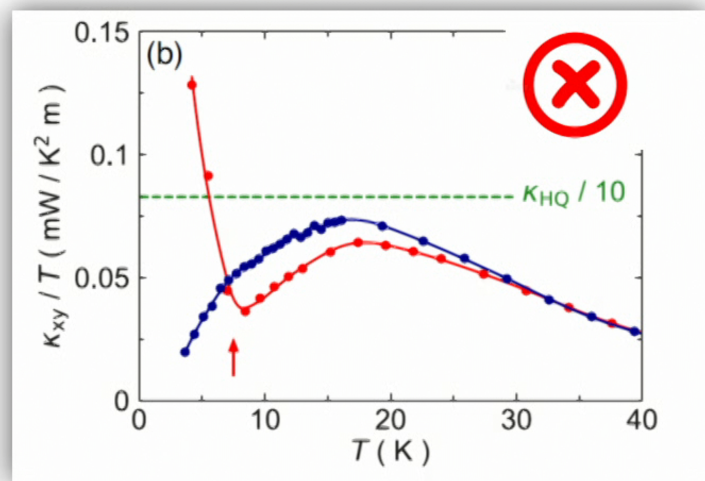
P. Czajka, N. P. Ong Nat. Phys. 2021



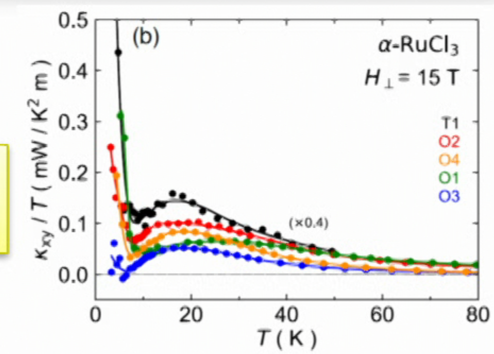
J. A. N. Bruin, H. Takagi, Nat. Phys. 2022



