Overview Interdisciplinary Science Department

Esther S. Takeuchi

Chair, Interdisciplinary Science Department

Brookhaven National Laboratory

SUNY Distinguished Professor

William and Jane Knapp Chair of Energy and the Environment

Co-Director Institute for Electrochemically Stored Energy

Stony Brook University

Amy C. Marschilok

Manager, Energy Storage Division, Energy Systems Division, Interdisciplinary Science Department, BNL

Associate Professor, Co-Director IESE, Stony Brook University

September 9, 2021

@BrookhavenLab

NY’s Ambitious Clean Energy Goals Align with Federal Direction

Targets in NY’s Climate Leadership and Community Protection Act (CLCPA)

- 85% reduction in greenhouse gas emissions by 2050
- 100% zero-emission electricity by 2040
- 70% renewable energy by 2030
- 9,000 megawatts of offshore wind by 2035
- 3,000 megawatts of energy storage by 2030
- 6,000 megawatts of solar by 2025
- 22 million tons of carbon reduction through energy efficiency and electrification

https://climate.ny.gov/

Interdisciplinary Science Department

Grid Modernization

- Grid modeling and simulation
- Data analytics and machine learning applications
- Probabilistic risk assessment
- Methods and tools for dynamic assessment and control design

Energy Efficiency

- Building efficiency
- Alternative fuels including biofuels and hydrogen
- Emissions measurement and analysis
- Geothermal materials

Energy Storage

- Operando studies
- Batteries for electric vehicles – fast charge, higher capacity materials
- Battery systems suitable for large scale applications
- EFRC – science of scalable batteries

Grid Modernization: Challenges in the Grid

Increasing challenges in power grid

- Increasing renewables and demand
- Vulnerabilities in complex and coupled infrastructures: Damage during weather events, E.g., Texas cold snap in 2021, cyber attacks

Electric energy industry is transforming rapidly

- Need to seamlessly integrate conventional and renewable sources, storage, central and distributed generation
- Deliver resilient, reliable, flexible, secure, sustainable, and affordable electricity to consumers where, when, and how they want it.

Achieving New York targets demands rapid change

- **Solar Goal:** 2GW solar installed and a total of 6GW solar expected by 2025.
- **Energy Storage Goal**: initiative for 3GW by 2030.
- **Wind Goal**: Initiative for addition of 9GW offshore wind development by 2035.
- **NYREV**: Effort to improve grid performance by developing a distribution level energy market and giving customers more control over their energy use.

Need to address both regional and national issues related to the transforming power grid

Brookhaven National Laboratory

Grid Modeling: Current Capabilities

Grid modeling and simulation

- Steady-state and dynamic impacts of high penetrations of renewables

Data analytics and machine learning applications

- Data-analytics and model-based anomaly detection and mitigation for cybersecurity
- Damage forecasting under severe weather conditions
- Online data-driven stability assessment, trajectory prediction, and control

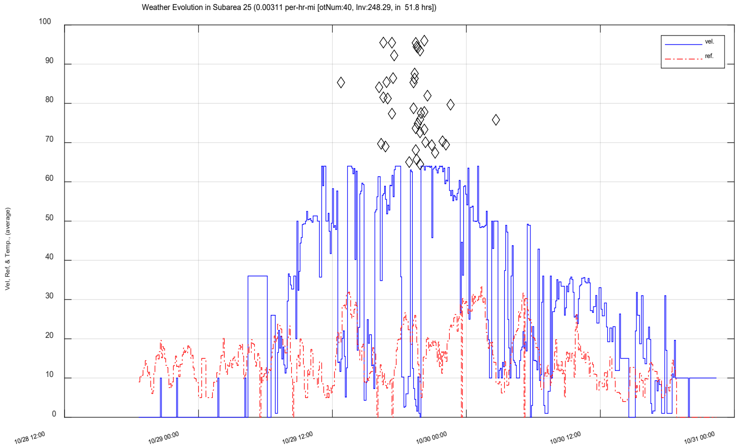
Probabilistic risk assessment

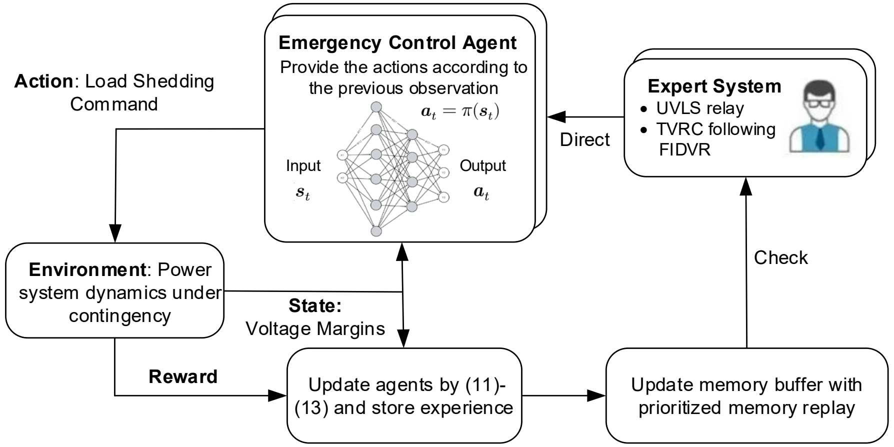
- Uncertainty modeling, quantification, and propagation
- Probabilistic contingency analysis and stochastic optimization for expansion studies and energy storage system sizing and siting.
- Probabilistic damage modeling for enhanced grid damage forecasting

