Studying-Polymers-On a-Chip (SPOC): Increased Alkaline Stability in Anion Exchange Membranes

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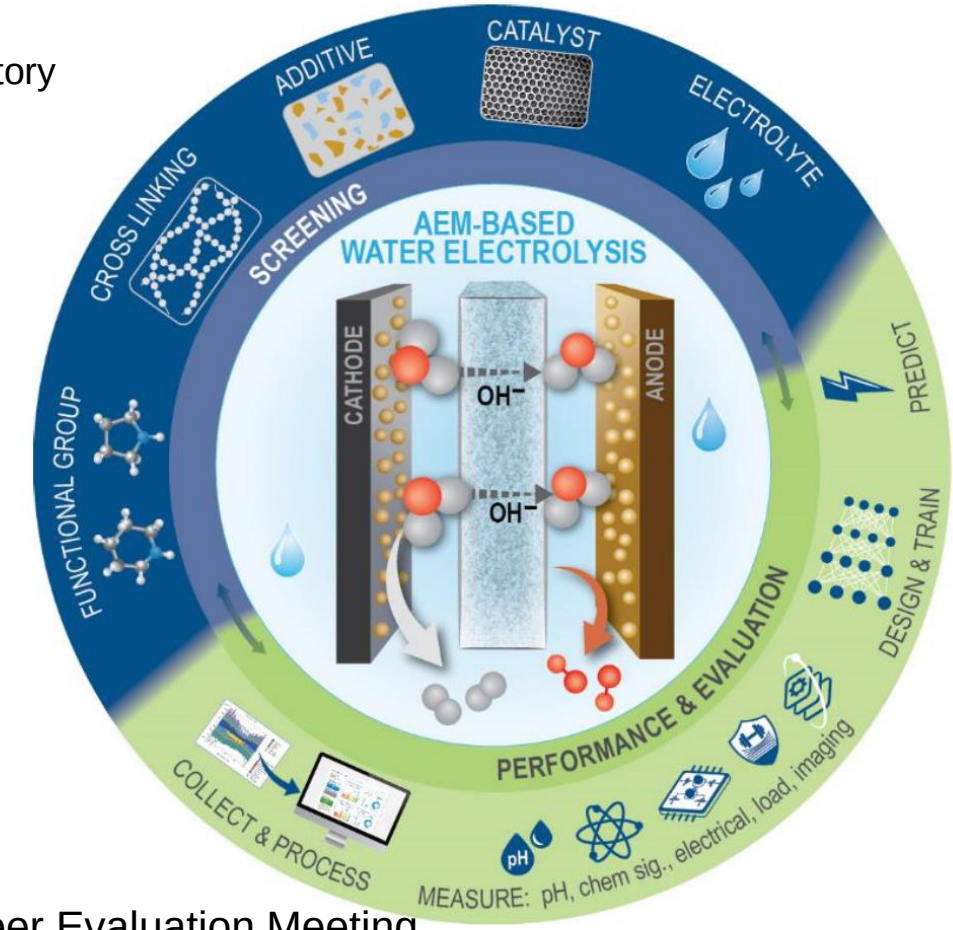

DOE Hydrogen Program

2024 Annual Merit Review and Peer Evaluation Meeting

AMR Project ID # **ELY-BIL005**

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LLNL-PRES-861356

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Project Goals

We will use an automated high-throughput Studying-Polymer-On a-Chip (SPOC) screening and aging platform and accelerate Anion Exchange Membrane (AEM) advancement by systematically modifying polymer compositions and comparing compositional effects on performance and lifetime. We will prioritize improving alkaline stability in AEMs.

We will do so by coupling 1) High-throughput screening and aging, 2) Integrated in- operando characterization, and 3) active learning-feedback models and high-performance computing (HPC) simulations to **vastly accelerate the identification of AEM formulations with co-optimized performance and lifetimes for further study toward scale-up.**

Overview

Timeline and Budget

- Project Start Date: 01/02/2024
- Funds Received: 02/25/2024
- FY24 DOE Funding: $867k
- FY25 Planned DOE Funding : $1,067k
- Total DOE Funds Received to Date: $867k