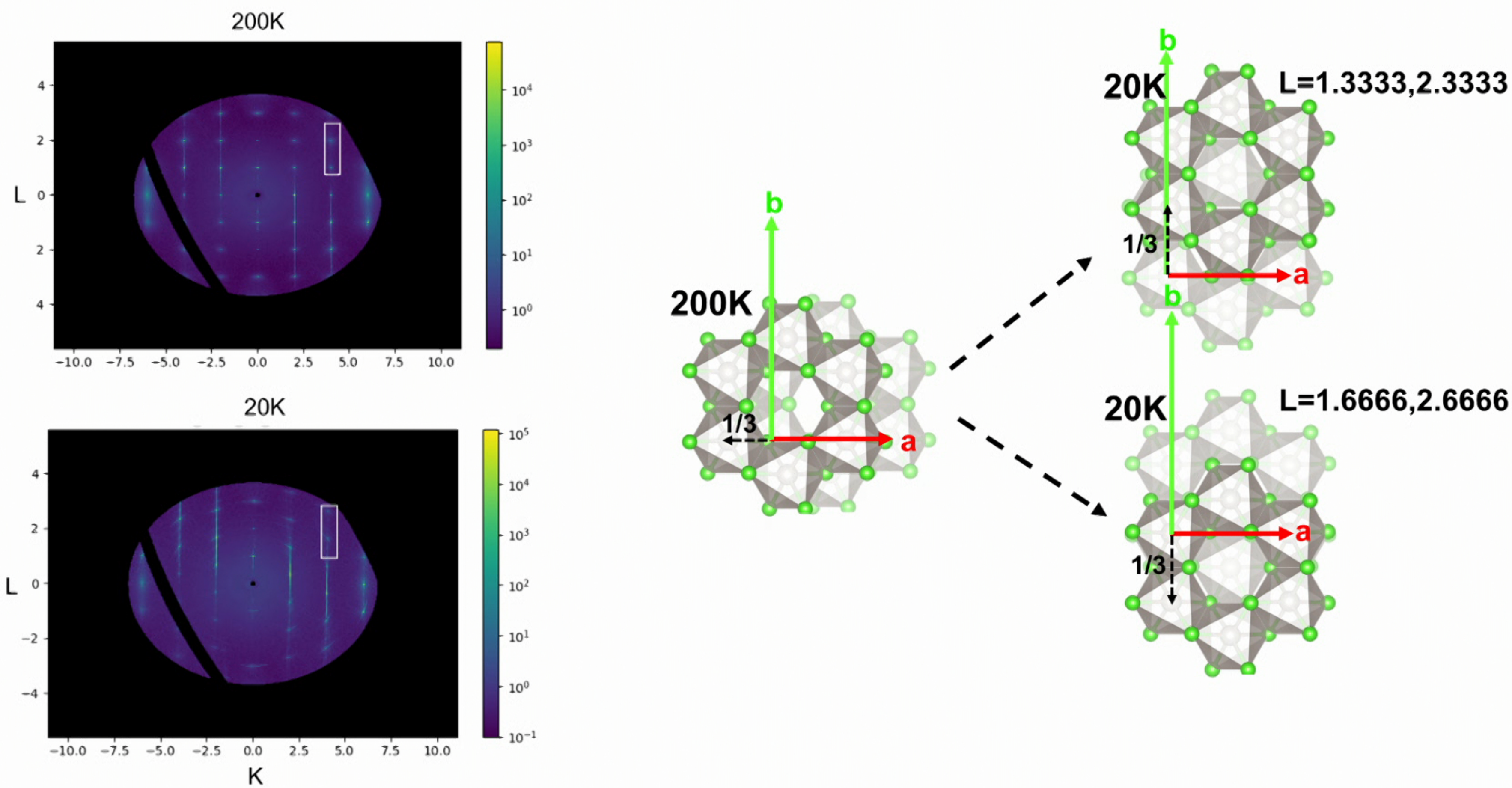
É. Lefrançois, L. Taillefer PRX 2022



However,
Strong sample dependence

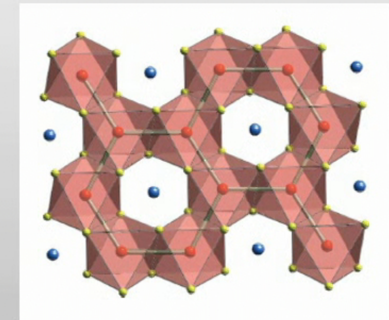


Structural Transition



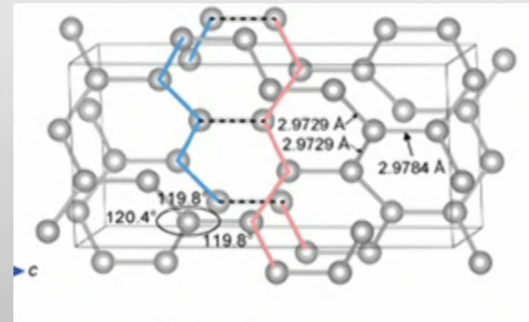
Kitaev materials

Na_2IrO_3 / α-Li_2IrO_3



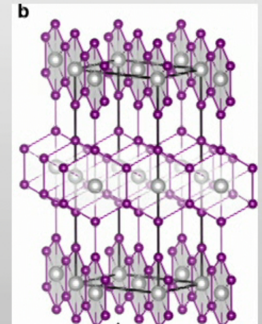
Singh & Gegenwart
