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Economical Production of Hydrogen through Development of Novel, High Efficiency Electrocatalysts for Alkaline Membrane Electrolysis

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Organization: Proton OnSite

Date: May 15, 2013

Project ID: PD094

Overview

Timeline

- Project Start: 20 Feb 2012
- Project End: 19 Nov 2012
- Percent complete: 100% (Phase II pending)

Budget

- Total project funding
  - DOE share: $1,150,000
- Funding for FY13
  - DOE share: $500,000 (pending)

Barriers

- Barriers addressed

  G: Capital Cost

Table 3.1.5 Technical Targets: Central Water Electrolysis Using Green Electricity [a,b]				
Characteristics	Units	2011 Status [c]	2015 Target [d]	2020 Target [e]
Hydrogen Levelized Cost (Plant Gate) [f]	$/kg H_2	4.10	3.00	2.00
Total Capital Investment [b]	$M	68	51	40
System Energy Efficiency [g]	%	67	73	75
	kWh/kg H_2	50	46	44.7
Stack Energy Efficiency [h]	%	74	76	78
	kWh/kg H_2	45	44	43
Electricity Price [i]	$/kWh	From AEO '09	$0.049	$0.031

Partners

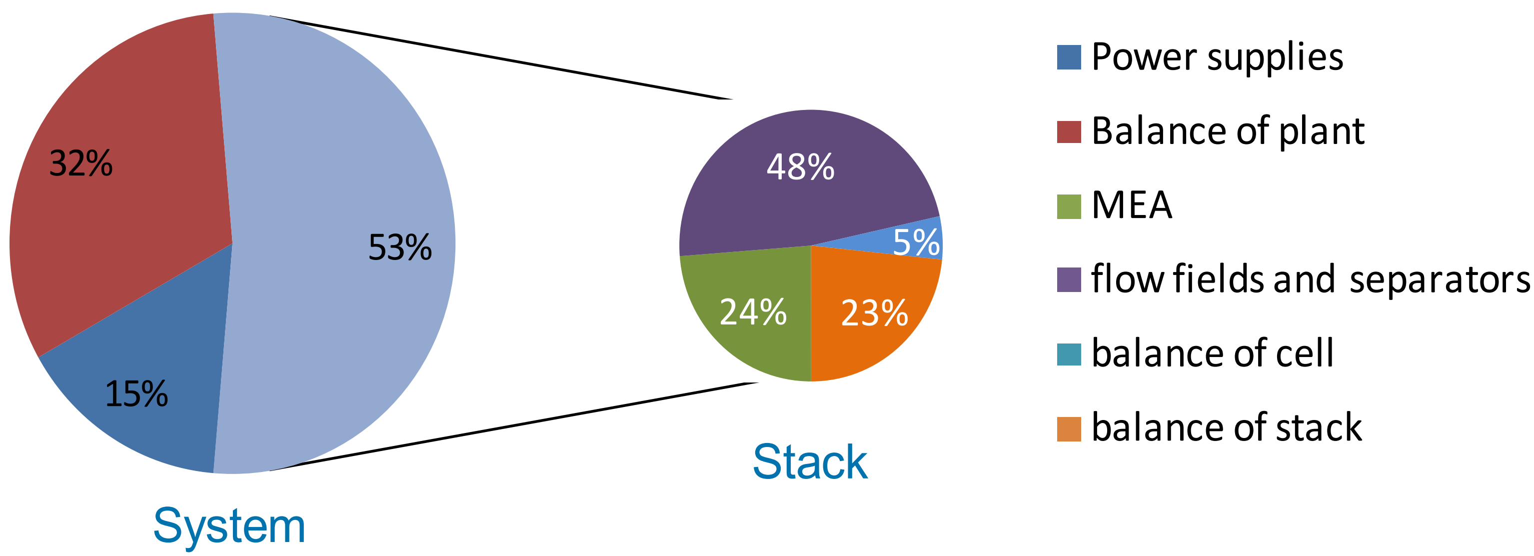
- Illinois Institute of Technology

Relevance: Project Objectives

- Demonstrate high activity of pyrochlore catalysts for oxygen evolution
- Optimize catalyst composition and microstructure
- Form and characterize new anion exchange membranes and demonstrate acceptable conductivity for electrolysis
- Process promising membrane and catalyst materials into MEAs
- Scale up to a relevant stack active area and height and operate in a relevant environment.

