Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Breakout Session Summaries
Photoelectrochemical Water Splitting (PEC)

June 11 – 12, 2024

Pacific Northwest National Laboratory

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ASU Arizona State University

Caltech

PEC Breakout Sessions

Session ID	Topic	Lead	Note Taker
P1	Priority Research Opportunities: Light absorber, Catalysts and Membranes	Joel Haber (Caltech)	Todd Deutch (NREL)
P2	PEC System Demonstration and Validation: what does a successful PEC pilot system look like in 2030	Zetian Mi (U. Michigan)	Sol A Lee (Caltech)
P3	PEC HydroGEN Seedling Projects Cross-Cutting Discussion	Todd Deutsch (NREL)	Joel Haber (Caltech)
P5	Hybrid PEC systems and New Opportunities (alternative oxidation or redox chemistry, coupling with STCH or CO2 conversion, etc)	Shane Ardo (UC Irvine)	Aaron Kaufman (Univ of Oregon)

Session Summary

Session ID: P1
Title: PEC Priority Research Opportunities

Summary

Topics Open for Discussion: top 3 Mural Boarded in bold

- Priority: Efficiency or Durability?
- **Need for Earth-Abundant, acid tolerant OER catalysts (replace IrO_x)?**
- PV-EC configuration, what are the main challenges and opportunities?
- PEC, does borrowing the carrier-selective contact concept from PV generate new approaches to protection and catalysis?
- Particle-based PEC system, what are the main challenges and opportunities?
- **Scale-up device size or ease of manufacturability (unit kg H2/hour)**
- **Different Membranes/selective transport layers including other than polymers**
- Diurnal Durability

Consensus or dissenting opinions

Consensus

- Need to define a minimum viable product, relevant for practical application.
- Durability remains the key challenge

Disagreement

- Reducing costs of light absorber, catalysts, membranes critical—Others felt demonstrating a working device took priority over costs
- Should focus on unique materials needs of PEC—others felt leveraging the LTE efforts most important for demonstrating device

Take Aways

- Largest PEC demo only made 50 grams of H2 per hour
- Need to get away from fluorinated polymers, lifetime required is much greater than for Fuel Cell Membranes
- Consider materials with lower efficiency but more durability to reduce cost
- Ability to produce/obtain high performing, lab-scale dual-junction PV for device development and demonstrations a real challenge

Action items

- There were no action items.

Session Attendee List

Session ID: P1
Title: PEC Priority Research Opportunities

Name	Affiliation
Bradley Layne	UC Irvine
Honghao Liu	UC Irvine
Siari Sosa	SoCalGas
Xiaohan Ma	Yale University
Joel Ager	LBNL
Haoran Chen	University of Toledo
Tingting Zhu	University of Toledo
Sol A Lee	Caltech
Kai Outlaw-Spruell	UH Manoa, hawaii
Lily Shiau	Caltech
YuYang Pan	University of Michigan
Zetian Mi	University of Michigan
Aaron Kaufman	University of Oregon
James Vickers	DOE

Session Attendee List

Session ID: P1
Title: PEC Priority Research Opportunities

Name	Affiliation
Shane Ardo	UC Irvine
Tadashi Ogatsu	LLNL
Huyen Dinh	NREL
Mason Jang	Caltech
Tom Jaramillo	SLAC
Henry Peel	TDA Research
Ryan Jones	Caltech

Session Summary

Session ID: P2-PEC

Title: PEC System Demonstration and Variation: what does a successful PEC pilot system look like in 2030

Summary of discussion

- Discussed key pilot demonstration metrics
  (1) stability: ~10,000 h
  (2) Efficiency: >10% or lower (5-8%)
  (3) Size: m^2-scale, kW-scale
- PEC system has distinct advantages over electrolysis: ease of deployment, more agnostic to electricity price, off-grid

Consensus and/or dissenting opinions

- Although the efficiency is not the best, achieving a durable PEC system can be more competitive.
- Safety issues (using strong acid or base electrolytes) should be considered.
- Extended period of testing under extreme weather conditions: can refer to accelerating aging tests done in LTE.

Key Take-Aways

- Achieving long-term "Stability" is important for the pilot PEC system.
  -elucidate the degradation mechanism
- For PEC pilot system, the costs (components, system), safety, and lifetime should be advantageous for the market adoption.
- Using small unit-cell with high efficiency and stability can be the platform for scale-up.

Action Items

- Dive into developing stable pilot PEC systems.
  -understand the possible factors affecting the stability
- Develop durability test and AST protocols.
- Understand scale-up challenges and get TEA & figure out key performance indicators.

Session Attendee List

Session ID: P2-PEC
Title: PEC System Demonstration and Variation: what does a successful PEC pilot system look like in 2030

Name	Affiliation
Zetian Mi	University of Michigan
Yuyang Pan	University of Michigan
Sol A Lee	Caltech
James Vickers	DOE
Honghao Liu	UC Irvine
Bradley Layne	UC Irvine
Aaron Kaufman	University of Oregon
CX Xiang	Caltech
Joel Haber	Caltech
Tadashi Ogitsu	LLNL
Ryan Jones	Caltech
Karl Gross	H2 Technology Consulting
Siari Sosa	SoCalGas
Mason Jang	Caltech
Lily Shiau	Caltech
Kai Outlaw-Spruell	Univerity of Hawaii
Shane Ardo	UC Irvine