Methods and tools for dynamic assessment and control design

- Machine-learning and physics-based transient simulator
- Deep reinforcement learning emergency control
- Reachability assessment of integrated transmission and distribution (T&D)

Distribution automation, micro-grids, and networked microgrids for improving grid resilience and how to manage

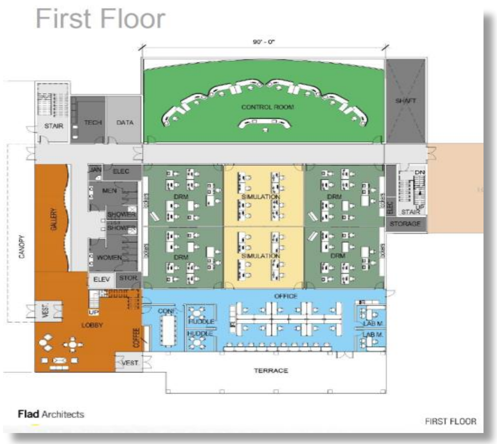


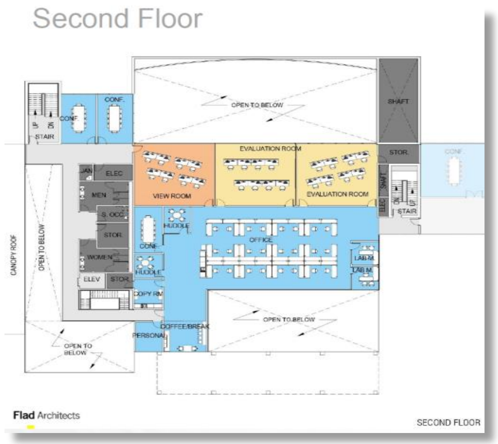


Brookhaven National Laboratory

Grid Enhancement and Modernization Center (GEM)

A New Grid Research Facility to Address the Challenges of Grid Modernization in the Northeast





Facility Vision

A versatile research, development and testing center to promote industry and university collaboration, both from the public and private sector, in the area of electric energy and grid modernization.

Simulation laboratory to test and validate new technologies in order to reduce risk prior to deployment

Provides the research capabilities needed to enable New York’s clean energy goals

Strong focus on understanding and addressing the dynamics and challenges of the modern electric grid

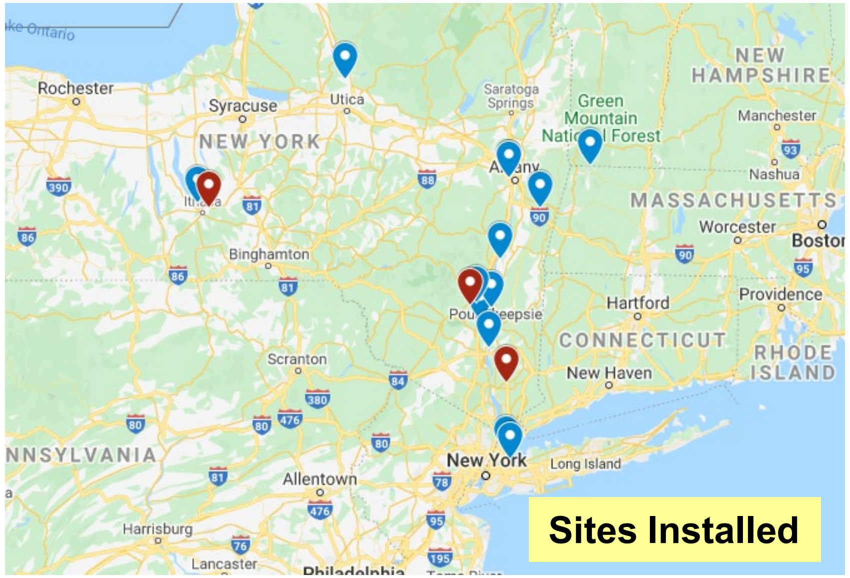
A “one-stop” venue for demonstrating new technologies to all New York stakeholders

Building Efficiency – Current Status

- Commercial / residential buildings consume 75% of generated electricity in the U.S. and account to 39% of carbon emissions.
- Building decarbonization is a megatrend with heat pumps driven by renewable power.
- Impractical unless building energy consumption can be dramatically reduced in parallel.
- Grid reliability, integration and energy storage extremely important.
- Fossil fuel industries making strong counter-thrusts with renewable fuels.
- IS Department capabilities, and experience include: combustion; emissions; solid, liquid, gaseous biofuels; performance mapping in lab and field of energy conversion equipment; development of novel systems; commercial and industrial systems; thermofluid science.
- BNL has a strong collaborations with SBU (and others).
- Efficiency is a team sport. Being part of community is critical.