Relevance: Cost

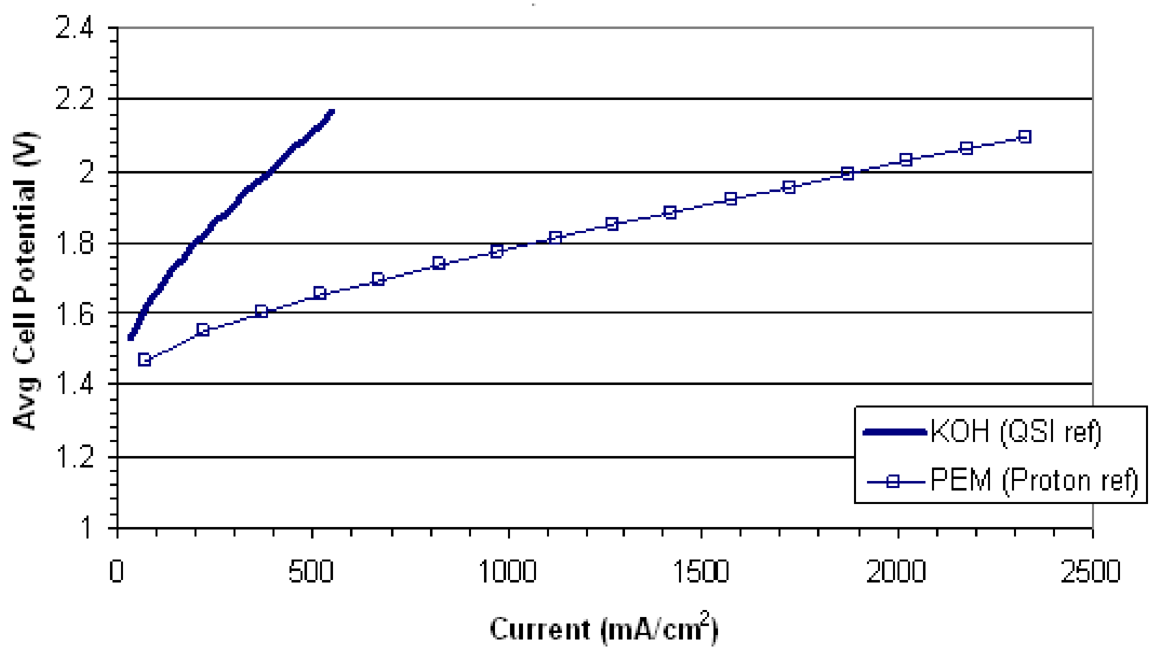
- Metal flow fields and separators represent almost half of stack cost



- Alkaline media enables transition from titanium to stainless steel: eliminates 75% of part cost
- Also enables less expensive catalysts

Relevance: Efficiency

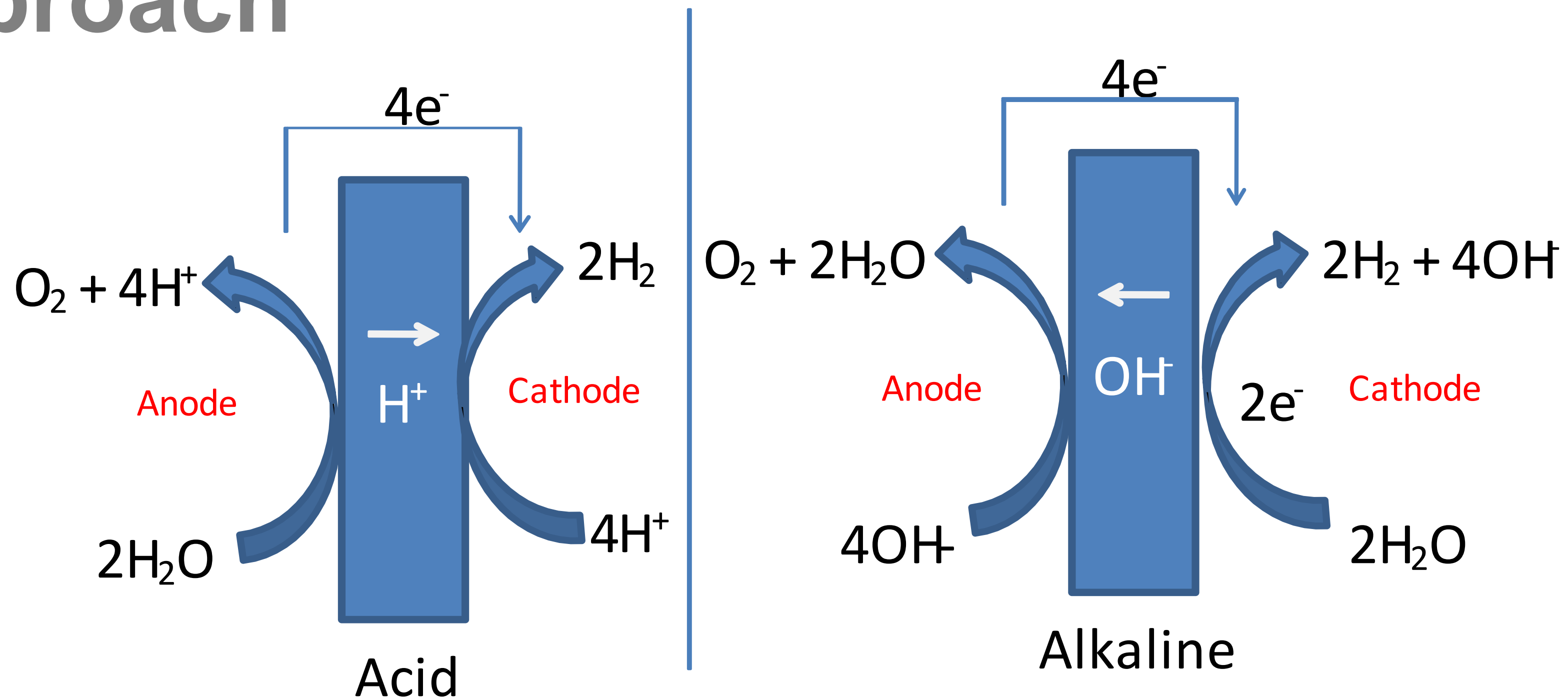
- Liquid KOH electrolyte systems much less efficient than membrane-based systems
- Expect AEM hybrid to fall between existing technologies
- Advanced catalysts and membranes help to close gap



