SAND2020-10172PE

Zn-based Batteries

Timothy. N. Lambert, Matthew B. Lim, D. J. Arnot, Igor V. Kolesnichenko, Noah B. Schorr, Rachel L. Habing, Logan S. Ricketts, Elijah I. Ruiz

PRESENTED BY

Timothy N. Lambert

DOE-OE Peer Review, Virtual Presentation, Albuquerque, New Mexico, September 29 – October 31, 2020

SAND2XXXX-XXXX

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Session OVERVIEW – Zn-based Batteries

OE supports RESEARCH&DEVELOPMENT needs of battery chemistries that could impact Grid Storage: Reliable and resilient electricity system

03:35 – 03:55 PM	Session Summary / Zinc-Based Batteries	Timothy Lambert, *SNL*
03:55 – 04:10 PM	From Concept Through Product to Market: Rechargeable Zinc Manganese Dioxide Batteries	Sanjoy Banerjee, *CCNY*
04:10 – 04:25 PM	Engineering an Aqueous Energy Dense Manganese Dioxide|Zinc Battery to Challenge Lithium - Ion's Dominance	Yadav Gautam, *UEP*
04:25 – 04:40 PM	Operando Studies to Enumerate the Electrochemical Phase Transformations of MnO_2	Joshua Gallaway, *Northeastern University*
04:40 – 04:55 PM	Advanced Aqueous Zn Batteries	Xiaolin Li, *PNNL*
04:55 – 05:10 PM	Mechanistic Probes of Zinc Anode Aqueous Electrolyte Batteries	Esther Takeuchi, *Stony Brook University*

Conversion Cathode Chemistry

Intercalation Cathode Chemistry

PROJECT OVERVIEW – Zn Batteries (Re: Cost, Safety & Reliability)

Alkaline zinc batteries are one of the core DOE/OE technologies for grid storage and feature energy-dense, safe, abundant, low-cost materials

Alkaline-Zn/MnO_2 Batteries Today

Wikipedia, user Aney, 2005

- Well-established supply chain for consumer products
- >10B units produced, \$7.5B global market (2019)
- Traditional primary alkaline batteries ~ < \$20/kWh
- Aqueous, long shelf life, EPA certified for disposal
- High achievable energy density
  - Zn/MnO_2 ~ 400 Wh/L
  - Zn/Ni ~ 300 Wh/L
  - Zn/Air ~ 1400 Wh/L

Zn

- 13M tons (2019)
- ~ \$1.25/lb (2019)

γ-MnO_2

- 19M tons Mn ores (2019)
- < \$2/lb (2012)

USGS Mineral Commodity summaries, 2020

KOH

- Potash ~ 61M tons (2019)
- ~\$400/ton (2020)
- Aqueous, non-flammable

Reversibility and Cycle life are the Challenges/Opportunities

PROJECT TEAM – Sandia National Laboratories and Collaborators

Sandia National Laboratories

Timothy Lambert

Alkaline Batteries for Grid Storage

Stephen Budy, Igor Kolesnichenko, Matthew Lim, Noah Schorr, David Arnot, Rachel Habing, Logan Ricketts, Elijah Ruiz, Nelson Bell

CUNY The City University of New York Energy Institute

Prof. Sanjoy Banerjee

Stable Zinc Anodes for High-Energy-Density Rechargeable Aqueous Batteries

Damon Turney, Michael D’Ambrose, Jungsang Cho, Brendan Hawkins, Jinchao Huang, Snehal Kolhekar, Michael Nyce, Xia Wei, Prof. Rob Messinger

NM STATE UNIVERSITY

Prof. Igor Vasiliev

Theoretical Studies of the Electrochemical Behavior of Solid-State Cathode Materials in Rechargeable Alkaline Zn/MnO$_2$ and Zn/Cu$_2$S Batteries

Birendra A. Magar, Nirajan Paudel

Prof. Joshua Gallaway

Understanding Phase Change Processes of Energy Storage Materials

Andrea Bruck, Matthew Kim

Prof. Esther Takeuchi

Advanced Materials for Next Generation Batteries

Amy Marschilok, Ken Takeuchi

Stony Brook University

PROJECT TEAM – Sandia National Laboratories and Collaborators

Gabe Cowles

Gautam Yadav

Advanced Manufacturing Research ***(FY19/20 Funding)***
Advanced Manufacturing Research - Second electron Research Extension ***(FY21 Funding)***
Gabe Cowles, Gautam Yadav, Jinchao Huang, Aditya Upreti, Meir Weiner, Valerio DeAngelis, Sanjoy Banerjee

Amalie Frischknecht

Membrane Modeling

In FY21 also ……….

Prof. Yang-Tse (YT) Cheng

Collaborative research to advance solid state ion conductors for emerging batteries
Ryan Hill, Andrew Meyer, w/Erik Spoerke (SNL)

In FY21 also ……….

Three-dimensional printing of architected Zinc electrodes for rechargeable Zn-MnO_2 batteries

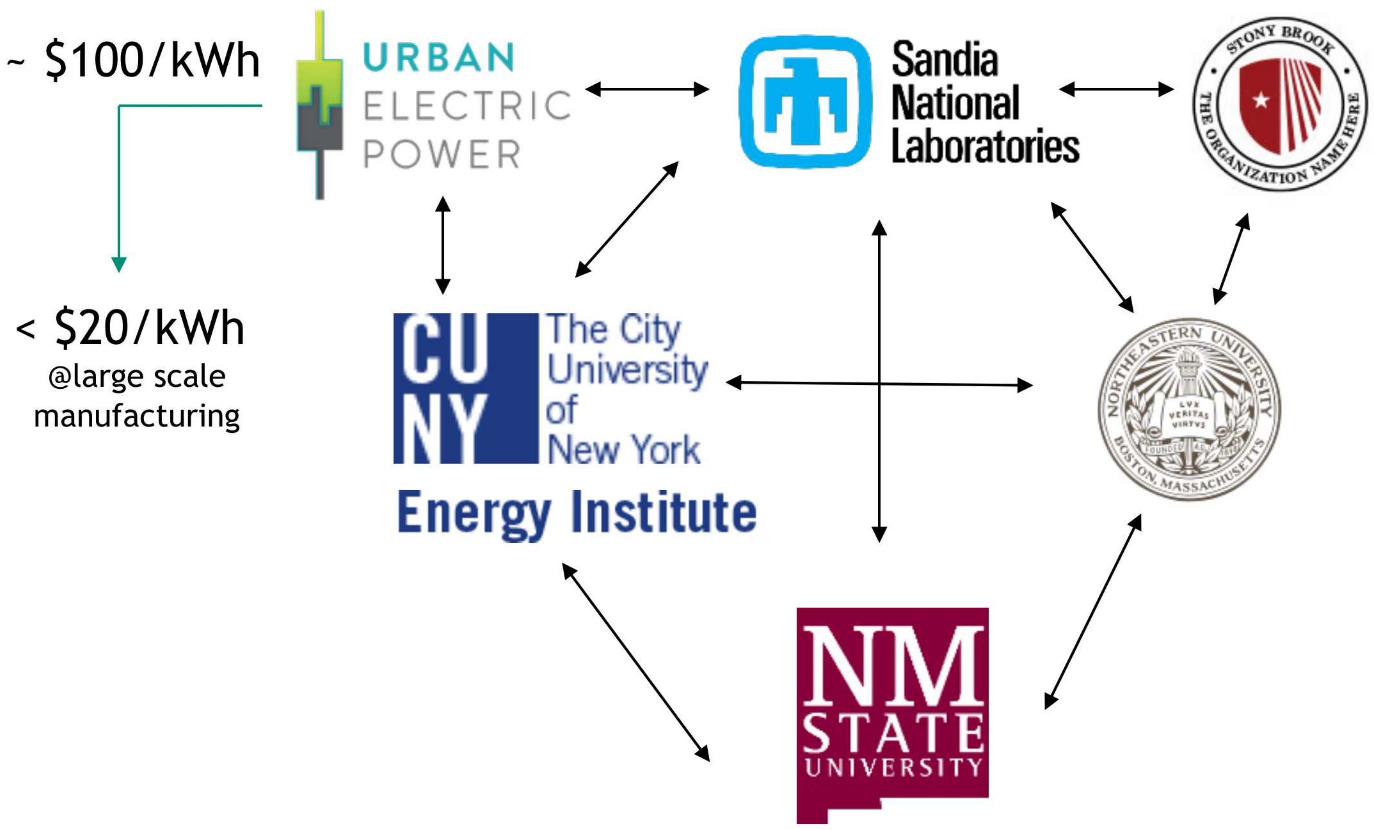
Cheng Zhu

Marcus Worsley

PROJECT TEAM – Sandia National Laboratories and Collaborators

OE supports RESEARCH & DEVELOPMENT, MANUFACTURING and DEMONSTRATION of Potentially Wide Impact, Low Cost Energy Storage Technologies

<u>Collaborative Efforts on Zn-batteries</u>



<u>2020 OE Peer Review Team Presentations</u>

S. Banerjee (CUNY-EI/UEP)

From Concept Through Product to Market: Rechargeable Zinc Manganese Dioxide Batteries

G. Yadav (UEP)

Engineering an Aqueous Energy Dense Manganese Dioxide|Zinc Battery to Challenge Lithium-Ion's Dominance

J. Gallaway (NEU)

Operando Studies to Enumerate the Electrochemical Phase Transformations of MnO_2

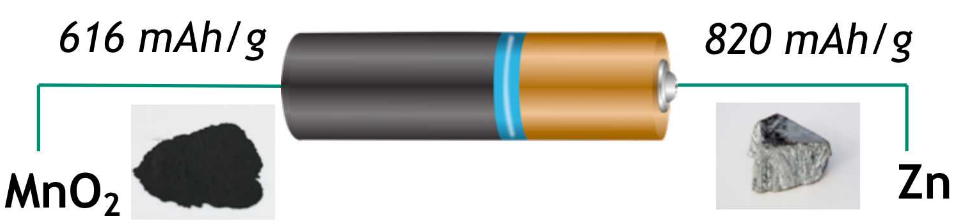
E. Takeuchi (SBU)

