Thin, highly selective polymer membrane separators for advanced liquid alkaline water electrolysis

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DOE Hydrogen Program
2024 Annual Merit Review and Peer Evaluation Meeting

Project ID: ELY-BIL007

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Project Goal

- Our team will develop novel, dense, polymer electrolyte separators based on polybenzimidazole (PBI) derivatives that will enable tuning of water/KOH uptake in mechanically robust films for advanced liquid alkaline water electrolysis (LAWE).
- These material advances will enable thinner separators with increased selectivity (hydroxide conductivity/hydrogen permeability).
- In overall, the project will enable **higher operating currents**, increased **dynamic operating high-temperature stability**, and catalyst-coated membranes (**zero-gap design** advantages) in direct alignment with stated lab call goals

Overview

Timeline and Budget

<u>For Lab Projects funded annually</u> <u>through AOPs:</u>

- Project Start Date: 04/01/2024
- FY24 DOE Funding to NREL: $364,775
- FY25 Planned DOE Funding to NREL $736,043
- Total DOE Funds Received to Date**: $0

  ** Since the project started

TEAM

- Abhishek Roy (PI, NREL)
- Mou Paul, Bryan Pivovar
- Oak Ridge National Lab – Structural Characterization

Barriers

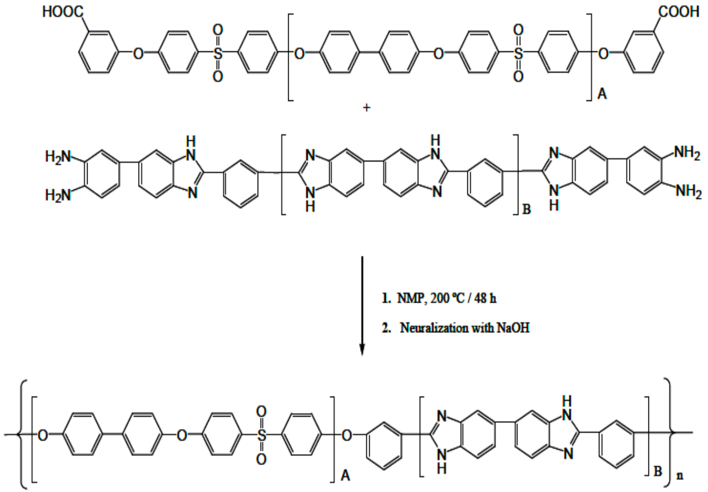
- Synthesize novel PBI copolymer and demonstrate reduction of H2 crossover compared to Zirfon
- Establish trade-off between resistance and crossover and chemistry and identify the 2–3 PSF-PBI block polymers
- Demonstrate and achieve performance ≥2.0 A/cm2 at 1.7 V/cell with ≤1.6-mV/kilohour degradation rate in concentrated, heated (80°–85°C) potassium hydroxide (5–10 M)
- Demonstrate and achieve performance ≥2.0 A/cm2 at 1.7 V/cell with ≤1.6-mV/kilohour degradation rate in concentrated, heated (80°–85°C) potassium hydroxide (5–10 M) duplicate

Potential Impact

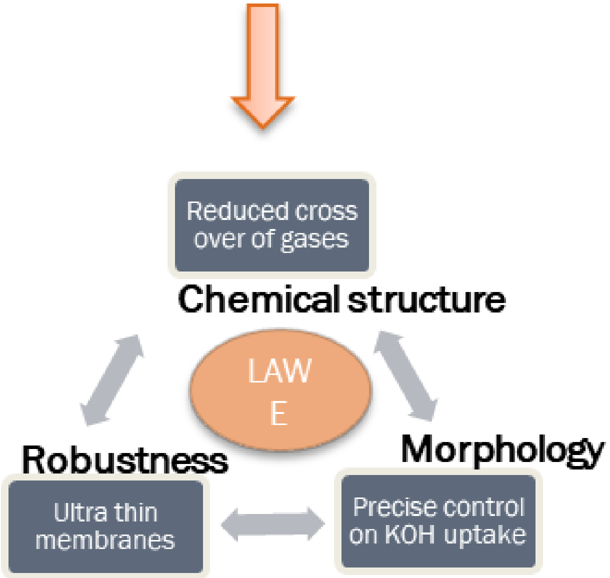
The project will deliver the following Impact