Current Programs

- Field study of the performance of air-source heat pumps in cold climates.
- Development of novel, low-cost methods for evaluating emission and efficiency performance of advanced wood burning appliances which are in development.
- Support for the Development of Next Generation Certification Test Methods for Wood Heaters.
- Development of air pollutant emission factors for emerging building heat and power technologies and fuels.
- Performance of solid oxide fuel cells with natural gas and gas/hydrogen blends.



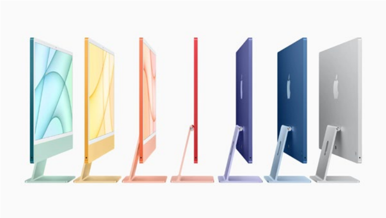
Wood Stove Event in DC – BNL Providing All Testing

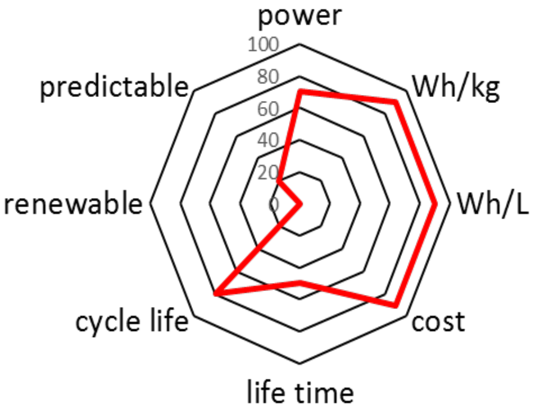
Brookhaven National Laboratory

Current and Future Energy Storage Technologies

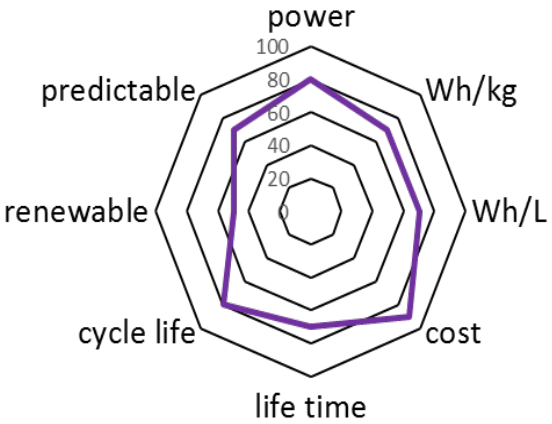
Current → **Future**

Consumer Electronics

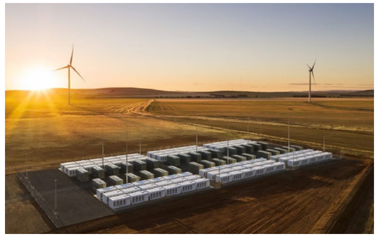


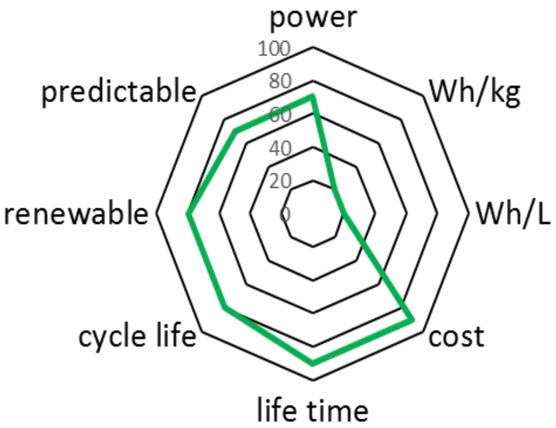


Electric Vehicles



Grid-Level Storage





Application specific development begins with understanding

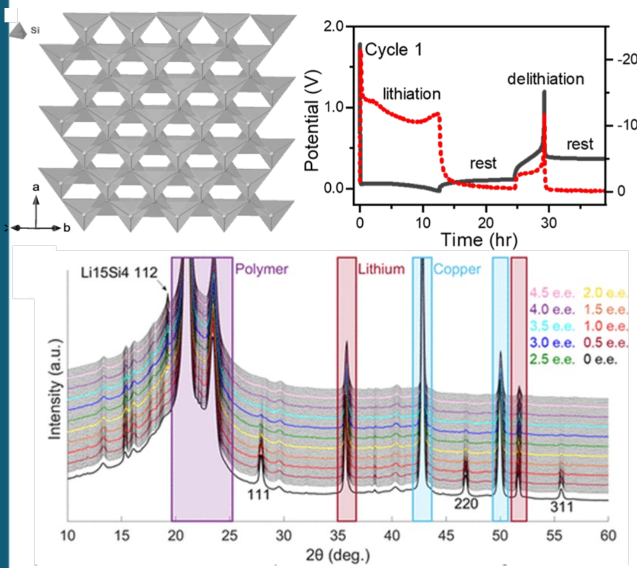
Brookhaven National Laboratory

E. S. Takeuchi, Ashton Cary Lecture, "From Medical Applications to the Environment: The Important Role of Energy Storage", Georgia Institute of Technology, Atlanta GA, March 4, 2020.