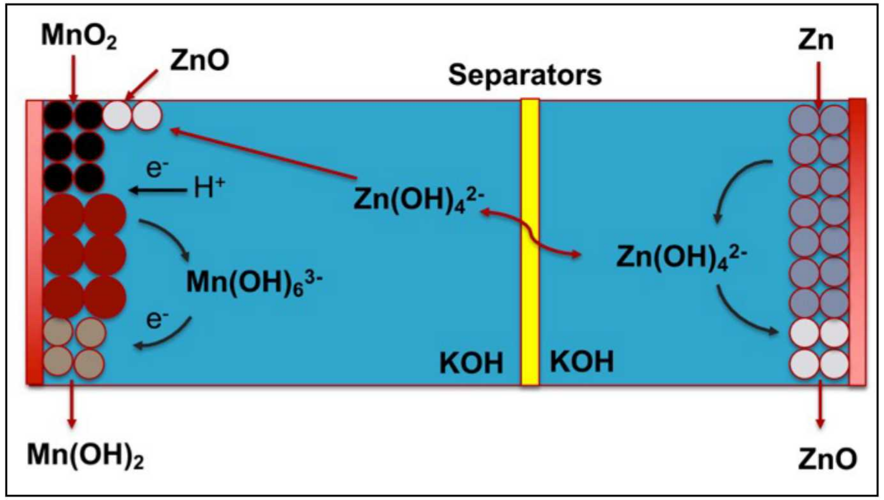
Mechanistic Probes of Zinc Anode Aqueous Electrolyte Batteries

I. Vasiliev (NMSU), D. Turney (CUNY-EI), A. Frischknecht (SNL)

Poster Presentations

PROJECT OVERVIEW

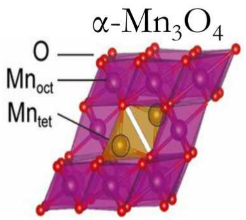




(Image adapted from CCNY)

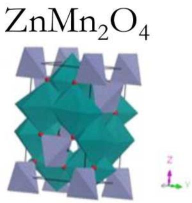
Technical Challenges Facing Zn/MnO_2

Cathode:
- Irreversibility of Cathode
- Susceptibility to Zinc poisoning



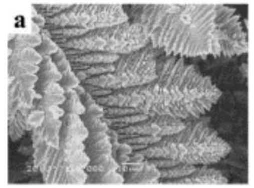
PNAS 115 (23), E5261 (2018)

Separator:
- Zincate crossover



Mater. Chem. Phys. 130, 39 (2011)

Anode:
- Shape Change
- Dendrite Growth
- Irreversible ZnO Passivation



J. Electrochem. Soc., 163 (9), A1836 (2016)

Problem: *Cycling Zn/MnO_2 (both electrodes) at high capacities for thousands of cycles - not realized*

Limiting Depth of Discharge has been shown to be a viable approach → 125 Wh/L to 170 Wh/L @$80-110/kWh

N. D. Ingale, J. W. Gallaway, M. Nyce, A. Couzis and S. Banerjee, *J. Power Sources*, 276, 7 (2015).

R&D: Full 2e⁻ equivalent can be realized, susceptible to zinc poisoning

G. G. Yadav, J. W. Gallaway, D. E. Turney, M. Nyce, J. Huang, X. Wei and S. Banerjee, *Nat. Commun.*, 8, 14424 (2017).

R&D: > 2V High Voltage system offers promise of increased Energy Density → 40% Zn/50% MnO_2 @ 2.4V ~ 760Wh/L ~ $20/kWh *(estimated)*

G. G. Yadav, D. Turney, J. Huang, X. Wei and S. Banerjee, *ACS Energy Lett.*, *4*, 9, 2144 (2019).

URBAN ELECTRIC POWER

Founded 2012

PROJECT TEAM - RESULTS

RESULTS: (SNL) Zn Battery Posters - DOE OE Energy Storage Virtual Peer Review 2020

A total of 18 Posters

SNL led Posters:
- D. Arnot et al. “Anodic Stripping Voltammetry Detection of Bismuth, Copper and Zinc and its Role in Evaluating Battery Separators”
- I. V. Kolesnichenko et al. “Polysulfone-Based Zincate-Blocking Separators for Secondary Zn-MnO_2 Batteries”
- M. Lim et al. “Flexible Ion-Selective Separators for Alkaline Zinc Batteries”
- A. Frischknecht et al. “Atomistic Simulations of Sulfone-based Polymer Electrolytes for Alkaline Batteries”

CCNY led Posters:
- D. Turney et al. “In operando synchrotron observations of aqueous Zn-MnO_2 materials evolution”
- S. Kolhekar et al. “Effect of KOH concentration on Mn(III) dissolution in Rechargeable γ-MnO_2 cathodes”
- M. D’Ambrose “Failure Mechanisms of Zinc Anodes in Rechargeable Alkaline Cells”
- B. Hawkins et al. “Reversible Electrochemical Control of ZnO Electronic Properties and Defect Structure in Zn Alkaline Batteries”
- D. Dutta et al. “Molecular-Level Investigation of Concentrated Acetate Electrolytes for High-Voltage Aqueous Zinc Batteries using NMR Spectroscopy”
- J. Huang et al. “Electrochemical Evaluation of the Application of Hydrogel Electrolytes to Rechargeable Zn|MnO_2 Alkaline Batteries”

NEU led Posters:
- A. Bruck et al. “Bismuth Enables the Formation of Disordered Birnessite in Rechargeable Alkaline Batteries”
- M. A. Kim et al. “Synthesis of birnessite with inserted cations and its application in rechargeable batteries”

NMSU led Posters:
- B. A. Magar et al. “Ab Initio Studies of the Cycling Mechanism of MnO_2 Cathodes Modified with Bi, Cu, and Mg in Rechargeable Zn/MnO_2 Batteries”
- N. Paudel et al. “Influence of Surfaces and Structural Defects on the Electrochemical Properties of MnO_2 in Rechargeable Zn/MnO2 Batteries”

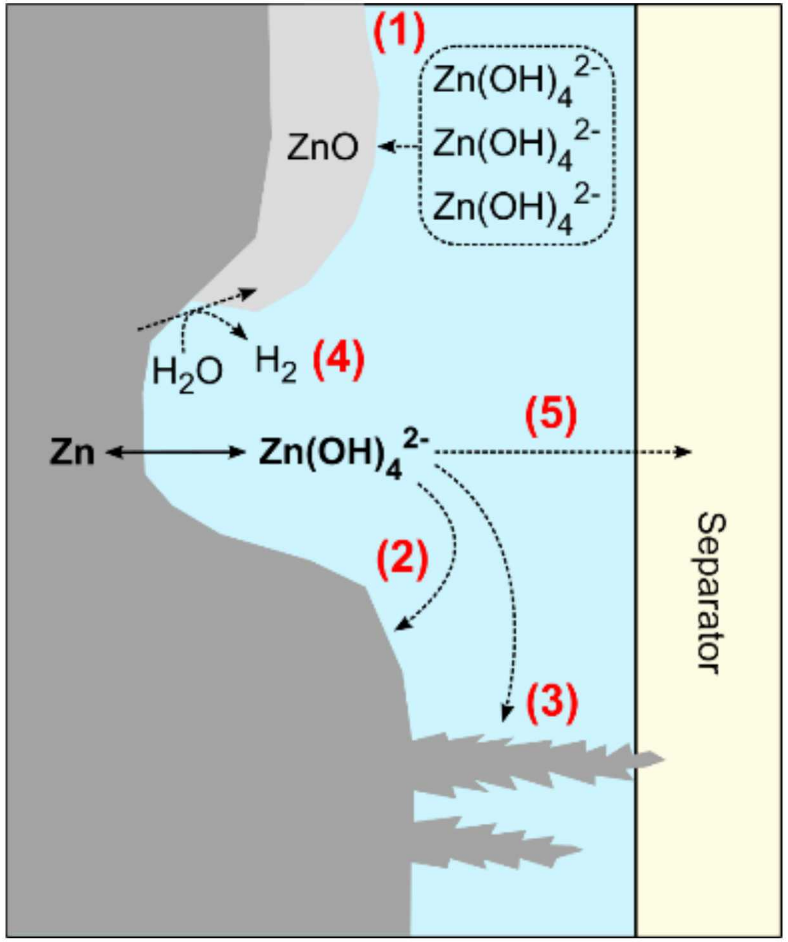
StonyBrook led Posters:
- E. Takeuchi et al. “Vanadium Oxide Cathodes for Beyond Li-Ion Energy Storage”
- E. Takeuchi et al. “Manganese Oxide Cathodes for Aqueous Zinc Anode Batteries”

UEP led Posters:
- M. Weiner et al. “Investigating electrochemical reactions of MnO_2 and Mn ions in Acidic Electrolyte”
- A. Upreti et al. “Functional hydrogels with enhanced physiochemical properties for highly energy dense rechargeable Zn-MnO_2 batteries”

PROJECT OBJECTIVES

SNL FY Objective 1 - INCREASE UNDERSTANDING and the DEPTH OF DISCHARGE (CAPACITY) OF Zn ELECTRODE

PROBLEM: Zn Capacity has not be realized for thousands of cycles at high DOD



Performance-Limiting Issues

1) Passivation
2) Shape change
3) Dendrite formation
4) H_2 evolution
5) Zincate crossover

Caused by solubility of ZnO in KOH (as $Zn(OH)_4^{2-}$) and subsequent precipitation of ZnO and Zn

Restricting migration of zincate is key

RESULTS - FOUR POSTERS:
M. Lim et al., M. D'Ambrose et al. B. Hawkins et al., J. Huang et al.

