# Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

## Breakout Session Summaries
## *Photoelectrochemical Water Splitting (PEC)*

**March 2 – 3, 2021**

# PEC Breakout Sessions

| Session ID | Topic | Lead |
|---|---|---|
| PEC-1 | Device and System Integration: New opportunities and Design Spaces for PEC Water Splitting | Todd Deutsch (NREL) |
| PEC-2 | Strategic Analysis TEA Review | Brian James (Strategic Analysis) |
| PEC-3 | Durability in Materials and Devices | Francesca Toma (LBNL) |
| PEC-4 | Photocatalyst and Particle Based Systems | Shane Ardo (UCI) |
| PEC-5 | Roadmap Review and Discussion | Daniel Esposito (Columbia)<br>Frances Houle (LBNL) |
| PEC-7 | Standard Hardware for Bench-Scale and Sub-Scale Testing | James Young (NREL) |

# Session Summary

**Session ID: PEC -01**

**Title: PEC-Device and System Integration: New opportunities and Design Spaces for PEC Water Splitting**

- **Summary of discussion**
  - Topic 1 : Energy islands, military applications, valorize $O_2$, water vapor splitting,
  - Topic 2: New reactor designs, manufacturability, $H_2$ carriers, water vapor, HPEV, optical engineer
  - Topic 3: Understand how PEC systems scale, optics research, thermal integration, lifetimes

- **Consensus and/or dissenting opinions**
  - Mostly consensus on the urgency to push out systems to understand scaling challenges
  - We still need more basic research on components (absorbers, membranes, catalysts, etc.) and interfaces between components because the ideal PEC system has not yet been identified

- **Key Take-Aways**
  - Several opportunities were identified that could increase the value proposition for PEC vs. PV/EC
  - New reactor designs are needed with novel approaches to $H_2$ collection and pressurization
  - There is a need for understanding how PEC systems scale in addition to materials research on component lifetimes and costs

- **Action Items**
  - Continue momentum from this Workshop by gathering folks in additional discussions, first late spring 2021
  - Gather community to write a perspective paper on the new science/research agenda identified targeting submission summer 2021

# Session Attendee List

**Session ID: PEC -01**

**Title: PEC-Device and System Integration: New opportunities and Design Spaces for PEC Water Splitting**

| Name | Affiliation |
|---|---|
| Nicolas Gaillard | Univ. of Hawaii |
| Olivia Alley | LBNL |
| Roel Van de Krol | HZB |
| Shu Hu | Yale |
| Sophia Haussener | EPFL |
| Vikash Kumar | EMPA |
| William Stinson | Univ. of Columbia |
| Yanfa Yan | Univ. of Toledo |
| Zejie (Justin) Chen | UC Irvine |
| Zhaoning Song | Univ. of Toledo |
| James Vickers | DOE |
| Aditya Mohite | Rice |
| Alex King | Univ. of Berkeley |
| Artur Braun | EMPA |

# Session Attendee List

Session ID: PEC -01

Title: PEC-Device and System Integration: New opportunities and Design Spaces for PEC Water Splitting

| Name | Affiliation |
|---|---|
| Brian James | Strategic Analysis Inc. |
| Todd Deutsch | NREL |
| Isaac Holmes-Gentle | EPFL |
| Shane Ardo | UC Irvine |
| CX Xiang | Caltech |
| John Lewis | NREL |
| Micha Ben-Naim | Stanford |
| Nico Gaillard | HNEI |
| Bruce Parkinson | Univ. of Wyoming |
| Jennie Huya-Kouadio | Strategic Analysis |
| Katie Hurst | NREL |
| Mark Ruth | NREL |
| Mark Spitler | Former DOE |
| Nathan Neale | NREL |

