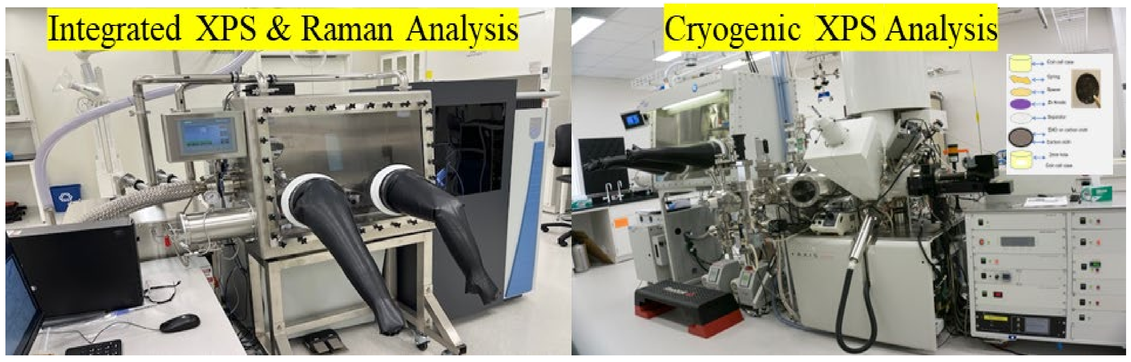
Battery Materials Reliability Analytics

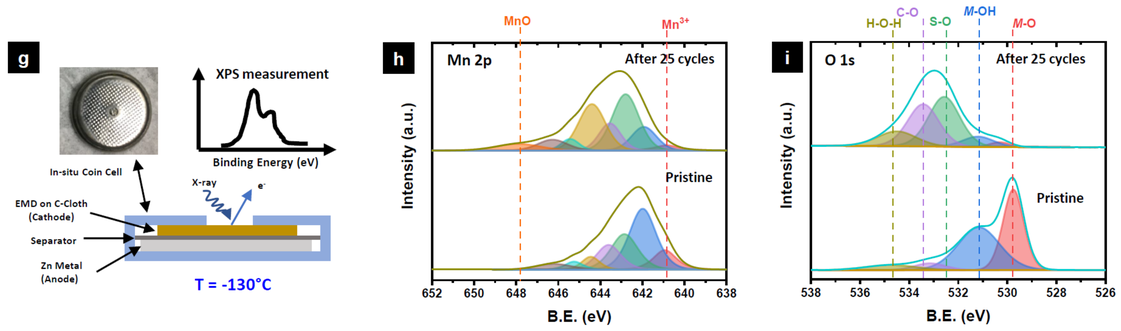
Bhuvana M. Sivakumar, Matthew Fayette, Edwin Thomsen, Daiwon Choi, Vijay Murugesan, Xiaolin Li, David Reed

Materials Reliability Platform

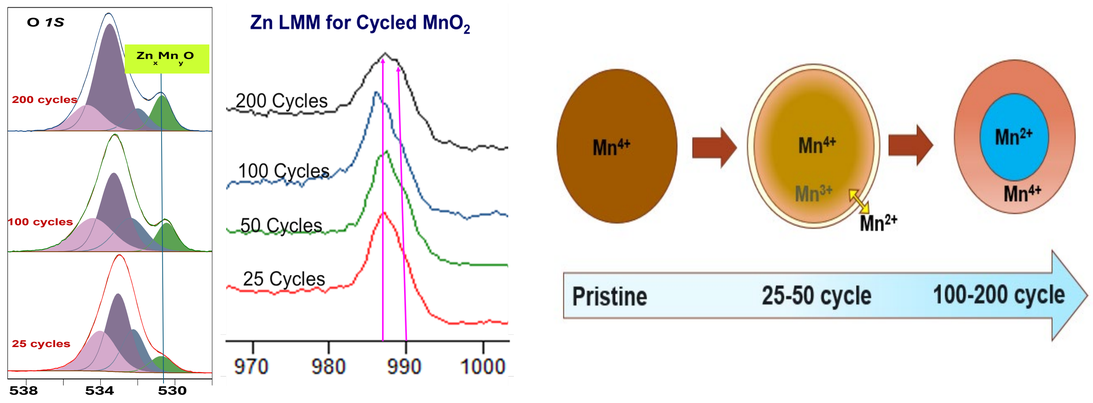


We are building a predictive analytics platform that detects early failure signs in battery materials—from chemical functionality of carbon electrodes to structural changes in intercalation cathodes. This will enable "materials-by-design" approach by providing predictive capabilities for battery degradations pathways and long-term performance to develop resilient electric grid.

