SAND2020-12979PE

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GRID ENERGY STORAGE R&D AT SANDIA

BATTERY MATERIALS

Large portfolio of R&D projects related to advanced materials, new battery chemistries, electrolyte materials, and membranes.

DEMONSTRATION PROJECTS

Work with industry to develop, install, commission, and operate electrical energy storage systems.

CELL & MODULE LEVEL SAFETY

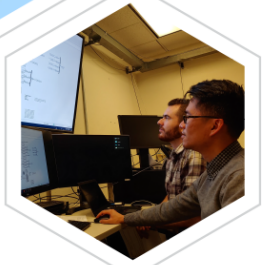
Evaluate safety and performance of electrical energy storage systems down to the module and cell level.

STRATEGIC OUTREACH

Maintain the ESS website and DOE Global Energy Storage Database, organize the annual Peer Review meeting, and host webinars and conferences.

POWER CONVERSION SYSTEMS

Research and development regarding reliability and performance of power electronics and power conversion systems.



GRID ANALYTICS

Analytical tools model electric grids and microgrids, perform system optimization, plan efficient utilization and optimization of DER on the grid, and understand ROI of energy storage.

SYSTEMS ANALYSIS

Test laboratories evaluate and optimize performance of megawatt-hour class energy storage systems in grid-tied applications.

Wide ranging R&D covering energy storage technologies with applications in the grid, transportation, and stationary storage

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A COMMITMENT TO SNL STORAGE ENGAGEMENT

Sandia believes in partnership with industry, utilities, government agencies, and academic partners.

A strong relationship between SNL and UT has led to a robust hiring pipeline at SNL:

OE Program Hires:

Tim Lambert (U.G.)
Stephen Percival (PD, now staff)
Martha Gross (PD)
Bryan Wygant (PD)
Melissa Meyerson (PD)
Igor Kolesnichenko (PD)
Claudina Cammack (PD)

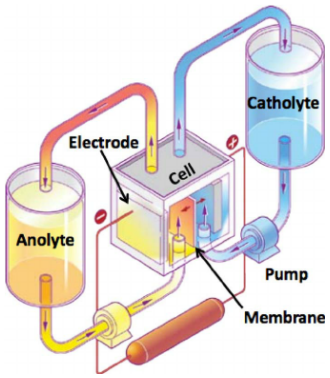
Additional SNL Energy Storage Hires:

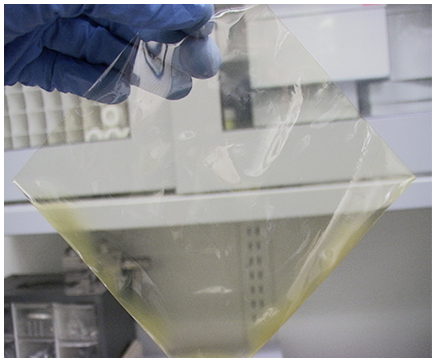
Katie Harrison
Eric Allcorn
Kyle Klavetter

Battery Research Workshop: SNL Membranes, Fujimoto

Problem Statement: Electrochemical cells requires membranes which separate electroactive species while providing ion conduction. In low temperature cells, this membrane is either a porous separator (no selectivity) or high cost Nafion type material.

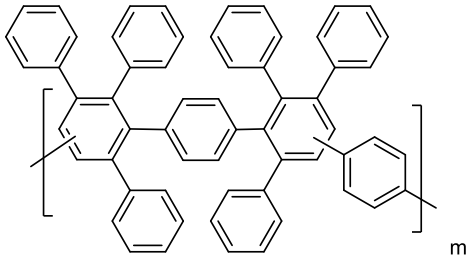
Objective: At SNL, developing hydrocarbon membranes for flow batteries to lower cost and improve performance which will facilitate commercialization.





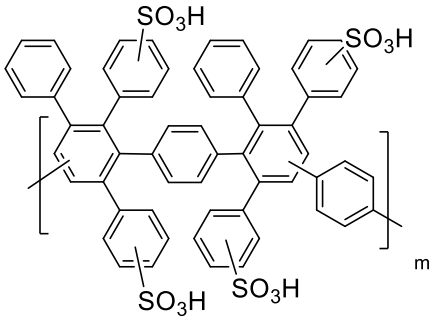
- 19 years have developed and patented ion conducting membranes based on stable Diels Alder poly(phenylene) [DAPP] backbone.
- 10 patents based on DAPP cation and anion exchange membrane.
- Membranes being explored for fuel cells, electrolysers and flow batteries with partners such as LANL, PNNL, ORNL and industry.

