

# ENERGY MATERIALS

## Add the power of neutrons to your energy research

**Oak Ridge National Laboratory (ORNL)** is the US epicenter of neutron scattering, a powerful technique for studying the nature of materials for increasing energy security.

Both scientists and non-scientists can access ORNL's leading research facilities via the U.S. Dept. of Energy's **User Program**. ORNL's two world-leading, complementary neutron research user facilities — the **High Flux Isotope Reactor (HFIR)** and the **Spallation Neutron Source (SNS)** — are available to facilitate studies in science and technology. Together, HFIR and SNS offer users 30 advanced instruments and their supporting laboratories for a wide range of materials research experiments.

*"Neutron scattering at ORNL enabled us to study the atomic structure of novel battery materials and understand how ions – such as lithium and sodium – move within their structures. These insights are helping us design new materials with desirable properties for next-generation energy storage devices."*

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Photo credit: Colorado School of Mines



### No neutron science experience is necessary

Oak Ridge National Laboratory's neutron sciences User Program invites you to collaborate with us, onsite or remotely, to achieve greater success. No neutron science experience is necessary, as our experts work closely with users to ensure the success and safety of their experiments. We can help you find the neutron techniques and instruments best suited for your research.

### Neutron users can achieve research success – at little or no cost

Beam time is granted through a proposal system managed by the User Program and is free of charge (with the exception of travel costs, if necessary) if researchers intend to publish their results to the scientific community. A fee is charged only for proprietary research that will not be made public.



### Contact the Neutron Users Office

Web: [neutrons.ornl.gov/users](http://neutrons.ornl.gov/users)

Email: [NeutronUsers@ornl.gov](mailto:NeutronUsers@ornl.gov)

Phone: 865-574-4600 or 865-341-4451

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## Neutrons are ideal for studying energy materials

Each year, our neutrons help scientists gain a better understanding of the processes and properties of energy-related materials, whether for batteries, solar cells, plant-based fuels, and fission and fusion reactors. From their ability to penetrate dense materials and probe light elements, to their neutral charge and magnetic moment, neutrons facilitate studies that are difficult or impossible for other research techniques. Neutron scattering is also often used as a complementary technique to x-ray scattering, NMR, Raman, and DFT, for example, to better understand the structure-property relationships in energy materials. Neutron scattering in energy includes a variety of materials and techniques as seen below.

## There are many sample environments that support energy experiments including cryostats, furnaces, sample changers, gas flow cells, magnets, battery cyclers, and much more.

### Fuel cells

- Reflectivity provided the structure of Nafion thin films before and after water uptake in different environments.
- Quasielastic scattering used isotopic substitution between H and D to understand proton diffusion through membranes.
- Diffraction showed how oxygen defects created an oxygen transport pathway in electrodes.

### Batteries

- Imaging showed spatial distribution of chemical oxidation at Li-cathodes to understand how redox occurs.
- Total scattering helped determine the types and quantities of defects in amorphous hard carbon in Na-ion battery anodes.
- Quasielastic scattering was used to understand proton uptake and removal in electrodes.

### Other types of energy storage

- Imaging confirmed areas of density fluctuations and cracks in an automotive-scale hydrogen storage tube.
- Quasielastic scattering in an MXene pseudocapacitor found the dynamics of methyl groups in a tunnel for ion transport remain unchanged with temperature.
- A method was developed using total scattering to determine the size of polar nanodomains in the capacitor  $\text{Bi}(\text{Mg}_{0.5}\text{Ti}_{0.5})\text{O}_3\text{-PbTiO}_3$ .

### Solar energy

- Small angle neutron scattering helped to understand the morphology and aggregation behaviors in organic solar cell materials.
- Total scattering found evidence that an oxyhalide only had long-range order in 2D with significant disorder in the third dimension.
- Neutron and x-ray diffraction were combined to fully understand the complex structure of a high entropy oxide.

### Biomass

- An imaging methodology was developed to determine correlations between hydrogen and carbon release dynamics for better quantitative analysis.
- In situ small angle neutron scattering was performed on cellulose samples to study their dissolution dynamics under various conditions.
- Diffraction and pair distribution function analysis on MgO revealed structural influences on catalytic properties.

### Thermoelectric energy conversion

- Inelastic scattering was used to understand the contribution of phonons to a material's low thermal conductivity.
- Neutron spectroscopy and x-ray scattering was used to understand the lattice dynamics of a single crystal as a function of temperature.
- Pair distribution function analysis revealed short-range cation distortions that contribute to low thermal conductivity in a material.

### Nuclear energy

- Pair distribution function was used to understand how bonding in a nuclear fuel influenced its properties at high temperatures.
- The densities of eutectic salts were determined by radiography, which led to a phenomenological understanding of the salts' behavior.
- A moderator material was studied with quasielastic scattering to determine the motion of hydrogen as a function of hydrogen stoichiometry at high temperatures.

### Superconductivity

- Single crystal diffuse scattering was performed on a material to understand the role of homogeneity in the fundamental physics behind the properties.
- Beamline development has enabled improved location of hydrogen atom positions at high pressures to aid in the search for room temperature superconductivity.
- Inelastic scattering was used to show that superconductivity in a unique material is coupled to a sharp magnetic excitation at a boundary near antiferromagnetic order.