Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Breakout Session Summaries
Photoelectrochemical Water Splitting (PEC)

May 3 – 4, 2022

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PEC Breakout Sessions

Session ID	Topic	Lead
P1	Priority Research Opportunities - Materials, Components and Devices	Tom Jaramillo (Stanford); Frances Houle (LBNL)
P2	PEC Stability and Durability Testing under Day/Night light Cycled Conditions	Adam Neilander (SLAC); Zetian Mi (Michigan)
P4	PEC Protocols Published to Date and Plans for Validation	Francesca Toma (LBNL); Shu Hu (Yale)
P5	Indirect Water Splitting and New Design Spaces	Todd Deutsch (NREL); Shane Ardo (UCI)
P-6	Wrap-up Session: PEC Status, Challenges, Action Items, and Outlook	Aditya Mohite (Rice); Nathan Nesbitt (NREL)

Session Summary

Session ID: P1
Title: Priority Research Opportunities – Materials, Components and Devices

Summary of topic:

- ***Device Integration***: How do we best manage light and heat integration into a device?
- ***Scale-up***: How do we establish economic methods for larger-scale PEC systems (e.g. III-V systems are usually ~0.1 cm^2 scales)?
- ***Real-world testing***: How does the real-world environment affect operation (e.g. weather)?
- ***Semiconductor durability***: What do we need to protect from and how do we do it?

Consenting and/or dissenting opinions

- ***Consenting***: There is a lack of controlling temperature in most papers.
- ***Consenting***: Need to understand how performance is impacted at larger-scales.
- ***Consenting***: Need to establish standard protocols for real-world testing of PEC devices
- ***Dissenting***: III-V photostability not realistic, so we should focus on material discovery. Can protective layers really work at scale?

Key takeaways

- Thermal considerations are important for benchmarking systems and to improve efficiency.
- Need protocols for scaling from lab scale to useful scale.
- Need protocols for 'real-world' conditions.
- Need to understand what electrolyte systems will be in real-world operation to determine effective protection strategies.

Action items

- Experimentation needs to control/monitor temperature to quantify thermal effects.
- Need more projects/funding working towards scaling-up of systems.
- Need to determine standardized real-world testing conditions and a standard reactor setup for benchmarking studies.
- Need to determine if large scale inorganic protective layers are feasible.

Session Summary

Session ID: P2
Title: PEC Stability

Summary of discussion

- Interest in protocols for PEC stability under day/night cycling - not currently described in literature
  - Very few experiments in this space
  - Degradation mechanisms may be chemically/electrochemically dependent on light intensity/current density
- A 'certification center' for PEC must measure H2, O2, use solar simulator akin to PV testing facilities
  - Measuring stability beyond current density challenging

Consensus and/or dissenting opinions

- Standard devices/cells difficult to identify
  - Too many 'classes' of PEC cell to easily identify a standard
- Protocols for 'equivalent' day/night cycling worthwhile

Key Take-Aways

- Developing accelerated stress test protocols need systems that last longer than 1000 hours to serve as model systems. 1000 hours can serve as a reasonable 'endpoint' for highly stable devices
- Day/night cycling should take into account the changing solar spectrum (re: wavelength, intensity, and direct/diffuse light)
  - On sun testing also relevant

Action Items

- Explore PEC Cell database akin to databases for solar fuels results
- How can we encourage publication of 'non-champion' electrode stability?
  - Process variability plays an important role in semiconductor processing, probably playing a key role here too.
- Develop day/night cycling protocols

Session Summary

Session ID: P4

Title: PEC Protocols Published to Date and Plans for Validation

Summary of discussion

1) Status updates for PEC protocols

2) Ideas for plans for validation

3) Synergy among various PEC database

Consensus and/or dissenting opinions

Needs for validation? How? Round-robin testing beyond III-V photoabsorbers for PEC? How to leverage data analysis and repository capabilities?

Key Take-Aways

1) All planned PEC protocols completed;

2) Protocols or best practices, broadly disseminated to help new researchers enter the field;

3) Strength/weaknesses of current DB

Action Items

1. Video (YouTube) / JofVE/social media
2. Design and implement new validation modes for PEC protocols
3. Incentivize dissemination of PEC best practices
4. Protocol about “on sun testing” (EPFL/NREL/LBNL)
5. Protocol on 2vs3 electrode testing (NREL/LBNL)

Session Summary

Session ID: P5
Title: Indirect Water Splitting and New Design Spaces

Summary of discussion

- Oxidative chemistry to add value
  - H_2O_2 for water treatment
  - Biomass (Glycerol) oxidation
- Immediate use of H_2, storage or utilization for chemical process (e.g., hydrogenation)
- Lower cost BOS materials
- Higher pressure

Consensus and/or dissenting opinions

Consensus.

Key takeaways

- Identify Unique ways to use sunlight
- TEA isn't everything, LCA can capture the value of anode reactions, need figure of merit besides STH
- Leverage areas with higher H_2 cost for market entry, capitalize on excitement around PEC for early adopters

Action Items

- Perspective paper
- Establish/continue international efforts to keep the discussion on new design spaces going

Session Summary

Session ID: P6

Title: Wrap-up Session: PEC Status, Challenges, Action Items, and Outlook

Summary of discussion

- A standard reactor design is desired.
- Durability is important. Solid electrolytes offer increased options beyond liquid electrolytes.
- Diurnal stability is rarely reported on, but crucially important.

Consensus and/or dissenting opinions

- Different PV materials have different electrolyte and reactor requirements.
- PV fabrication can necessitate front or back contact.
- PV material can require acid, base, or neutral electrolyte pH.

Key Take-Aways

- There is not consensus on optimal and flexible reactor designs that work for all device types.

Action Items

- There is need for standardized tests to demonstrate durability, especially diurnal.
- Hands-on workshops or bootcamps might help train the research community on good practice.
- Publication and effective publicization/dissemination of CAD drawings of standard cells would help research community.