

Title: Honeycomb lattice quantum magnets with strong spin-orbit coupling

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Abstract: In recent years, there has been much interest in honeycomb lattice quantum magnets described by Kitaev-Heisenberg Hamiltonian. For example, honeycomb lattice iridates, such as Na_2IrO_3 and Li_2IrO_3 have been intensely scrutinized. Recently, we proposed that a 4d honeycomb magnet $\hat{\Gamma}_2\text{-RuCl}_3$ is a promising candidate material in which Kitaev physics could be studied. I will give an overview of the physics of $\alpha\text{-RuCl}_3$, and talk about recent experimental and theoretical advances.

4 Corners May 12, 2016

Honeycomb Lattice Quantum Magnets with strong SOC

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Acknowledgements

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H. Gretarsson



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K. Plumb



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X-ray/Neutron

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Samples/ARPES

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Theory

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Heungsik Kim
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Jeroen van den Brink
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Advanced
Photon
Source



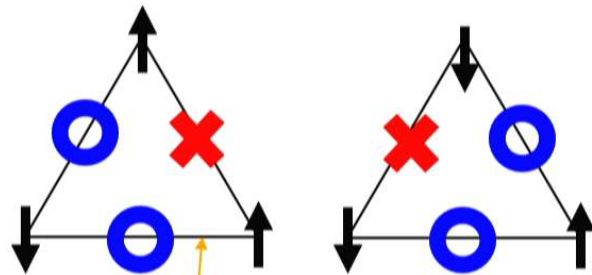
UNIVERSITY OF
TORONTO



Canada Foundation
for Innovation
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pour l'innovation

Frustration suppresses order

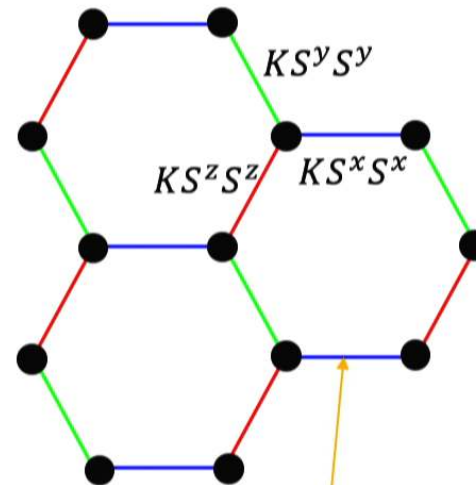
Bond frustration



Heisenberg interaction

- + single ion anisotropy
- + exchange anisotropy
- + Dzyaloshinsky-Moriya

Site frustration



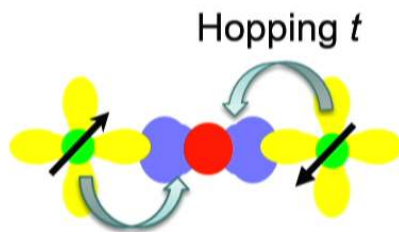
Kitaev interaction
– bond dependent anisotropic interaction

Kitaev model

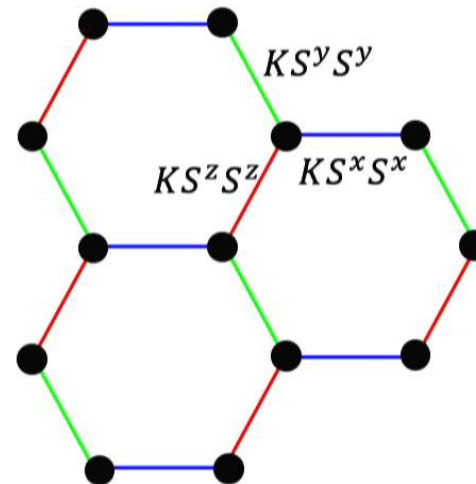
$$\mathcal{H}^{Kitaev} = - \sum_{i,\gamma} K_\gamma S_i^\gamma S_{i+\vec{e}_\gamma}^\gamma$$

- Exactly solvable model
- Gapless Spin liquid ground state due to frustration
- Elementary excitation - Majorana fermion

Heisenberg superexchange

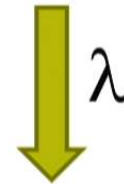


Alexei Kitaev, Ann. Phys. 2006

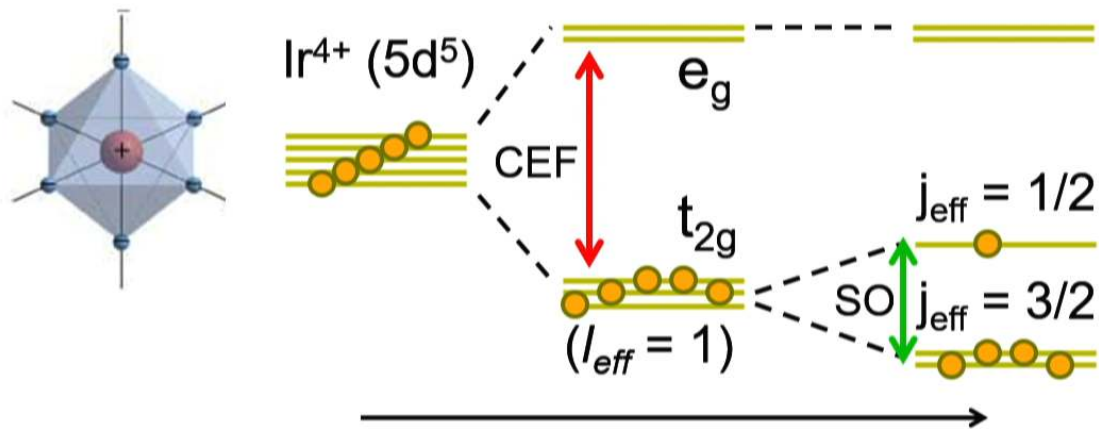


Why iridates?