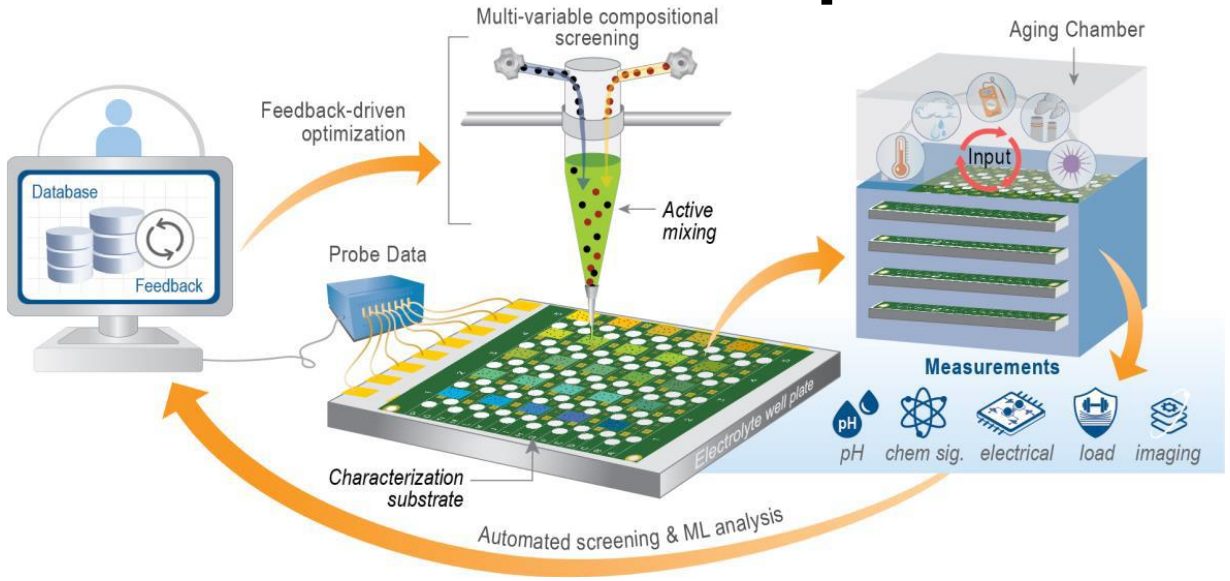
Partners

- **Project lead:** Dr. Johanna J. Schwartz, Lawrence Livermore National Laboratory
- **Partner organization and role:** University of Utah, subcontract, computational simulations
- **Potential collaborators (as part of H2LinkSc):** CENT, CIWE, and CABES

Barriers

- **Need:** AEMs with improved alkaline stability and lifetime
  - **Barrier:** Current material optimization approaches slow, time-consuming and needs excessive amounts of materials
    - **Target:** Accelerate optimization via coupled high throughput screening and in-operando analysis
  - **Barrier:** A wide range of compositional and processing variables to choose from
    - **Target**: Utilize multiscale simulations to predict and integrate with experiment and further accelerate advancement
  - **Barrier:** Large database from high throughput experimentation and application-based data analysis are not comparable in some cases
    - **Target**: Coupled machine learning modeling to automate and reduce barrier to optimization

Potential Impact



- AEM alkaline stabilities and lifetimes need to be improved to reach the Clean Hydrogen Electrolyzer Program goal of $2/kg H2 by 2026 and $1/kg by 2031.
- Our LLNL-invented Studying-Polymers-On a-Chip platform is uniquely situated to address the identified barriers via *automated high-throughput screening and in-operando aging* that reduces manpower, time, and the need for ex-situ characterization
- This project will complement ongoing activities within DOE Hydrogen Program, including Enabling High Efficiency, Durable AEM Electrolysis Performance within the HydroGEN Advanced Water Splitting Materials Consortium, as well as predicting and controlling polymer degradation in H2NEW Consortium and Center for Ionomer-based Water Electrolysis

