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 Na2IrO3 and Li2IrO3 have been intensely scrutinized. Recently, we proposed that a 4d honeycomb magnet Î±-RuCl3 is a promising candidate material in which Kitaev physics could be studied. I will give an overview of the physics of alpha-RuCl3, and talk about recent experimental and theoretical advances.

4 Corners May 12, 2016

Honeycomb Lattice Quantum Magnets with strong SOC

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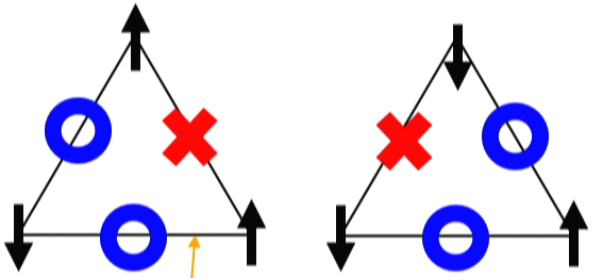
Frustration suppresses order

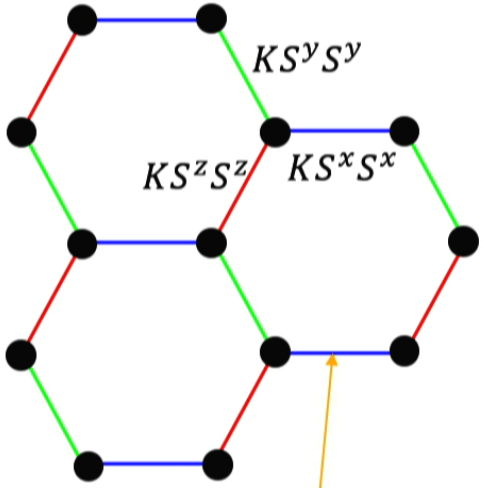
Bond frustration



Heisenberg interaction

+ single ion anisotropy
+ exchange anisotropy
+ Dzyalloshinsky-Moriya

Site frustration



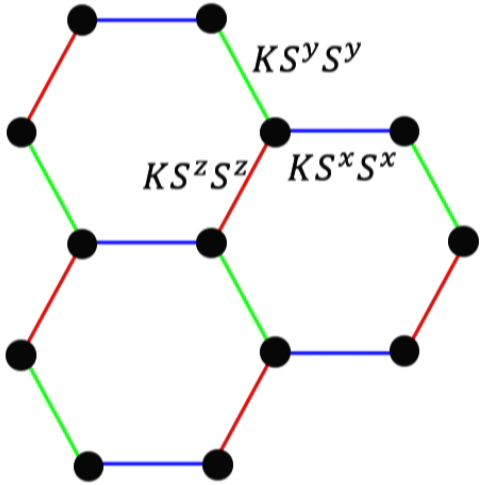
Kitaev interaction
– bond dependent anisotropic interaction