Programs on Lithium-based Technologies

Energy Density

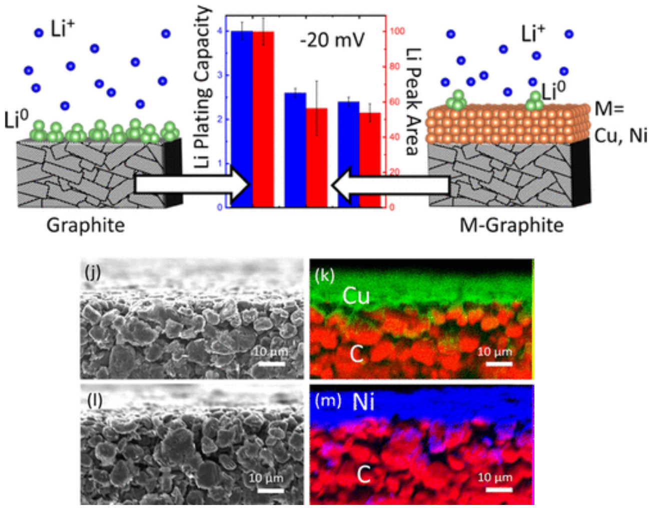
Conversion/Alloying Materials



L.M. Housel, W. Li, C.D. Quilty, M.N. Vila, L. Wang, C.R. Tang, D.C. Bock, Q. Wu, X. Tong, A.R. Head, K.J. Takeuchi, A.C. Marschilok, E.S. Takeuchi, *Appl. Mater. Inter.* 2019, *11* (41), 37567-37577.

Fast Charge

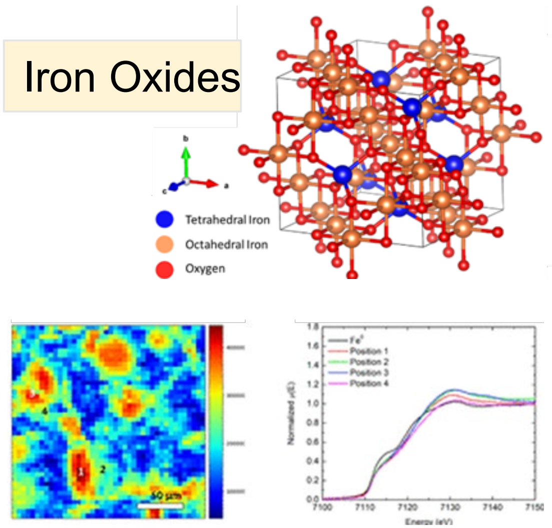
Surface Modifications



K.R. Tallman, B. Zhang, L. Wang, S. Yan, K. Thompson, X. Tong, J. Thieme, A. Kiss, A.C. Marschilok, K.J. Takeuchi, D.C. Bock, E.S. Takeuchi, *ACS Appl. Mater. Inter.* **2019,** *11* (50), 46864-74.

Cost Effective

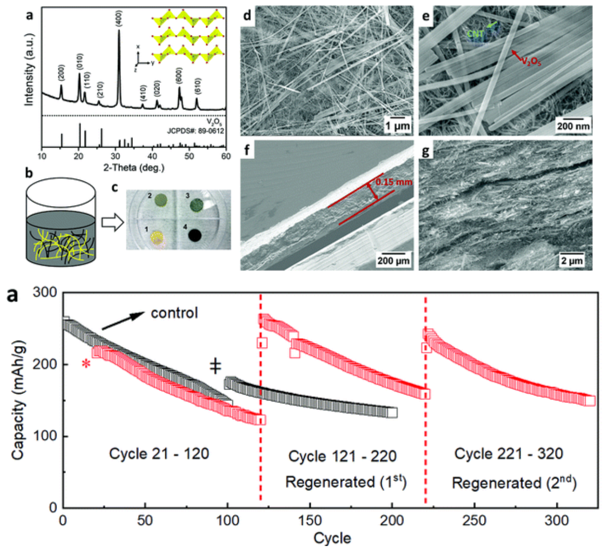
Earth Abundant Materials



M.M. Huie, D.C. Bock, A.M. Bruck, K.R. Tallman, L.M. Housel, L. Wang, J. Thieme, K.J. Takeuchi, E.S. Takeuchi, A.C. Marschilok, *ACS Appl. Mater. Inter.* **2019,** *11* (7), 7074-7086.