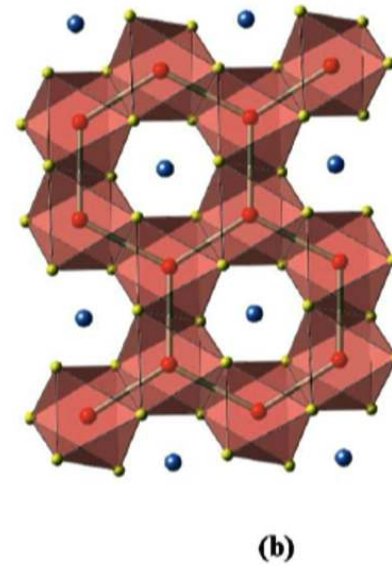
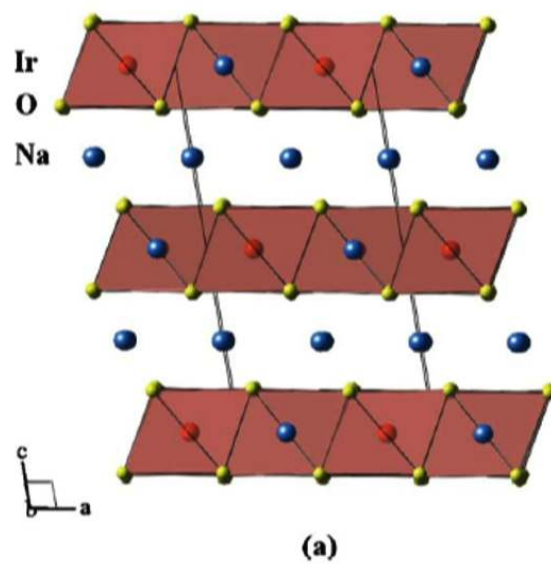
Group →	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	
↓ Period																			
1	1 H																		2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	
6	55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	
7	87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Fl	115 Uup	116 Lv	117 Uus	118 Uuo	
Lanthanides			57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu		
Actinides			89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr		



Physics of Ir^{4+} ($5d^5$) in cubic CEF



A₂IrO₃ (A=Na, Li)



Li₂IrO₃ **powder**
Na₂IrO₃ **crystal**

~2x2 mm²

- Honeycomb lattice of Ir⁴⁺
- Heisenberg-Kitaev model?

$$\mathcal{H}_{ij}^{(\gamma)} = -J_1 S_i^\gamma S_j^\gamma + J_2 \mathbf{S}_i \cdot \mathbf{S}_j$$

Singh, Gegenwart

Honeycomb iridates

PRL **105**, 027204 (2010)

PHYSICAL REVIEW LETTERS

week ending
9 JULY 2010

Kitaev-Heisenberg Model on a Honeycomb Lattice: Possible Exotic Phases in Iridium Oxides $A_2\text{IrO}_3$

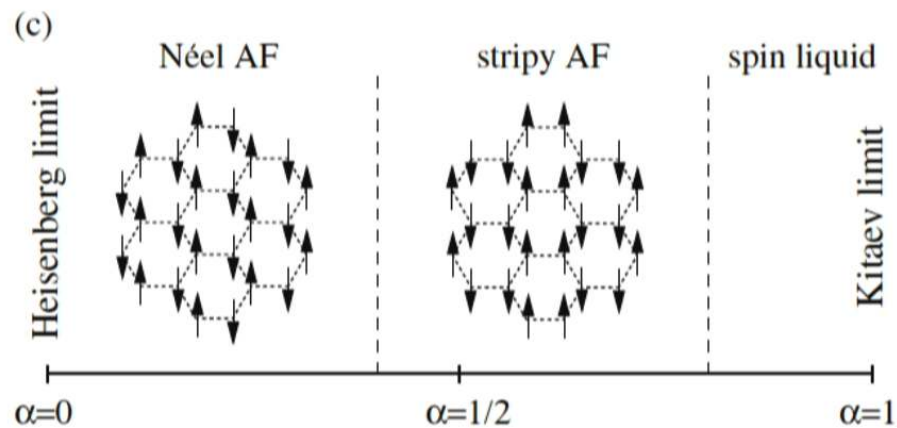
Jiří Chaloupka,^{1,2} George Jackeli,^{2,*} and Giniyat Khaliullin²

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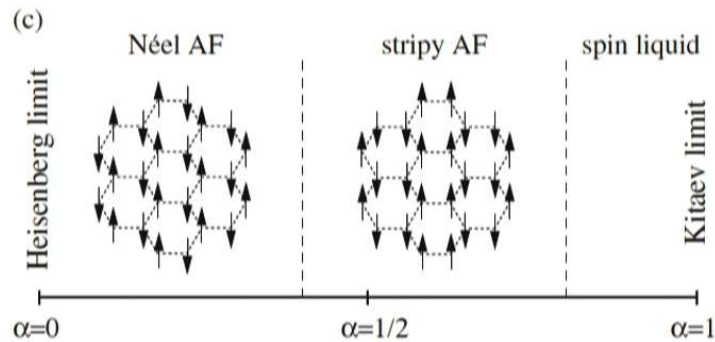
(Received 16 April 2010; published 9 July 2010)

$$\mathcal{H}_{ij}^{(\gamma)} = -J_1 S_i^\gamma S_j^\gamma + J_2 \mathbf{S}_i \cdot \mathbf{S}_j.$$



However...