Kitaev model

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

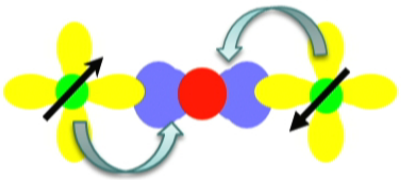
Alexei Kitaev, Ann. Phys. 2006

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

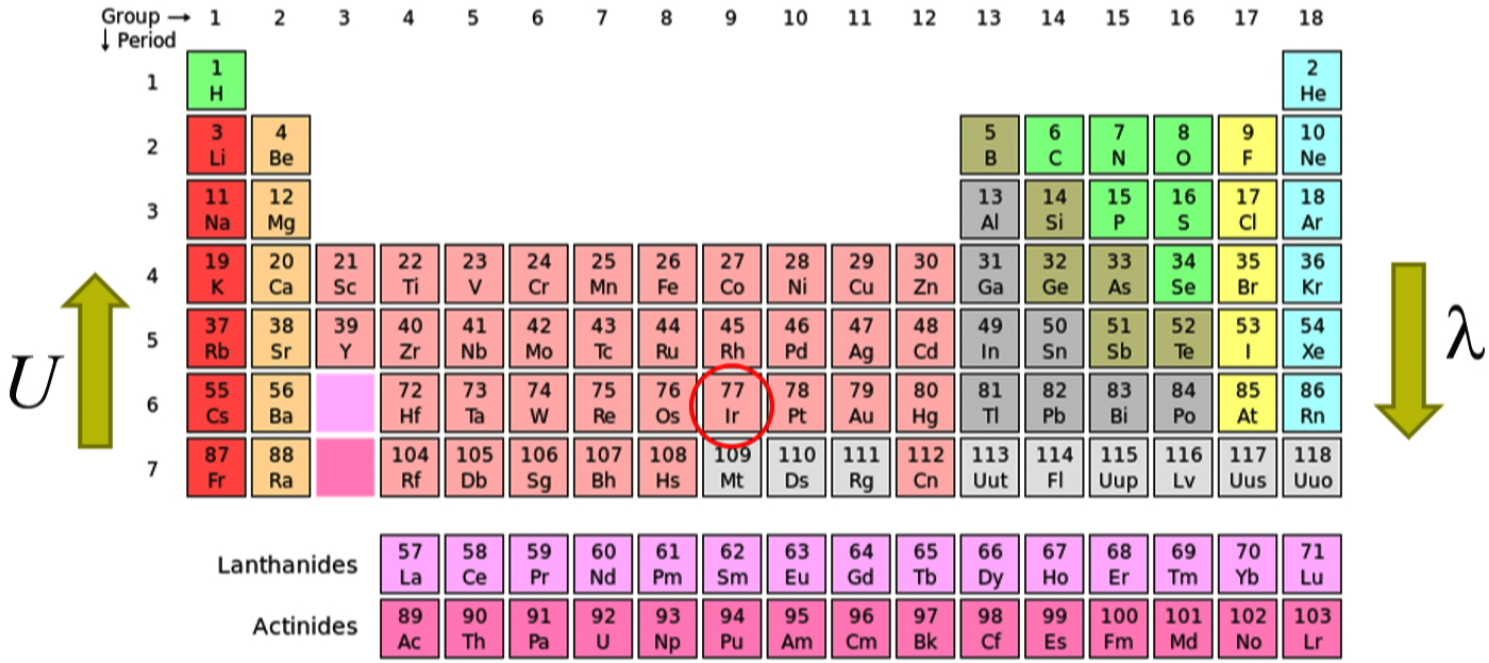


Heisenberg superexchange

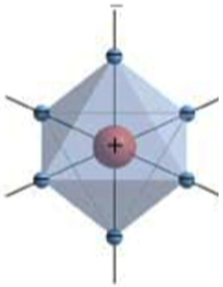
Hopping t

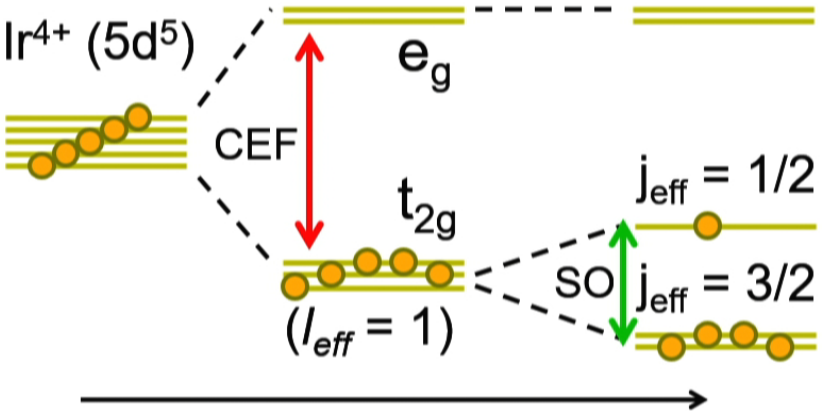


Why iridates?

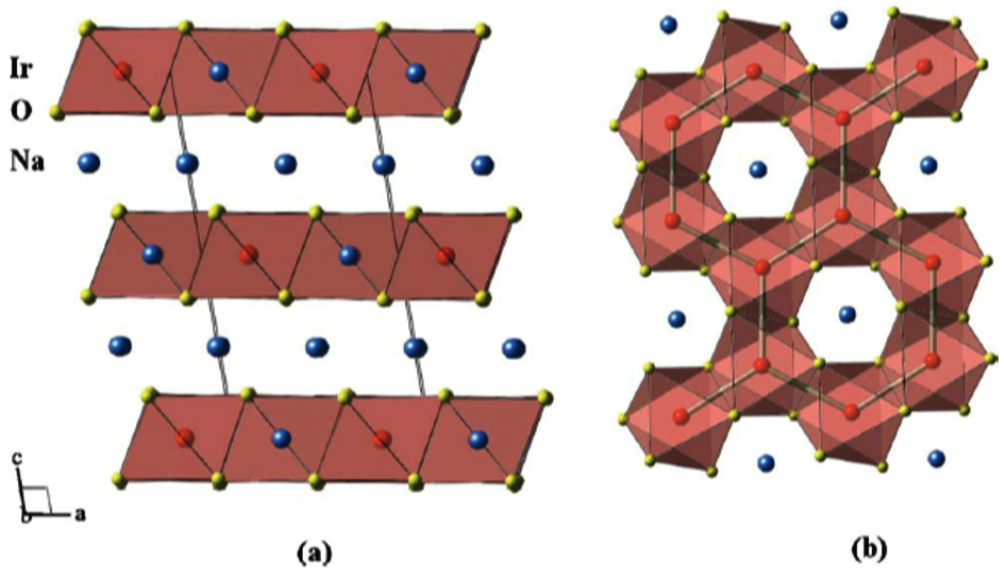


Physics of Ir^{4+} ($5d^5$) in cubic CEF





A_2IrO_3 (A=Na, Li)



Li_2IrO_3 powder
Na_2IrO_3 crystal

~2x2 mm^2

- Honeycomb lattice of Ir^{4+}
- Heisenberg-Kitaev model?

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

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_2IrO_3

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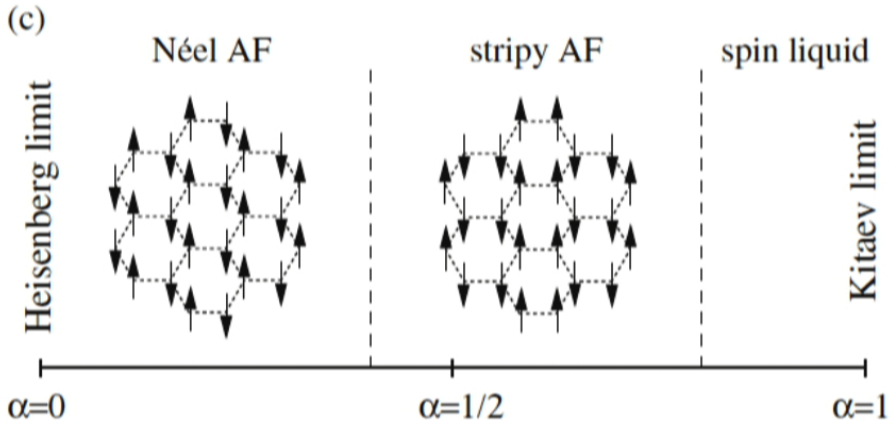
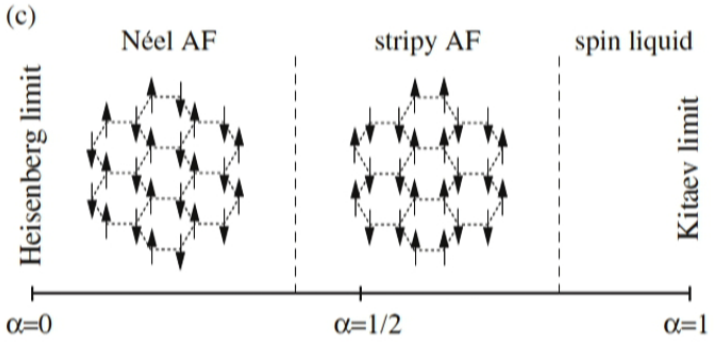
$$\mathcal{H}_{ij}^{(\gamma)} = -J_1 S_i^\gamma S_j^\gamma + J_2 \boldsymbol{S}_i \cdot \boldsymbol{S}_j.$$