Battery Research Workshop: SNL Membranes



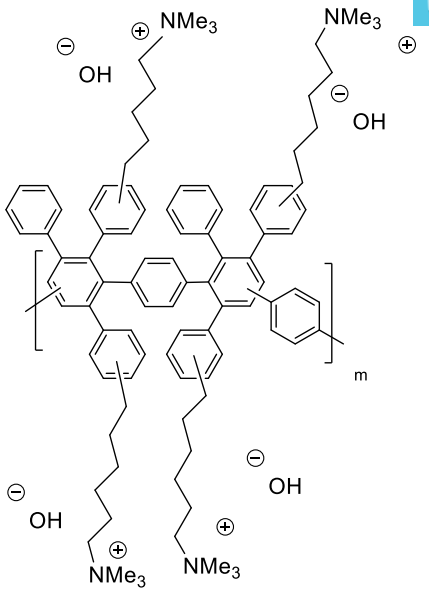
Diels Alder Poly(phenylene)
DAPP

Functionalize



Cation exchange Membrane

OR



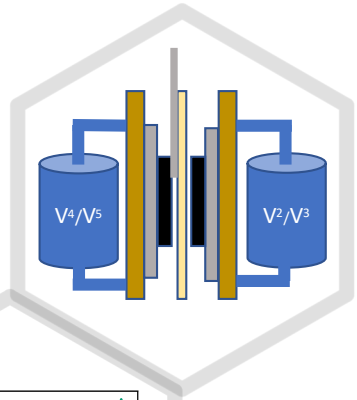
Anion exchange Membrane

Relevant Publications:

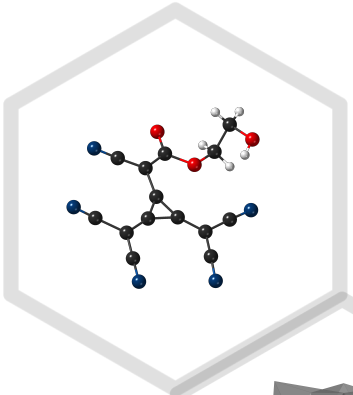
- Ionomeric Poly(phenylene) Prepared by Diels-Alder Polymerization. Fujimoto, C.; Hickner, M.; Cornelius, C.; Loy, D. Macromolecules (2005), 38(12), 5010-5016.
- Vanadium redox flow battery efficiency and durability studies of sulfonated Diels Alder poly(phenylene)s. Fujimoto, C.; Kim, S.; Stains, R.; Wei, X. Li, L.; Yang, G. Electrochemistry Communications (2012), 20, 48-51.
- Evaluation of Diels-Alder poly(phenylene) anion exchange membranes in all-vanadium redox flow batteries. Sun, C.; Tang, Z.; Belcher, C.; Zawodzinski, T.; Fujimoto, C. Electrochemistry Communications (2014), 43, 63-66.
- Alkaline stability of poly(phenylene)-based anion exchange membranes with various cations. Hibbs, M. Journal of Polymer Science, Part B: Polymer Physics (2013), 51(24), 1736-1742.

FLOW BATTERY MATERIALS R&D AT SANDIA

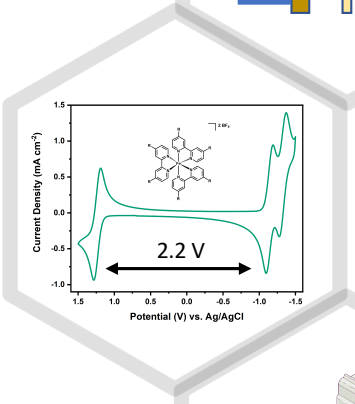
Travis Anderson



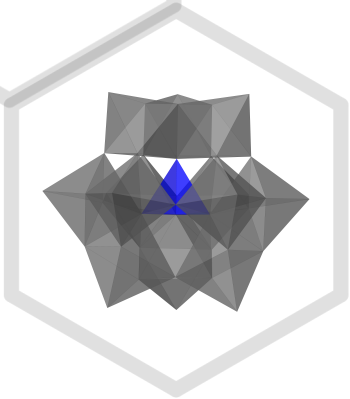
Membrane and Safety Testing for Aqueous Vanadium Flow Batteries