Recyclability

Process Development



J. Huang, L.M. Housel, L. Wang, A.M. Bruck, C.D. Quilty, A. Abraham, D.M. Lutz, C.R. Tang, A. Kiss, J. Thieme, K.J. Takeuchi, E.S. Takeuchi, A.M. Marschilok, *Sustain. Energy Fuels* **2019,** *3* (10), 2615-26.

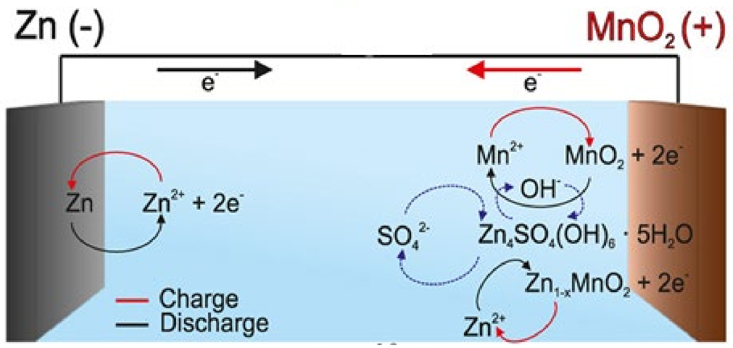
Brookhaven National Laboratory

Future Electrochemical Energy Storage

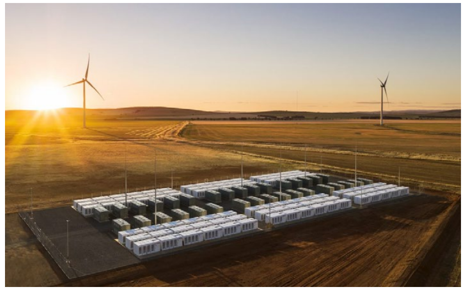
Current → Future

- scalable
- low cost
- high operational safety
- abundant, environmentally benign components
- ambient manufacturing

Zinc-Ion Aqueous Batteries



M. Chamoun, W.R. Brant, C.-W. Tai, G. Karlsson, D. Noréus, *Energy Storage Mater.* **2018,** *15*, 351-360.



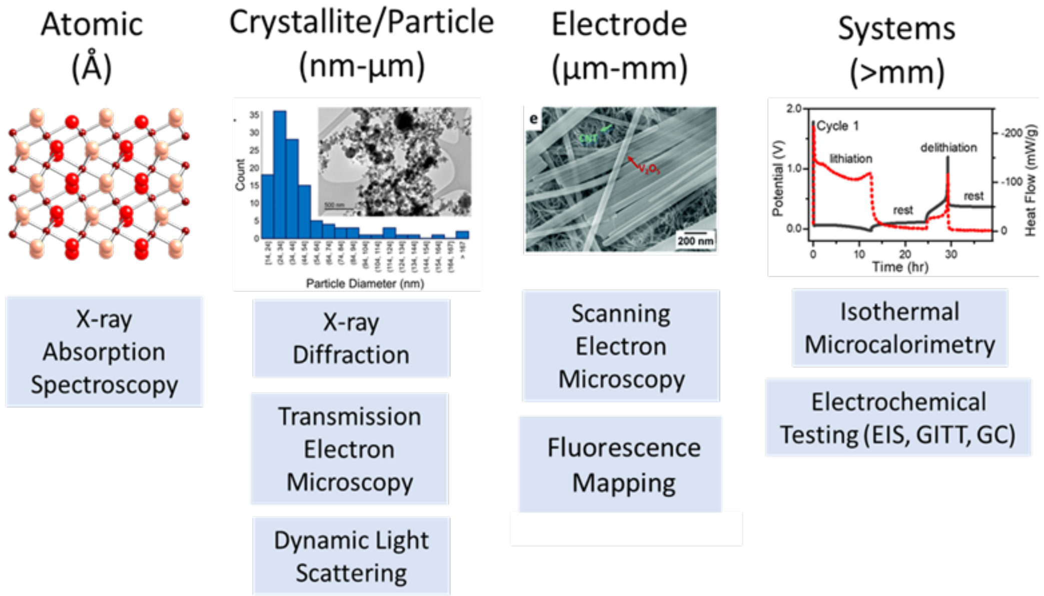
Brookhaven National Laboratory

Center for Mesoscale Transport Properties (EFRC)

Mission: to **enable deliberate design of materials and components** to achieve higher performing, longer life, and **scalable** energy storage systems through acquisition of new **fundamental knowledge** about **ion and electron transport** properties of energy relevant materials, **over multiple length scales, across interfaces and over time**.