1. Novel PSF-PBI functionalized thin polymeric dense separator for LAWE meeting FOA's target (≥2.0 A/cm2 @ 1.7 V/cell with ≤1.6 mV/khr degradation rate in concentrated, heated (80-85 °C) potassium hydroxide (5-10 M))
2. Thin polymeric dense separator with improved selectivity (hydroxide conductivity/gas cross over) over Zirfon
3. New classes of functionalized PBI material with tunable polymer parameters to control and design LAWE performance metrics
4. Synthetic and fabrication design for scaling up to higher TRL and potential market introduction
5. A strong community plan specific to project to address DEIA, energy equity and workforce implementation plan

Approach



Synthesis scheme of PS-PBI copolymers



Lee, Hae-Seung, Abhishek Roy, Ozma Lane, and James E. McGrath. *Polymer* 49, no. 25 (November 2008): 5387–96.

Approach -Project timeline and task

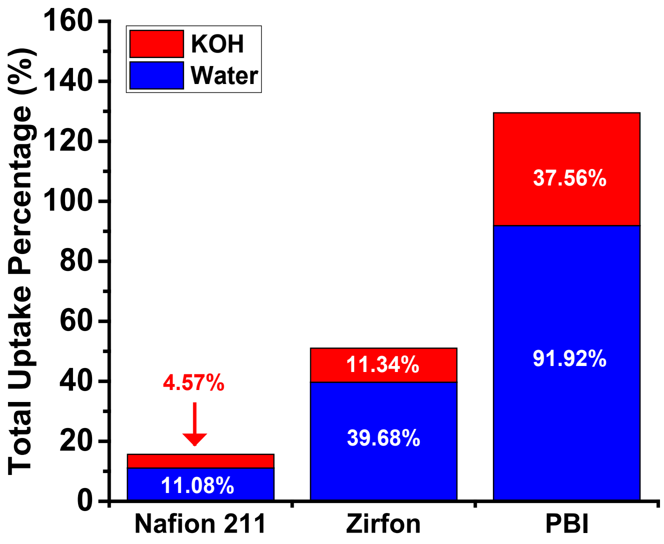
Task #	Description	Year 1				Year 2				Year 3			
		Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4	Q1	Q2	Q3	Q4
1	**Novel polymer separator synthesis**												
1.1	Synthesis of random PBI copolymers												
1.2	Synthesis and characterization of PSF-PBI block copolymers												
1.3	Synthesis and characterization of functionalized PSF-PBI												
2	**Membrane fabrication and characterization**												
2.1	Fabrication of membrane with varying thickness												
2.2	Morphological characterization of block copolymers												
2.3	Intrinsic membrane properties evaluation												
2.4	Electrochemical characterization (HFR and H_2 crossover)												
	Selection of candidates for H2NEW												

Approach: Safety Planning and Culture

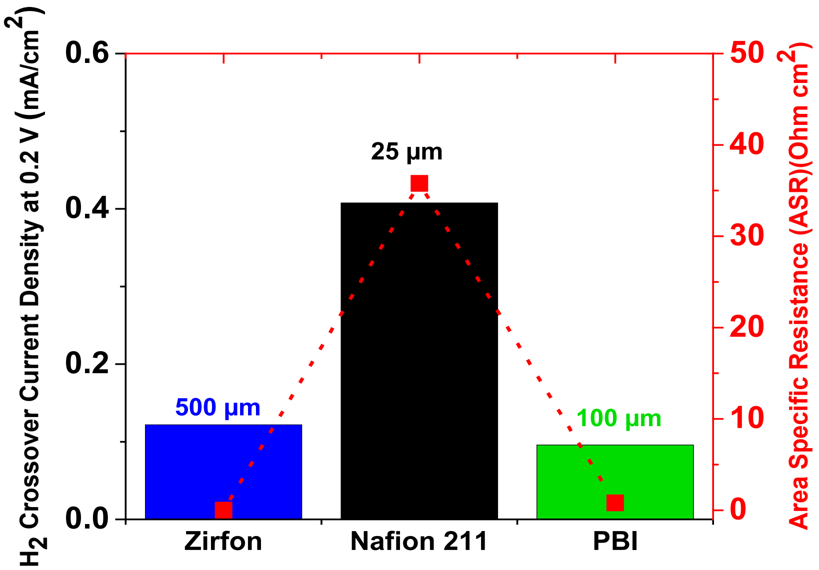
- Was your project required to submit a safety plan to the Hydrogen Safety Panel (HSP)?
  - No

- The team will follow NREL's and ORNL's safety protocols and standards
- The team will follow safety reviews, implement standard operating procedure for new equipment start ups and polymer synthesis
- Safety review for any potential concerns, near miss and incident at team meeting level and elevate/report based on standard safety protocol
- Review safety data sheet and take follow appropriate PPE guidelines for introduction of any new chemicals and communicate to other lab workers as needed.

