Benchmarking Advanced Water Splitting Technologies: Best Practices in Materials Characterization

HydroGEN PEC Questionnaire
(Distributed May 8, 2018)
Summary of Responses
38 responses as of November 2018

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The PEC Questionnaire can be found at: https://datahub.h2awsm.org/dataset/benchmarking-pec-survey-response/resource/c1b431a9-415b-4447-b6da-d4eb5ef3625e

Background and motivation: We aim to develop standards for benchmarking performances, comparisons between devices from different research groups can be made in future. Three sections were included in this questionnaire: (I) What standard conditions should we use to benchmark devices for unassisted photoelectrochemical water splitting? (II) What standard materials would be the most useful? (III) What sort of standard chassis would be the most useful? The background and motivation for each section were included in the summary report below.

A questionnaire was sent to EMN project leads, National Lab Node Leads, Industry, academic and international experts in the Spring of 2018. The goal of this effort was to collect broad feedback across the water splitting community with a specific target of obtaining at least a 50% response rate from EMN Level 1 Node Leads and Project PI's.

As part of the questionnaire, respondents were asked if they wished to provide feedback to the proposed test framework. Access to the draft framework documents was provided for those interested and they will be able to add comments/edits. Following the collection of feedback, the framework will be reviewed and updated.

The following table illustrates the feedback received to date (November 2018). See attached summary report for detailed feedback.

Affiliations	Sent	Received	Response Rate (%)
EMN (Level 1 PEC Node experts and Seedling PIs)	28	23	82%
Domestic (Non-EMN)	54	8	15%
International	25	7	28%
Total	107	38	36%

Acronyms

FF – fill factor
OER – oxygen evolution reaction
PEC – photoelectrochemical
PV – photovoltaic
STH – solar to hydrogen
V(OC) / V_{OC} – open circuit voltage

Summary of PEC Questionnaire Responses

Section 1: What standard conditions should we use to benchmark devices for unassisted photoelectrochemical water splitting?

Background and motivation*: We aim to develop standards for benchmarking performance, so comparisons between devices from different research groups can be made in the future. In addition to device-specific optimal operating conditions, community-accepted standard tests, developed through this exercise, are strongly encouraged to include in publications.*

1.) Do you think reporting the performance of devices at standard conditions, in addition to "favored" testing conditions, would be useful?

Yes: **94.6%**
No: **5.4%**
Main concerns about materials/devices underperforming at standardized conditions. Others suggested having a few options within standard conditions.

2.) Should we choose a minimal photoelectrode area for benchmarking un-assisted PEC water splitting? If so, what MINIMUM photoelectrode area should ALWAYS be reported for benchmarking? (choose one)

1.0 cm^2 : **34.3%**
0.5 cm^2 : **14.3%**
0.1 cm^2: **25.7%**
No: **11.4%**
Other: **14.3%**

Some suggested having levels of standardization at different sizes, and grouping results by size.

3.) Should we choose one or several standards for operating pHs? If so, what pH values should ALWAYS be reported for benchmarking? (choose all that apply)

0,7,14: **44%**
0, 14: **31%**
No: **25%**

Many suggested allowing groups to choose one of the standard pH values, rather than testing at multiple pHs. Some said pH should be part of device design, but that would be the difference between standard and favored conditions. Some indicated that PEC technology is not developed enough for these standards.

4.) What electrolyte(s) should ALWAYS be reported for benchmarking in acidic conditions? (choose all that apply)

H_2SO_4: **56%**
H_2SO_4, $HClO_4$: **19%**
H_2SO_4, $HClO_4$, HCL: **13%**

None: **13%**

Similar comments to 3), many said allow one of a few standard acids.

5.) What electrolyte(s) should ALWAYS be reported for benchmarking in neutral conditions? (choose all that apply)

Phosphate buffer solution: **41%**
None: **32%**
Unbuffered KCl or NaCl: **5%**
Other: **22%**

Similar comments to 3), other electrolytes, such as Na, K sulfate or Na, K perchlorate were also suggested.

6.) What electrolyte(s) should ALWAYS be reported for benchmarking in basic conditions? (choose all that apply)

KOH: **38%**
NaOH: **8%**
KOH, NaOH: **29%**
None: **25%**

Similar comments to 3), some insisted high purity NaOH or KOH electrolytes.

7.) Should standard illumination conditions be reported for benchmarking? If yes, what illumination intensities should ALWAYS be reported for benchmarking? (choose all that apply)

1 Sun: **86%**
Any standard intensity: **4%**
Other: **10%**

All "Other" answers included 1 Sun as well as other intensities. Some commented on a need to make the standard more like real world conditions.