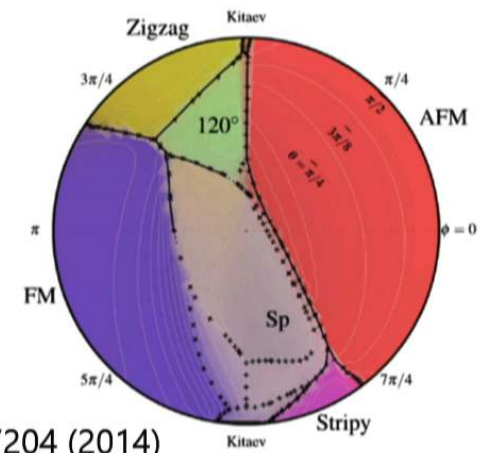
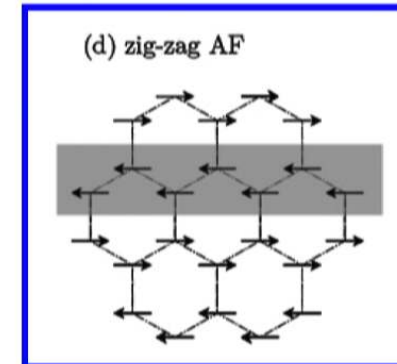
Chaloupka, Jackeli, and Khaliullin PRL 2010



- No zig-zag phase!
- Still a lot of confusion about the Hamiltonian
 - Large 2nd and 3rd nearest neighbor interaction
 - Antiferromagnetic Kitaev term (?)

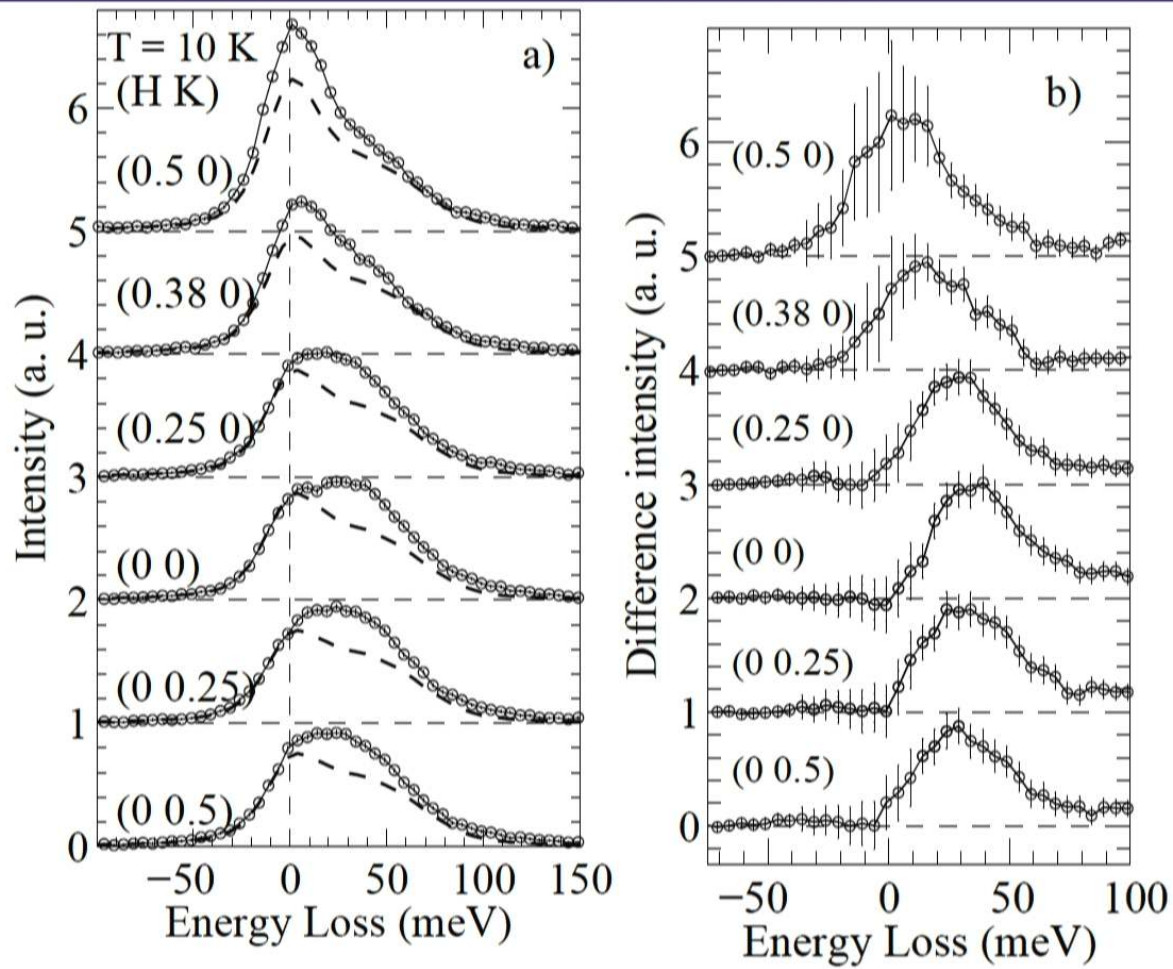
X. Liu, et al., PRB (2011)

Experimental structure



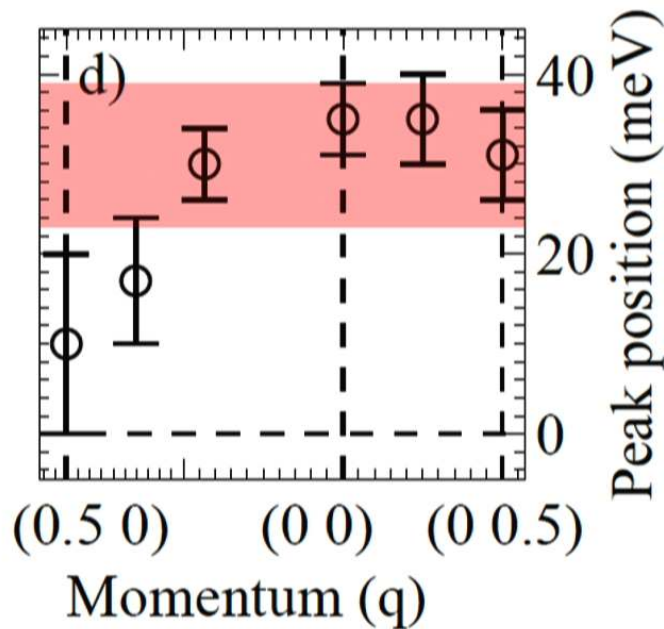
J. G. Rau et al., PRL 112, 077204 (2014)