Name	Affiliation
Tingting Zhu	University of Toledo
Haoran Chen	University of Toledo
Xiaohan Ma	Yale University
Joel Ager	LBNL and UCB
Huyen Dinh	NREL
Todd Deutsch	NREL
Peng Peng	

Session Summary

Session ID: P3

Title: PEC Seedling Cross-cuts

Summary

- NREL experience and challenges with scaling electrode to photoreactor were presented as they relate to seedling on-sun testing
- The Mural board was used to have participants answer several questions
  - For on-sun devices, should we prioritize innovation in designs or component comparability
  - Is it important to have periodic diagnostics (J-V) of device components over the course of on-sun testing?
  - What device metrics are important to track and at what rate should the data be collected?
- There was a discussion of whether all the seedling reactors should be tested concurrently or staggered

Consensus or dissenting opinions

- Dissenting: Some thought disrupting the 2-week on-sun tests my impact performance and shouldn't be done. Some thought a standard, reference component should be used to isolate/characterize individual components
- Consensus: Many voiced a preference for all systems to use MEAs as their electrolyzer component. It's too early to be prescriptive in device designs. It's important to gather diagnostics on components while the system is running to aid understanding and inform future approaches. Performance (of current-limiting junction) as a function of solar spectrum should be tracked, measuring H2 production isn't trivial. Measuring all 6 seedling devices simultaneously is desired but may not be possible

Take Aways

- We will learn a lot about how PEC devices perform under realistic conditions in the design of a testing platform and during 2-weeks of on-sun testing
- MEAs that can achieve high water-splitting currents at low voltages using DI water are a desirable option for the seedlings' electrolysis component
- Automated measurement of the hydrogen production rate will be challenging and require developing a robust method

Action items

- There were no action items.

Session Attendee List

Session ID: P3
Title: PEC HydroGEN Seedling Projects

Name	Affiliation
Bradley Layne	UC Irvine
Honghao Liu	UC Irvine
Siari Sosa	SoCalGas
Xiaohan Ma	Yale University
Joel Ager	LBNL
Haoran Chen	University of Toledo
Tingting Zhu	University of Toledo
Sol A Lee	Caltech
Kai Outlaw-Spruell	UH Manoa, Hawaii
Lily Shiau	Caltech
YuYang Pan	University of Michigan
Zetian Mi	University of Michigan
Aaron Kaufman	University of Oregon
James Vickers	DOE

Session Attendee List

Session ID: P3
Title: PEC HydroGEN Seedling Projects

Name	Affiliation
Shane Ardo	UC Irvine
Tadashi Ogitsu	LLNL
Huyen Dinh	NREL
Mason Jang	Caltech
Ryan Jones	Caltech
Chris Topping	Tetramer
Earl Wagener	Tetramer
CX Xiang	Caltech

Session Summary

Session ID: P5

Title: Hybrid and New Systems

Summary of discussion

Redox-chemistry-coupled indirect PEC water splitting

- Designs can decouple area, volume, and reaction rates, e.g. for time shifting or H_2 compression
- Enables redox that is incompatible with H_2 or O_2
- Reactor size and redox shuttle concentrations must be considered and carefully designed to mitigate mass transfer limitations
- Redox shuttle absorbance in the UV-Vis will hinder semiconductor performance; IR light absorption could speed reactivity via heating

Alternative oxidation reactions

- Designs can overcome slow O_2 evolution reaction kinetics and lack of value from the anodic reaction
- Entry or niche markets can increase value, but for scalability, large-volume products are desired such as partial oxidation of methane, biomass, glycerol, or for remediation

Synergy with CO_2 Reduction

- Designs could include photothermal reactions, such as using heat to drive C-C coupling reactions
- Could generally use H_2 as an "energy currency" for hydrogenation of CO_2 and for other reactions

Key Take-Aways

- Alternative cathodic reactions enable pressurization of H_2 without a costly compressor
- Alternative anodic reactions valorize oxidation chemistry, such as methane oxidation to methanol for ease of transportation
- Redox selectivity is a critical consideration, where low currently density operation may enable better control over it
- Having redox shuttle reactions could enhance durability
- "Particle-based designs," i.e. photocatalysis, could result in an increased STH efficiency due to operation at low current density per particle, and thus lower overpotential needs

Consensus and/or dissenting opinions

- Consensus

Action Items

- Possible perspective paper
- Funding to support new ideas

Session Attendee List

Session ID: P5

Title: Hybrid and New Systems

Name	Affiliation
Shane Ardo	UC Irvine
Aaron Kaufman	Univ. of Oregon
James Vickers	DOE
Tadashi Ogitsu	LLNL
Honghao Liu	UC Irvine
Huyen Dinh	DOE
Joel Haber	Caltech
Sol A Lee	Caltech
Lily Shiau	Caltech
CX Xiang	Caltech
Flavio de Cruz	SoCal Gas
Joel Ager	LBNL / UC Berkeley
Ryan Jones	Evolved Energy Research (?)
Todd Deutsch	NREL

Session Attendee List

Session ID: P5

Title: Hybrid and New Systems

Name	Affiliation
Bradley Layne	UC Irvine
Kai Outlaw-Spruell	Univ. of Hawaii

Session Action Item Assignments

Session ID: P5

Title: Hybrid and New Systems

Name	Affiliation	Action Item	Target Due Date
Shane Ardo & Shu Hu	UC Irvine & Yale Univ.	Perspective Paper on Photocatalytic Water Splitting	~2025 *(possible)*