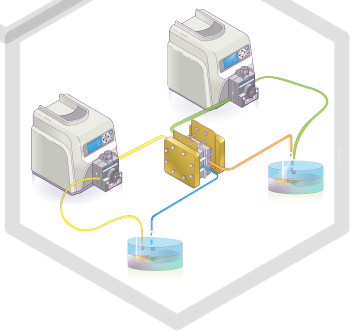
New Aqueous Organic Radialenes (collaboration with UNC-Charlotte)



New Metal Coordination Complexes (MCCs) for Higher Voltages



New Cluster Compounds (collaboration with U Rochester)



Prototyping Capabilities for Aqueous, Non-aqueous, and Hybrid Flow System Architectures

Sandia has a wide range of flow battery R&D capabilities including new energy storage materials validation and prototyping.

Alkaline Zn-based batteries

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

Sandia National Laboratories

Timothy Lambert

Babu Chalamala

Amalie Frischknecht

CUNY The City University of New York Energy Institute

Prof. Sanjoy Banerjee

Prof. Joshua Gallaway

NM STATE UNIVERSITY

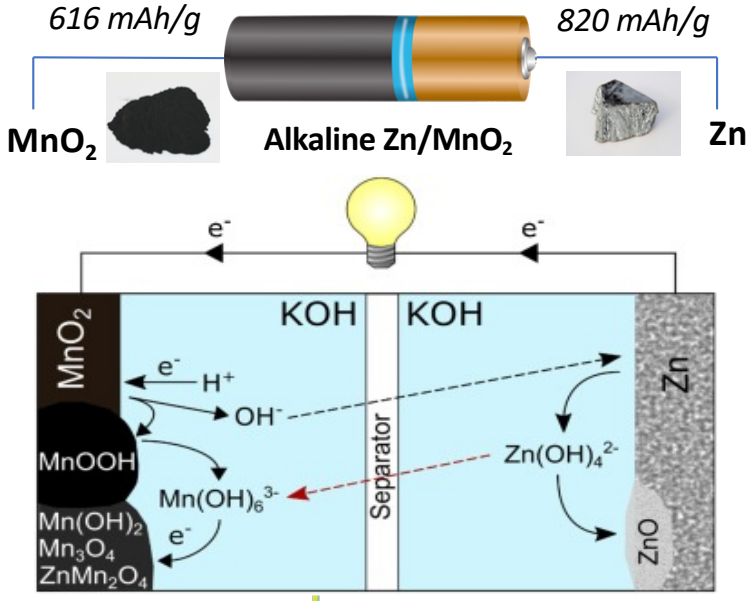
Prof. Igor Vasiliev

U.S. DEPARTMENT OF ENERGY

Imre Gyuk

Stony Brook University

Prof. Esther Takeuchi



Lawrence Livermore National Laboratory

Cheng Zhu

URBAN ELECTRIC POWER

Gautam Yadav

Gabe Cowles

< $20/kWh @large scale manufacturing

Review: M. B. Lim et al. "Rechargeable Alkaline Zinc–Manganese Oxide Batteries for Grid Storage: Mechanisms, Challenges and Developments" *Mater. Sci. Eng. R Rep.* **2020**. *https://doi.org/10.1016/j.mser.2020.100593*

Alkaline Zn-based batteries – SNL Efforts (TN Lambert)

Synthesis, Materials Processing, Electrochemistry and Battery Development:

