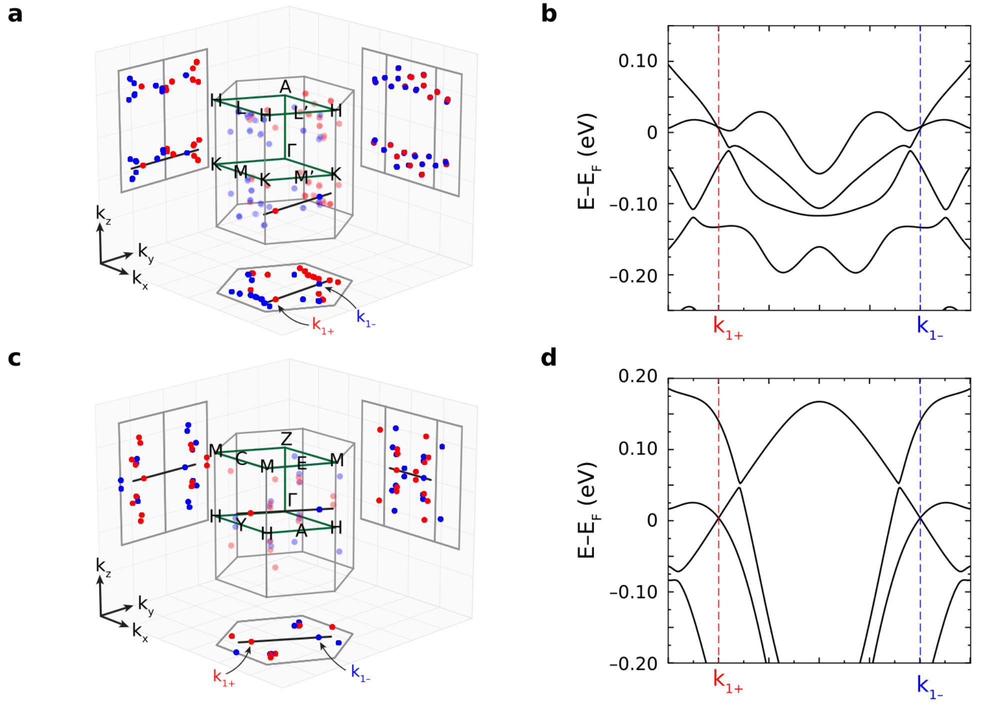
Integrated Neutron Scattering and First-Principles Modeling Reveal an Intrinsic Weyl Phase Transition in a Kagome Quantum Material



Integrated neutron scattering and first-principles modeling reveal how coupled crystal and magnetic symmetry breaking reorganizes Weyl nodes and drives an intrinsic topological phase transition in the kagome magnet Mn_3Ga.

Tsung-Han Yang, Satoshi Okamoto, D. Alan Tennant, Michael A. McGuire and Qiang Zhang. "Intrinsic topological Weyl phase transition induced by a magnetostructural transformation in a kagome magnet" *Nature Communications* 17, 5063 (2026)

Scientific Achievement

Established an integrated experimental–theoretical framework that combines neutron diffraction, symmetry analysis, and first-principles electronic-structure calculations to determine the microscopic magnetic Hamiltonian and predict topological Weyl phases in correlated quantum materials.

Significance and Impact

Demonstrates how accurate determination of crystal and magnetic structures provides the foundation for predictive discovery of topological quantum materials, enabling new pathways for identifying and engineering quantum phases for future spintronic and quantum technologies.

Research Details

- Combined high-resolution neutron diffraction, magnetic characterization, and density functional theory to determine the previously unresolved crystal and magnetic ground states of kagome Mn_3Ga.
- Established that a magnetostructural transformation near room temperature reconstructs the electronic topology, producing an intrinsic transition between distinct Weyl states.
- Developed a predictive framework linking experimentally determined magnetic structures to Berry curvature, anomalous Hall response, and topological electronic states for quantum materials discovery.

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- **NQISRC Intellectual Role:** *[Collaborator]*
  - The Quantum Science Center contributed the theoretical framework connecting experimentally determined magnetic structures with first-principles electronic structure, Berry curvature, Weyl topology, and predictive quantum materials discovery.
- **NQISRC Funding Role:** *[Shared]*
- **Explanation of Funding Institution Contributions:**
  - The Quantum Science Center supported theoretical modeling of magnetic order, electronic topology, and predictive quantum materials design. ORNL LDRD, DOE Basic Energy Sciences, and the Spallation Neutron Source supported materials synthesis, neutron scattering, magnetic characterization, and experimental validation.