https://www.stonybrook.edu/commcms/m2m/index.php

m2m/t
molecular to mesoscale over time

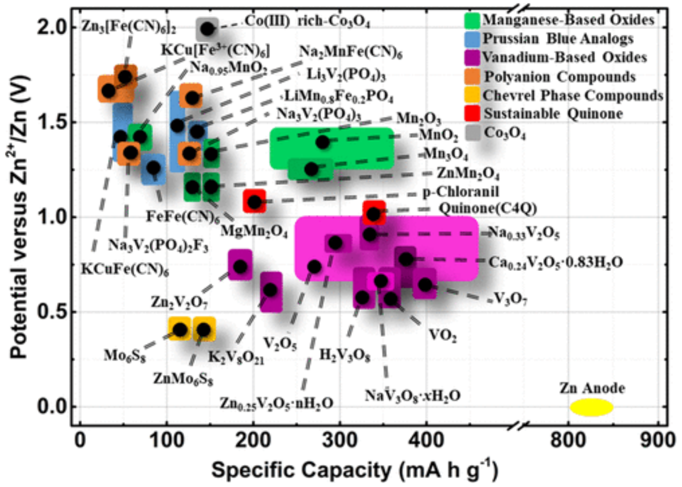


U.S. DEPARTMENT OF ENERGY | Office of Science

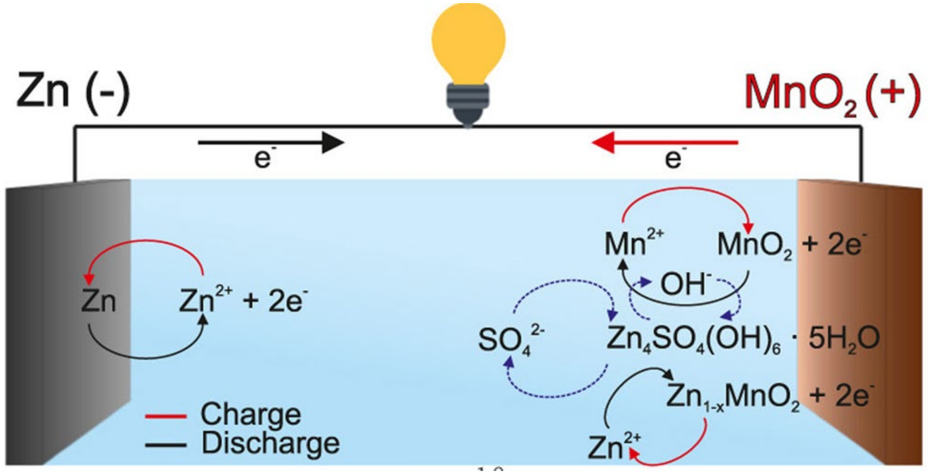
Brookhaven National Laboratory

W. Li, D. Lutz, L. Wang, K.J. Takeuchi, A.C. Marschilok, E.S. Takeuchi, *Joule* **2021,** *5* (1), 77-88.

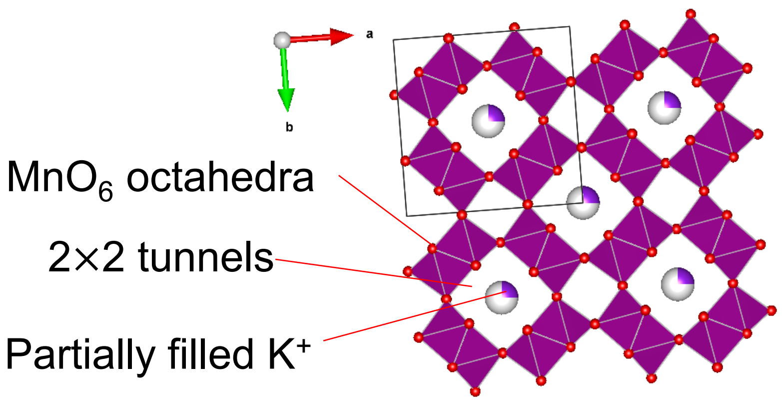
Aqueous Zn/α-MnO_2 Batteries



G. Fang, J. Zhou, A. Pan, S. Liang, *ACS Energy Lett.* **2018,** *3* (10), 2480-2501.



M. Chamoun, W.R. Brant, C.-W. Tai, G. Karlsson, D. Noréus, *Energy Storage Mater.* **2018,** *15*, 351-360.



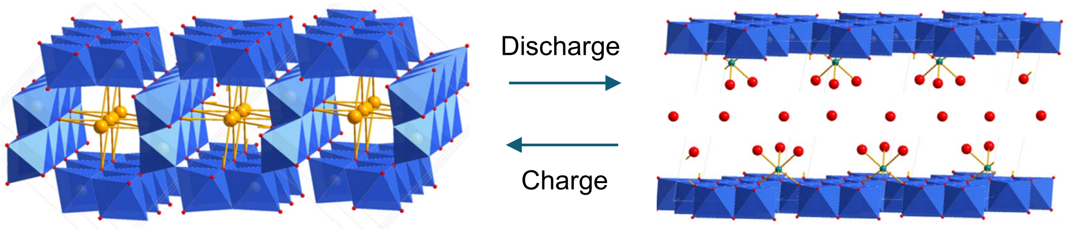
L.M. Housel,† L. Wang,† A. Abraham,† J. Huang, G.D. Renderos, C.D. Quilty, A.B. Brady, A.C. Marschilok, K.J. Takeuchi, E.S. Takeuchi, *Acc. Chem. Res.* **2018,** 51 (3), 575-582.