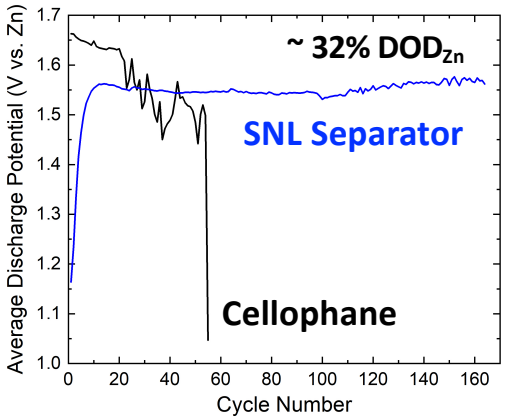
Small molecules, polymers, composites, electrospinning, electrocatalysis, electroanalysis, battery fabrication and testing

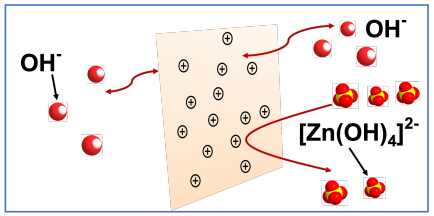
- Ion selective separators ($D_{Zn(OH)_4^{2-}} <<< D_{HO^-}$)
  (ASV of $Zn(OH)_4^{2-}$, $Bi(OH)_3^-$ and $Cu(OH)_4^{2-}$)
- Gelled polymer electrolytes
- Zn anodes – high capacity and cycle life
- New high capacity cathodes (Zn/Cu_2S and Zn/CuO)

<u>UT Austin Interactions</u>: B.S. Chemistry 1995, R. Ruoff (Graphene/Goodyear Rubber & Tire), SNL UT Austin Recruiting Team, MRSEC Industrial Mentor (T. FitzSimons, G. Partipilo)

<u>Hiring of Postdocs</u>:
OE: J. Duay, I. Kolesnichenko, B. Wygant, M. Meyerson (SNL-NM)
Other: A. Lapp, J. Trindell (SNL-CA)

High capacity High Cycle Life Zn



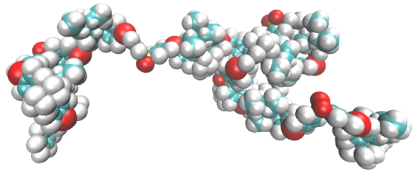


Molecular Simulations of Polymer Membranes

Amalie Frischknecht

Molecular dynamics simulations can reveal details of:

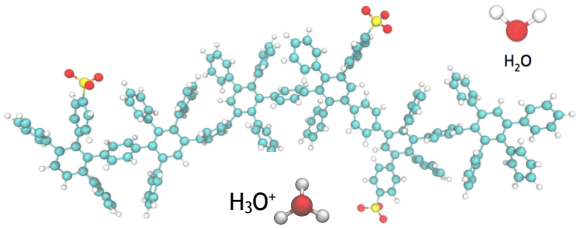
- nanoscale morphology of hydrophilic domains
- diffusion of ions
- partitioning of ions in membrane



Features:

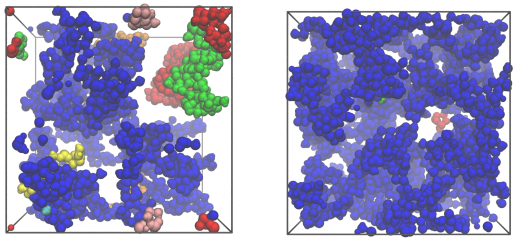
- fully atomistic simulations
- can compare to scattering, NMR, impedance spectroscopy
- procedures for annealing glassy polymers

SDAPP simulations



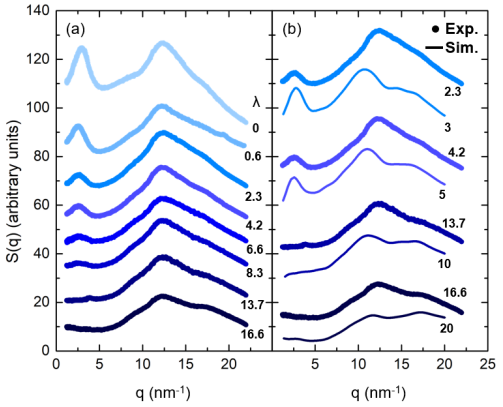
SDAPP research included collaboration with Prof. Nate Lynd, UT Austin