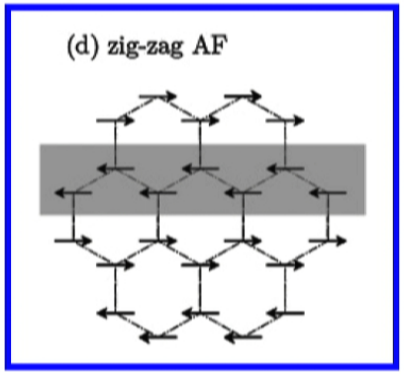
However…

Chaloupka, Jackeli, and Khaliullin PRL 2010

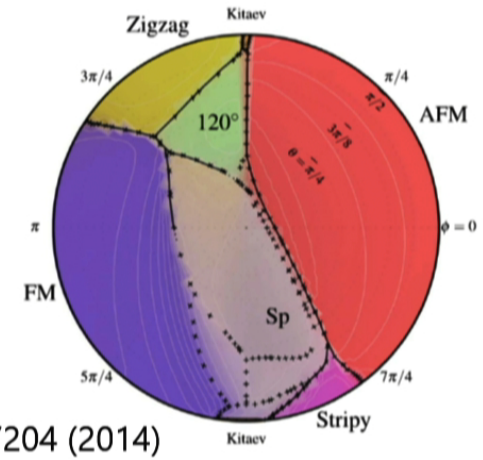


X. Liu, et al., PRB (2011)

Experimental structure

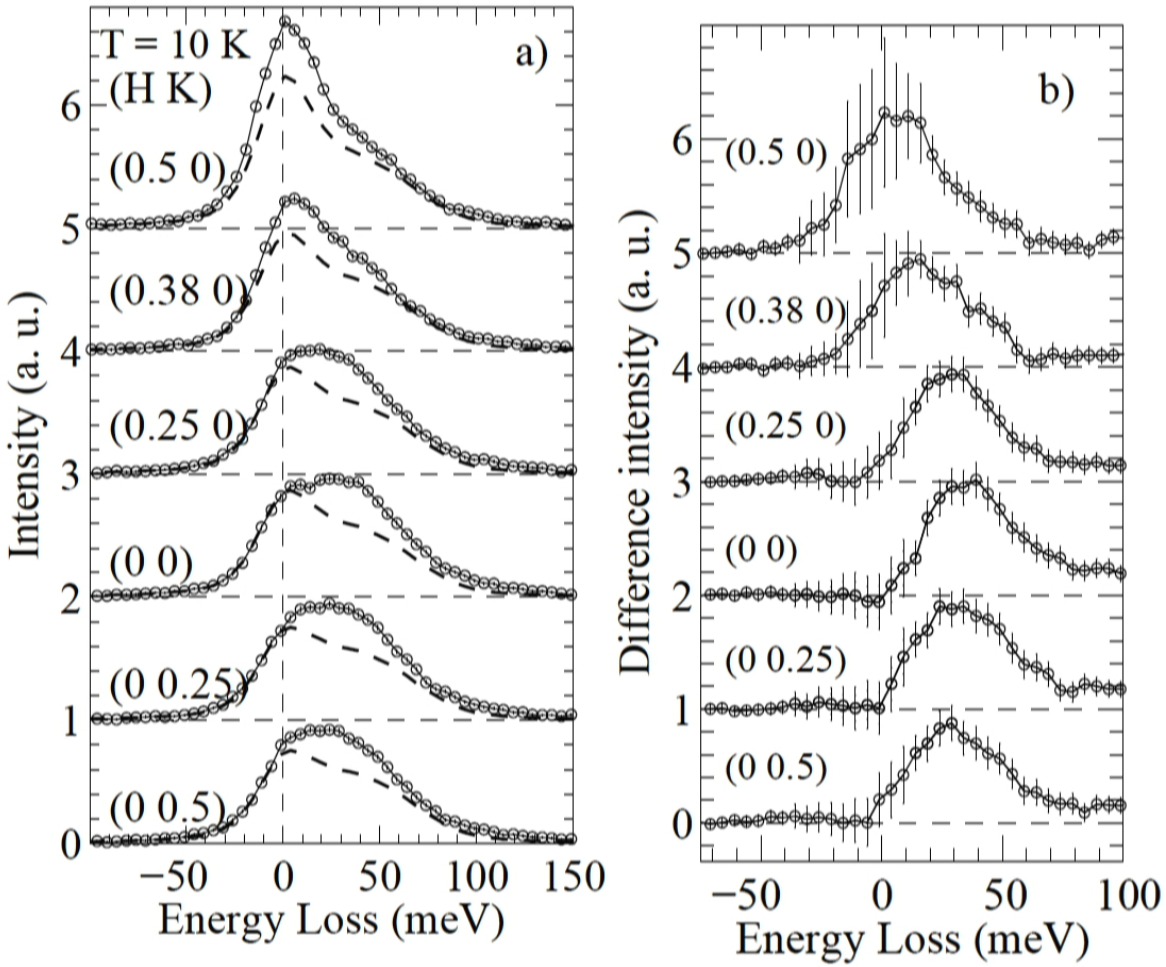


- No zig-zag phase!
- Still a lot of confusion about the Hamiltonian
  - Large 2nd and 3rd nearest neighbor interaction
  - Antiferromagnetic Kitaev term (?)