PRB 2010

β-Li_2IrO_3



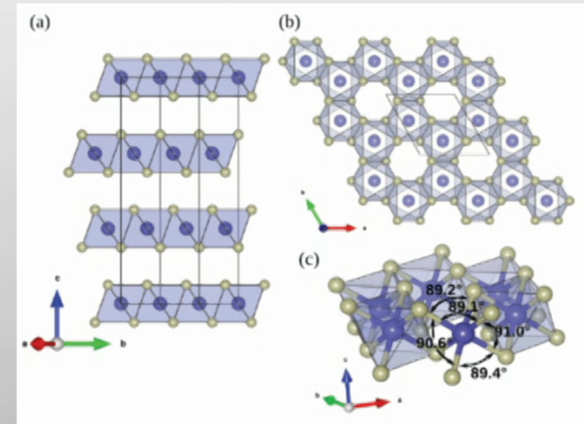
Takagi group
PRL 2015

γ-Li_2IrO_3



Analytis group
Nat. Comm. 2014

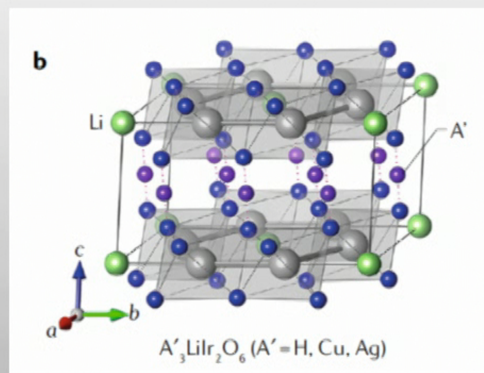
α-$RuCl_3$



Plumb, YJK, et al. PRB 2014

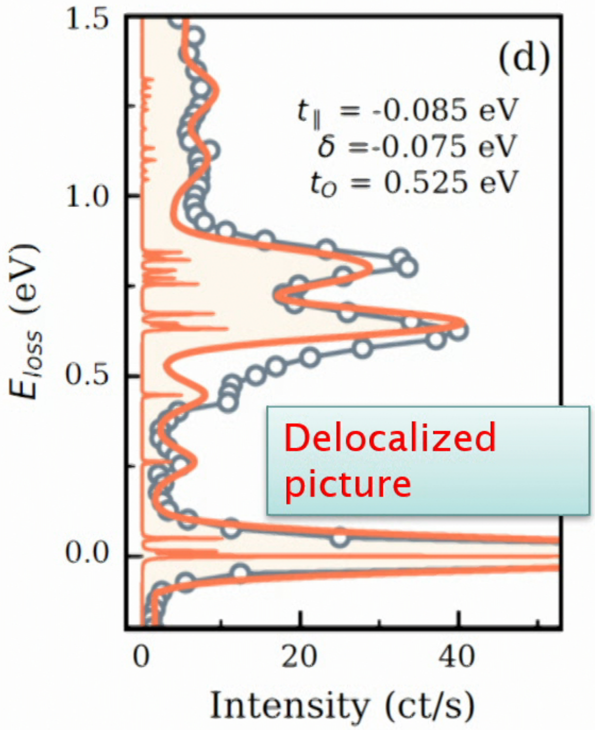
$A'_3LiIr_2O_6$

Takagi group
Nature 2018



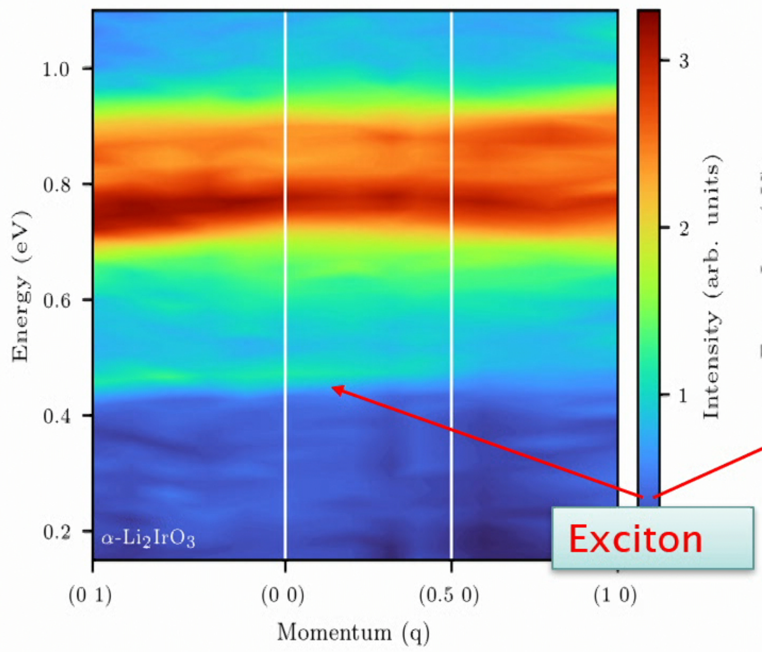