Na₂IrO₃ magnetic excitations (RIXS)

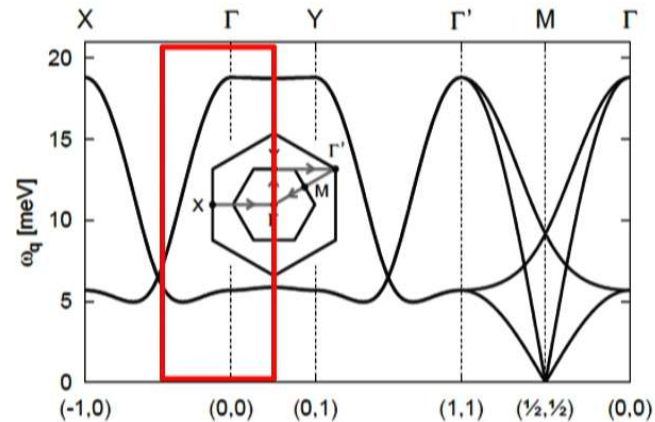


Dispersion relation

Gretarsson, YJK et al., PRB 87, 220407 (2013)



Chaloupka et al., PRL 110, 097204 (2013)



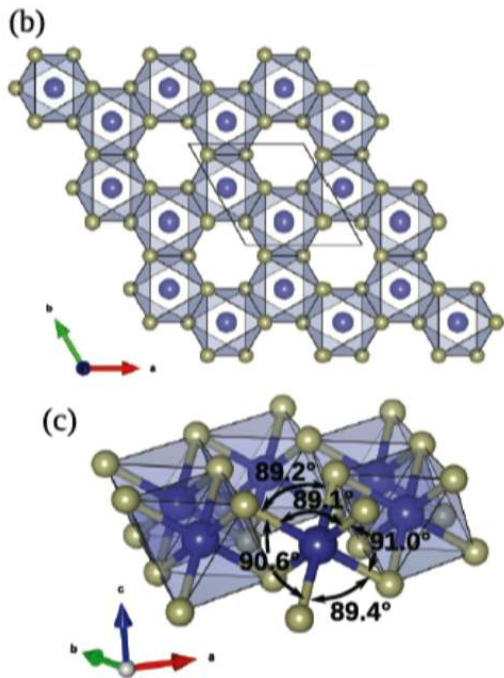
- Need a large energy scale ~ 30 meV
- Is this AF Kitaev term?

Difficulty due to poor energy resolution of RIXS

Wait till next gen instrumentation

α -RuCl₃ - neutron friendly

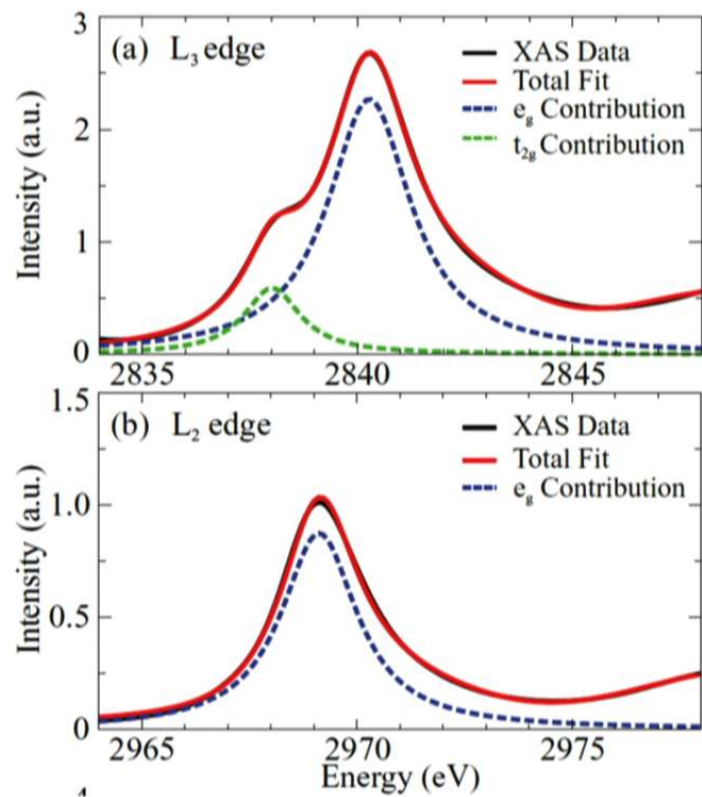
- Well-known semiconductor since 1960's.
- Used as a catalyst