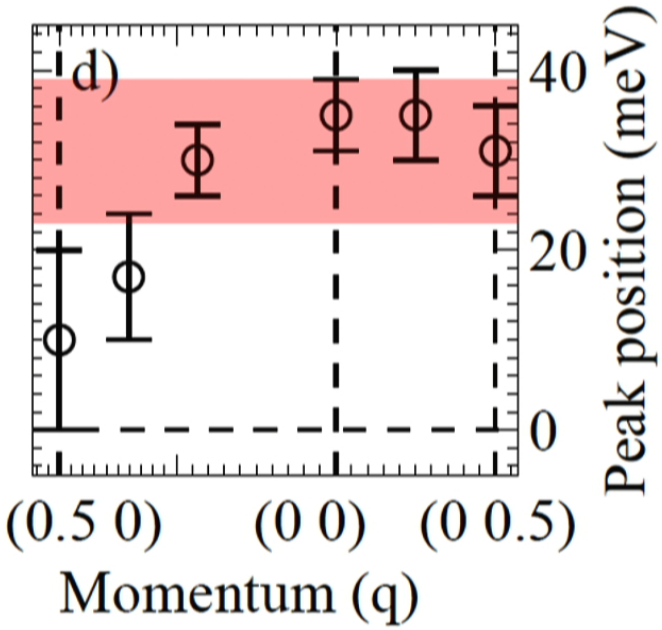
J. G. Rau et al., PRL 112, 077204 (2014)

Na_2IrO_3 magnetic excitations (RIXS)

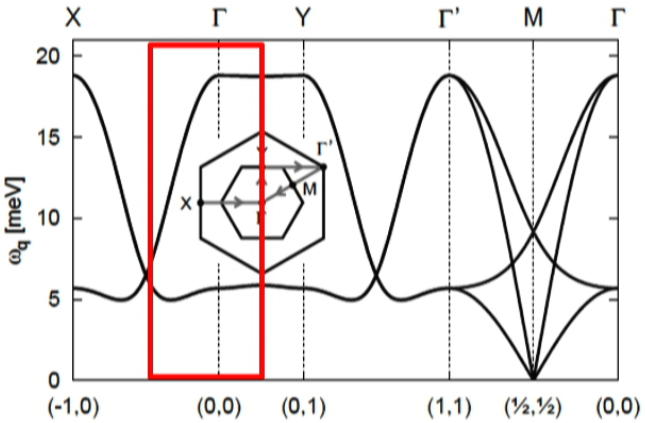


Dispersion relation

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



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



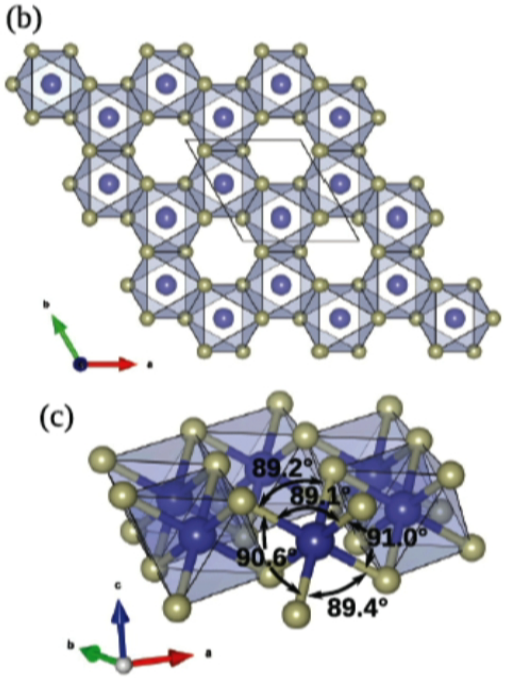
- Need a large energy scale ~30 meV
- Is this AF Kitaev term?

Difficulty due to poor energy resolution of RIXS

Wait till next gen instrumentation

α-$RuCl_3$ - neutron friendly

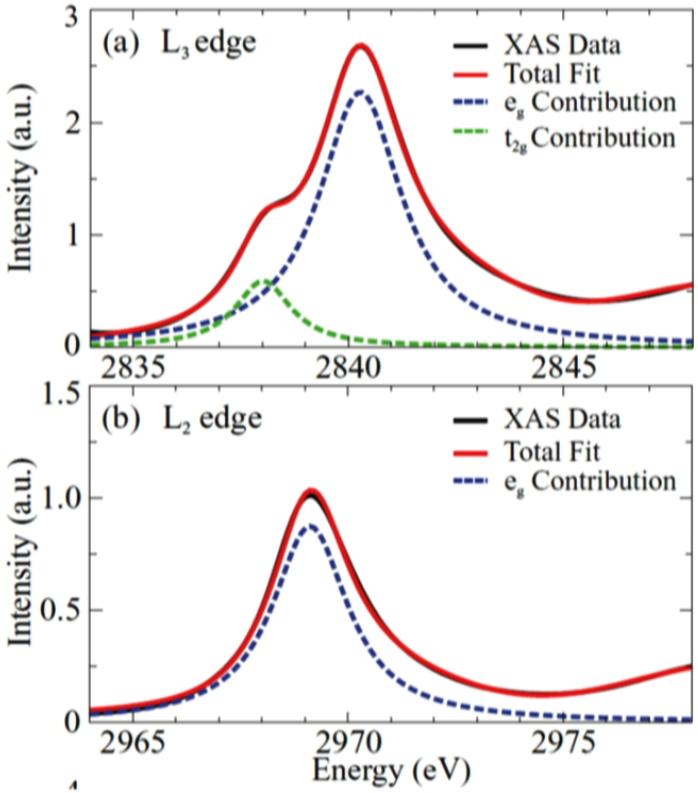
- Well-known semiconductor since 1960's.
- Used as a catalyst