Top Level Approach

- Task 1.0 Catalyst Development
  - 1.1 – Catalyst Synthesis
  - 1.2 – Catalyst Characterization
- Task 2.0 Membrane Development
  - 2.1 – Membrane Synthesis
  - 2.2 – Membrane Characterization
- Task 3.0 MEA Testing
  - 3.1 – Manufacturing Development
  - 3.2 – Electrochemical Characterization
  - 3.2 – Post Operational Assessment
- Task 4.0 Program Management

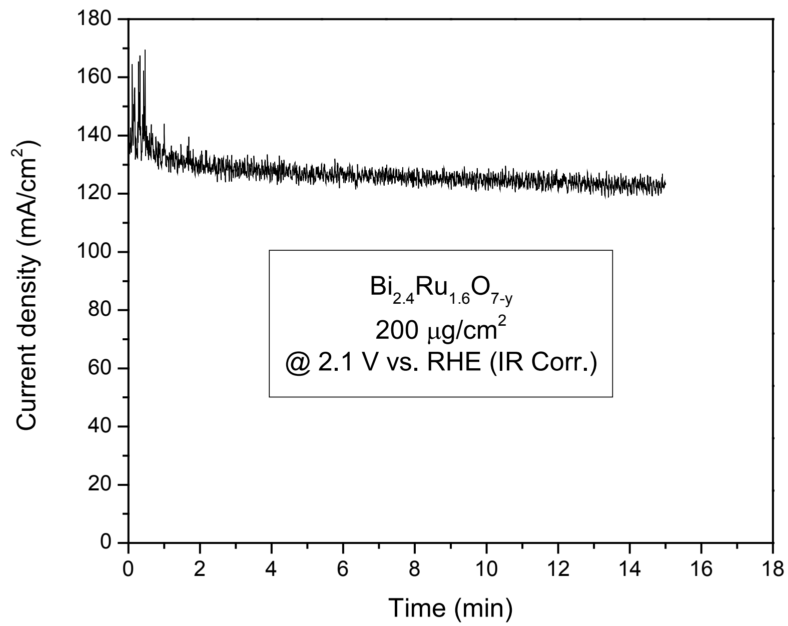
Approach



- Water management is a key consideration in determining operating point
- Phase separation easier with anode feed
- ARPA-E work shows 500 mA/cm^2 achievable with no water mass transport issues

Approach

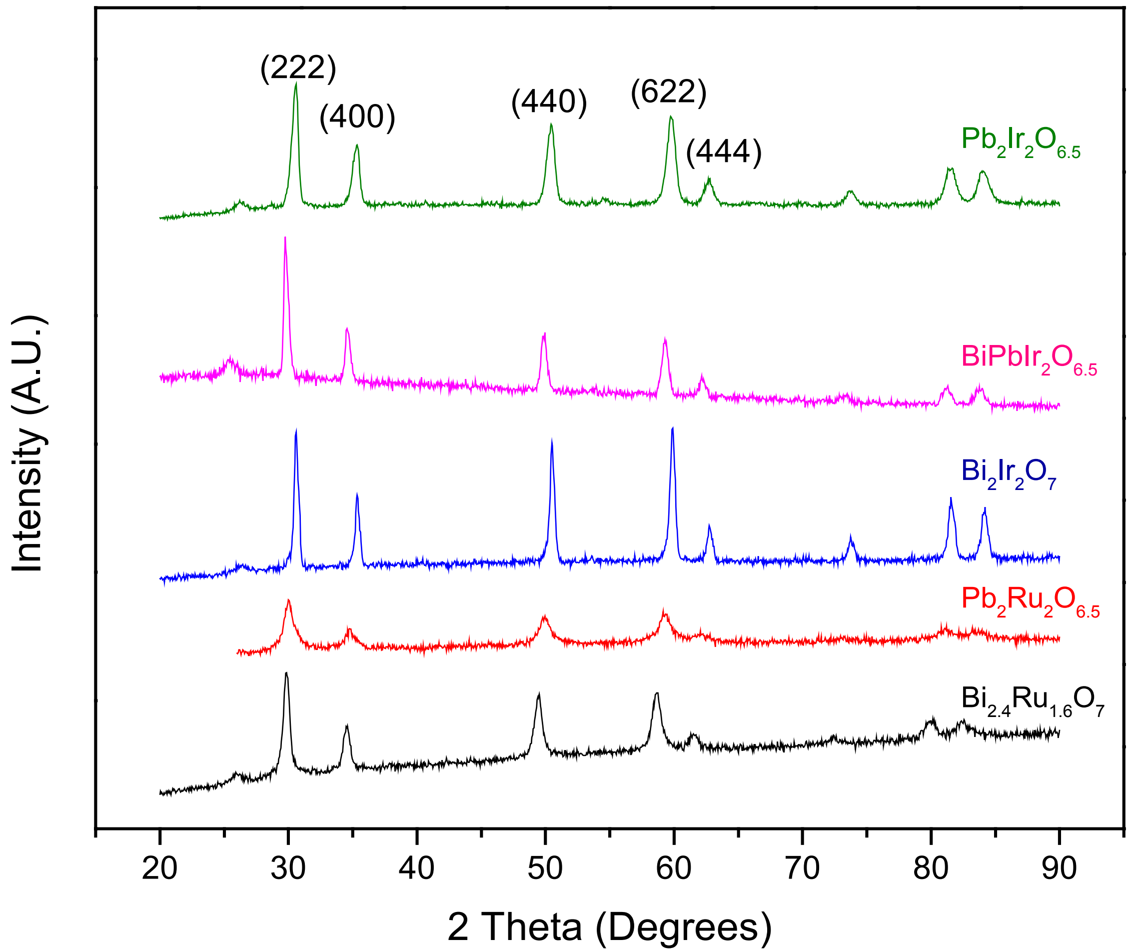
- Leverage pyrochlore class of catalysts ($A_2B_2O_{6-7}$)
  - Good kinetics for OER
  - Stable in base
  - Able to make as nanoparticles
- Investigate compounds with A = Bi, Pb; B = Ru, Ir