# Session Attendee List

**Session ID: PEC -01**

**Title: PEC-Device and System Integration: New opportunities and Design Spaces for PEC Water Splitting**

| Name | Affiliation |
| --- | --- |
| Austin Fehr | Rice |
| Cassidy Houchins | Strategic Analysis |
| Charles Mismukes | Rutgers |
| Chris Topping | Tetramer |
| Daiki Nishiori | ASU |
| Daniel Esposito | Univ. of Coumbia |
| Eric Miller | DOE |
| Frances Houle | LBNL |
| Huyen Dinh | NREL |
| Jason Cooper | LBNL |
| Hengfei Gu | Rutgers |

# Session Summary

**Session ID: PEC -02**

**Title: PEC TEA Review**

## Summary of discussion

- Validity of key parameters
  - T4 PEC absorber costs too low
  - Need more realistic/achieved lifetimes
  - Purity of water
  - Startup safety: purge H2 bed with N2?
  - Outdoor environment impact on cost (hail, etc.)
  - Get out of TEA
- Practical T4 absorber drives to high concentration
- BOP/concentrator is large cost contributor
  - Possibility of lower-cost solar concentrators
- Very far-off vision of magic low-cost perovskite

## Consensus and/or dissenting opinions

- TEA studies
  - Sensitivity to pressurization
  - Concentration: link capacity factor with optics cost, go to 1000x
  - Show impact of passive vs. forced convection
  - Clearly show materials vs. manufacturing costs
  - TEA in terms of energy input/output (in addition to cost)
  - Tradeoff between durable/expensive vs. cheap/replaceable materials. TEA on replacement interval.
  - Explore long-term operation cost (specifically plastic degrad. under sunlight and stretching)
- Very large gap between expensive T4 with concentration and vision of stable/low-cost materials (that don't currently exist). Need to do something different.

## Key Take-Aways

- Need to be innovative, very different ideas needed
  - Need to make something of high value (chlorine? )
  - Possibly operate at very low current density, made of cheap materials. Possibly vapor operation.
  - Solar Redox flow battery approach
- How can we leverage night-time to decrease costs?
- PV electrolysis is tough to beat. PV costs have come down significantly. Can we learn from that?
- When producing at pressure, biggest gain is the first 10 bars. (use mech. compression after that)
- Next big thing: Perovskites

## Action Items

- Access to tools to make manufacturing cost analysis more user-friendly. Often black box.

**Explore:**

- Redox couples to achieve compression
- Plug & Play/Modularity to reduce cost
- Maximize roll-to-roll processing
- Optical engineering
- Leverage advances in (TV) display technology? (TCO on glass)

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| Name | Affiliation |
|---|---|
| Brian James | Strategic Analysis Inc. |
| Todd Deutsch | NREL |
| Isaac Holmes-Gentle | EPFL |
| Shane Ardo | UC Irvine |
| CX Xiang | Caltech |
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| Micha Ben-Naim | Stanford |
| Bruce Parkinson | Univ. of Wyoming |
| Jennie Huya-Kouadio | Strategic Analysis |
| Katie Hurst | NREL |
| Hengfei Gu | Rutgers |
| Mark Ruth | NREL |
| Mark Spitler | Former DOE |
| Nathan Neale | NREL |

# Session Attendee List

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| Name | Affiliation |
|---|---|
| Nicolas Gaillard | Univ. of Hawaii |
| Olivia Alley | LBNL |
| Roel Van de Krol | HZB |
| Shu Hu | Yale |
| Sophia Haussener | EPFL |
| Vikash Kumar | EMPA |
| William Stinson | Univ. of Columbia |
| Yanfa Yan | Univ. of Toledo |
| Zejie (Justin) Chen | UC Irvine |
| Zhaoning Song | Univ. of Toledo |
| James Vickers | DOE |
| Aditya Mohite | Rice |
| Alex King | Univ. of Berkeley |
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| Chris Topping | Tetramer |
| Daiki Nishiori | ASU |
| Daniel Esposito | Univ. of Coumbia |
| Eric Miller | DOE |
| Frances Houle | LBNL |
| Huyen Dinh | NREL |
| Jason Cooper | LBNL |