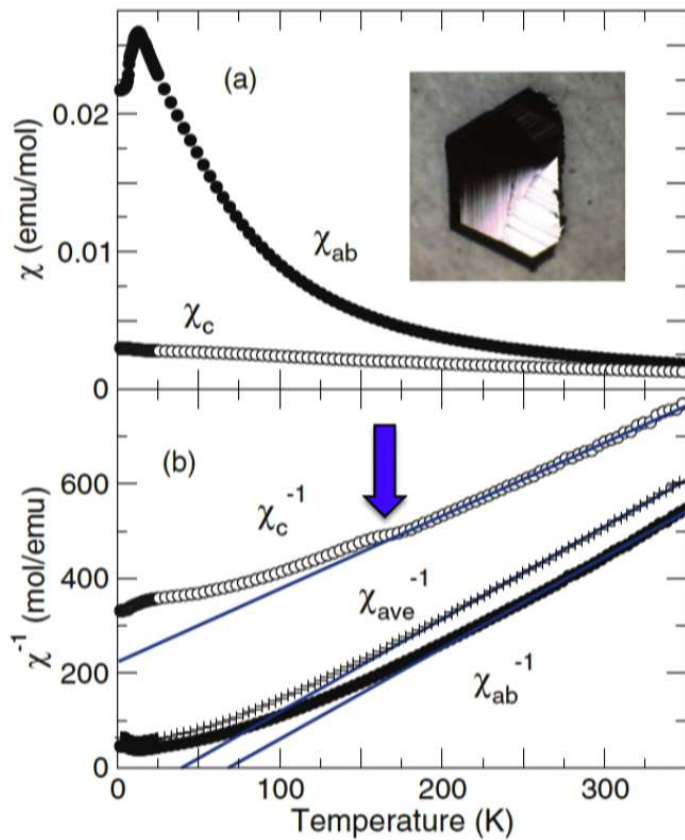
K. W. Plumb, YJK et al., Phys. Rev. B 90, 041112 (2014)

$J_{\text{eff}}=1/2$?