PROJECT OBJECTIVES

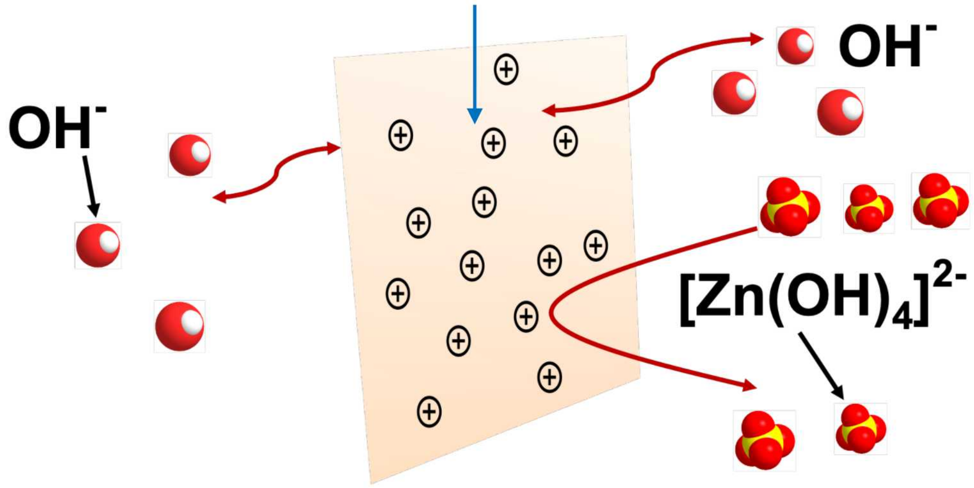
SNL FY Objective 2 – DEMONSTRATE ZINCATE BLOCKING SEPARATOR

PROBLEM: High Capacity Bi/Cu-MnO_2 only cycles well in absence of Zn –
Need to prevent Zincate [$Zn(OH)_4^{2-}$] Crossover to MnO_2 Cathode

Properties of an Effective Separator:

- Stability in alkaline electrolyte (pH >14)
- High ionic conductivity
- High hydroxide permeability
- Low zincate permeability
- Ease of Fabrication/Processing

Charge screening, size screening, and/or chelation results in a hydroxide selective membrane.

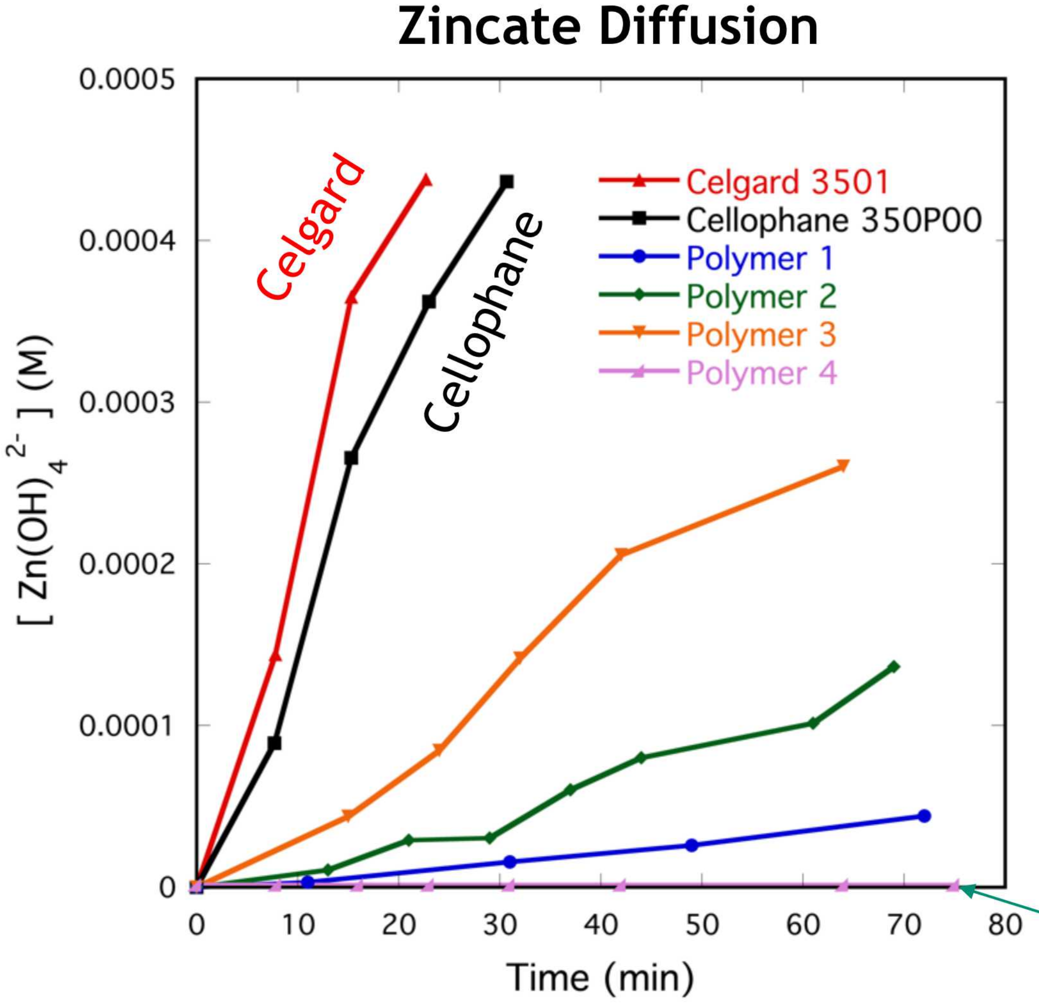


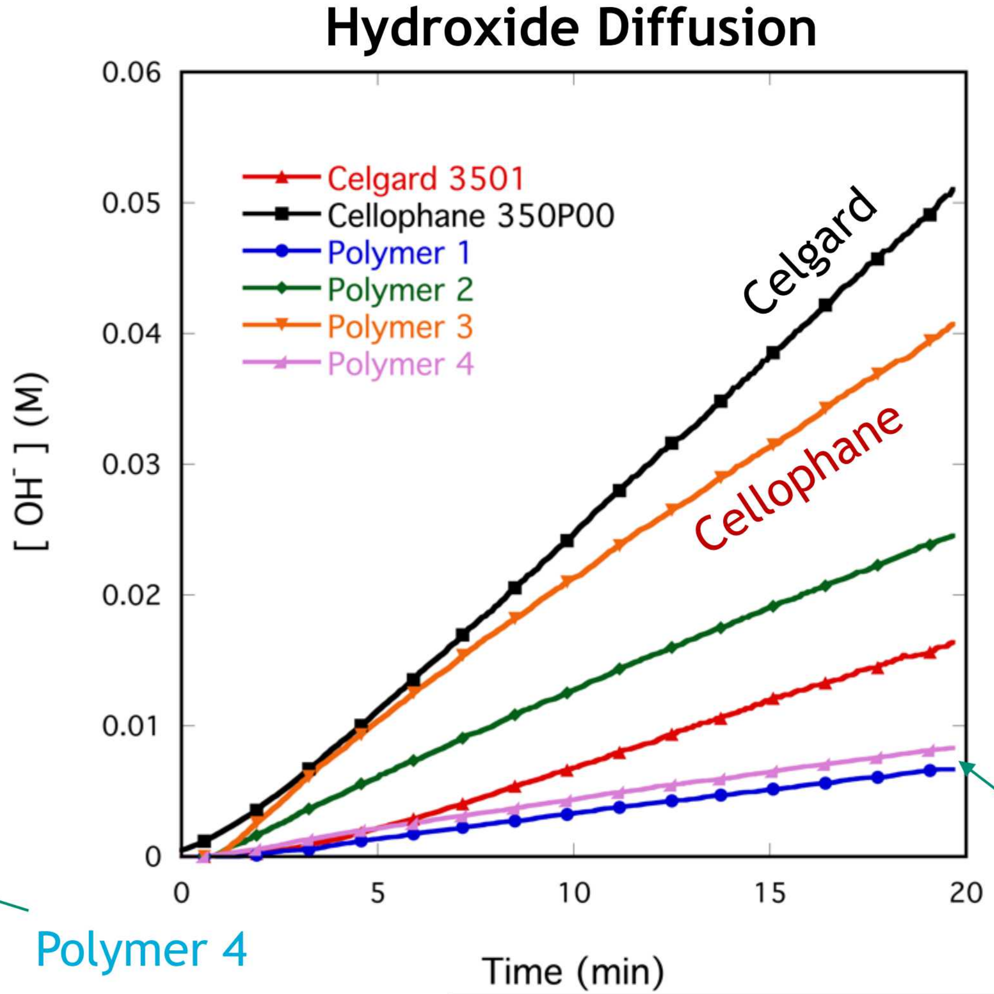
RESULTS - POSTERS:

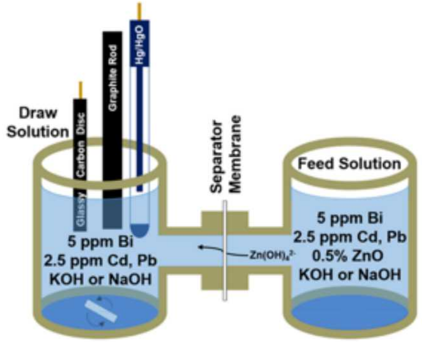
1. D. Arnot et al. “Anodic Stripping Voltammetry Detection of Bismuth, Copper and Zinc and its Role in Evaluating Battery Separators”
2. I. V. Kolesnichenko et al. “Polysulfone-Based Zincate-Blocking Separators for Secondary Zn-MnO_2 Batteries”
3. M. Lim et al. “Flexible Ion-Selective Separators for Alkaline Zinc Batteries”
4. A. Frischknecht et al. “Atomistic Simulations of Sulfone-based Polymer Electrolytes for Alkaline Batteries”

PROJECT RESULTS

Ex Situ – Hydroxide Selective Separator Successfully Developed







ASV Analysis of Zn, Cu and Bi in Alkaline conditions
J. Duay, et al.
Electroanalysis
DOI: 10.1002/elan.201700337
DOI: 10.1002/elan.201700526.
D. Arnot et al.
Electroanalysis
Bi ASV
Manuscript Submitted FY20