RIXS spectra for other Kitaev materials

$Ag_3LiIr_2O_6$



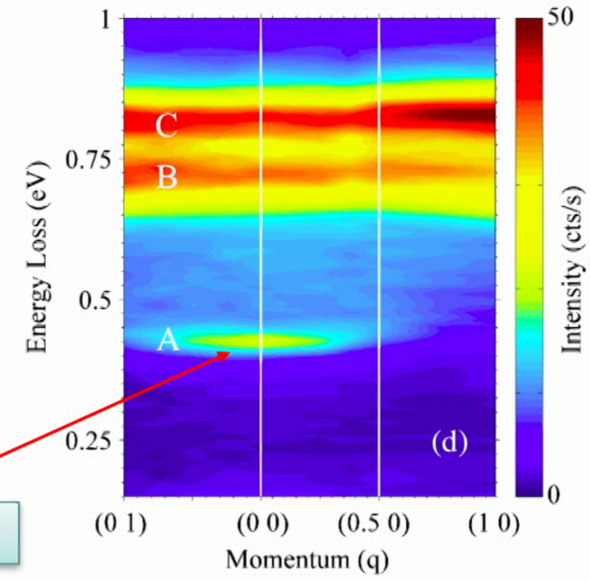
de La Torre, Plumb et al. PRB 2021

α-Li_2IrO_3



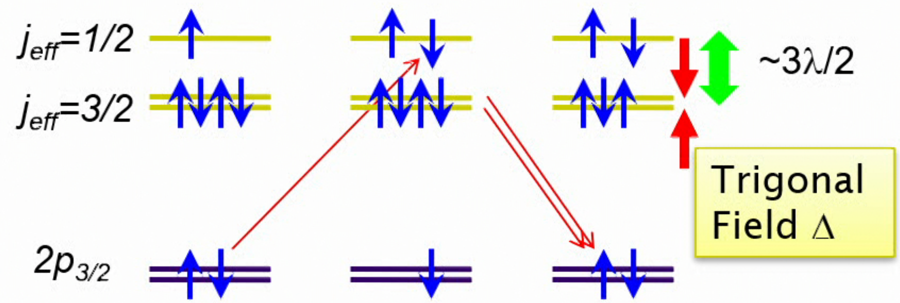
Lebert et al. unpublished

Na_2IrO_3



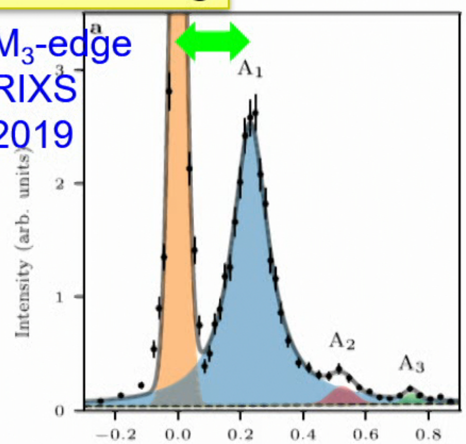
Gretarsson et al.
PRL 110, 076402 (2013)

