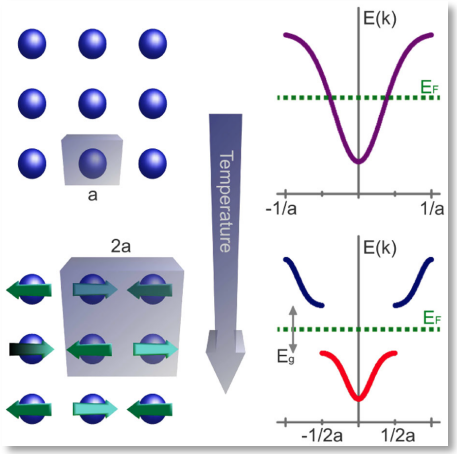
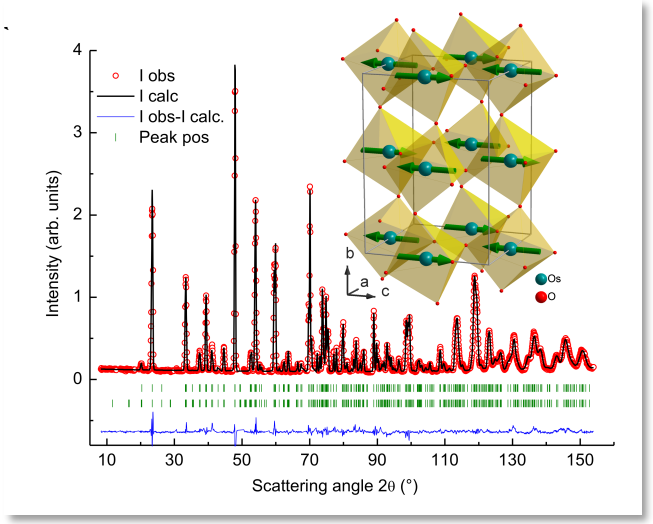
OAK RIDGE National Laboratory

Magnetically driven metal to insulator transition

Experimental demonstration of a novel pathway to transform a materials conducting properties first predicted 60 years ago, with the unique insulting state existing at room temperature.



- The metal-insulator transition (MIT) is one of the most dramatic manifestations of electron correlations in materials, enjoying both fundamental and technological interest.
- Various mechanisms producing MITs have been extensively considered, including the Mott (electron localization via Coulomb repulsion), Anderson (localization via disorder), and Peierls (localization via distortion of a periodic one-dimensional lattice).



The Slater MIT mechanism. Right: the electronic conduction band is shown. Left: the magnetic ions (blue spheres), with the green arrows denoting magnetic spins creating a magnetic structure. As the temperature is reduced, magnetic order develops. The type of ordering of the spins creates a periodic energy potential surrounding each ion. This has the consequence of breaking the electronic conduction band and transforming the material from a metal to an insulator solely due to magnetic order.

S. Calder et al., *Phys. Rev. Lett.* 108, 257209 (2012)

- One additional route to a MIT proposed by Slater in 1951, in which long-range magnetic order drives the MIT, has remained elusive.
- The *5d* transition metal oxides are undergoing increasing interest, showing many novel properties. Probing one such material, $NaOsO_3$, with neutron scattering from HB2A and HB1 at HFIR/ORNL and x-ray scattering at the APS uncovered the necessary magnetic ordering concurrent with the MIT.
- Our experimental methodology is the first definitive demonstration of the long predicted Slater MIT.

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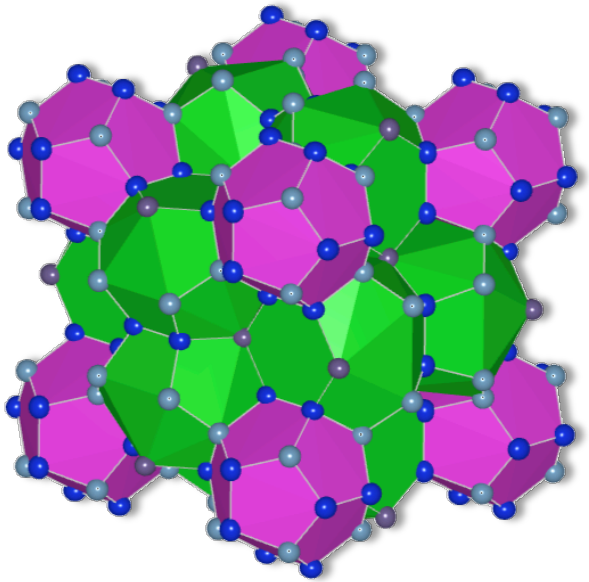
Tuning thermoelectric materials at the atomic level, guest-host interactions are important

New findings emphasize the importance of site occupancies in the framework sites nearest to the guest atom in the large cage. This correlation will help guide the search for new clathrate-type thermoelectric phases with improved physical properties.