Takeaway & Accomplishments



Water and KOH uptake of membranes equilibrated in 7M KOH



ASR and H_2 cross over trade off

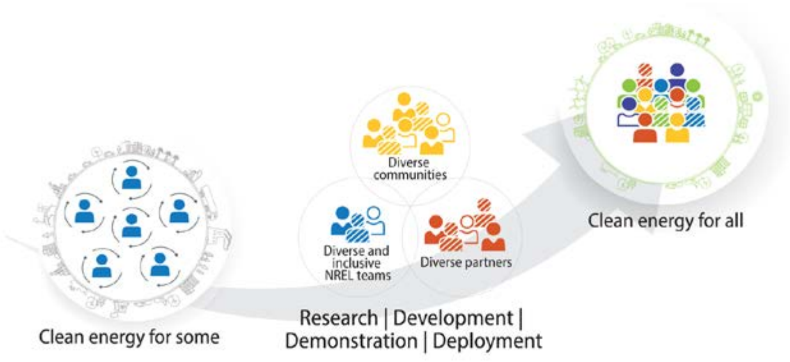
Collaboration

- Collaboration with Oak Ridge National Lab in characterization of the polymers
    - Scattering and microscopic techniques

- Collaboration with H2NEW in electrolysis performance testing

    - Cell Testing
    - Electrode Fabrication
    - Post –mortem characterization

DEIA/Community Benefits Plans and Activities



- DEIA (SM1, Q3 2024): A training plan will be designed and distributed across the project institutions and will include a statement of principles for research and collaboration that aligns with the DEIA objectives for this project.
    - Success criterion: Distribution of the training plan and statement of principles.

- Energy Equity (Q4 2025): Conduct an analysis make novel polymeric dense separator using green solvent during the polymerization process.
    - Success criterion: Demonstrate similar polymer properties using green solvent route during polymerization as compared to the current solvent used for making such polymers.

- Workforce Planning (Q4 2026): Workshop engagement between industry, academic, and participating organizations to raise awareness around topics like technical needs, opportunities, recruiting, and the importance of collaboration and student exchange programs.
    - Success criterion: Student and postdoc participation with report generation, presentation of research in front of industry representatives, and potential internships at an industrial setting.

Key Proposed Future work

- Synthesize novel PBI copolymer and demonstrate 2x reduction of H_2 crossover compared to Zirfon
- Establish trade-off between resistance and crossover and chemistry and identify the 2–3 PSF-PBI block polymers
- Demonstrate initial electrolysis performance of random and PBI-based multiblocks
- Generate structure–property relationships incorporating the effect of block copolymer morphology, hydrophilicity, and membrane thickness
- Demonstrate and achieve performance ≥2.0 A/cm^2 at 1.7 V/cell with ≤1.6-mV/kilohour degradation rate in concentrated, heated (80°–85°C) potassium hydroxide (5–10 M)
- Demonstrate and achieve performance ≥2.0 A/cm^2 at 1.7 V/cell with ≤1.6-mV/kilohour degradation rate in concentrated, heated (80°–85°C) potassium hydroxide (5–10 M)

Remaining Challenges and Barriers

- Demonstrating synthetic capabilities to synthesize PBI based multiblocks at NREL
- Investigate synthetic routes to improve chemical durability under operating conditions and developing corresponding durability testing protocols.

Summary

- Our team will develop novel, dense, polymer electrolyte separators based on polybenzimidazole (PBI) derivatives that will enable tuning of water/KOH uptake in mechanically robust films for advanced liquid alkaline water electrolysis (LAWE).
- Our target is to achieve Novel PSF-PBI functionalized thin polymeric dense separator for LAWE meeting FOA's target (≥2.0 A/cm2 @ 1.7 V/cell with ≤1.6 mV/khr degradation rate in concentrated, heated (80-85 °C) potassium hydroxide (5-10 M))
- The project will implement a strong community plan specific to project to address DEIA, energy equity and workforce implementation plan

Thank You

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