Decoding MnO_2 Degradation

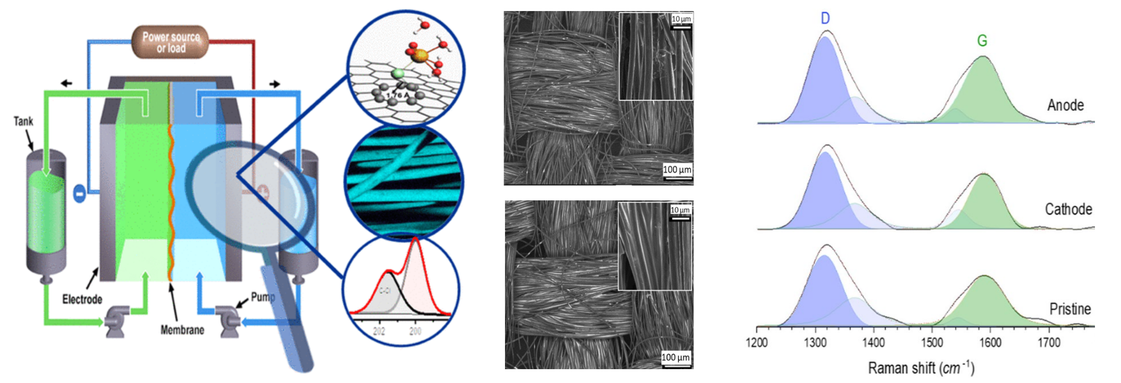


- **Structural Evolution**: Increased intensity of the binary metal oxide peak (~530 eV) at extended cycling indicates structural changes due to Zn^{2+} intercalation, suggesting phases like buserite and spinel $ZnMn_2O_4$.
- **Surface Hydration**: O1s peak at ~535 eV at 100 and 200 cycles confirms surface hydration on the electrode.
- **Electrochemical Support**: Strong peak for intercalated water (~533 eV) reinforces the role of Mn^{2+} dissolution in the electrochemical process

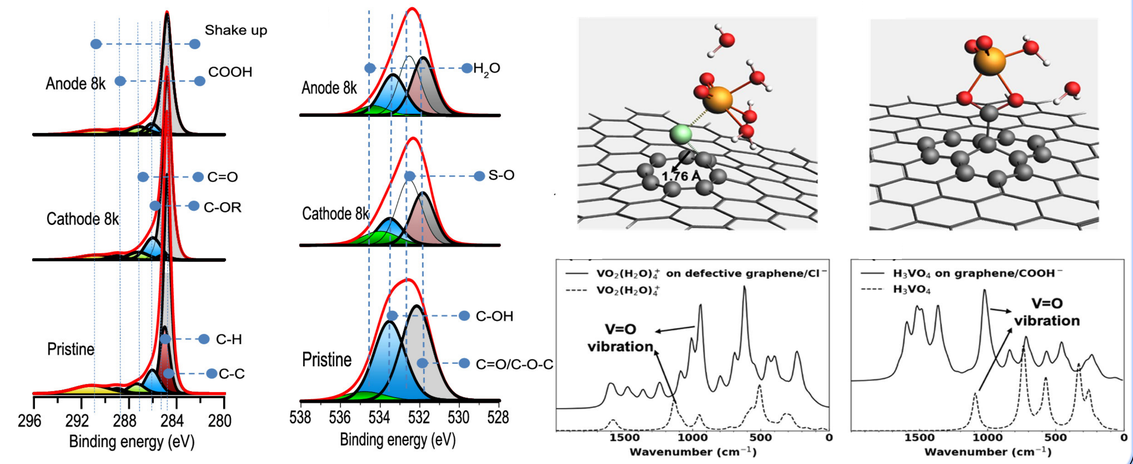


- ***Failure Indicator**: Mn^{2+} presence at 200 cycles signals a critical failure threshold in electrochemical materials.*
- ***Diffusion Limitations:** Formation of $ZnMn_2O_4$ suggests low Zn^{2+} diffusion kinetics, potentially hindering battery efficiency.*
- ***Enhanced Intercalation:** Detection of Mn^{4+} and Mn^{3+} at early cycles indicates a more favorable environment for aqua-Zn^{2+} and proton intercalation, essential for optimizing performance.*

Carbon Electrode Resiliency



Bulk structure is resilient: The core graphitic structure remains remarkably stable and unchanged even after 8,000+ cycles in redox flow battery.
Surface chemistry is vulnerable: Significant chemical changes, including new functional groups and point defects, dominate the degradation process.
Altered surface kinetics: Unique chemical evolution on the anode and cathode creates inconsistent hydrophilicity and slows down redox reactions.
Localized conductivity loss: The accumulation of point defects on the surface degrades local electronic conductivity, hindering overall performance.
Targeted anion attack: Counter-anions preferentially bind to defect sites ($Cl^- > HSO_4^-$), revealing a primary mechanism for chemical degradation.



Building Predictive Analytics

Fingerprinting failure modes: Building multimodal spectroscopic tool to precisely identify structural and chemical failure modes of battery materials.

Resiliency Prediction Tools: By correlating spectroscopic signals with performance data, we pinpoint critical failure triggers—such as anion-defect interactions in flow batteries and the onset of Mn^{2+} formation in Zn-ion cathodes.

Value of Material Analytics: The chemical and structural signatures act as early-warning indicators, enabling us to forecast material lifetime and accelerate the design of more robust, next-generation energy storage systems.

Acknowledgement
This material is based upon work supported by the U.S. Department of Energy, Office of Electricity (OE), Energy Storage Division.

This project is identifying degradation mechanisms in batteries which is crucial to meeting the Administration's goal of providing affordable, secure, and resilient energy.

For additional information, contact:
Bhuvana M. Sivakumar
bhuvana@pnnl.gov

U.S. DEPARTMENT of ENERGY
BATTELLE
PNNL is operated by Battelle for the U.S. Department of Energy

Pacific Northwest NATIONAL LABORATORY
www.pnnl.gov