percolating water domains with increasing water content



increasing water

x-ray MD and x-ray



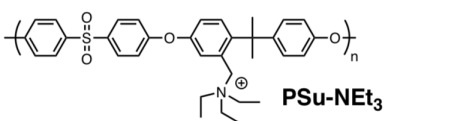
good agreement

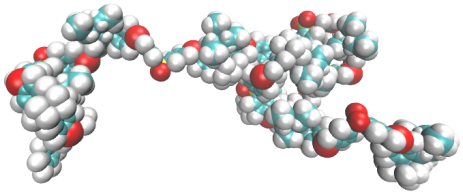
E. G. Sorte, B. A. Paren, C. G. Rodriquez, C. Fujimoto, C.Poirier, L. J. Abbott, N. A. Lynd, K. I. Winey, A. L. Frischknecht, and T. M. Alam, *Macromolecules* **52**, 857 (2019)

Current MD simulations

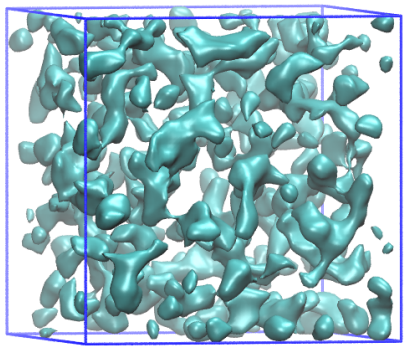
Polysulfone-based membranes for alkaline batteries
collaboration with Tim Lambert (Sandia)

- investigate molecular mechanisms of OH^- transport
- investigate exclusion of zincate ions
- roles of functional groups, water content, polymer blending

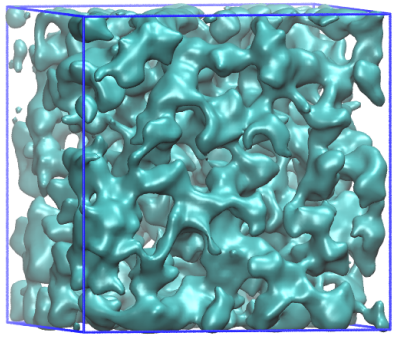




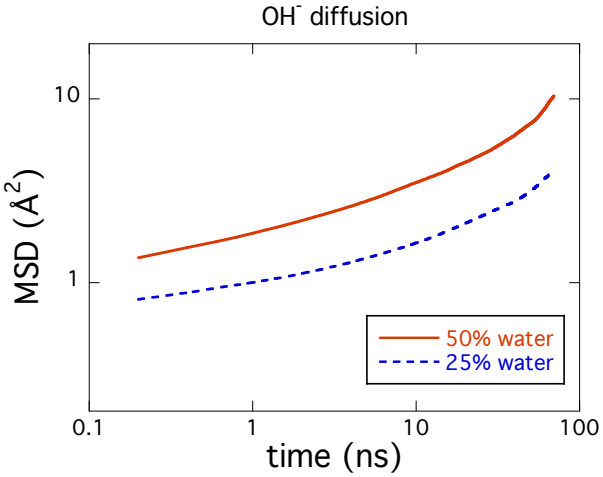
25% water
isolated water clusters



50% water
percolated water channels



snapshots show isodensity surfaces of water and hydroxide ions



- at 50% water: $D_{OH^-} \approx 1.6*10^{-9}$ cm^2/s
- smaller than in commercial membranes with larger pores

Low Temperature Molten Sodium Batteries

PI: Leo Small (ljsmall@sandia.gov)

Goal:

Develop enabling technologies for safe, low cost, molten sodium batteries. Principally, through development of materials that enable a reduction in operating temperature from 300 °C to near 100 °C.

Interests:

- Coatings on NaSICON separator to enable low resistance sodium-NaSICON interfaces at low temperatures
- Zero-crossover Na^+-selective separators
  - NaSICON (Na^+ Super Ion CONductor, $Na_3Zr_2Si_2PO_{12}$)
  - Scalable architectures that enable mechanically robust, very low resistance separators (collaboration with Prof. Cheng at UKy)
  - Chemical stability of separator materials
- Fully inorganic, redox-active molten salts
  - Flammability, safety during battery failure
  - Electrochemical and materials characterization of these molten salt-electrode interfaces