Technical Accomplishments: Phase 1

Task	Task Description	Progress Notes	Completion
1.0	Catalyst Development	• Synthesized desired pyrochlores and proved structure with XRD	100%
2.0	Membrane Development	• Focused on development of Tokuyama for catalyst screening • Investigated 2 additional polysulfone derivatives	100%
3.0	MEA testing	• Process trials completed for improved electrode adhesion and stability • Cells tested for up to 200 hours	100%
4.0	Program Management	• Project reporting completed • Phase II proposal completed with internal funds	100%

Technical Accomplishments: Synthesis

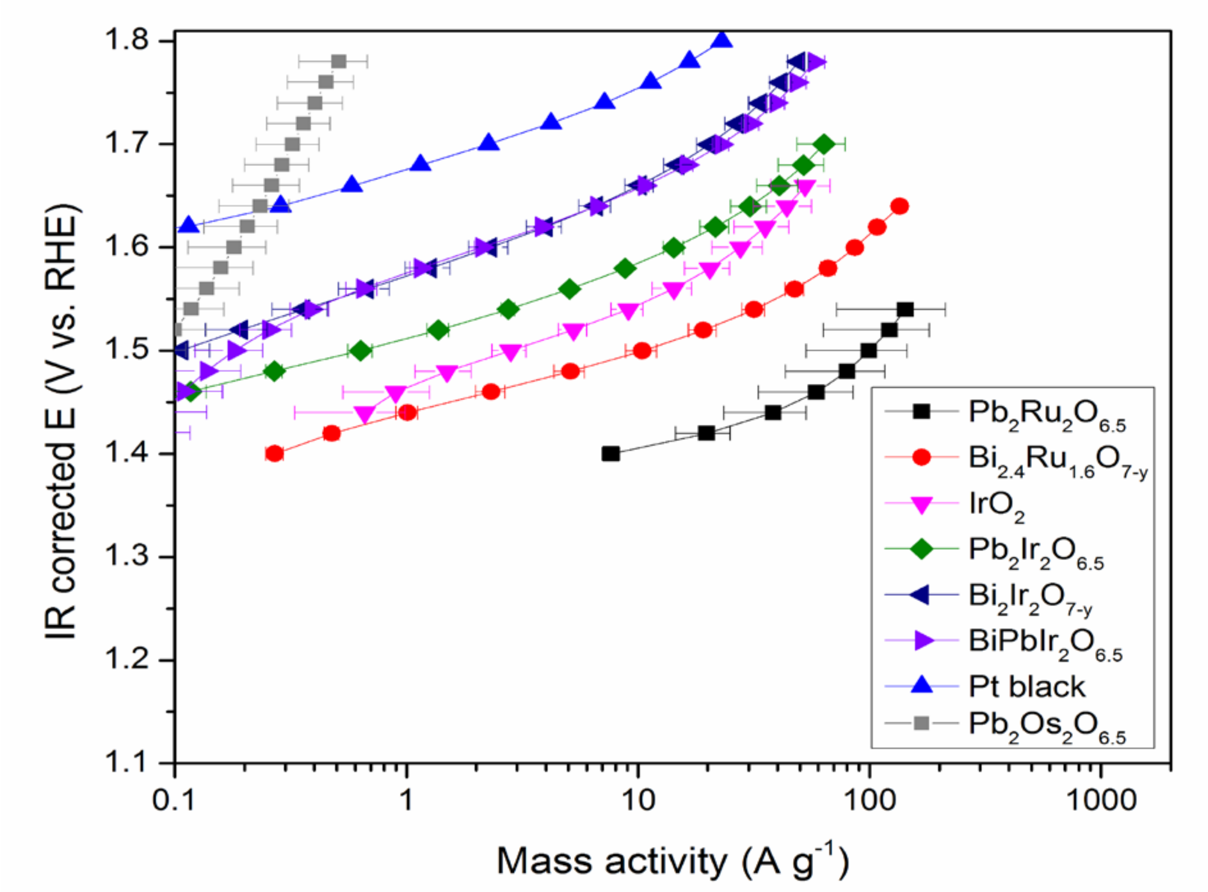


Catalyst	B.E.T. surface area (m^2/g)	Electronic conductivity S/cm
$Pb_2Ru_2O_{6.5}$	99±4	87
$Bi_{2.4}Ru_{1.6}O_7$	7.8±0.2	63
$Pb_2Ir_2O_{6.5}$	1.2±0.1	73±7
$Bi_2Ir_2O_7$	0.4±0.1	56±6
$BiPbIr_2O_{6.5}$	0.4±0.1	75±7
$Pb_2Os_2O_{6.5}$	0.8±0.3	