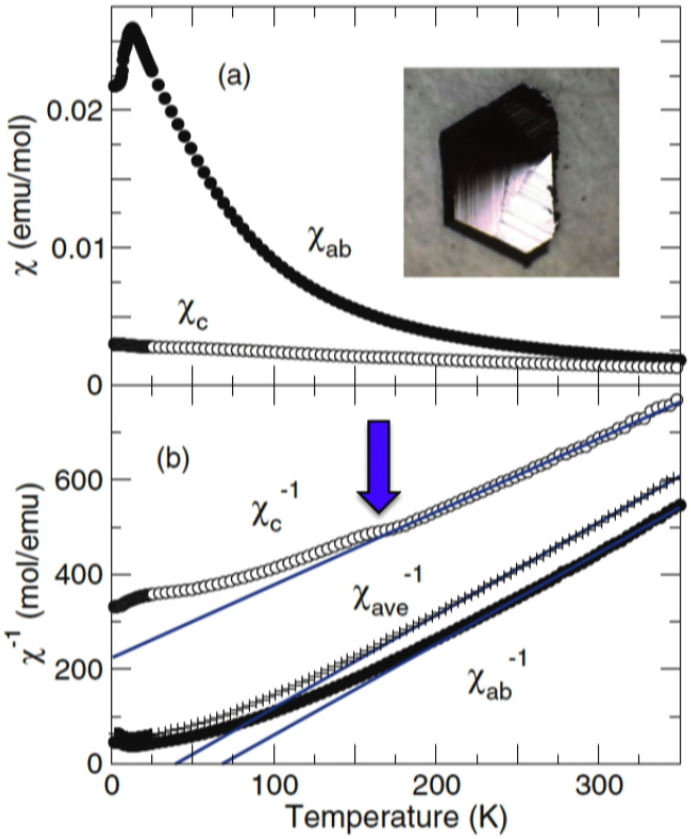
K. W. Plumb, YJK et al., Phys. Rev. B 90, 041112 (2014)

J_{eff}=1/2 ?