# Session Summary

**Session ID: PEC-03**

**Title: Durability in Materials and Devices**

## Summary

- Stability is a problem for numerous classes of high performing PEC materials
- Corrosion, dissolution, pitting, delamination
- Protocols needed for both material and device level characterizations, plus accelerated aging
- Theoretical calculations using combinatorics can and do predict new stable metal oxides
- Report a list of device characteristics in each publication, share data via data hub like HydroGEN's

## Consensus/dissenting opinions

- Value of using theory for materials development: Often Pourbaix diagram calculation predicts bulk stability; needs further work for surface predictions
- Do we need to accelerate aging? May be more important when 1,000 hours has been accomplished, and 10,000 hours is the aim
- What's the incentive for people to report data on a data hub like HydroGEN's?
- Consensus: require reporting of e.g. specific duration CA for materials during publication

## Key take-aways

- Protocols exist currently to draw from, incl. HydroGEN stability protocols. Open access of further publications should enhance uptake.
- Protocol specifics: report experimental protocol, device statistics and failure times
- Defined accelerated testing would allow long stability measurements to be reported for each device
- Coatings can improve stability of otherwise unstable materials. Variable defects make evaluation of protection strategies difficult.

## Action Items

- Protocol for durability measurements on representative samples: CX to speak with Francesca to coordinate a multi-authored paper.
- Put a stability testing/stress test protocol together. Francesca to coordinate -- Daniel Esposito and Roel van de Krol interested, among many others.
- Huyen Dinh will check on availability of HydroGEN data hub for international users
- Special issue on protocols in PEC in Frontiers in Energy Research: incl. best practices to increase consistency in field

# Session Attendee List

**Session ID: PEC-03**

**Title: Durability in Materials and Devices**

| Name | Affiliation |
|---|---|
| CX Xiang | Caltech |
| Francesca Toma | LBNL |
| Shane Ardo | UC Irvine |
| Sophia Haussener | EPFL |
| Bruce Parkinson | Univ. of Wyoming |
| Tom Jaramillo | Stanford |
| Eric Miller | DOE |
| Todd Deutsch | NREL |
| France Houle | LBNL |
| Adam Neilander | Stanford |
| Shu Hu | Yale |
| Roel van de Krol | HBZ |
| Zhaoning Song | Univ. of Toledo |
| Nathan Neale | NREL |

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|---|---|
| Isaac Holmes-Gentle | EPFL |
| Chris Topping | Tetramer |
| William Stinson | Univ. of Columbia |
| Daniel Esposito | Univ. of Columbia |
| Vikash Kumar | EMPA |
| Alex King | Univ. of Berkeley |
| Aditya Mohite | Rice |
| Charles Mismukes | Rutgers |
| Daiki Nishiori | ASU |
| Zejie (Justin) Chen | UC Irvine |
| Austin Fehr | Rice |
| Hengfei Gu | Rutgers |
| Nicolas Gaillard | Univ. of Hawaii |
| Jason Cooper | LBNL |

# Session Attendee List

**Session ID: PEC-03**

**Title: Durability in Materials and Devices**

| Name | Affiliation |
|---|---|
| Zetian Mi | Univ. Michigan |
| Olivia Alley | LBNL |
| Zachary Clifford | Rutgers |
| Katie Hurst | NREL |
| James Young | NREL |

# Session Summary

Session ID: PEC-4

Title: Photocatalysis

## Summary of Discussion

- Overview of field (reactors, theory, exps., etc.)
- What differs between photocatalysis (PC) and photoelectrochemistry (PEC)?
- Specific considerations for PC (vs. PEC) protocols at the level of (M)aterials, (C)omponents, and (D)evices
- Many inquiries about details of PC reactors, considerations, and types of measurements