- Desired compositions successfully made
- Surface area of some compositions still low

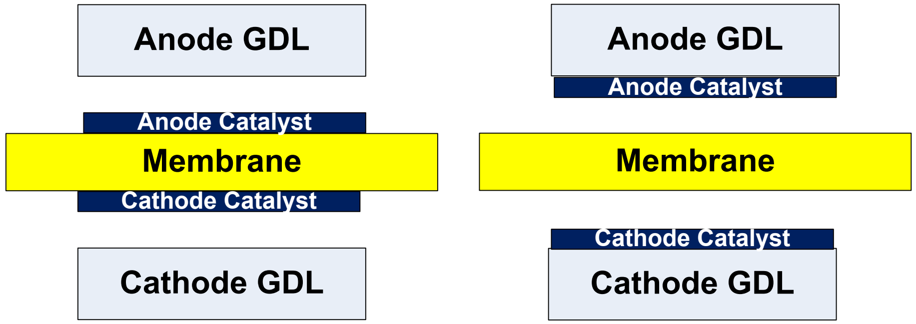
Technical Accomplishments: Bench Tests

- Mass activity shows good promise even with some catalysts at 10% desired surface area

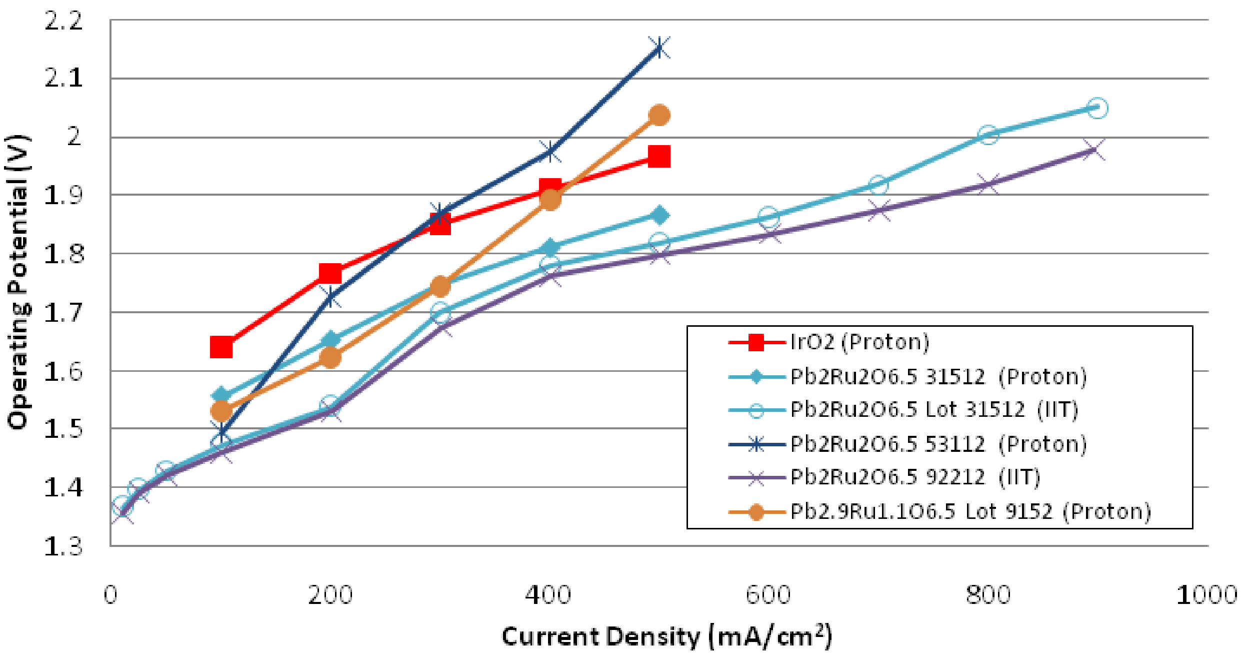


Technical Accomplishments: Electrode and Cell Fabrication

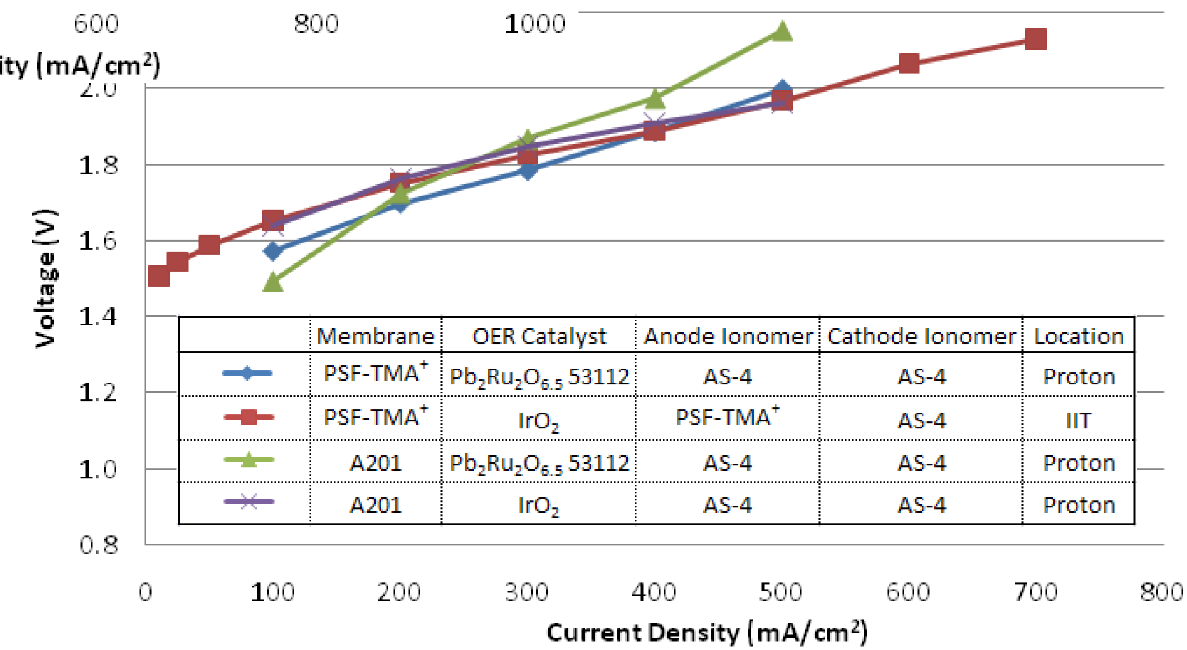
- GDE approach leveraged to mitigate stress on membrane