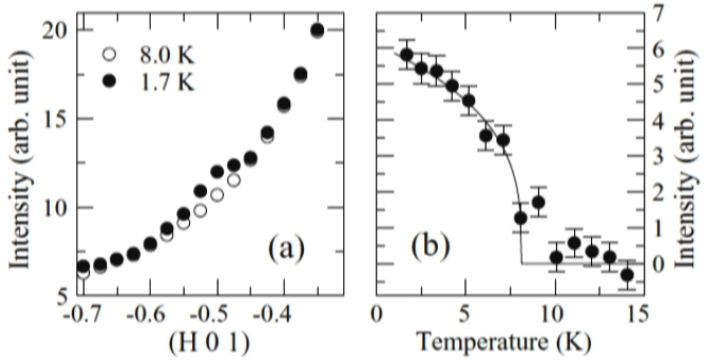
X-ray Absorption Spectroscopy

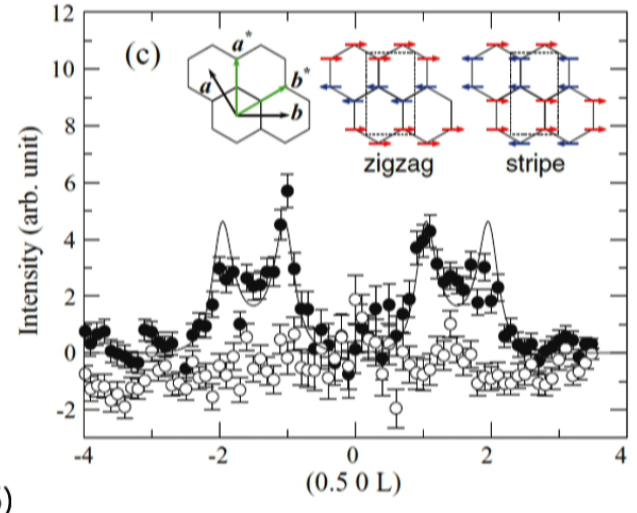


Magnetic properties



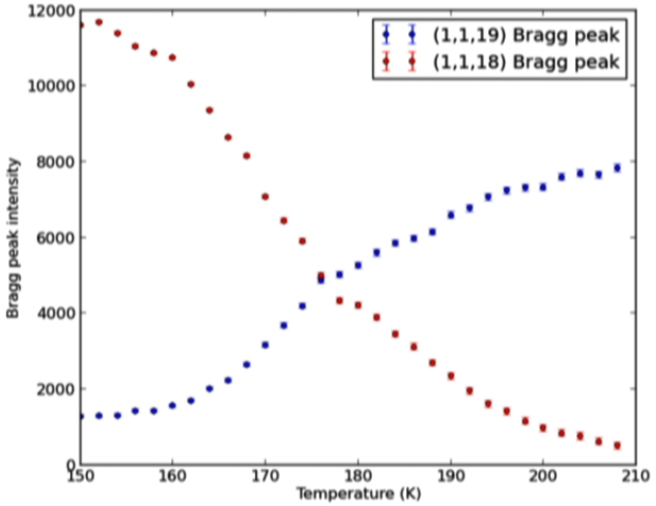
Neutron diffraction



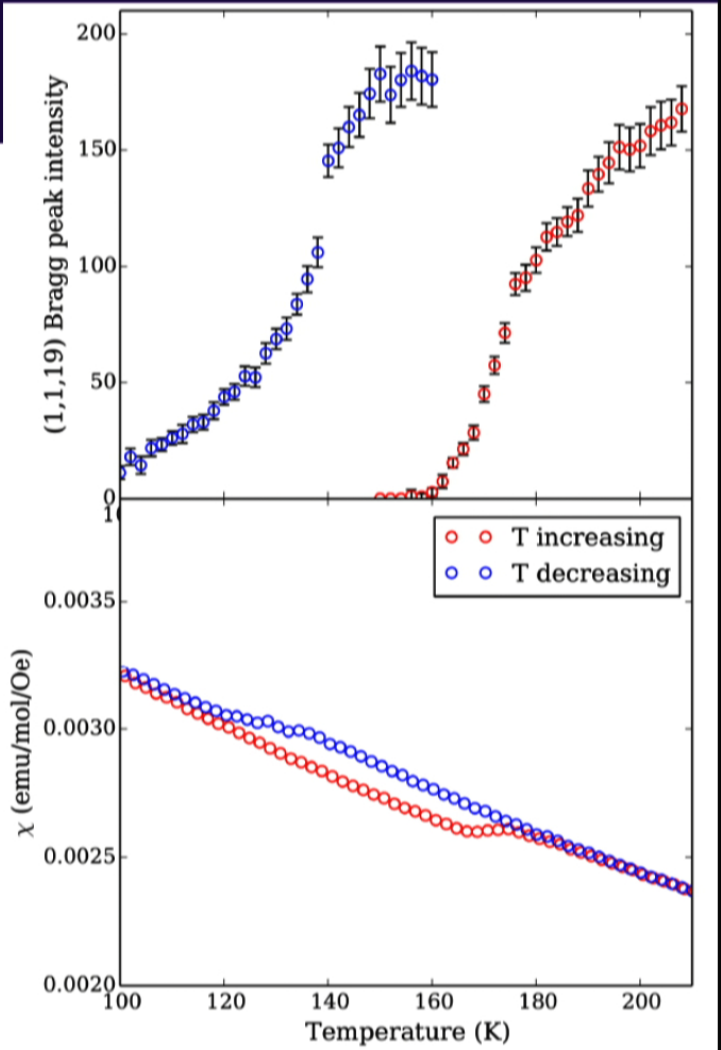


J. A. Sears, YJK et al., Phys. Rev. B 91, 144420 (2015)

Structural transition



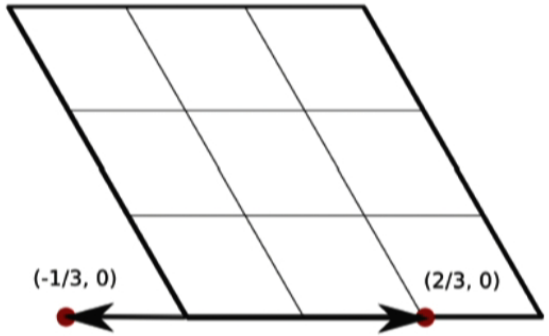
- Change in stacking pattern
- 1st order transition
- Large hysterisis