## Consensus and *(no major)* Dissenting Opinions

**Differences between Photocatalysis (PC) and Photoelectrochemistry (PEC):**

- electrochemically coupled tandem (shuttle diffusive transport, reaction selectivity, cocatalysts mediate back reactions, separator)
- large photoabsorber surface area (large recomb./generation SRVs, short charge-carrier collection lengths, thin-layer cocatalysts)
- isolated small particles (mobile photoabsorbers, possibly facile syntheses, isolated degradation points, possibly easy to replace materials, smaller absorbed photon flux from blackbody and sunlight sources, unique nano-optical properties)
- opportunities for new solar $H_2$ processes and reactor designs

## Key Take-Aways

- There is a lot of excitement to innovate on new ideas in PC and PEC
- Less is known broadly about the PC field than the PEC field
- Many more interrelated properties in PC than in PEC
- Key challenge is to determine how to bridge data from single-particle measurements to reactor-scale observations

## Action Items *(not discussed during session)*

**Session Chair**

- Read existing PEC protocols and identify those to update with PC
- *Contact attendees to determine who will help with the following:*
- Oversee updating, or generating new, ~10 PEC protocols, with PC

**Session Chair's Project Team, et al.**

- Develop protocols unique to PC
  (M1) Redox shuttle characterization
  (C1) Baggie material characterization
  (D1) STH Standards: stir rate, particle conc., light profile, $pH_2/pO_2$
  (D2) Modify/use Type 1 protocols from Feb. 2021 *Joule* article
- Write and publish detailed PC perspective paper

# Session Attendee List

Session ID: PEC-4

Title: Photocatalysis

| Name | Affiliation |
|---|---|
| Shane Ardo | UCI |
| Zejie Chen | UCI |
| Chengxiang Xiang | Caltech |
| Todd Deutsch | NREL |
| Adam Weber | LBNL |
| Alex King | LBNL |
| Aliya S. Lapp(Aslapp) | SNL |
| Bruce Alan Parkinson | University of Wyoming |
| Charles Dismukes | Rutgers University |
| Chris Topping(Ctopping) | Tetramer Technologies,L.L.C. |
| Daniel Esposito | Columbia University |
| Earl Wagener | Tetramer |
| Eric Garfunkel | Rutgers University |
| Eric Miller | DOE |

# Session Attendee List

Session ID: PEC-4

Title: Photocatalysis

| Name | Affiliation |
|---|---|
| Hengfei Gu(Hengfei) | Rutgers |
| Huyen Dinh | NREL |
| Isaac Holmes-Gentle | EPFL |
| James Vickers | DOE |
| Jason Cooper | LBL |
| James Young (Jyoung3) | NREL |
| Micha Ben-Naim | Stanford |
| Michael Wong | Rice |
| Olivia Alley | LBNL |
| Robert Stinson | Columbia University |
| Roel van de Krol | HZB |
| Rohini Bala Chandran | University of Michigan |
| Vikash Kumar | EMPA |
| William Stinson | Columbia University |

# Session Attendee List

**Session ID: PEC-4**

**Title: Photocatalysis**

| Name | Affiliation |
|---|---|
| Zetian Mi | University of Michigan |
| Zijie Chen | University of Michigan |
| Adam Nielander | Stanford |
| Zachary Clifford | Rutgers University |

# Session Summary

Session ID: PEC-5

Title: PEC Roadmap Review

## Summary

- Reviewed prev. roadmaps /performance targets PEC components and systems
- Discussion organized based on 4 key PEC elements and 3 PEC technology pathways
- Participants filled out a survey & MURAL board identifying and assessing key bottlenecks, as well as timelines needed to overcome those bottlenecks

## Consensus

- Wide range of progress across different components and pathways
- Pattern of gaps spanning all pathways that need to be systematically assessed
- Lacking expertise in failure analysis protocols for durability assessment
- **Dissenting view**: PV electrolysis is closer to practice; why do integrated PEC at all?