- Ionomer formulation and technique leveraged from ARPA-E program
- Cell design modified for thinner/stiffer membranes



Technical Accomplishments: Stack Testing



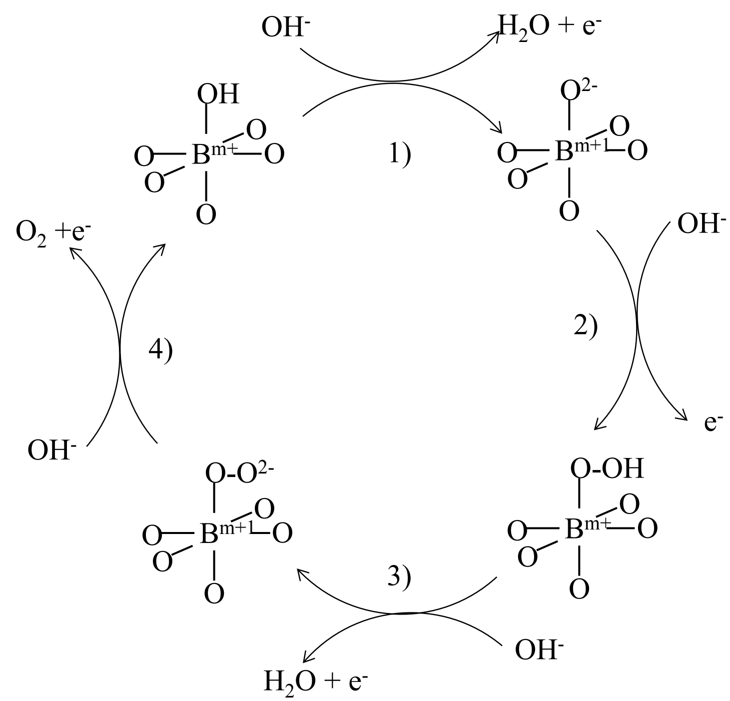
- RDE shows good translation to full cell
- IIT membranes show similar performance to commercial AEM



Technical Accomplishments: Modeling

- D-band orbital theory and density functional theory used to explain activity trends
- Larger metal-adsorbate repulsion (V^2) leads to lower OER activity