- The clathrate-type semiconductor, $Ba_8Al_xSi_{46-x}$, provides a controlled system to explore the role of the interactions between the guest atoms, barium in this case, and the host atoms, Al and Si, because the Al-content can be varied over a large range. We have used neutron diffraction to explore the detailed structural changes of the crystal structure of $Ba_8Al_xSi_{46-x}$ as a function of Al content using the HB-2A Neutron Powder Diffractometer at the High Flux Isotope Reactor, Oak Ridge National Laboratory (ORNL).
- The Ba atomic displacements increase with increasing cage size, but appear to be primarily dependent on the host framework site occupancies, specifically that displacement increases in the direction of host framework sites with the largest Al content.
- Differences in the physical properties, specifically thermal conductivity, have been linked to the displacement of the atom in the large cage.
- Thermoelectric materials are used in devices to generate power from waste heat or alternatively in devices to provide solid-state refrigeration. This research was from a collaboration between University of California – Davis and ORNL scientists.

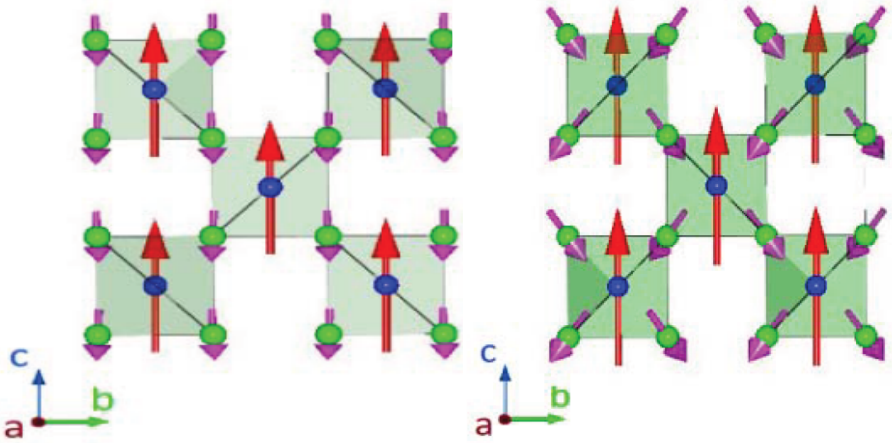


This clathrate crystal structure (at right) consists of a host framework of tetrahedrally linked Al and Si atoms (show as three differently colored balls), which form polyhedral cages (green and purple) that enclose one Ba atom in each.

J. Roudebush, et al, Inorganic Chemistry. 51, 1201-1976, (2012)

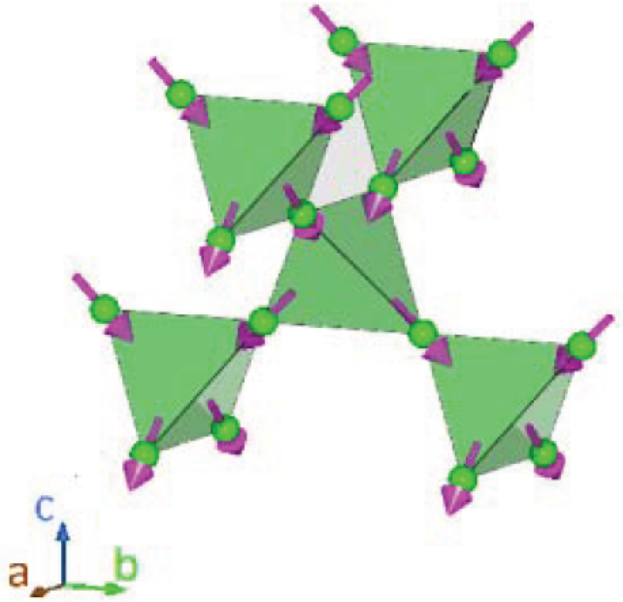
Magnetic order and ice rules in the multiferroic spinel FeV_2O_4

Neutron diffraction study done at HB2A of FeV_2O_4, which is rare in exhibiting spin and orbital degrees of freedom on both cation sublattices of the spinel structure., showing that the direction of ordered vanadium spins at low temperature obey `ice rules' more commonly associated with the frustrated rare-earth pyrochlore systems



(left) Sketch of the collinear ferrimagnetic state in the FCO phase, as seen along the cubic (001) direction.
(right) A similar sketch of the canted state seen in the LTT phase.

G. J. MacDougall, et al, arXiv: 1204.2812v2



A view of V 3+ moments in low-temperature ordered state clearly demonstrating the 2-in-2-out spin structure on the pyrochlore sublattice.