## Key Take-Aways

- H2 makes sense for PEC and reasonable to create a meaningful roadmap
- Roadmap should account for needed progress in both components & devices (sub-roadmaps helpful too!)
- Today: Type IV > Type III >> Type II, although "entitled technology" not clear

## Action Items / Recommendations

- R: Regularly updated pathway-specific road-maps based on latest technical progress is needed, and should be an intl' effort
- R: 1 $m^2$ + demos are essential to both R&D efforts & accurate long range roadmap
- R: Consolidated list of intl. PEC program
- A.I.: Short summary report of survey that captures comments of MURAL board

# Session Attendee List

**Session ID: PEC-5**

**Title: PEC Roadmap Review**

| Name | Affiliation |
|---|---|
| Dan Esposito | Univ. of Columbia |
| Todd Deutsch | NREL |
| Tom Jaramillo | Sandford |
| Katie Randolph | DOE |
| James Young | NREL |
| CX Xiang | Caltech |
| Adam Nielander | Stanford |
| James Vickers | DOE |
| William Stinson | Univ. of Columbia |
| Shu Hu | Yale |
| Zhaoning Song | Univ. of Toledo |
| Zetian Mi | Univ. of Michigan |
| Huyen Dinh | NREL |
| Isaac Holmes-Gentle | EPFL |

# Session Attendee List

**Session ID: PEC-5**

**Title: PEC Roadmap Review**

| Name | Affiliation |
|---|---|
| Karl Gross | H2 Technology Consulting |
| Roel Van De Krol | HZB |
| Waseer Mohamed | Univ. of Columbia |
| Shane Ardo | UCI |
| Frances Houle | LBNL |
| Charles Dismukes | Rutgers |
| Earl Wagnerer | Tetramer |
| Bruce Parkinson | Wyoming |
| Francesca Toma | LBNL |
| Krishani Teeluck | Rutgers |
| Micheal Wong | Rice |
| Robert Stinson | Univ. of Columbia |
| Ned Stetson | DOE |

# Session Attendee List

**Session ID: PEC-5**

**Title: PEC Roadmap Review**

| Name | Affiliation |
|---|---|
| Sixuan Hou | Columbia |
| Zejie Chen | UCI |

# Session Summary

**Session ID: PEC-07**

**Title: Standard bench- and sub-scale hardware**

- Summary of discussion
  - Discussed bench- and sub-scale definitions appropriate for current status of PEC
  - Discussed design needs for bench- and sub-scale standard hardware
  - Discussed the continuing development of two hardware examples that may facilitate standard testing configurations
  - Discussed subscale demonstration targets the field should strive to reach within 5 years and the critical barriers to meeting these targets

- Consensus and/or dissenting opinions
  - PEC-specific bench- and sub-scales by vote:
    - Current bench scale definition: 1-10 $cm^2$
    - Current subscale definition: >0.1-1 $m^2$
  - Within 5 years, the field should strive to achieve demonstrations with STH >10% and >100-hr durability at 0.1-1 $m^2$ scale. Particle photocatalyst systems have less stringent 5-yr targets.

- Key Take-Aways
  - Standardization is helpful for systematic progress, but the field should also explore novel photoreactor concepts
  - Lack of standard hardware not a hindrance to scaling studies which are necessary regardless
  - Scaling studies with model integrated PV-E needed to understand future challenges
  - Although there are general DOE $H_2$ production definitions for bench- and sub-scale, PEC-specific definitions at smaller scale may be more useful to classify near-term PEC scaling efforts

- Action Items
  - Those in the PEC community are encouraged to make their hardware design files public to facilitate open-source development of hardware

# Session Attendee List

**Session ID: PEC-07**

**Title: Standard bench- and sub-scale hardware**

| Name | Affiliation |
|---|---|
| James Young | NREL |
| Todd Deutsch | NREL |
| CX Xiang | Caltech |
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| Adam Nielander | Stanford |
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| Zhaoning Song | Toledo |