Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Breakout Session Summaries
Cross Cutting Topics

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Cross Cutting Breakout Sessions

Breakout Session #	Session ID	Technology	Topic	Lead
1	C1-A	PEC/LTE	Membrane operating at different regimes	Cy Fujimoto
1	C1-B	STCH, LTE, PEC	Theory on catalytic reactions with metal oxides and other materials	Tadashi Ogitsu, Hector Colon-Mercado
1	C1-C	STCH, PEC, LTE, HTE	Standards development and crosscutting measurement issues	Karl Gross
6	C6-A	PEC/STCH, LTE/HTE	Comparative analysis on key cross-cutting metrics (definition and discussion of device efficiency, cost of hydrogen, etc)	Huyen Dinh, Michael Sanders

Session Summary

Session ID: C1-A

Title: Membrane operating at different regimes

Summary of discussion

- Nafion is commonly agreed upon standard membrane in an acid system.
- In alkaline environments, there is no good commercial source of stable, alkaline membranes.
- Ongoing development of alkaline stable membranes by universities and national labs, but how to define a standard of an experimental membrane is still under discussion.
- What are the metrics of determining which membrane, who makes that decision and who will scale an experimental membrane is still an issue.

Consensus and/or dissenting opinions

- Nafion is standard PEM LTE membrane.
- Consensus that there are no good AEM LTE standard. There was mention that Fumatech AEM membrane is consider by some as an AEM standard, but everyone agrees that this membrane is not suitable for alkaline environment.
- Consensus that there is little to leverage between LTE and PEC in both PEM and AEM.
- Dissenting opinions on how to select a standard AEM in terms on what physical properties are most important. Conductivity (should it be base on hydroxide conductivity or chloride?), water uptake (at what temperature taken), durability (what conditions to measure?).

Key Take-Aways

- No AEM standard.
- There are experimental membranes being developed but still in evaluation stage, path on how or when to down select these experimental membranes and then how or who will scale the materials is still a question.
- What is also slowing this decision is the fact that there are no strong pull or industry need that would absorb and financially drive this endeavor (scaling).

Action Items

- Small group agreed that AEM membranes are still being filtered/tested by the community.
- Byron Pivovar has an ARPA-E project that is looking at characterizing various experimental membranes, he is willing to screen membranes from the community, but will need to think about what are the physical properties that will weigh heaviest in determining a standard membrane.

Session Summary

Session ID: C1-B

Title: Theory on catalytic reactions with metal oxides and other materials

Summary of discussion

- Relevance of theory
- Applicability of theory
- Limit of theory
- Relevance of theory-experiments interaction

Consensus and/or dissenting opinions

- Theory is increasingly becoming important
- Theory-characterization interaction is very important

Key Take-Aways

- Ab-initio modeling can take the most of effects (pH, electrolytes, bias potential) into consideration, however, limited by size and their validations are far from complete
- Multiscale modeling is in infancy
- Theory-experiment collaboration is the key for enabling its full potential

Action Items

- Need experimental data protocols for reliable model construction and cross validation

Session Summary

Session ID: C1-C

Title: Standards development and crosscutting measurement issues

Summary of discussion

- Underlying problem is the limited resources and limited time to enable cross technology comparisons
  - How to compare data based on best practices
  - How to identify the common crosscutting issues
- How to develop standards across water splitting technologies
- Identification of relevant metrics for reporting results

Consensus and/or dissenting opinions

- Standardizing vs harmonizing protocols – Standards seem more appropriate.
- Need to clearly define efficiency – standardizing reporting – how to really compare approaches is efficiency the right measure
- *Developing system level tools to describe overall exergetic efficiency – this should be based on a definitional structure for what is efficiency*
- Need to not constrain basic research so there may be more discrete standards for basic studies

Key Take-Aways

- Targets at different levels – materials, device, system all need some definitions – this phase is critical
- Need more validated tech to market analysis to compare costs of eventual H2 production
  - Need to have a list of what goes into tech to market
- Use cost of hydrogen as the metric that drives this as a comparison across technology areas at the system level – also look at the more intangible benefits of sustainability
- Life cycle analysis – cradle to grave – what is lifetime?
- Need to develop a cross cutting tech to market tools that will help communicate between areas.

Action Items

- Need to clearly define a standard, a metric and basic comparison – how to ensure basic results are robust – need to have best practices in this area. These vary from technology to technology
- How to define pressure, temperature and materials even within a technology area to compare efficiency?
  - Agreement on water and pH
  - Purity of starting materials and hydrogen
  - Can define based on thermodynamic properties of what goes in and what comes out and chemical purity
  - Need to look at the cell in a box
  - Need to have well defined reporting in this respect
  - Should you look at the pressure of hydrogen for end use application (not device output pressure)?

Session Summary

Session ID: C6-A
Title: Comparative analysis on key cross-cutting metrics

Summary of discussion

- How to compare solar to hydrogen efficiencies
- Cross-cutting metrology, synthesis, and analysis capabilities
- Difficulties and opportunities in directly comparing systems

Consensus and/or dissenting opinions

- For comparing technologies, kWh thermal and electric are not comparable inputs for efficiency calculations
- These comparisons break down when you zoom too far in on the component systems
- These technologies are continually evolving

Key Take-Aways

- Draw 5 boxes around system (4 for each tech, 1 in general)
  - Heat / electricity / solar in
  - Room temperature H2O in
  - H2 out at pressures and purities called for
  - Compare $/kg H2
- Plenty of metrics comparable between high T and low T technologies
- May be tests we can run to cross test technologies
  - For STCH from THE: can you do a TGA test under the right conditions
  - For HTE from STCH: is a material also conductive
  - Comparable PEC and LTE corrosion tests

Action Items

- Circulate analysis cost range assumptions and see how reasonable they are
- Work to develop cross-cutting metrics between high and low T
- Perspective paper comparing these technologies in context of H2@scale
  - Include co-production of H2 and electricity
- Definition written down for terms of art in each field to assist communication between fields.