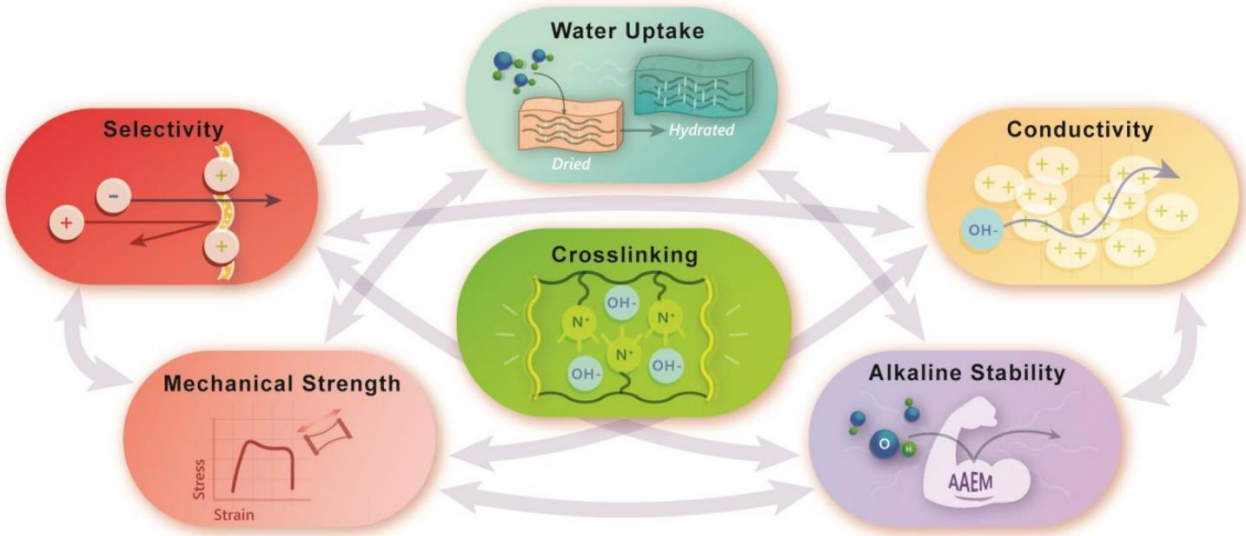
Approach

Technical Approach

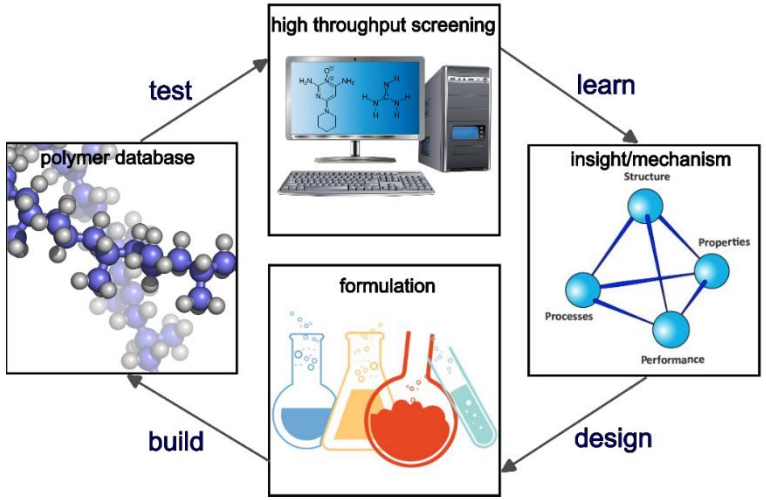
- Utilize multiscale computational simulations to predict trends in performance and stability in AEMWEs
- Screen water electrolysis membranes using SPOC platform
- Monitor electrolysis (electrical), water uptake (mechanical), and composition (Raman) during aging
- Use machine learning and living database for feedback and further acceleration in optimization

Compositional variables:

- functional group
- crosslinking
- electrolyte (pH)
- catalyst and additive
- composite and multimaterial (assembly)



Simple schematic of complex interplay of composition effects (such as crosslinking) on material properties. SPOC will enable us to quickly screen and optimize formulations prioritizing improved alkaline stability.



Approach

Milestones and Deliverables

Q1: Purchase all major materials for AEM chamber integration.

Q2: Populate experimental matrix of membrane performance in relation to functional group variables.

Q3: Utilize hybrid DFT-continuum solvent method and multiscale simulations to predict additional effects of factors such as pH, ionic strength, solution gradients, and interfacial fields for up to ten polymers.

Q4: Validate compositional ionic conductivity trends against ex-situ EIS.

Year 1 go/no go: SPOC chamber is built. Up to 500 mA/cm2 electrochemical testing with couple in-operando compositional analysis. Functional groups down-selected for future membrane compositional SPOC screenings and durability testing.

CBP: Have student interns present on their results (poster or internal presentation) in the summer.

Integration with HydroGEN, H2NEW, and H2LinkSc:

- Leverage crosscuting modeling capabilities in HydroGEN to predict and optimize AEM performance
- Coordinate with CIWE through the H2LinkSc program to predict AEM degradation. Activities include data sharing, student exchange and development of joint projects.