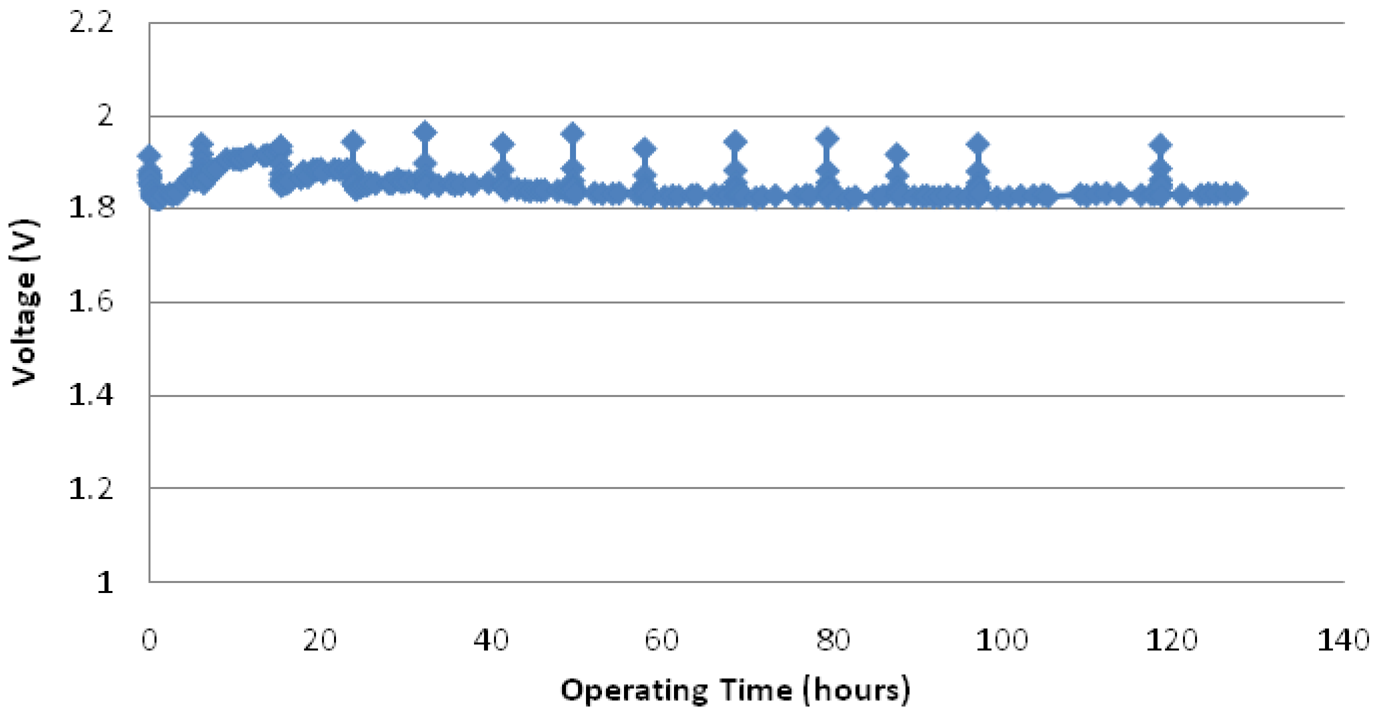
Catalyst	B cation	d band center* (ε_d, eV)	V^2_{ad}*	i_m(A/g)	i_s(A/m^2)
$Pb_2Ru_2O_{6.5}$	Ru	-1.41	3.87	100±40	1.0±0.5
$Bi_{2.4}Ru_{1.6}O_{6.9}$	Ru	-1.41	3.87	10±2	1.3±0.2
$Pb_2Ir_2O_{6.5}$	Ir	-2.11	4.45	0.6±0.1	0.5±0.1
$Bi_2Ir_2O_{6.8}$	Ir	-2.11	4.45	0.11±0.03	0.3±0.1
$BiPbIr_2O_{6.5}$	Ir	-2.11	4.45	0.18±0.06	0.5±0.2
$Pb_2Os_2O_{6.5}$	Os	------	5.13	0.08±0.03	0.1±0.05