X-ray Absorption Spectroscopy

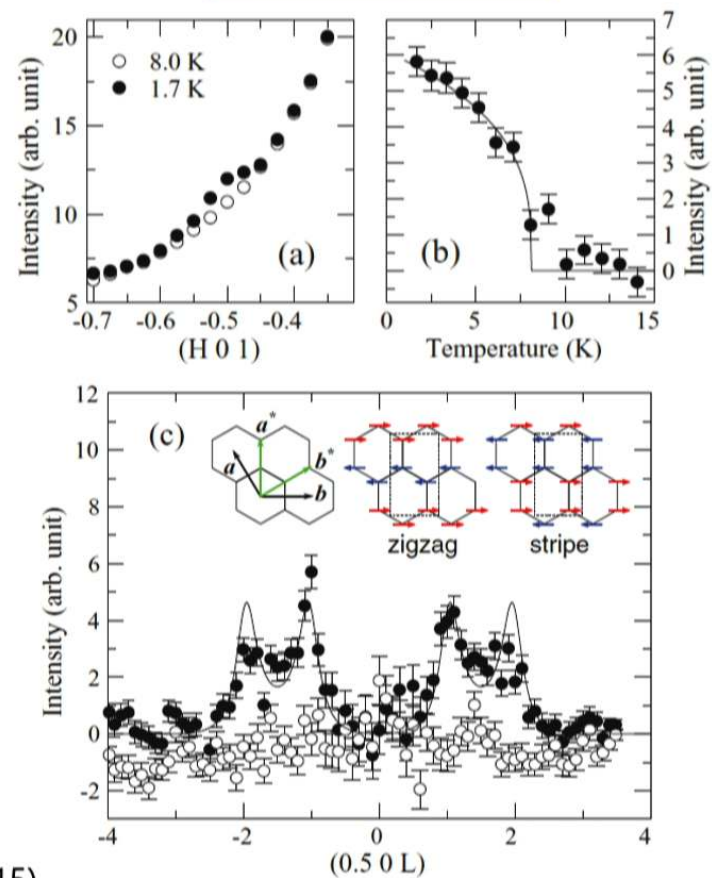


Magnetic properties

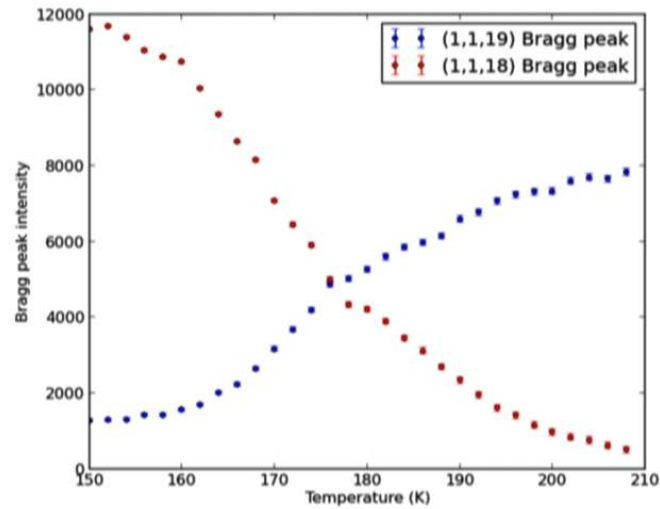


J. A. Sears, YJK et al., Phys. Rev. B 91, 144420 (2015)

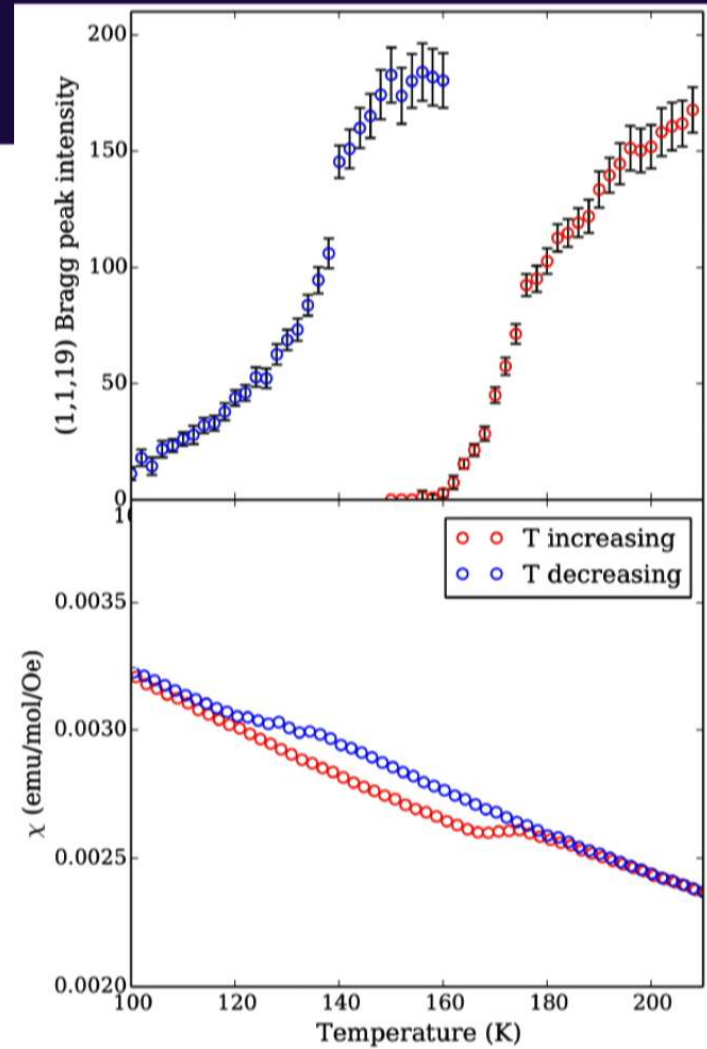
Neutron diffraction



Structural transition



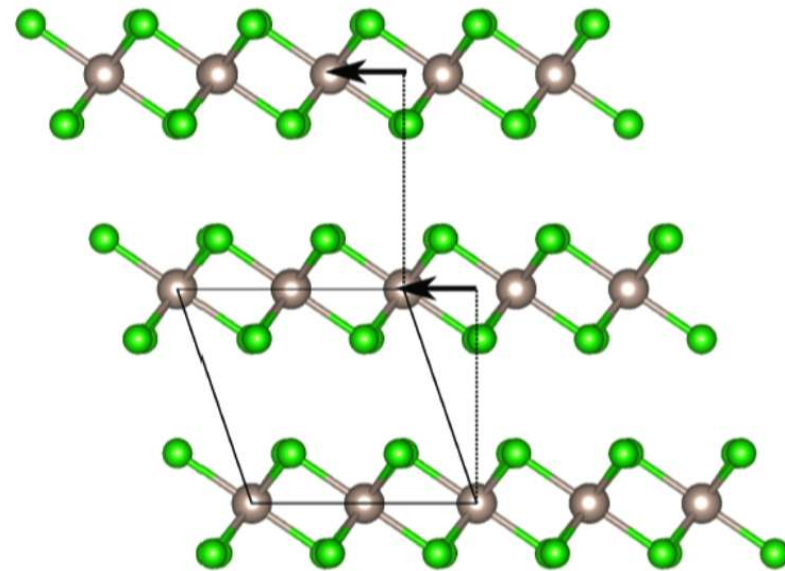
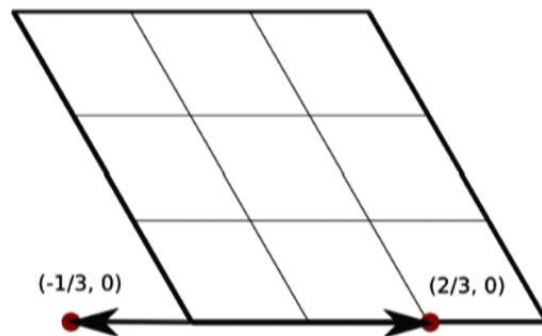
- Change in stacking pattern
- 1st order transition
- Large hysteresis