Polymer 4: $D_{HO^-}/D_{Zn(OH)_4^{2-}}$ ~ 10,000
ASV LOD for zincate ~ 0.026 mM

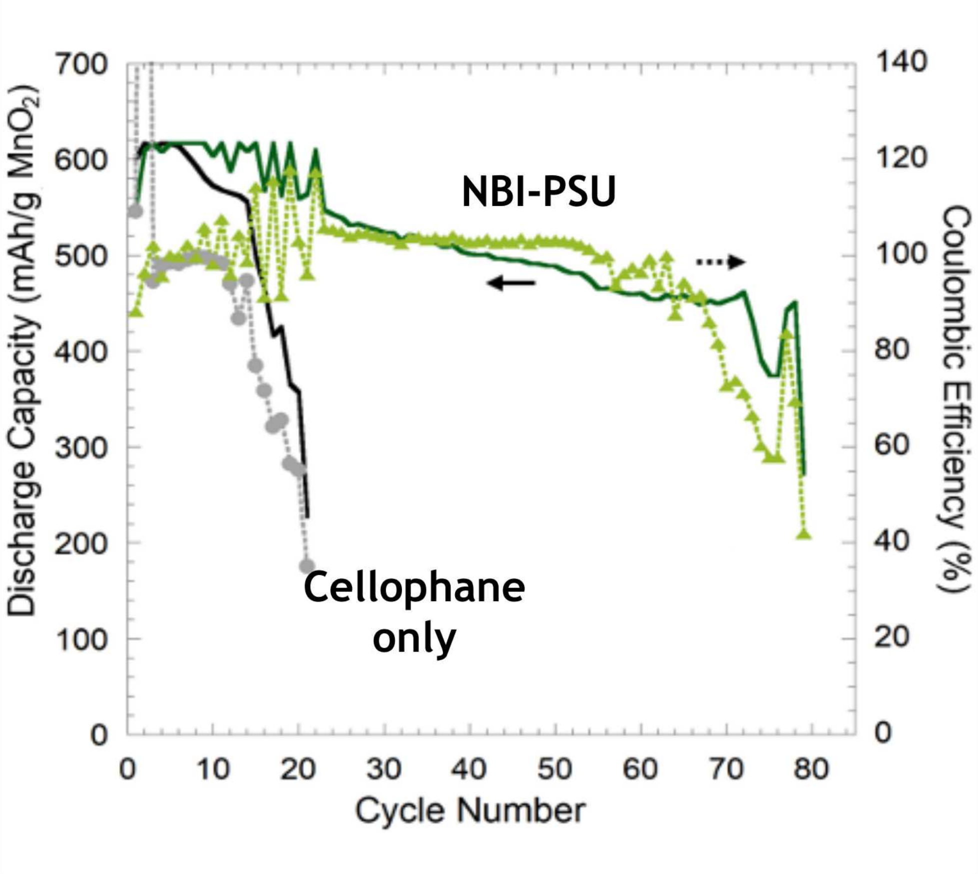
RESULTS

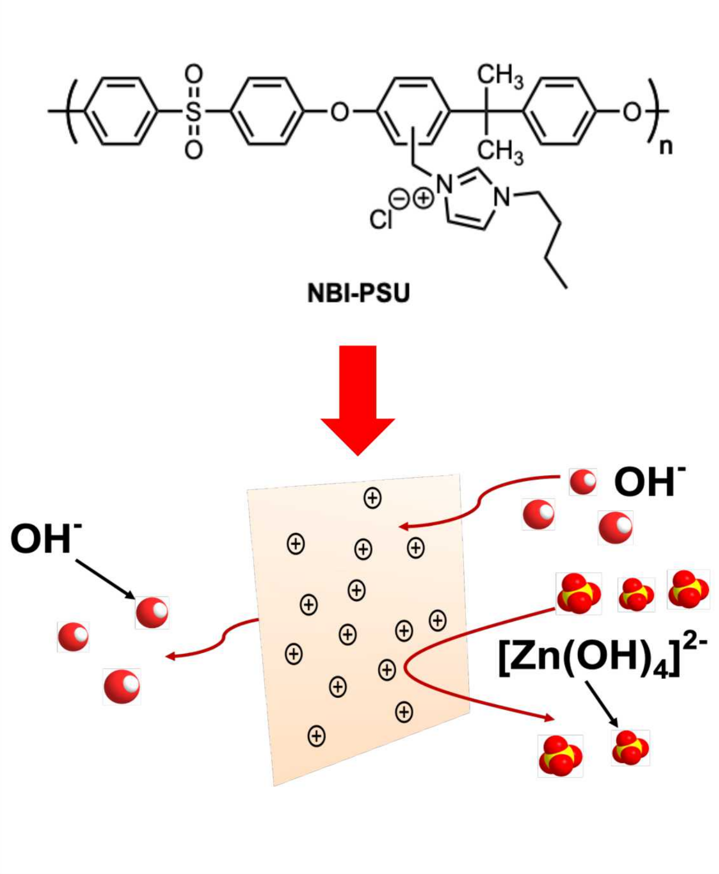
3 POSTERS: I. Kolesnichenko et al. , M. Lim et al., D. Arnot et al.

PROJECT RESULTS (for Objective 2)

In Situ - Hydroxide Selective Separator leads to 4-fold increase in Cycle Life

- Synthesized new PSU polymer
- Cast into Flexible Membrane
- More selective than COTS separators
- C/10 (2e- of MnO_2) cycling data under 'low electrolyte' conditions provides a 4-fold increase in cycle life





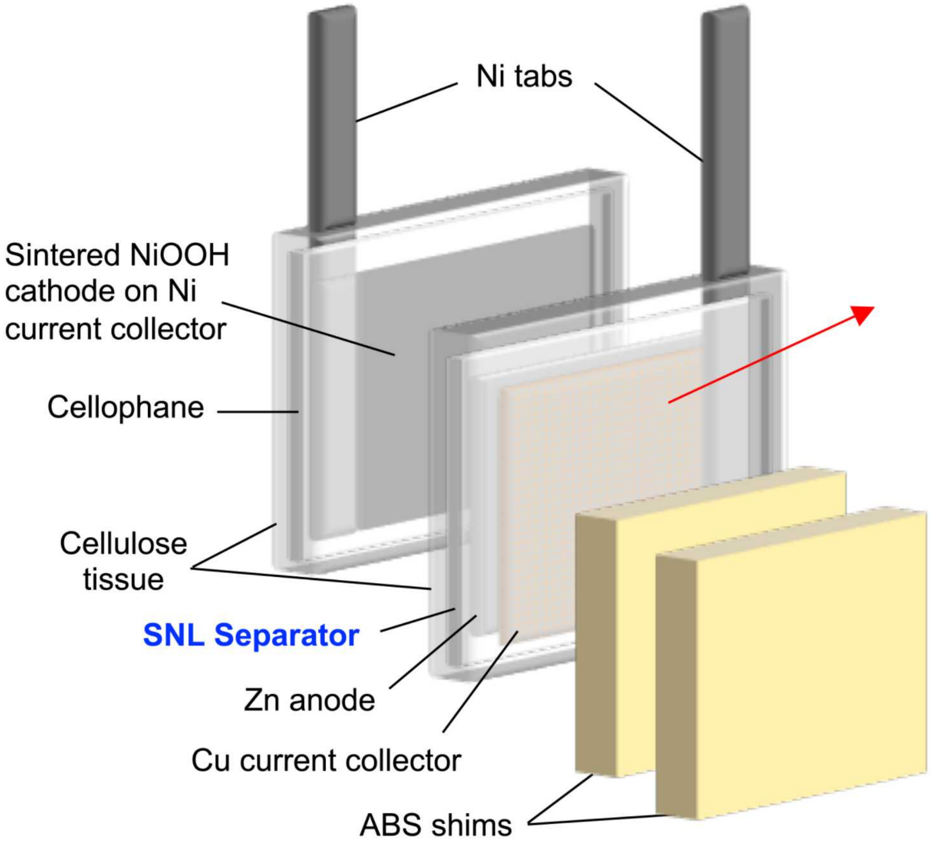
RESULTS (in collaboration with CCNY and UEP)

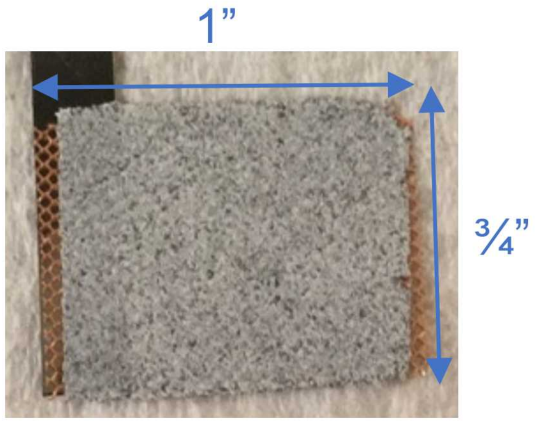
Manuscript: I. V. Kolesnichenko et al. "Zincate-Blocking Functionalized Polysulfone Separators for Secondary Zn/MnO_2 Batteries" *manuscript under review*.