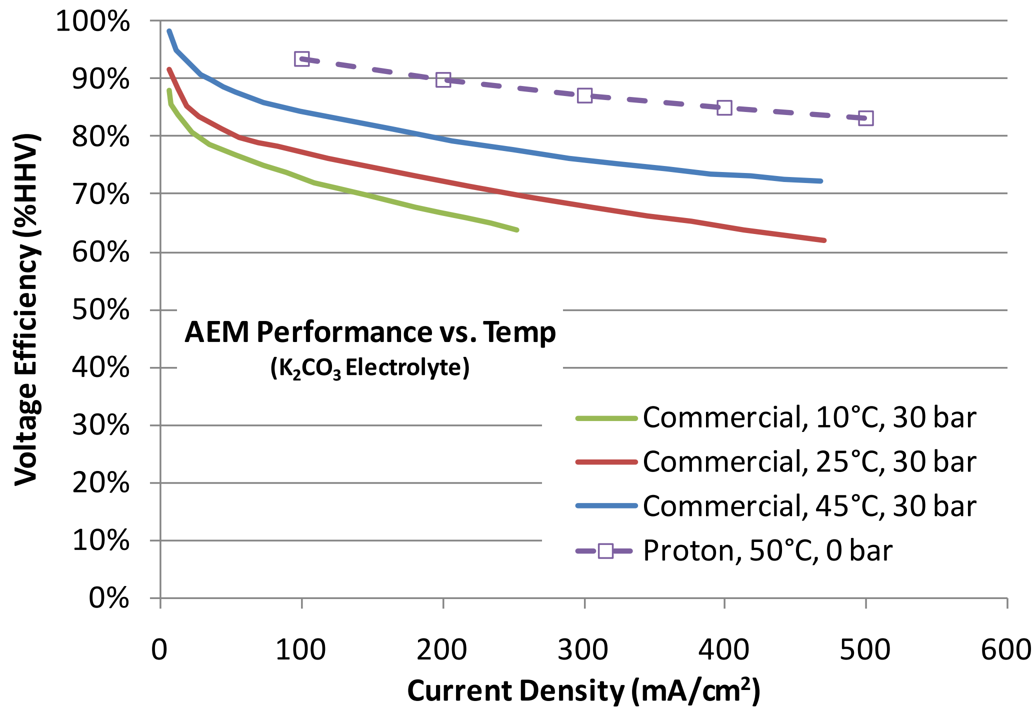
Proposed mechanism

Technical Accomplishments: Durability

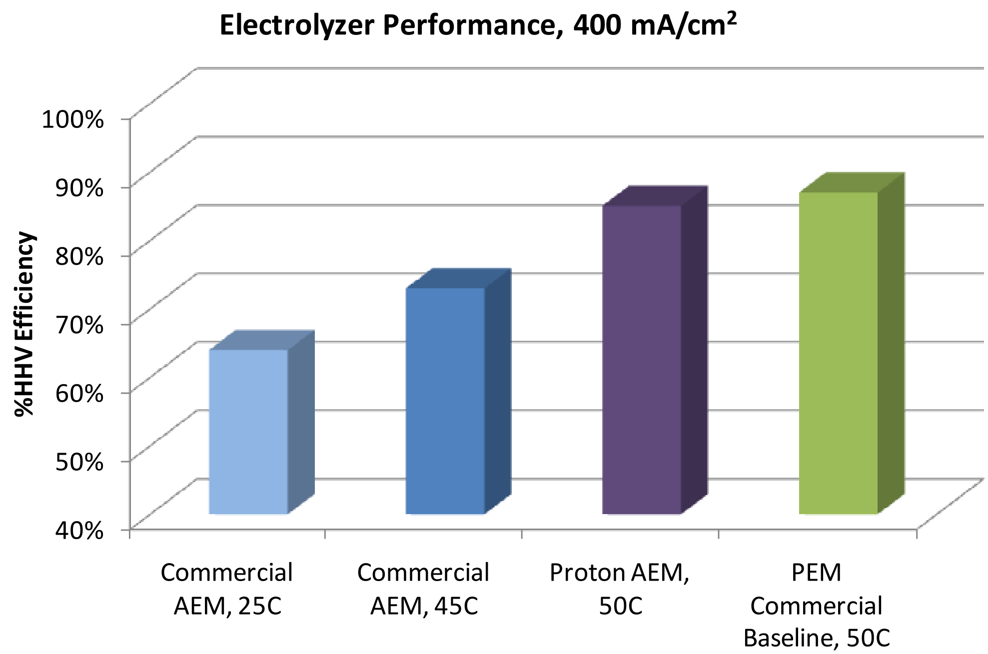
- Voltage stability good with carbonate recirculation
- Phase II will focus on pure water



Comparison to State of the Art



- Exceeds existing AEM and approaches legacy PEM performance

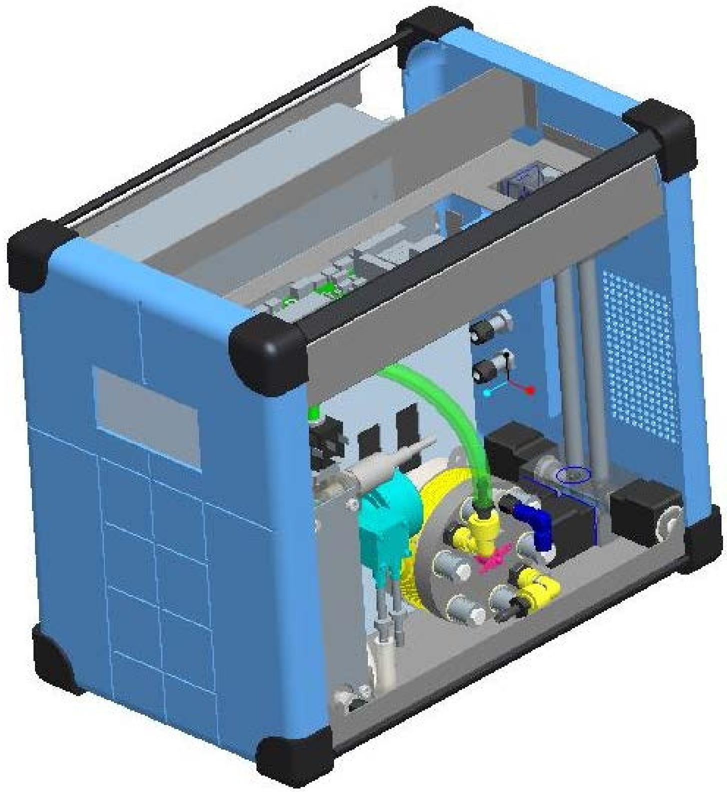


Collaboration

- IIT major subcontractor on Phase 1
  - Catalyst synthesis and structural characterization
  - Molecular bonding theory
- Phase II to focus on continued synthesis optimization of particle size and composition
- Tuning of properties for membrane and ionomer stability

Future Work:

- Determine influence of composition on pyrochlore microstructure, physical properties, and activity
- Determine the impact of key AEM properties (conductivity, water uptake, gas crossover) on AEM performance and synthesize optimized AEMs
- Complete system trade study of electrolyte vs. cost and stability and develop prototype lab system
- Provide a product cost analysis for lab scale and large scale AEM electrolysis systems



Summary

- **Relevance:** Alternate electrolysis chemistry for capital cost reduction
- **Approach:** Leverage AEM expertise to reduce cell part cost with efficient catalyst and membrane materials to offset lower operating current
- **Technical Accomplishments:**
  - Improved OER and model development for improved prediction
  - Initial membrane performance equivalent to baseline
  - Stability of AEM electrolysis and improvement over existing technology
- **Collaborations:**
  - IIT: Catalyst and membrane synthesis; modeling
- **Proposed Future Work:**
  - Leverage model to optimize catalyst performance
  - Optimization of membrane properties for stable performance
  - System prototype and cost analysis