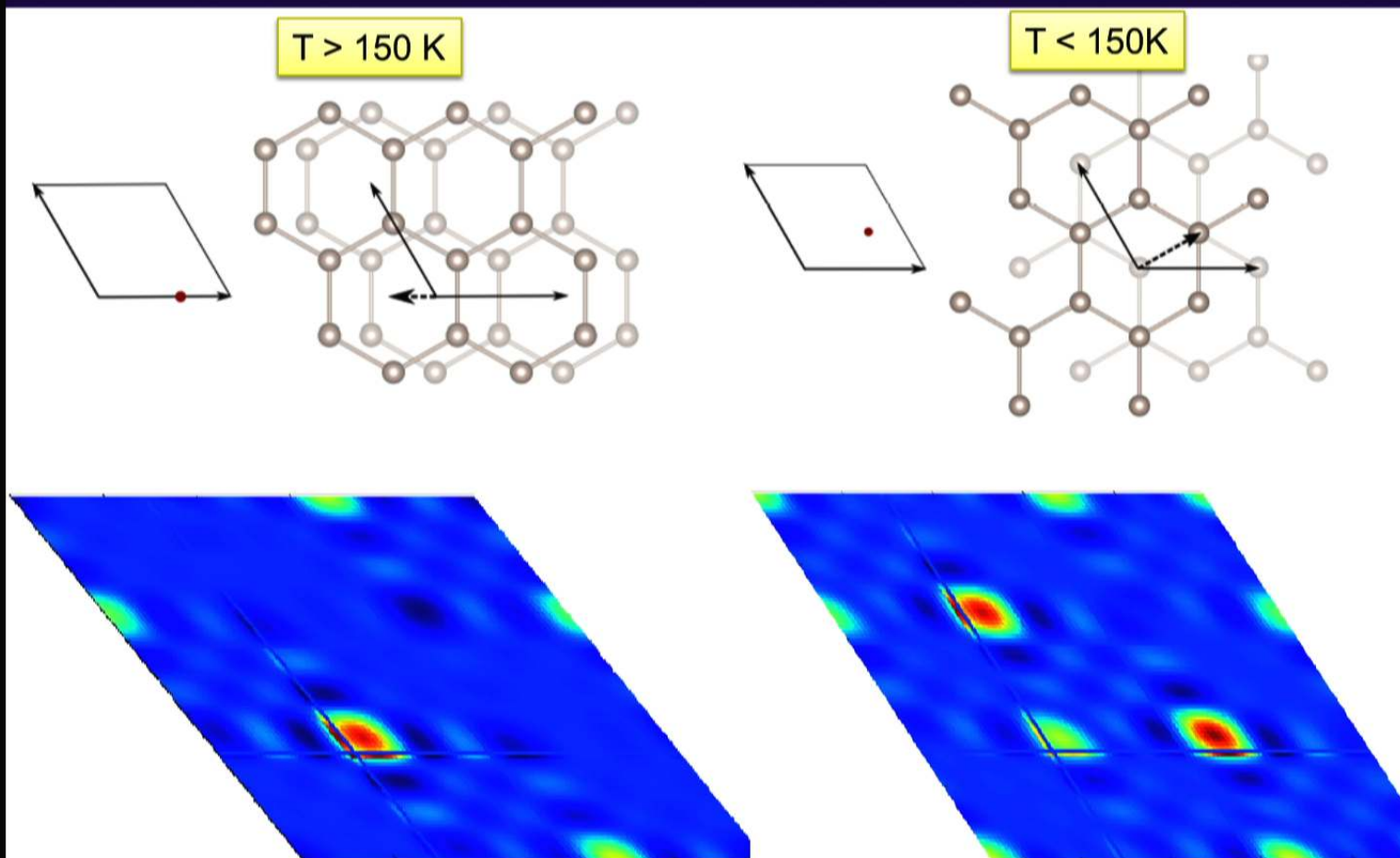
Room temperature structure

In perfect C2/m structure only 1 type of shift between nearest neighbours:

$(-1/3, 0)$ in hexagonal notation



Fourier analysis of stacking

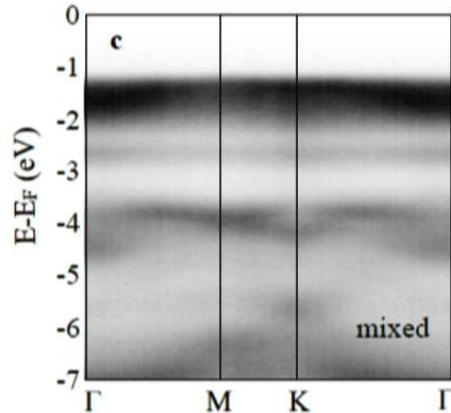


Electronic structure

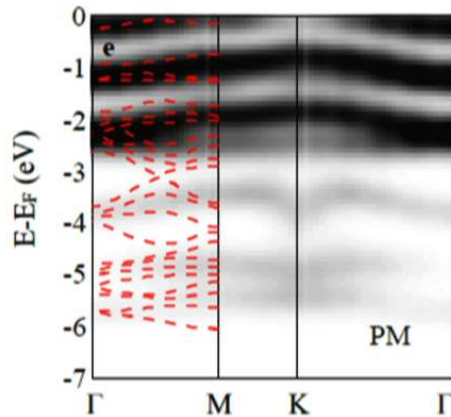
ARPES (Dessau group U of Colorado)

DFT (Kee group U of Toronto)

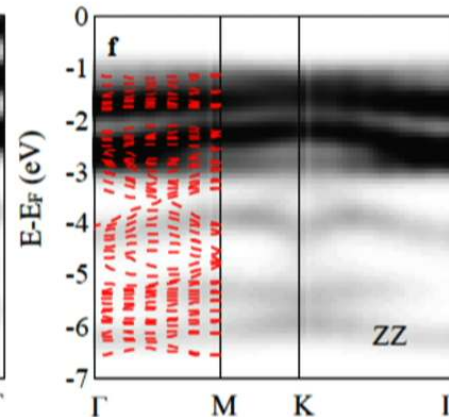
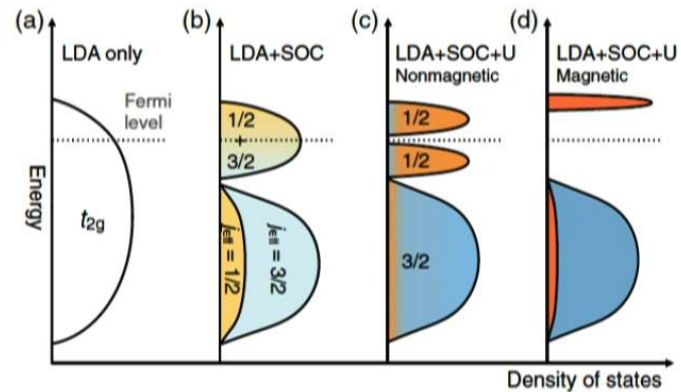
Expt.



Calc.