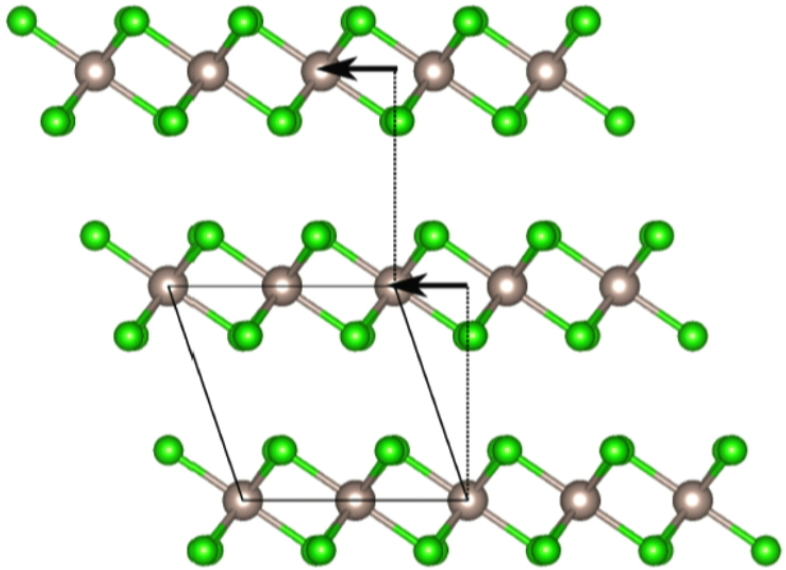


Room temperature structure

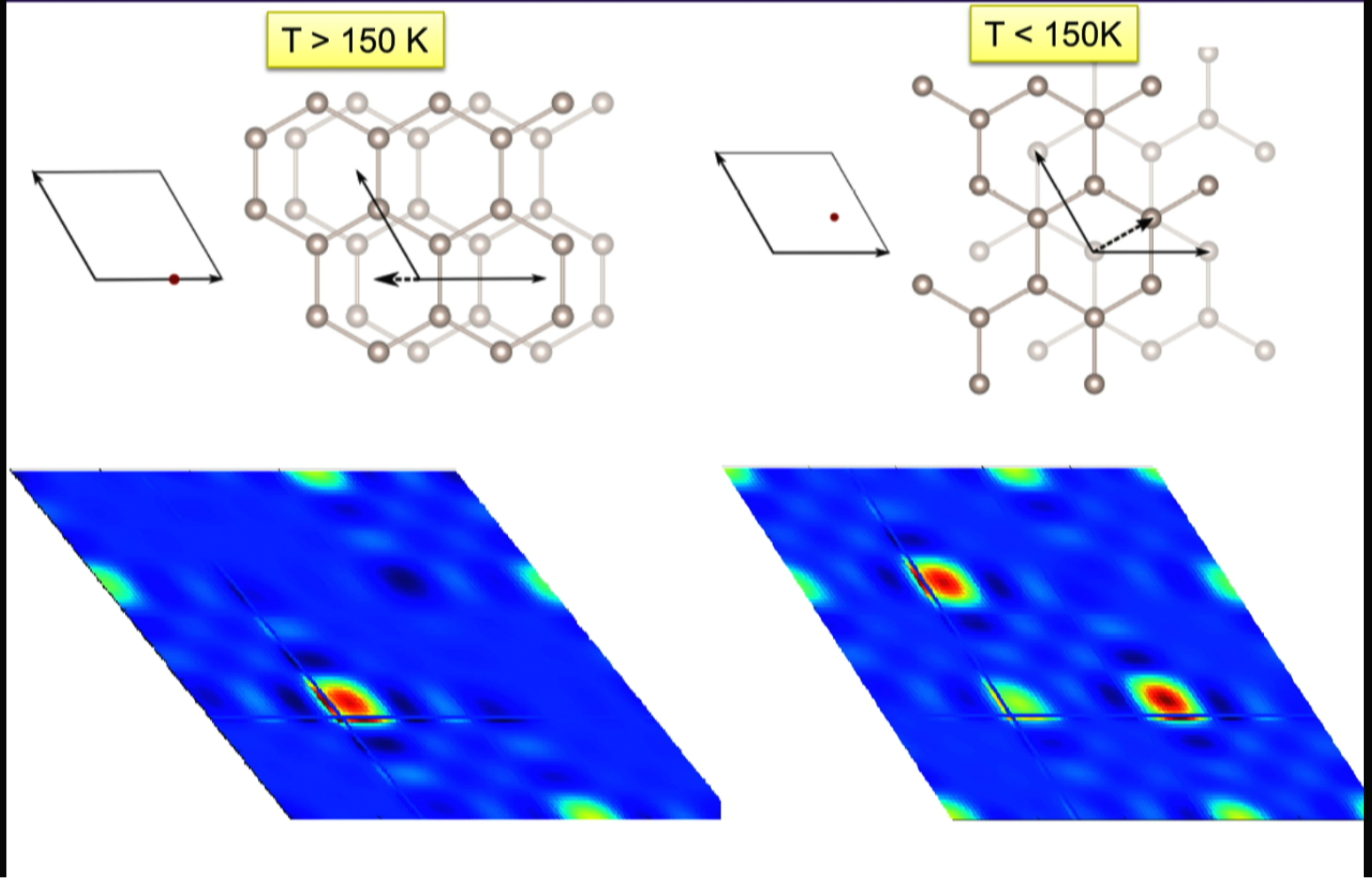
In perfect C2/m structure only 1 type of shift between nearest neighbours:

(-1/3, 0) in hexagonal notation





Fourier analysis of stacking

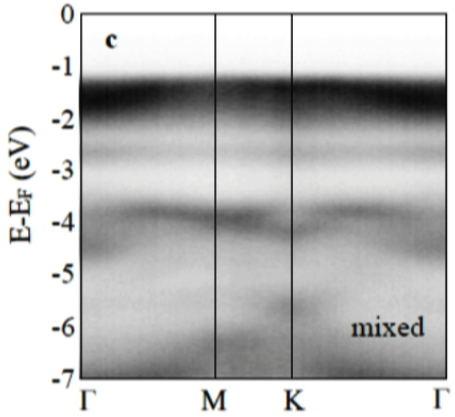


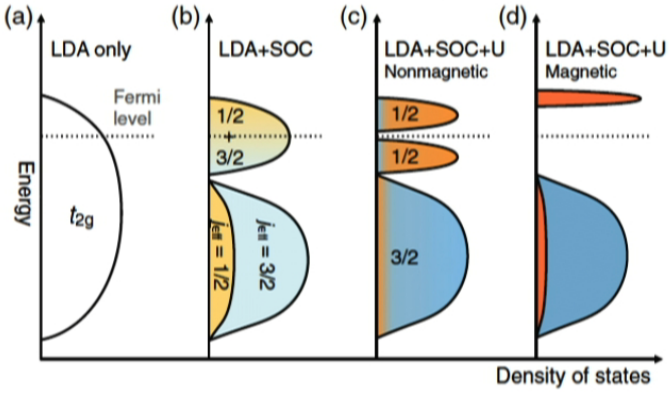
Electronic structure

ARPES (Dessau group U of Colorado)

DFT (Kee group U of Toronto)

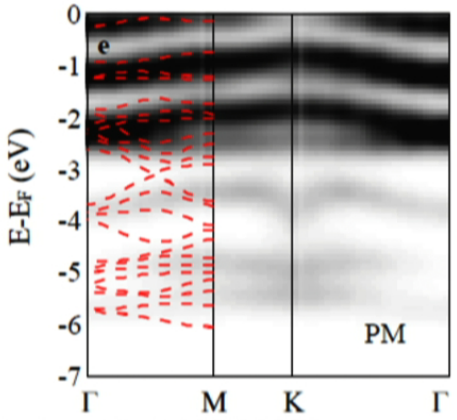
Expt.

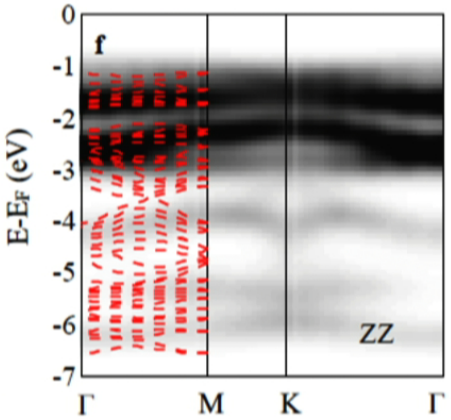




H. Kim et al.
PRB 91, 241110 (2015)

Calc.