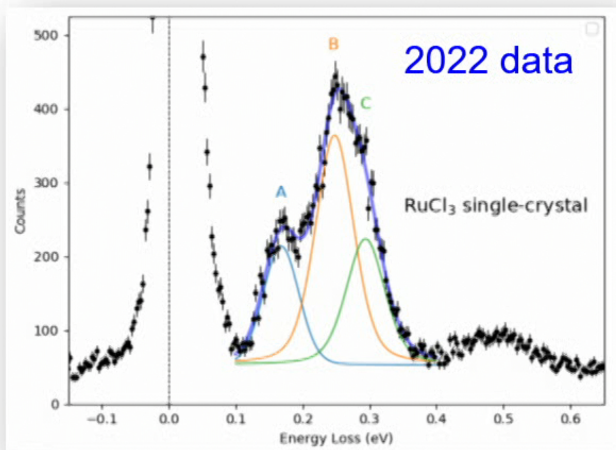
What about α-$RuCl_3$



α-$RuCl_3$

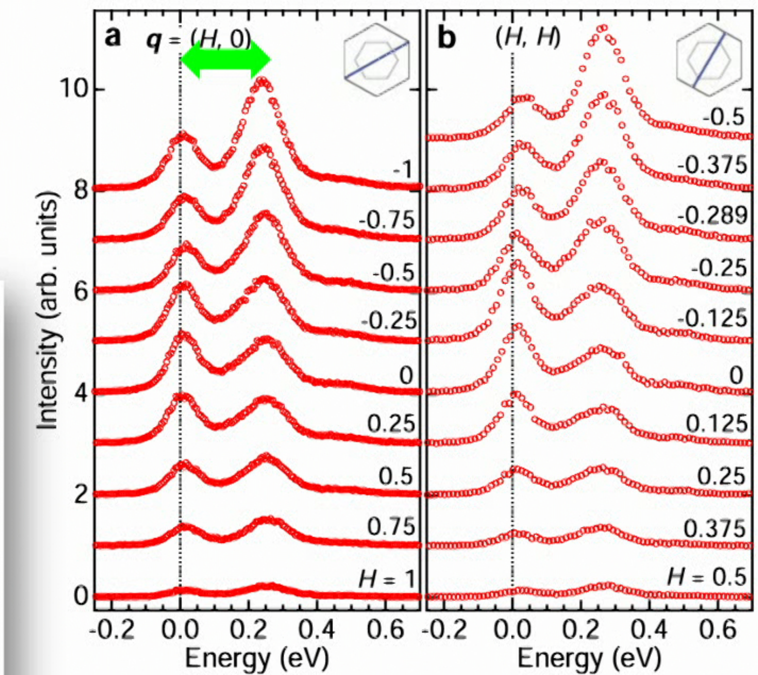
M$_3$-edge RIXS 2019





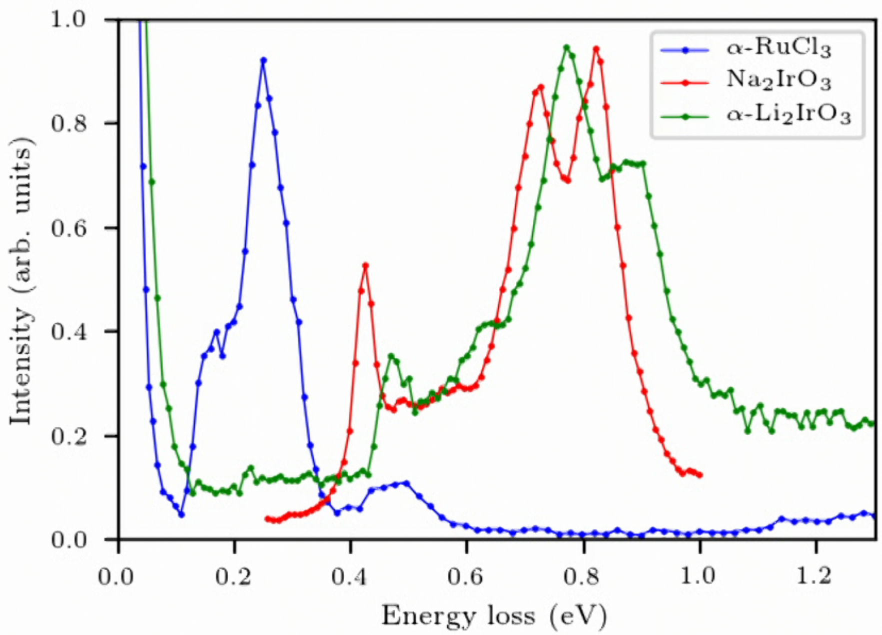
B. Lebert, YJK et al. JPCM 32, 144001 (2020)