- Scalable due to earth abundant components and non-flammable aqueous electrolyte
- α-MnO_2 most studied cathode material for Zn-ion due to large 2x2 tunnels for ion storage
- Mildly acidic $ZnSO_4$ electrolytes have enabled reversible cycling of Zn/MnO_2 cells
- Cycle life of Zn/α-MnO_2 remains limited

Brookhaven National Laboratory

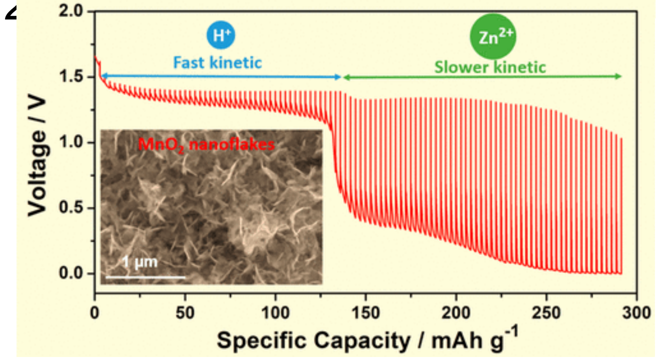
Understanding Charge Storage within Zn/α-MnO_2 Batteries

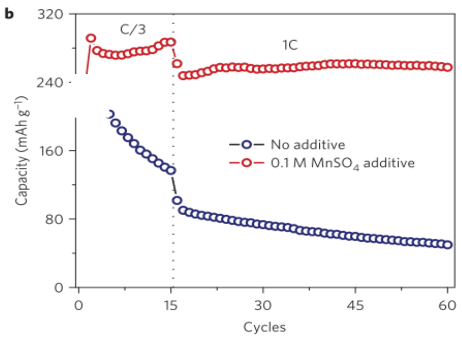
Multiple reported charge storage mechanisms



1. Zn-insertion reaction[1]

2. H^+ insertion/chemical conversion reaction[2]





3. H^+ and Zn^{2+} co-insertion/conversion[3]

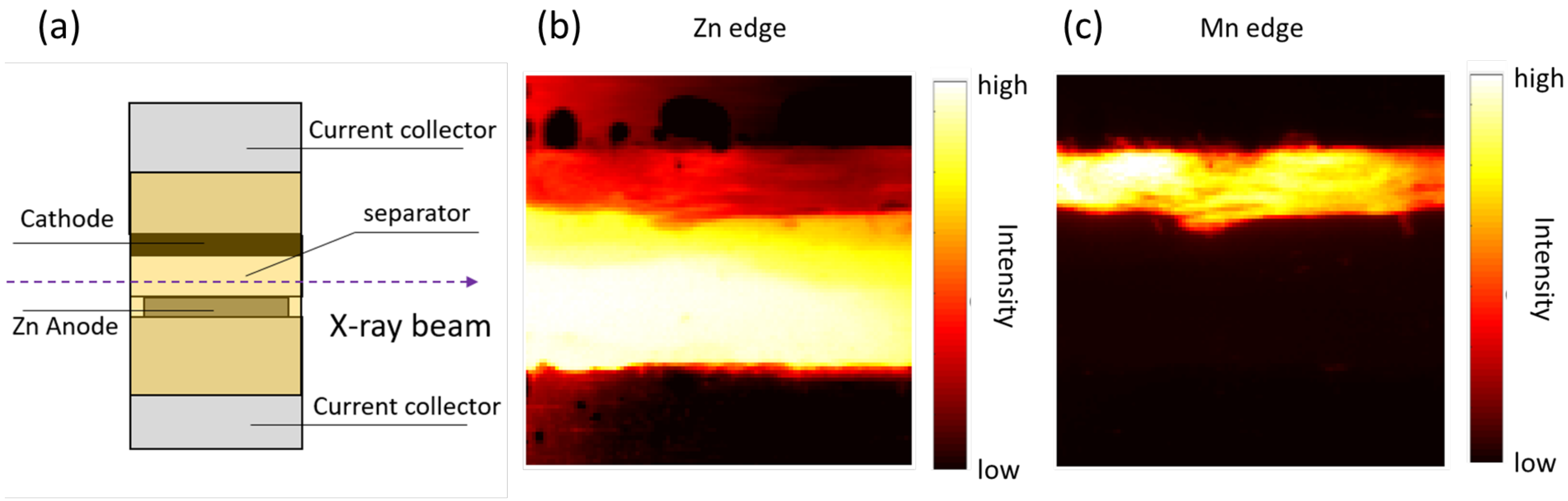
4. Mn^{2+} additives improve capacity retention[3,4]