Approach: Safety Planning and Culture

A Hydrogen Safety Plan was not required for our project submission.

- **Our automated systems** are regularly assessed for safety hazards prior to operation, including:
- Standard operating procedures (SOPs) for users and best safety practices when running equipment
- Communications with Environment, Safety, and Health team members prior to use of equipment (such as aging chamber) and understanding of AEM chemical SDS's
- Communication with LLNL's cybersecurity and Electrical Authority Having Jurisdiction Program for safe database storage and equipment usage
- Regular meetings for effective material handling and problem-solving, and effective team communication

Accomplishments and Progress

This is new project and has not been reviewed at AMR before:

- Project Start Date: 01/02/2024
- Funds Received: 02/25/2024

Early Accomplishments:

- Scheduled first internal workshop on project (March 11th)
- Started initial discussions with CIWE, HydroGEN, and identified scope for collaboration

We are very excited to make progress on this effort!

Collaboration and Coordination

DOE-EERE

- Leverage modeling capabilities for predicting AEM degradation and performance within HydroGEN
- Coordinate with on-going activities within H2NEW for optimizing polymers for improved durability

H2LinkSc: Targets for initial efforts and strengthening EERE-BES integration

DOE-BES

- Leverage modeling capabilities developed by CENT EFRC for predicting the impact of transport
- Coordinate with CIWE through jointed activities, data sharing and student exchange to control polymer degradation

Collaboration and Coordination

- **Current project collaborators:**
  - Prof. Valeria Molinero, University of Utah, subcontract
  - **Role:** Perform molecular simulations to elucidate the impact of various pathways of chemical degradation on the physical properties and performance of anion exchange membranes. Molinero and the Postdoctoral Scholar will use the results from the simulations to propose new polymer designs and strategies to increase the resistance of polymer membranes to degradation in highly alkaline medium.
  - Coordination: biweekly team meetings and regular email correspondence
- **Potential project collaborators:**
  - CIWE · Center for Ionomer-based Water Electrolysis: **Dr. Adam Weber**
  - CENT · Center for Enhanced Nanofluidic Transport: **Dr. Michael S. Strano**
  - CABES · Center for Alkaline-Based Energy Solutions: **Dr. Kevin Noonan and Dr. Geoff Coates**
  - **Prof. Mengyang Gu** (UCSB) – machine learning and automation
  - **Prof. David Hoezle** (Ohio State) – mechanical engineering automation

DEIA/Community Benefits Plans and Activities

Within my team

- For this project I will bring on two summer students each year from minority serving institutions, GEM fellows, or the pipelines I have established.
- Commit to one professional development training course per year to remove implicit bias from my teaching methods, research practices, and project management.
- Develop an active mentorship style and inclusive and welcoming lab dynamic
- Approach the hiring process of students, postdoctoral researchers, and research scientists using an equity lens.

Within my community

- Engage in at least two outreach events a year within my local community and nationally.
- Create new internship and LLNL engagement pipelines and show community LLNL resources.

Energy Equity

- One of my SMART goal targets for **the third year of this project** is to conduct technoeconomic and environmental-impact analyses of targeted AEMWE formulations to validate the potential of these materials for widespread use.
- If viable, engage with industrial manufacturers, distributors, and energy infrastructure users for scaling up and testing these materials within the Central Bay and broader community.

Remaining Challenges and Barriers

Project is just beginning

- Fundamental challenge is building and integrating AEM aging chamber into existing SPOC screening and automation infrastructure
- Additionally, need to integrate predictive computation for further acceleration of AEM optimization

Proposed Future Work

FY24:

- Build chamber
- Screen AEM materials experimentally using SPOC and traditional methods
- Identify trends in experimental and computational results, focusing on AEM functional group and alkaline stability, for future screenings.

FY25:

- Begin AEM cyclic aging experiments
- Incorporate variable effects of crosslinking and additives on AEM performance and stability
- Improve computational simulations and machine learning models

FY26-27

- Tailor AEMWEs for improved alkaline stability
- Integrate with consortia for cell testing of improved formulations
- Technoeconomic analysis

SPOC Summary

Project has just started

Our Studying-Polymers-On a-Chip (SPOC) screening platform will accelerate AEM co-optimization of performance and lifetime by coupling:

1) High-throughput screening and aging
2) Integrated *in-operando* characterization
3) active learning-feedback models and high-performance computing (HPC) simulations