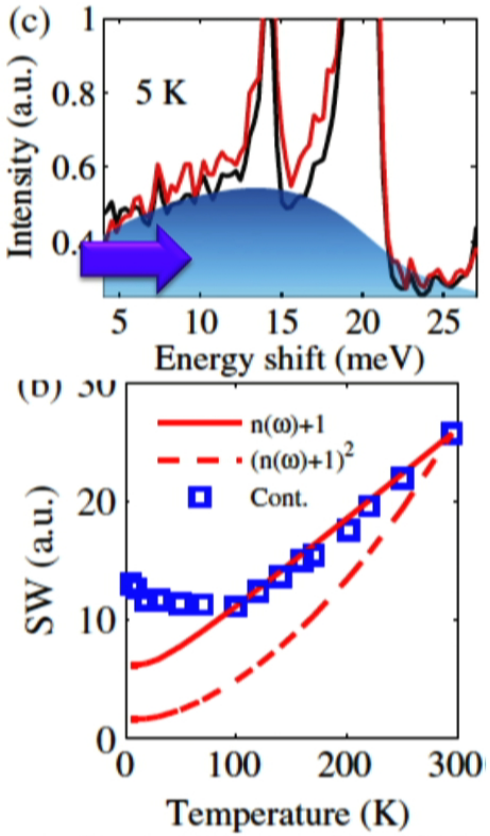




X. Zhou et al., arXiv:1603.02279

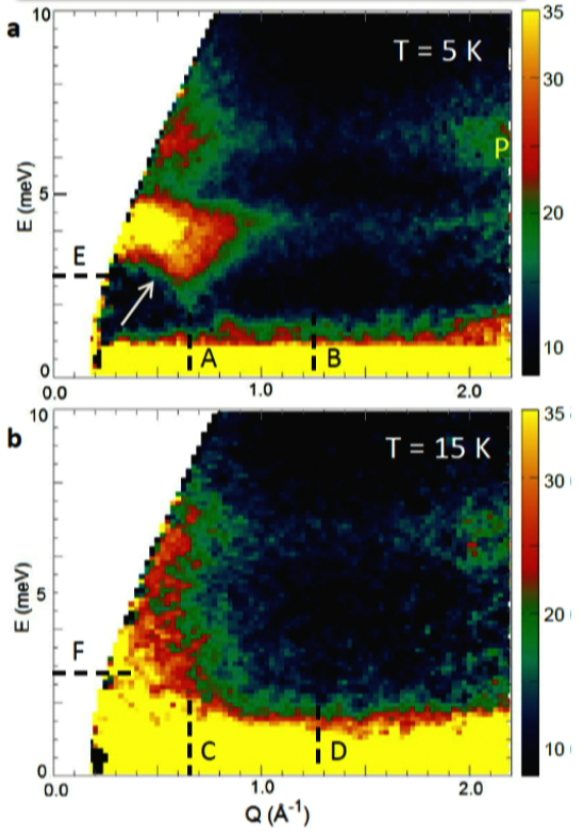
Close to Quantum Spin Liquid?

Magnetic Raman Scattering



Sandilands, Burch, YJK et al., PRL 2015

Inelastic Neutron Scattering

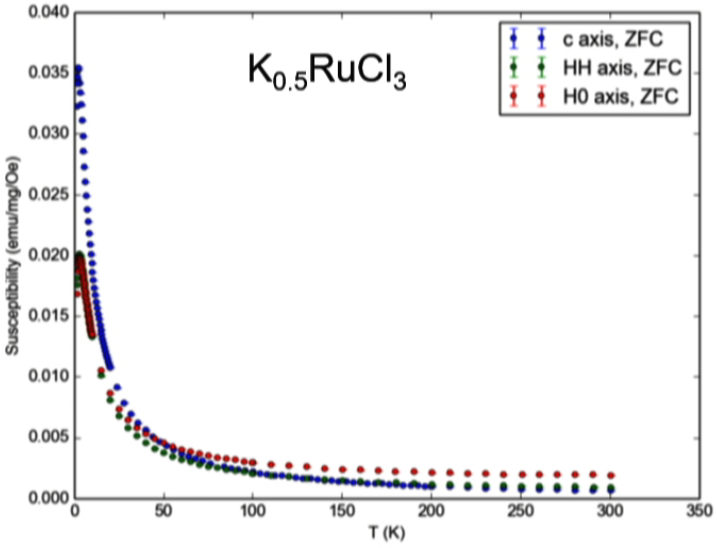


Banerjee et al., arXiv:1504.03087

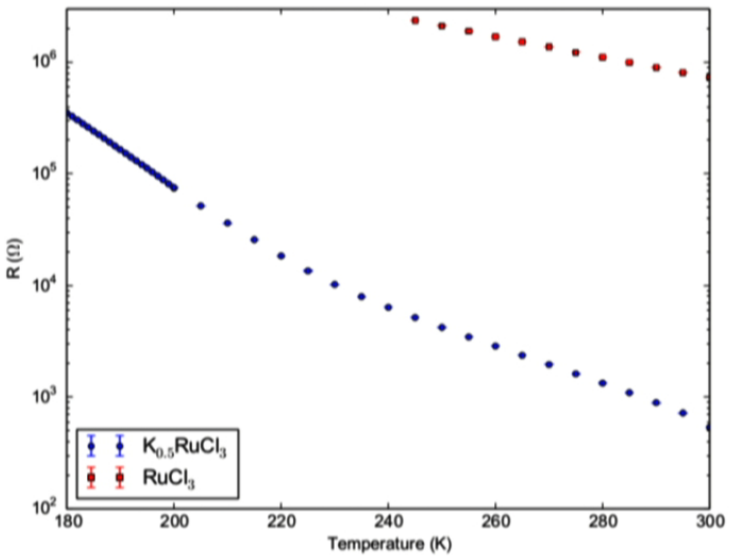
What about doping?

- 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)

Magnetic susceptibility



Electrical Resistance



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
  - α-$RuCl_3$ – Continuum magnetic excitations around 10 meV.
- α-$RuCl_3$ is also a van der Waals Mott insulator
  - Proliferation of stacking faults
  - Graphite-like mechanical properties
  - Intercalation of K^+ possible