1. B. Lee, H.R. Lee, H. Kim, K.Y. Chung, B. Cho, W. Oh, *Chem. Commun.* **2015**, *51*, 9265-9268.
2. H. Pan, Y. Shao, P. Yan, Y. Cheng, K.S. Han, Z. Nie, C. Wang, J. Yang, X. Li, P. Bhattacharya, K. Mueller, J. Liu, *Nat. Energy* **2016**, *1*, 16039.
3. W. Sun, F. Wang, S. Hou, C. Yang, X. Fan, Z. Ma, T. Gao, F. Han, R. Hu, M. Zhu, C. Wang, J. Am. Chem. Soc. 2017, 139 (29), 9775-9778..
4. M. Chamoun, W.R. Brant, C.-W. Tai, G. Karlsson, D. Noréus, *Energy Storage Materials* **2018,** *15*, 351-360.

Brookhaven National Laboratory

Operando characterization of Zn/α-MnO_2 cells

NSLS II at BNL



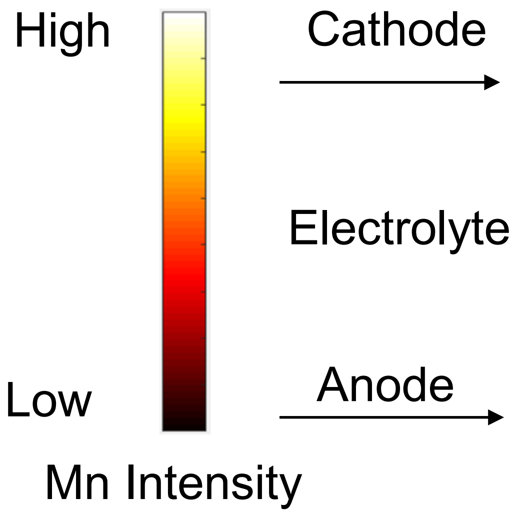
Beamline 4-BM, X-ray Fluorescence Microprobe (XFM) at NSLS-II

Spatially and Temporally resolved x-ray fluorescence maps collected continuously during Galvanostatic cycling of an Zn-α-MnO_2 cell at the Mn K-edge.

Brookhaven National Laboratory

D. Wu, L.M. Housel, S-J. Kim, N. Sadique, C.D. Quilty, L. Wu, R. Tappero, S.L. Nicholas, S. Ehrlich, Y. Zhu, A.C. Marschilok, E.S. Takeuchi, D.C. Bock, K.J. Takeuchi, Energy & Environmental Science (2020). DOI: 10.1039/d0ee02168g.

Direct Observation of Reversible Mn Dissolution-Deposition



Zn/α-MnO_2 *operando* cell cy

Mn fluorescence maps collected every ~9 minutes

Mn intensity increases in electrolyte during discharge

Mn intensity decreases in electrolyte during charge

Mn dissolution is reversible

Video Graphic by: Daren Wu (SBU)

Brookhaven National Laboratory

D. Wu, L.M. Housel, S-J. Kim, N. Sadique, C.D. Quilty, L. Wu, R. Tappero, S.L. Nicholas, S. Ehrlich, Y. Zhu, A.C. Marschilok, E.S. Takeuchi, D.C. Bock, K.J. Takeuchi, Energy & Environmental Science (2020). DOI: 10.1039/d0ee02168g.

Interdisciplinary Science Department: Relevant to NY State and Federal Goals

Grid Modernization

- Grid modeling and simulation
- Data analytics and machine learning applications
- Probabilistic risk assessment
- Methods and tools for dynamic assessment and control design

Energy Efficiency

- Building efficiency
- Alternative fuels including biofuels and hydrogen
- Emissions measurement and analysis
- Geothermal materials

Energy Storage

- Operando studies
- Batteries for electric vehicles – fast charge, higher capacity materials
- Battery systems suitable for large scale applications
- EFRC – science of scalable batteries

Acknowledgements

U.S. DEPARTMENT OF ENERGY | Office of Science

U.S. DEPARTMENT OF ENERGY | OFFICE OF ELECTRICITY

U.S. DEPARTMENT OF ENERGY
Office of TECHNOLOGY TRANSITIONS

OFFICE OF
Cybersecurity, Energy Security, and Emergency Response

U.S. DEPARTMENT OF ENERGY
Energy Efficiency & Renewable Energy

VTO, AMO, BTO

NEW YORK STATE OF OPPORTUNITY. | NYSERDA

nationalgrid

Brookhaven National Laboratory