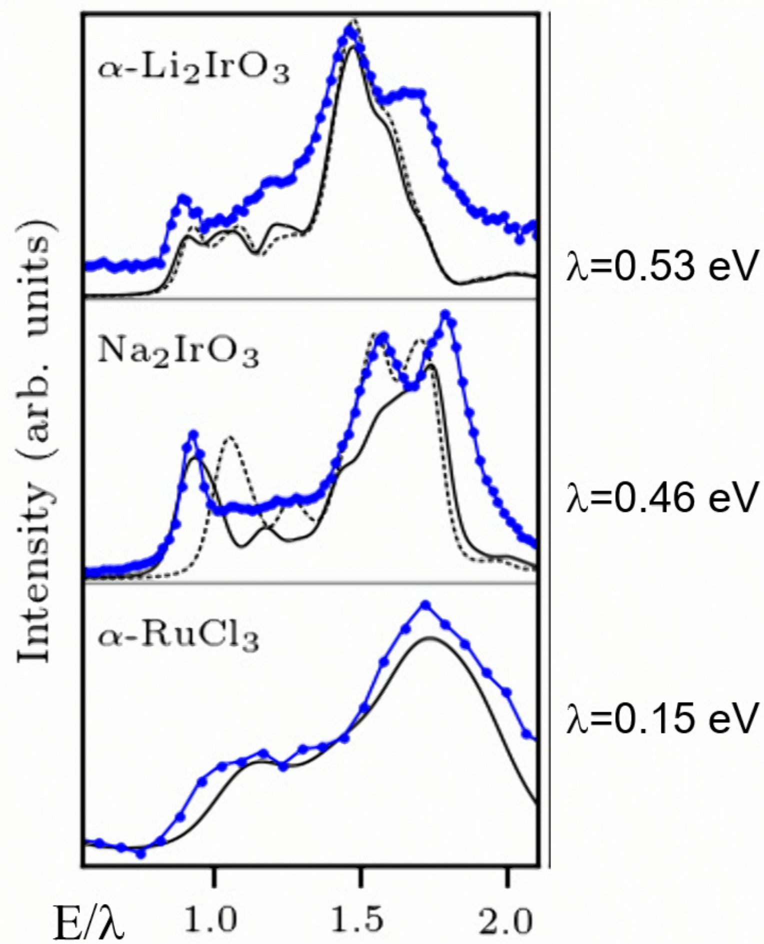
L3-edge RIXS (IRIXS)