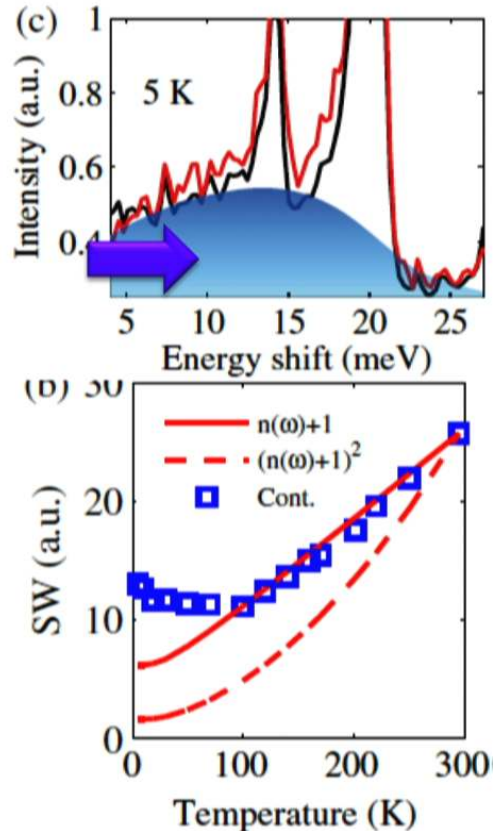
X. Zhou et al., arXiv:1603.02279



H. Kim et al.
PRB 91, 241110
(2015)

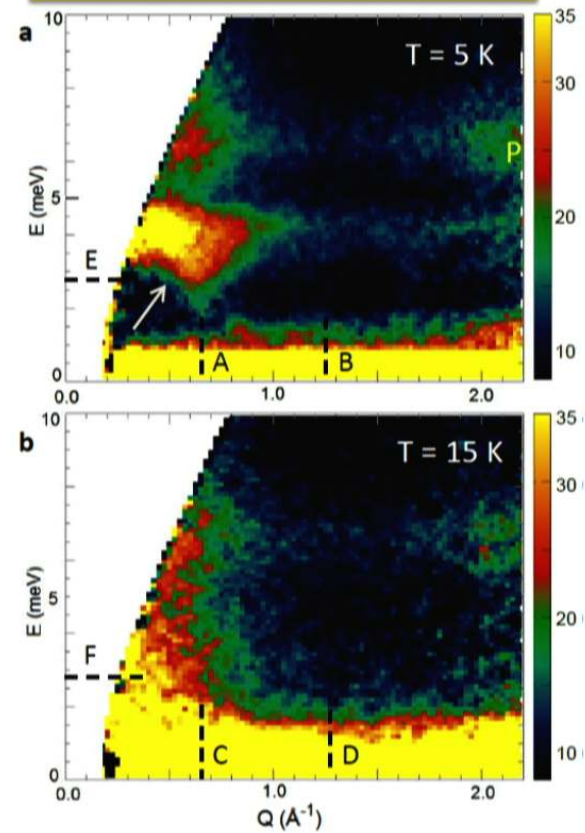
Close to Quantum Spin Liquid?

Magnetic Raman Scattering



Sandilands, Burch, YJK et al., PRL 2015

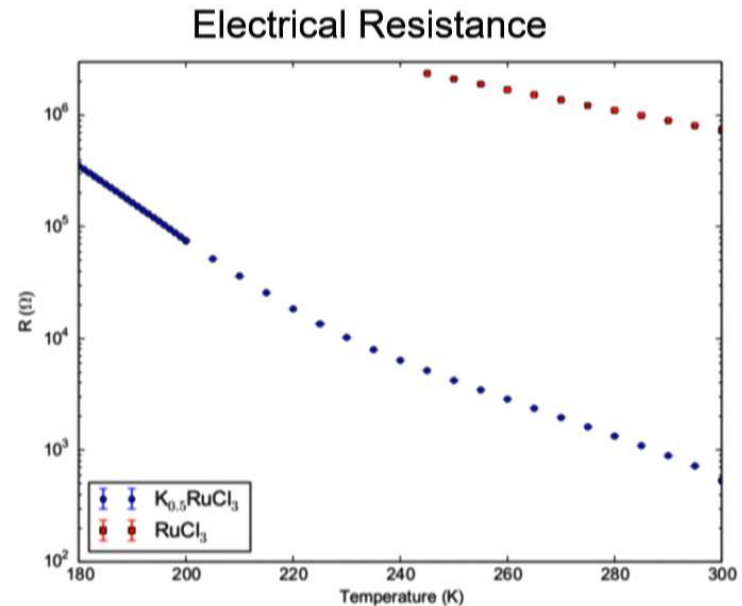
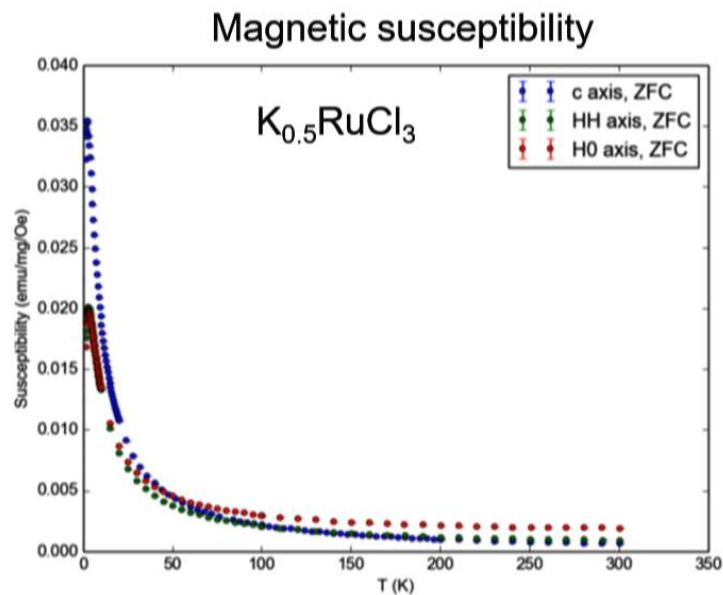
Inelastic Neutron Scattering



Banerjee et al., arXiv:1504.03087

What about doping?

- Doped Heisenberg-Kitaev model exhibits topological p-wave or d-wave superconductivity – T. Hyart et al. PRB 85, 140510 (2012); You et al., 86, 085145 (2012); Okamoto PRB 87, 064508 (2013)
- Intercalation of K^+ ions
- Localized carriers (still insulating)



Summary

- Strong spin-orbit coupling is required to realize Kitaev interaction in real materials
- Kitaev QSL Candidates: Iridates, RuCl_3
- Magnetic excitations
 - Na_2IrO_3 – Magnetic excitation around 30-40 meV
 - $\alpha\text{-RuCl}_3$ – Continuum magnetic excitations around 10 meV.
- $\alpha\text{-RuCl}_3$ is also a van der Waals Mott insulator
 - Proliferation of stacking faults
 - Graphite-like mechanical properties
 - Intercalation of K^+ possible