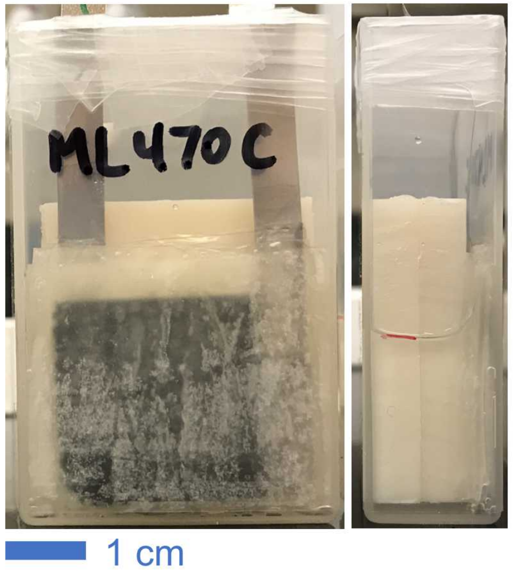
POSTER: I. Kolesnichenko *et al*. "Polysulfone-Based Zincate-Blocking Separators for Secondary Zn-MnO_2 Batteries"

PROJECT RESULTS (for Objective 1)

Utilization of flexible separator (Polymer 4) to enable increased Zn DOD







Scalable Zn/ZnO powder-based anode (very similar to UEP electrode)

Polymer Separator – minimal volume change or complexity to cell

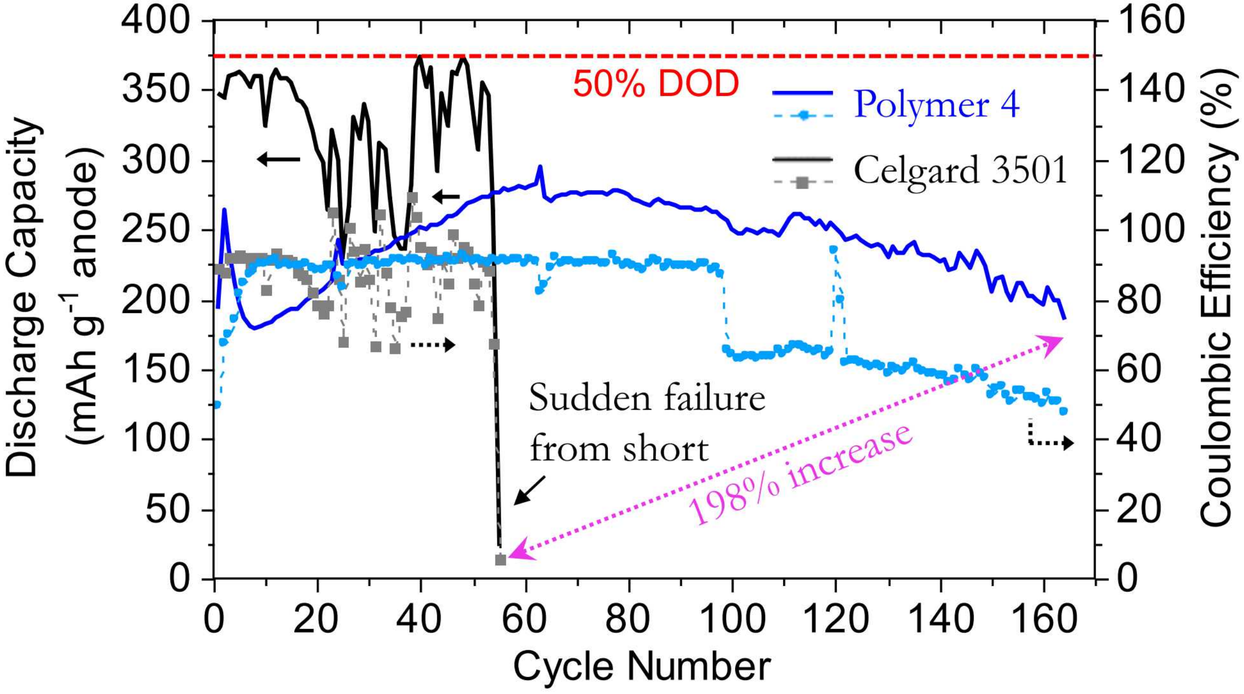
RESULTS

POSTER: M. Lim *et al.* “Flexible Ion-Selective Separators for Alkaline Zinc Batteries”
MANUSCRIPT: D. Arnot and M. Lim et al. *manuscript in preparation*.

PROJECT RESULTS (for Objective 1)

Flexible separator (Polymer 4) enables increased Zn DOD and cycle life

C/20 (3.0 mA/cm²), 50% Zn DOD limit



(rate based on total anode capacity)

Selective Separator prevents zincate crossover and impedes Zn growth enabling longer cell life

- Selective Separator enables > 150 cycles
- Achieves Average DOD of 32%
- 198% Increase in cycle life is obtained
- Achieves average Energy Density of 180 Wh L^{-1}

Increased cycle life of energy-dense Zn electrodes without adding significant volume, complexity (or cost?) to the system

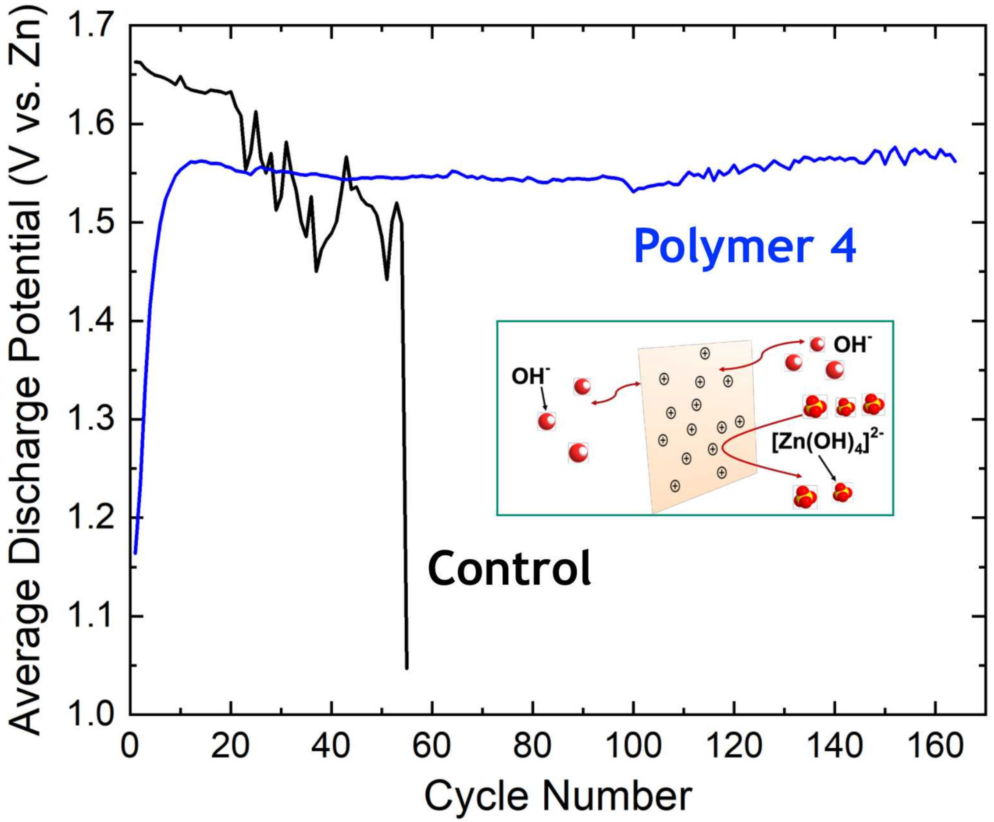
RESULTS

POSTER: M. Lim *et al.* "Flexible Ion-Selective Separators for Alkaline Zinc Batteries"
MANUSCRIPT: D. Arnot and M. Lim et al. *manuscript in preparation.*

PROJECT RESULTS (for Objective 1)

Flexible separator (Polymer 4) enables increased Zn DOD

Average Potential During Discharge at (nominally) 50% DOD



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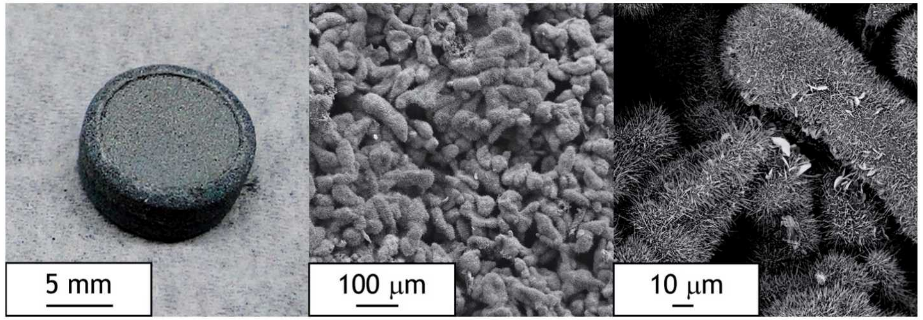
RESULTS

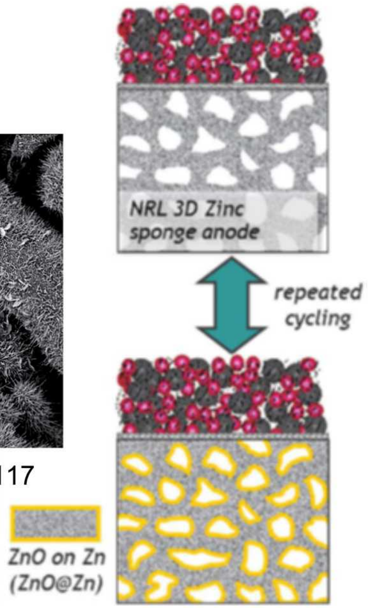
Manuscript: D. Arnot and Matthew Lim *et al*. manuscript in preparation

Poster: M. Lim et al. "Flexible Ion-Selective Separators for Alkaline Zinc Batteries"

COMPARISON TO OTHER HIGH DOD Zn ANODES

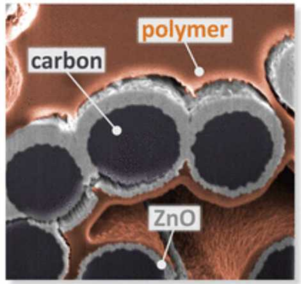
- Parker et al., Science 2017, 356 (6336), 415.
  - 3D Zn sponge
  - 111 cycles above 20% DOD (including 85 cycles at 40% DOD limit)
  - Anode capacity ~ 100 mAh/cm^2





