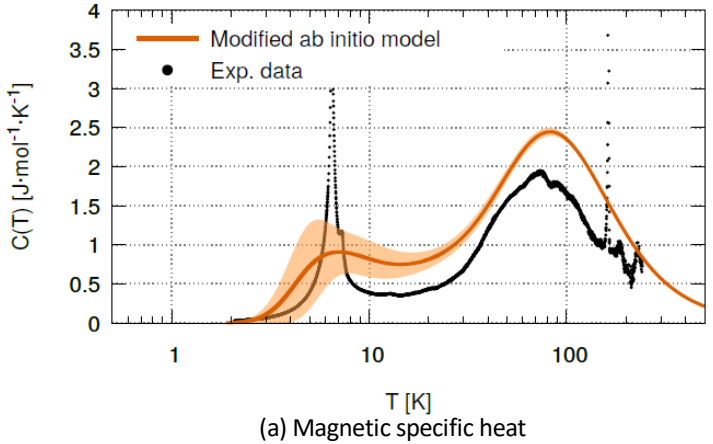
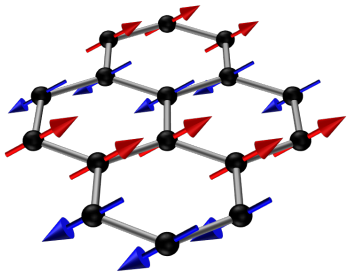
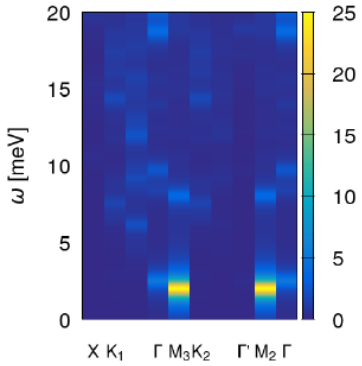
A coherent theoretical description of Kitaev-candidate material α-$RuCl_3$



(a) Magnetic specific heat


(b) Magnetic ground state.



(c) Inelastic neutron scattering spectrum

Theoretical results of (a) magnetic specific heat, (b) magnetic ground state, and (c) inelastic neutron scattering spectrum. The energy scales in (a) and (c), and ordering pattern in (b) are consistent with experimental results reported earlier.

P. Laurell and S. Okamoto, Dynamical and thermal magnetic properties of the Kitaev spin liquid candidate α-RuCl3, *npj Quantum Mater*. **5**, 2 (2020).

Scientific Achievement

A new theoretical model found that the Kitaev term is the largest contribution to the low-energy spin Hamiltonian of α-$RuCl_3$, a candidate for the Kitaev spin liquid.

Significance and Impact

The model resolves a conflict in energy scales reported from different experiments in α-$RuCl_3$ for the first time, and may answer the fundamental question: is the Kitaev spin liquid realized in α-$RuCl_3$?

Research Details

- The theoretical model is derived from first principles calculations, which provide material-specific hopping matrices and Coulomb interactions.
- Kitaev interaction ~15meV is found to be the largest, consistent with the magnetic specific heat results.
- Yet, magnetic excitations appear at low energies ~2meV due to quantum fluctuations of local spins, consistent with inelastic neutron scattering results.

Work was performed at Oak Ridge National Laboratory.