H. Suzuki, Keimer et al.
Nat. Comm. 12, 4512 (2021).

Common features of spin-orbit excitations



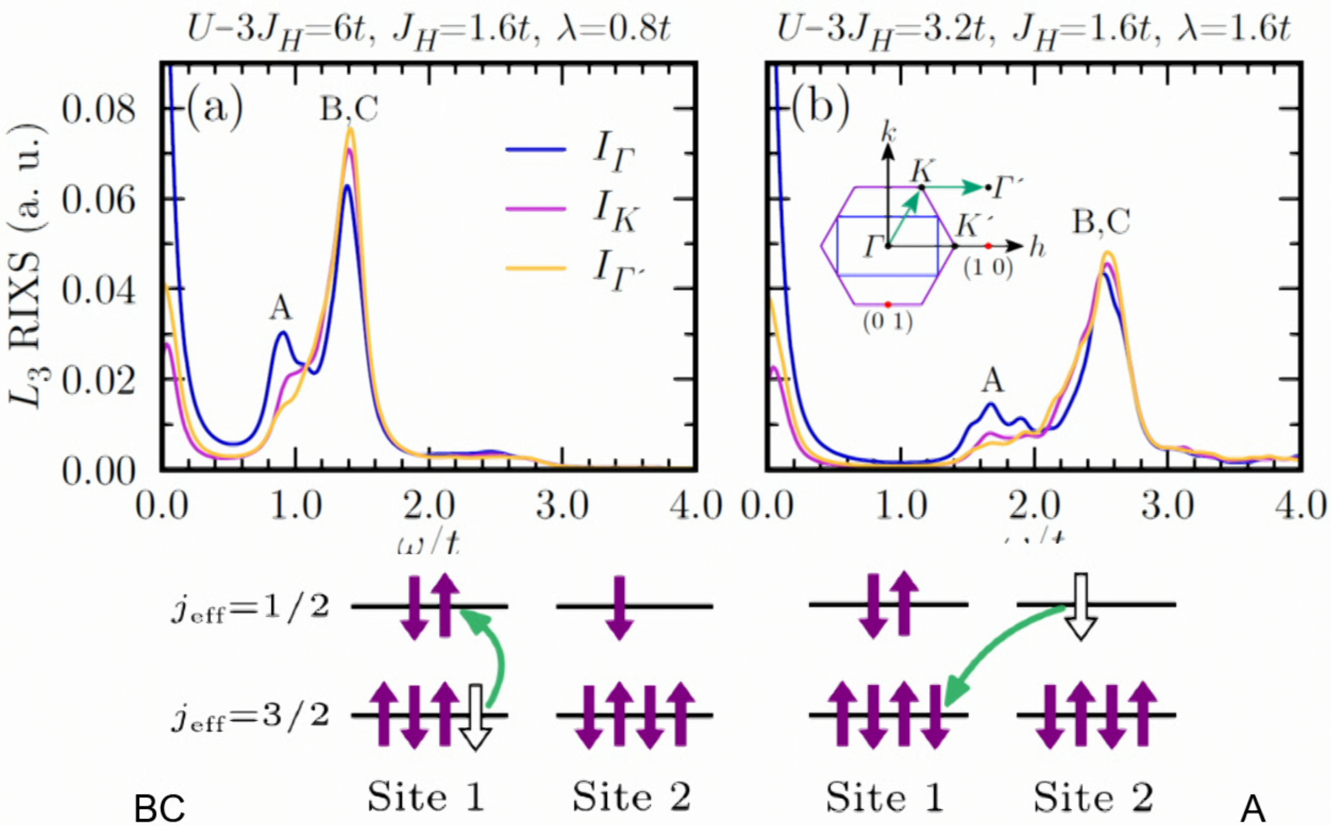


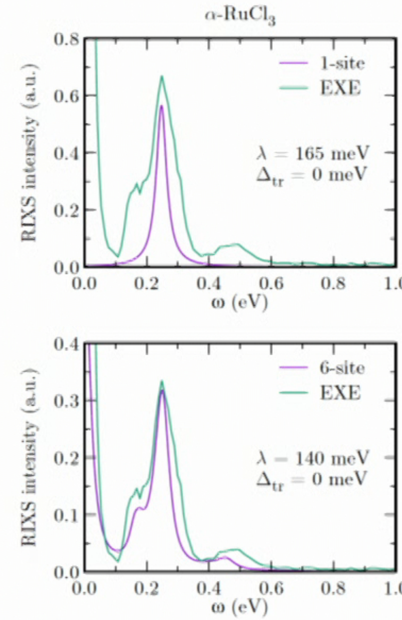
The charge gap is ~1 eV for $RuCl_3$
~0.4 eV for Na_2IrO_3 and Li_2IrO_3

Non-local effect

B. H. Kim, T. Shirakawa, and S. Yunoki, PRL 117 187201 (2016)

- Cluster calculation (ED) – 3 band Hubbard model





Holon-doublon bound state?

Conclusions

- Spin-orbit excitons in Kitaev materials studied with RIXS
  - α-$RuCl_3$ (Ru M_3-edge)
  - Na_2IrO_3 (Ir L_3-edge)
  - α-Li_2IrO_3 (Ir L_3-edge)
- Characteristic 3 peak features are observed in all three compounds
  - Intensity of these peaks show strong momentum dependence
  - The energy scale is more or less determined by SOC only!
  - Can be captured with ED calculation of 3-band model
    - A-peak is not electron-hole exciton (Charge gap of α-$RuCl_3$ is much larger than those of the other two materials)
    - A is due to non-local physics (holon-doublon excitation)