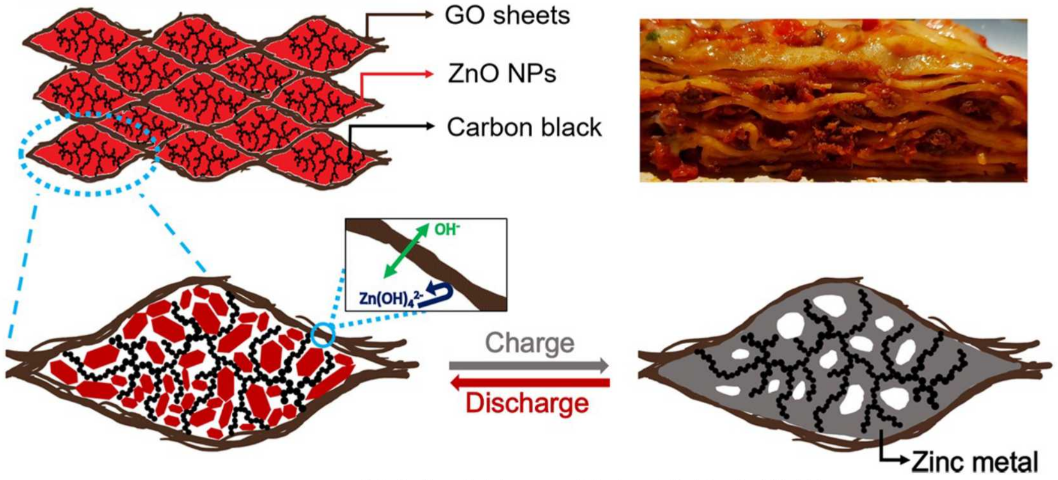
Energy Environ. Sci. 2014, 7, 1117
Science 2017, 356, 415

- Stock et al., ACS Applied Energy Materials 2018, 1 (10), 5579-5588.
  - C mesh/ZnO/anion-exchange ionomer core-shell structure
  - 67 cycles with 40.5% average DOD
  - Anode capacity ~ 5.7 mAh/cm^2



ACS Appl. Energy Mater. 2018, 1, 5579

- Yan et al., ACS Applied Energy Materials 2018, 1 (11), 6345-6351.
  - ZnO nanoparticles in "lasagna-like" GO matrix
  - 150 cycles with 82.2% average DOD
  - Anode capacity ~0.66 mAh/cm^2



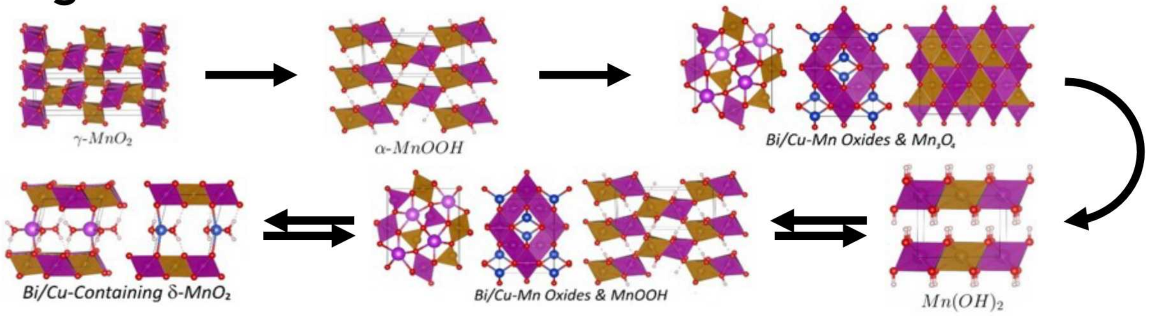
ACS Appl. Energy Mater. 2018, 1, 6345

- **Our work**
  - **Scalable Zn/ZnO powder-based anode w/flexible separator (i.e. similar to UEP Zn-electrode)**
  - **164 cycles above 25% DOD with 32.4% average DOD**
  - **Anode capacity ~ 60 mAh/cm^2**

PROJECT OBJECTIVES

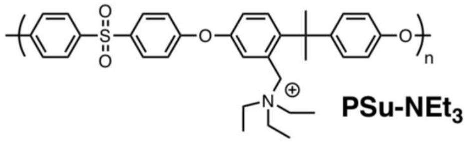
SNL FY Objective 3 – USE MODELING TO UNDERSTAND CATHODE MECHANISMS AND ION TRANSPORT

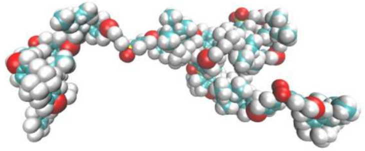
PROBLEM: Cathode cycling mechanism are not well understood

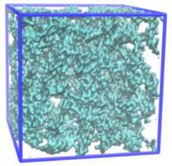


Prof. Igor Vasiliev

PROBLEM: Selective ion transport mechanisms are not well understood







Amalie Frischknecht

RESULTS

MANUSCRIPT: B. A. Magar et al. "Ab Initio Studies of Discharge Mechanism of MnO_2 in Deep-Cycled Rechargeable Zn/MnO_2 Batteries" J. Electrochem. Soc. 2020, 167, 020557. DOI:10.1149/1945-7111/ab6eec.

POSTER: B. Ale Magar et al. "Ab Initio Studies of the Cycling Mechanism of MnO_2 Cathodes Modified with Bi, Cu, and Mg in Rechargeable Zn/MnO_2 Batteries"

POSTER: N. Paudel et al. "Influence of Surfaces and Structural Defects on the Electrochemical Properties of MnO_2 in Rechargeable Zn/MnO_2 Batteries"

POSTER: A. Frischknecht et al. "Atomistic Simulations of Sulfone-based Polymer Electrolytes for Alkaline Batteries"

PROPOSAL: ** NEW CINT User Proposal (2020AU0134):*** T. N. Lambert, A. Frischnecht et al. Nanoscale Morphology and Ion Transport in Membrane Separators for Rechargeable Alkaline Batteries ***

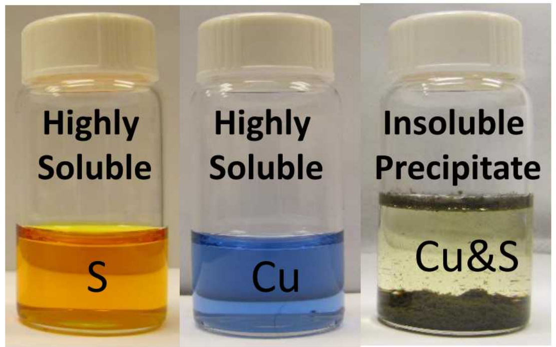
PROJECT Results (FY19)

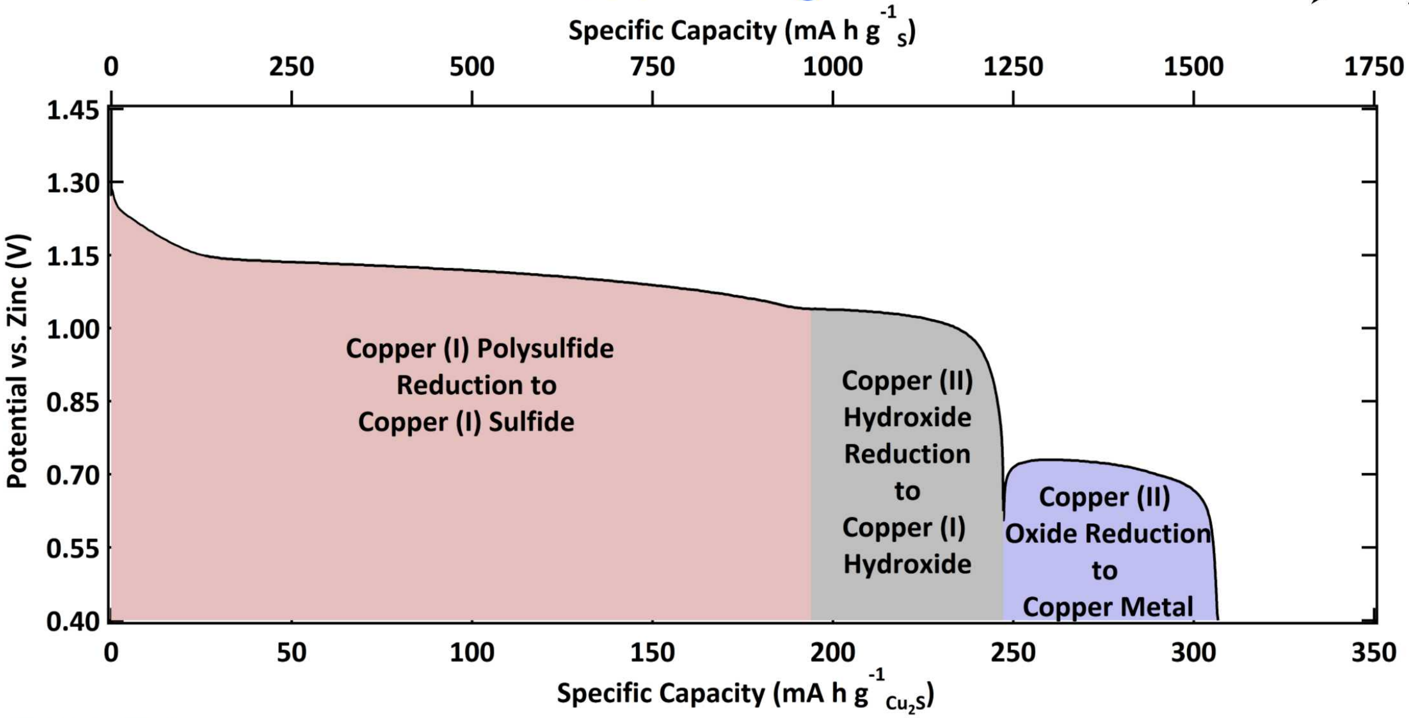
SNL FY Objective 4 – DEVELOPMENT OF NEW LOW COST HIGH CAPACITY BATTERY CHEMISTRIES

Zn/Cu_2S

Sulfur is known to have a high theoretical specific capacity:
1650 mA h g^{-1}

- ~1500 mAh g^{-1} (S)
- ~300 mAh g^{-1} (Cu_2S)
- ~ 23 mAh cm^{-2}
- >135 Wh L^{-1}
- ~ 250 cycles





Electrode transitions from Sulfur electrochemistry to Copper Electrochemistry

Copper electrochemistry is not sufficiently stable to cycle well

Leads to failure

RESULTS

Manuscript: J. Duay et al. *J. Electrochem. Soc.* **2019** *166 (4)*, A687-A694. DOI:10.1149/2.0261904jes.

