

# THE BEST X-RAY TOOLS FOR BATTERY DEVELOPMENT AND TESTING

*The Advanced Photon Source is your one-stop shop for nanoscale to bulk analysis beyond the reach of industry* 



Argonne physicist Mahalingam Balasubramanian loads a lithium-ion battery into the low-energy resolution inelastic X-ray (LERIX) system at the Advanced Photon Source. This multi-element X-ray scattering instrument is helping Argonne researchers understand the fundamental mechanisms that limit the performance of batteries.

Researchers optimizing today's batteries and designing the highperformance batteries of tomorrow need more than just the tools found in modern industry and university laboratories. To overcome big hurdles and eliminate costly trial and error design practices, researchers need big machines such as the U.S. Department of Energy Office of Science's Advanced Photon Source (APS) that can see deeper into battery materials with higher spatial, temporal, and chemical resolution. To optimize battery performance and manufacturing processes as quickly as possible, researchers need access to Argonne's experts in the fields of chemistry, physics, materials science, and x-ray science to augment their home research staffs.

As the nation's largest synchrotron x-ray user facility, the APS offers the perfect tools to study chemical reactions across length scales, microstructures of materials under stress and strain, and the dynamics of batteries operating in real and extreme conditions.

Research at the APS will optimize today's battery materials and contribute to the design of novel materials to reduce manufacturing costs and unwanted byproducts. New designs for lighter weight and smaller batteries can lead to expanded uses of batteries in a myriad of industries including construction, medical devices, aerospace, automotive, defense, consumer electronics, and utilities. The Advanced Photon Source has a suite of best-in-class x-ray techniques and lab space to tackle the most difficult challenges in battery design and production to:

- Improve battery chemistry to extend lifespan, speed charging and discharging, increase power capacity and density, and ensure safety.
- Improve material design to minimize failures, endure harsh conditions, and reduce size, weight, and cost
- Improve processing to eliminate defects and reduce unwanted byproducts.

## ADVANCED TECHNOLOGY PROVIDES A WINDOW TO NEW SOLUTIONS

Complementary to neutron sources, high-energy synchrotrons offer deeper penetration and more photons to typically provide higher spatial resolution x-rays. High-energy x-rays are the only way to see inside operating battery cells and casings to watch catalytic reactions as the cell cycles. This revelatory process is the key to optimizing battery chemistry and materials processing in many applications.

Argonne's APS provides the brightest storage-ring generated x-ray beams available in this hemisphere. This can help unravel the complexities of atomic-scale defects often associated with performance degradation as well as potentially control or optimize a material's properties.

## POTENTIAL APPLICATIONS OF X-RAY ANALYSIS

- Unlock the high rate capability of layered cathode material
- Create novel design strategies of nano-structured complex materials for cathodes to extend charge-discharge cycle rates, decrease charging time, and expand energy storage capacity and density
- □ Enable longer battery life spans
- Increase charge capacity to design electrical vehicles that can travel farther
- Enhance density and storage capabilities to enable better load-balancing capabilities and the expanded use of wind and solar power on utility grid systems
- Design new cathode materials that are cheaper and more environmentally friendly than the metals used today
- Design new battery materials that can operate in harsh conditions
- Optimize properties of existing battery materials such as siliconbased materials, which have the potential to double or triple the energy storage in conventional batteries, but have limited lifespans
- Generate better overall energy output through improved cathodes with greater discharge capacity and voltage response

## THE APS AND BATTERY DEVELOPMENT

The following are examples of synchrotron x-ray techniques used for battery studies.

X-ray fluorescence can pinpoint defects caused by elemental contaminants introduced during processing.

X-ray microscopy enables liquid-solid interface insights on complex materials such as a lithium battery. This makes visible the interface of an electrode as it charges and discharges under real operating conditions.

X-ray Absorption Fine-edge Spectroscopy (XAFS) can probe the environment around atoms of all states of matter and X-ray Absorption Near-edge Structure (XANES) can determine the average oxidation state and local symmetry of the elements in all phases. This allows the monitoring of the state of charge, which can reveal insights about fundamental mechanisms, including the solubility and stability of the electrolytes.

X-ray diffraction enables real-time monitoring of the dynamic chemical and structural changes in commercial cells under realistic cycling conditions to better understand processstructure-property relationships.

**LERIX spectroscopy** is the only reliable method for bulk sensitivities studies of chemicals on the low absorption edge, such as Li-K-edge and O-K-edge. To map the Ta-L edge spectra in many electrochemical systems, XANES is required.

## Pair distribution function x-ray

**scattering** can map the movement between atoms to reveal the structure and dynamics of ion solvation in electrolytes.

### **RESEARCH OPPORTUNITIES**

- Redox targeting reactions to both anode and cathode materials and the matched redox mediators and conducting membranes
- Map impurities introduced into batteries
- Characterize the interfaces and structures in fundamental materials as they operate
- Trace chemical reactions across layers during cycling
- Analyze how electronic conductivity is affected by the lithiation/delithiation mechanism and electronic structure of materials subjected to different heat treatments
- Characterize the solvation shell of multivalent ions in organic electrolytes
- Analyze irreversible phase transitions on deep discharge that limit the use of cathode materials, such as vanadium pentoxide

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