PROJECT RESULTS (FY 20)

SNL FY Objective 4 - DEVELOPMENT OF NEW LOW COST HIGH CAPACITY BATTERY CHEMISTRIES

Anode: $Zn^0 + 4OH^- \rightarrow [Zn(OH_4)]^{2-} + 2e^-$ $E^o = 1.285$ V

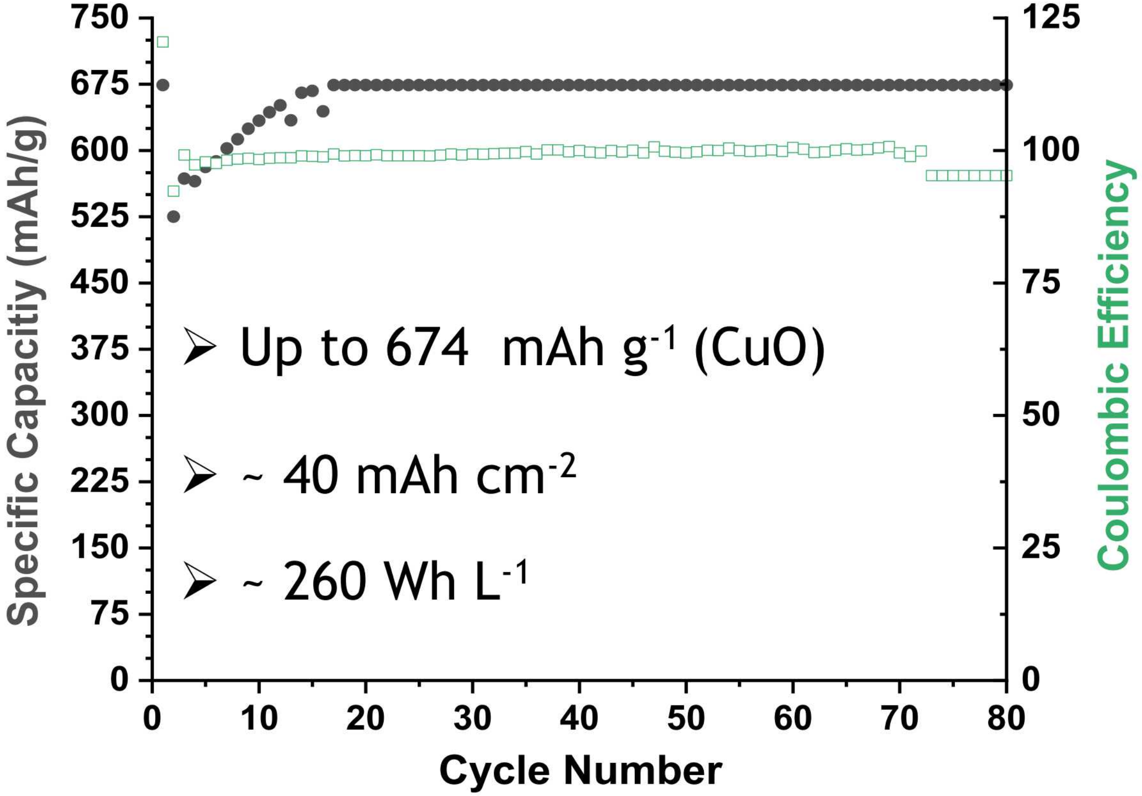
Cathode: $CuO + H_2O + 2e^- \rightarrow Cu^0 + 2OH^-$ $E^o = - 0.29$ V

$Zn^0 + CuO + H_2O + 2\ OH^- \rightarrow [Zn(OH_4)]^{2-} + Cu^0$ Cell Voltage: 0.995 V

Edison-LaLalande Battery.
PAT. Mar. 20, 1883.
OTHER PATENTS APPLIED FOR

Edison-Lalande Battery (Primary Cell)

FY 20: 1st rechargeable Alkaline Zn/CuO Battery



RESULTS

PATENT APPLICATION: T. N. Lambert and J. Duay

PUBLICATION: N. Schorr *et al*. manuscript submitted (In Collaboration with NEU).

PLAN: FUTURE WORK TO INCLUDE DEVELOPMENT WITH UEP

PROJECT RESULTS - Summary

FY 20 Accomplishments

1. **Demonstrated Increased Cycle life of Energy Dense Zn:**
   > 150 cycles at Average DOD_{Zn} 32% @ 180 Wh L^{-1} (198% lifetime increase over control)
   > 350 cycles at Average DOD_{Zn} = 17% @ 132 Wh L^{-1} (897% lifetime increase over control)

   Use of selective separator = No significant volume or complexity added to the system

2. **Demonstrated Increased Cycle life of Energy Dense Zn/(Cu/Bi-MnO_2) cells:**
   Synthesis of new cationic polysulfone-based separator and membranes
   (Partial) Zincate screening demonstrated
   Four-fold increase in cycle life under low electrolyte conditions

3. **Developed the first Zn/CuO re-chargeable battery**
   Energy density of ~ 260 Wh L^{-1}
   Among the highest Energy Density reported for Zn/Conversion cathode battery

(not shown in detail, see Poster, D. Arnot et al.)

4. **Developed Anodic Stripping Voltammetry for Bi in Highly Alkaline Electrolyte**
   Limit of DOD ~ 8.5 ppb
   Can now more efficiently screen separators for Zn, Cu and Bi crossover

PROJECT RESULTS

FY 20 Manuscripts (15 total = 8 published, 6 in peer review, 1 in preparation)

SNL led manuscripts

1. R. M. Wittman et al. "A materials perspective on the reliability and safety of grid-scale aqueous batteries" J. Electrochem. Soc. 2020, 167, 090545. https://iopscience.iop.org/article/10.1149/1945-7111/ab9406/meta
2. M. B. Lim et al "Rechargeable Alkaline Zinc–Manganese Oxide Batteries for Grid Storage: Mechanisms, Challenges and Developments" Mater. Sci. Eng. R Rep. 2020, manuscript submitted.
3. I. V. Kolesnichenko et al. "Zincate-Blocking Functionalized Polysulfone Separators for Secondary Zn/MnO_2 Batteries" manuscript submitted.
4. D. J. Arnot et al. "Bismuth Detection in Alkaline Electrolyte via Anodic Stripping Voltammetry for Battery Separator Evaluation" manuscript submitted.
5. M. B. Lim et al. "Rechargeable Zinc Batteries for Grid Storage" Book Chapter in U.S. Department of Energy (DOE) Energy Storage Handbook, 2020.
6. N. B. Schorr et al "Rechargeable Alkaline Zinc/Copper Oxide Batteries" manuscript submitted.
7. B. E. Hawkins et al. "Reversible Electrochemical Control of Conductivity, Color, and Native Defect Structure of ZnO" manuscript submitted.
8. M. D'Ambrose et al. "Failure Mechanisms of Rechargeable Zinc Conversion Electrodes in Alkaline Electrolyte" manuscript submitted.
9. D. E. Turney et al. Book Chapter: Aqueous Mn-Zn and Ni-Zn batteries for sustainable energy storage in eds. M. Alston, T. Lambert, Energy – Sustainable Advanced Materials, in Press, Springer Nature, London, 2020 https://www.springer.com/gp/book/9783030574918.

PROJECT RESULTS

FY 20 Manuscripts continued…

10. G. G. Yadav et al. “Going beyond Intercalation Capacity of Aqueous Batteries by Exploiting Conversion Reactions of Mn and Zn electrodes for Energy-Dense Applications” Adv. Energy Materials, 2019, https://onlinelibrary.wiley.com/doi/abs/10.1002/aenm.201902270
11. G. G. Yadav et al. “Rechargeable Manganese Dioxide-Zinc Batteries” Chemical & Engineering News, 98 (19), 41-47, 2020.
12. G. G. Yadav et al. “The Advent of Membrane-less High Voltage Zinc Anode Batteries” manuscript in preparation.
13. A. M. Bruck "Bismuth Enables the Formation of Disordered Birnessite in Rechargeable Alkaline Batteries." Journal of the Electrochemical Society, 2020, 167, 110514. DOI:10.1149/1945-7111/aba075. https://iopscience.iop.org/article/10.1149/1945-7111/aba075/meta
14. A. C. Marschilok et al. "Energy dispersive X-ray diffraction (EDXRD) for operando materials characterization within batteries" Physical Chemistry Chemical Physics, 2020. DOI:10.1039/D0CP00778A. https://pubs.rsc.org/en/content/articlehtml/2020/cp/d0cp00778a?casa_token=LWjji-kV7QAAAAAA:y9TvijTJ94WIAYIil33yQFCkatRhOavhhE1C0kIeOYxy5VbF7r7dGwNMGt3U0sjCDFJGEVYu93vC
15. B. A. Magar et al. “Ab Initio Studies of Discharge Mechanism of MnO_2 in Deep-Cycled Rechargeable Zn/MnO_2 Batteries” Journal of the Electrochemical Society, February 5, 2020, Vol. 167, Issue 2, 020557, doi: 10.1149/1945-7111/ab6eec. https://iopscience.iop.org/article/10.1149/1945-7111/ab6eec

PROJECT RESULTS

FY 20 Presentations (37 Presentations)

1. M. B. Lim, I, Kolesnichenko, D. Arnot and T. N. Lambert “Effect of ZnO-Saturated electrolyte on Rechargeable Alkaline Zinc Batteries at High Depth-of-Discharge” 2019 Postdoc Research Symposium and Career Fair, Los Alamos, NM, August 27th, 2019.
2. Invited Talk: T. N. Lambert “Recent Progress in Alkaline Zn/MnO_2 Batteries” NAATBatt International Workshop on Zinc Battery Technology II, the Advanced Science Research Center at CUNY, New York, New York, November 7, 2019.
3. D. J. Arnot et al. “Permselective Separators for Rechargeable Alkaline Zn/MnO_2 Batteries” 2019 Annual AIChE Student Conference Poster Competition, Orlando, Florida, November 8-11, 2019.
4. B. Hawkins et al. “The Electrochemical Activity of Zinc Oxide Discharge Product in Zinc Alkaline Electrodes” 2019 AIChE Battery and Energy Storage Workshop, New York, New York, October 21-22nd, 2019.
5. J. Cho et al. “The Study on the Factors Affecting the Single Discharge Curve of the Zn/MnO_2 Primary Battery and Their Effects on the Energy Density Performance” 2019 AIChE Battery and Energy Storage Workshop, New York, New York, October 21-22nd, 2019.
6. M. B. Lim et al. “Effect of ZnO-Saturated Electrolyte on Rechargeable Alkaline Zn–Ni and Zn–MnO_2 Batteries at High Zinc Depth-of-Discharge” 236th Electrochemical Society Meeting, Atlanta, Georgia, October 13-17, 2019.
7. M. D'Ambrose et al. “Zinc Anode Discharge Study in Alkaline Electrolyte for Rechargeable Battery Applications, 2019 AIChE Annual Meeting, https://aiche.confex.com/aiche/2019/meetingapp.cgi/Paper/575378
8. G.G. Yadav “Highly Energy-Dense, Rechargeable, Alkaline Birnessite-Zinc Batteries for Grid-Scale Applications” ECS Conference, November 2019, https://iopscience.iop.org/article/10.1149/MA2019-02/1/47/meta

FY 20 Presentations continued…

9. BE Hawkins et al. "Investigating the Dynamic Behavior of Zinc Oxide Discharge Product in Rechargeable Zinc Electrodes" 236th ECS Meeting (October 13-17, 2019), https://iopscience.iop.org/article/10.1149/MA2019-02/6/457/meta
10. J Gallaway et al. "On the fly EIS tracking of rechargeable alkaline Zn-MnO^2 batteries for large-scale use" ECSarXiv. May 13, https://iopscience.iop.org/article/10.1149/MA2017-02/2/167/meta
11. D.E. Turney et al. "Elucidating Battery Reaction Mechanisms in Aqueous Rechargeable Mn-Zn Cells By Advanced Computational and Experimental Approaches" AIChE Annual Conference Talk, San Francisco, November 2020, accepted, proceedings not public yet, https://www.aiche.org/conferences/aiche-annual-meeting/2020
12. B. E. Hawkins et al. "A Mechanistic Study of Proton Insertion and Defects in Electrochromic Zinc Oxide Formed in Alkaline Electrolytes by Solid-State NMR Spectroscopy" 61st Experimental Nuclear Magnetic Resonance Conference (ENC), 8-13 Mar. 2020, Baltimore, MD., https://www.enc-conference.org/DesktopModules/inmAbstractAdmin/inmAbstractAdminDisplay.aspx?Conference=ENC2020&Session=PB
13. B. E. Hawkins et al. "The Electrochemical Activity of Zinc Oxide Discharge Product in Zinc Alkaline Electrodes" American Institute of Chemical Engineers (AIChE) 2019 Battery and Energy Storage Workshop, 21-22 Oct. 2019, New York, NY., https://www.aiche.org/cei/conferences/battery-and-energy-storage/2019/technical-program
14. B. E. Hawkins et al. "The Dynamic Behavior of the Discharge Product in Zinc-Alkaline Batteries" 2019 MRS Fall Meeting, 1-6 December 2019, Boston, MA. https://mrsfall2019.zerista.com/event/member/612488
15. M. D'Ambrose "Zinc anode discharge study in alkaline electrolyte for rechargeable battery applications" American Institute of Chemical Engineers (AIChE) Battery and Energy Storage Workshop, 21 October 2019, New York, NY. [Poster], https://www.aiche.org/conferences/aiche-annual-meeting/2019/proceeding/paper/696d-zinc-anode-discharge-study-alkaline-electrolyte-rechargeable-battery-applications

FY 20 Presentations continued…

16. J. Cho et al. “The Study on the Factors Affecting the Single Discharge Curve of the Zn/MnO_2 Primary Battery and Their Effects on the Energy Density Performance," 2019 Battery & Energy Storage Workshop, 21-22 October 2019, New York, NY.
17. J. Cho, "Electrochemical Evaluation of the Application of Hydrogel Electrolytes to Rechargeable Zn|MnO_2 Alkaline Batteries" American Institute of Chemical Engineers (AIChE) Annual Meeting, 15-20 Nov. 2020, San Francisco, CA.
18. G. Yadav, “Highly Energy Dense Cu-Intercalated Birnessite/Zn Battery for Grid Applications” 2019 AIChE Annual Meeting.
19. G. Yadav “Going Beyond Intercalation Capacity of Aqueous Batteries By Exploiting the Conversion Reactions of Mn and Zn-Based Electrodes for Energy Dense Applications” 2019 AIChE Annual Meeting.
20. G. Yadav “Going Beyond Intercalation Capacity of Aqueous Batteries By Exploiting the Conversion Reactions of Mn and Zn-Based Electrodes for Energy Dense Applications” ECS Conference, November 2019.
21. Invited Talk: G. G. Yadav, Engineering an Aqueous Energy Dense Manganese Dioxide|Zinc Battery to Challenge Lithium-Ion’s Dominance, Invited Talk at the American Institute of Chemical Engineers (AIChE) Battery and Energy Storage Workshop, 21 October 2019, New York, NY.
22. Invited Talk: G. G. Yadav, Engineering an Aqueous Energy Dense Manganese Dioxide|Zinc Battery to Challenge Lithium-Ion’s Dominance, Invited Talk at NAATBATT Zinc Workshop, November 2019, New York, NY.
23. Invited Talk: G. G. Yadav “High Voltage Zinc|Manganese Dioxide Batteries for Electric Vehicles” Invited Talk at NAATBATT Zinc Workshop, February 2020, New York, NY.
24. Invited Talk: J. W. Gallaway et al. "Operando Characterization of Rechargeable Alkaline MnO_2 Batteries" AIChE Center for Energy Initiatives, 2019 Battery and Energy Storage Workshop, New York NY, 22 October 2019

PROJECT RESULTS

FY 20 Presentations continued…

25. J. W. Gallaway, "Operando Studies to Enumerate the Electrochemical Phase Transformations of MnO_2" 1E - Electrochemical Fundamentals, American Institute of Chemical Engineers Fall Meeting, Orlando FL, November 2019.
26. M. Kim “Operando Energy Dispersive X-Ray Diffraction (EDXRD) of Bulk Cathode Material for Multivalent Secondary Batteries” The Electrochemical Society 236th Meeting, Atlanta GA, Oct 2019.
27. E. Takeuchi, “From Medical Applications to the Environment: the Important Role of Electrochemical Energy Storage,” Cary lecture, Georgia Institute of Technology, March 4-5, 2020, Atlanta, GA.
28. E. Takeuchi “Parasitic Reactions and their Impact on Electrochemistry” Gordon Research Conference on Batteries February 16-20, 2020, Ventura, CA.
29. E. Takeuchi “From Medical Applications to the Environment: The Important Role of Electrochemical Energy Storage” Tufts University, October, 7, 2020.
30. A. C. Marschilok “Benefits of Complementary Ex-situ, In-situ and Operando Characterization of Electrochemical Energy Storage Systems” 2019 Battery and Energy Storage Workshop, Center for Energy Initiatives and American Institute of Chemical Engineers, New York, New York, October 21, 2019.
31. A. C. Marschilok “Fundamental Investigations Toward Safe Electrochemical Energy Storage Systems” LIB Consumer Safety: Strategies & Standards Meeting, Battery Safety Summit, Alexandria, Virginia, October 23, 2019.
32. A. C. Marschilok. “Energy Storage and Distribution” 2019 National Lab Day, The University of Toledo, Toledo, Ohio, October 11, 2019.
33. N. Paudel et al. “Theoretical Studies of Zinc Contamination of ¤-MnO2 in Deep-Cycled Rechargeable Zn/MnO_2 Batteries” Four Corners Section Meeting of the American Physical Society, Prescott, AZ, October 11-12, 2019. http://meetings.aps.org/Meeting/4CS19/Session/E02.6

FY 20 Presentations continued…

34. B. A. Magar et al. "Bi- and Cu-Modified-MnO2 Electrodes in Rechargeable Zn/MnO2 Batteries: An Ab Initio Study" Four Corners Section Meeting of the American Physical Society, Prescott, AZ, October 11-12, 2019. http://meetings.aps.org/Meeting/4CS19/Session/F01.24
35. N. Paudel et al. "Influence of Structural Defects on the Electrochemical Properties of MnO2 in Rechargeable Zn/MnO2 Alkaline Batteries: An Ab Initio Study", March Meeting of the American Physical Society, Denver, CO, March 2-6, 2020. https://meetings.aps.org/Meeting/MAR20/Session/A21.10
36. B. A. Magar et al. "Ab Initio Study of the Discharge Mechanism of Bi- and Cu- Modified MnO_2/Zn Rechargeable Batteries" March Meeting of the American Physical Society, Denver, CO, March 2-6, 2020. https://meetings.aps.org/Meeting/MAR20/Session/B21.13.
37. Invited Seminar: I. Vasiliev, "Discharge Mechanism of MnO_2 in Rechargeable Alkaline Zn/MnO_2 Batteries" Apple Inc., San Jose, CA, December 16, 2019.

Proposals:

1. NEW CINT User Proposal (2020AU0134): T. N. Lambert, A. Frischnecht et al. Nanoscale Morphology and Ion Transport in Membrane Separators for Rechargeable Alkaline Batteries.

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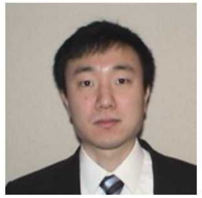

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ACKNOWLEDGEMENTS

Imre Gyuk

THIS WORK WAS SUPPORTED THROUGH THE ENERGY STORAGE PROGRAM, MANAGED BY DR. IMRE GYUK, WITHIN THE U.S.DEPARTMENT OF ENERGY'S OFFICE OF ELECTRICITY

&

OUR MANY COLLABORATORS!

This work was supported by the U.S. Department of Energy, Office of Electricity, and the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia National Laboratories is a multi-program laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. Dr. Imre Gyuk, Director of Energy Storage Research, Office of Electricity is thanked for his financial support. The views expressed herein do not necessarily represent the views of the U.S. Department of Energy or the United States Government.