8.) What MINIMUM number of diurnal cycles should ALWAYS be reported for benchmarking? (choose one)

20 cycles: **11.4%**
4 cycles: **20%**
1 cycle: **17.1%**
None: **14.3%**
Other: **37.2%**

Some had concerns about this disqualifying materials before stability has been worked out. Many wanted more basic research into diurnal cycling before setting a standard.

9.) Do we need to benchmark operating temperature? If so, what temperatures should ALWAYS be reported for benchmarking? (choose all that apply)

30°C: **84%**
70°C: **8%**
30°C and 70°C: **8%**

Some comments worried about the challenge of precise thermal control, while others said it was necessary. Some said that proper reporting of temperature was more important than control.

10.) Which parameters other than solar-to-hydrogen efficiency should ALWAYS be reported for ALL benchmarking conditions? (choose all that apply)

7% of respondants said STH only
Of the remain answers, the breakdown was
Total H_2 in kg: **29%**
Faradaic efficiency for HER and OER: **43%**
Spectral response: **29%**

11.) Comments and/or questions that we missed regarding benchmarking conditions?
Some respondents had concerns about whether these standards would apply to other types of PEC systems (particulate, vapor, etc.)
Some respondents indicated a need for measurement of conditions during benchmarking tests. Light source calibration was stressed.

Section2: What standard materials would be the most useful?

Background and motivation*: Working with HydroGEN Lab nodes, we aim to develop standard materials and/or devices that can be used to compare conditions between different labs and enable rapid prototyping.*

1.) Would standard light absorbers that produce enough voltage for unassisted water splitting be useful for testing catalysts or protecting layers? If yes, which would be most useful?

Triple junction amorphous silicon: **14.7%**

Tandem junction III-V: **8.8%**

Triple junction III-V from Spectrolab Inc: **14.7%**

Custom tandem III-V: **14.7%**

Not useful: **17.6%**

Other: **29.5%**

Other comments include: Some suggested perovskite solar cells, possibly as hybrids with these kinds of materials. Some suggested materials should be commercially available and reproducible. Some suggest integration of protective coatings and catalysts onto light absorbers is challenging and should do it in partnership. Some explained that all the key parameters can be obtained using 3-electrode measurements, and hence, light absorbers that are capable of un-assisted water-splitting is not useful for benchmarking purpose.

2.) Would a standardized photocathode or photoanode be useful to characterize or integrate catalysts or protective coatings? If yes, which would be most useful? (J-V characteristicss for the referenced electrodes are shown below)

n-p+-Si: **13.3%**

p-n+-Si: **3.3%**

p-Si: **6.7%**

n-Si: **6.7%**

np+-GaAs: **0%**

p-GaAs: **0%**

n-GaAs: **3.3%**

Not useful: **30%**

Other: **6.7%**

Some suggested InGaP, some suggested degenerate wafers for stability test, some suggested commercially available and reproducible materials for this purpose, some expressed the difficulty in obtaining the standard materials with robust performances.

3.) Would you find any of these catalysts useful as a standard dark anode for OER to test photocathodes?

None, these are readily available: **12.1%**

Ni/NOx for pH=14: **3.3%**

IrO2 for pH=0: **36.4%**

RuO2: **12.1%**

NiFeOx: **6.1%**

Other: **30%**

Some expressed the difficulty in obtaining standard materials in terms of contamination, morphology, etc., some explained that dark cathode or anode are not useful since 3-electrode measurements can tell all the key parameters for the light absorber. Other research materials were also suggested.

4.) Would you find any of these catalysts useful as a standard dark anode for HER to test photocathodes?

None, these are readily available: **18.2%**

Pt: **57.6%**

Pd: **3%**

Other: **21.2%**

Very similar comments to 3).

5.) Comments and/or questions that we missed in this topic?

Most topics were covered, several suggested that we should not limit to specific electrode or catalyst materials, and each system needs to be considered differently.

Section 3: What sort of standard chassis would be the most useful?

***Background and motivation**: We aim to design a standard chassis that will facilitate rapid testing of devices. The goal would be to widely distribute these and ensure benchmarking is consistent as possible. Depending on the cost of production, we may be able to distribute these beyond the labs directly involved in this initiative.*

1.) Would a standardized chassis design be useful?

Yes: **76.5%**

No: **5.9%**

Other: **17.6%**

Some suggested that chassis is part of the device/design and should not be standardized. Some expressed the challenge in access to such standard chassis and active size limitations.

2.) What chassis material should be used for benchmarking in acidic solutions? (choose one)

Teflon: **48.5%**

Acrylic: **3%**

Polycarbonate: **9.1%**

High density polyethylene: **12.1%**

Other: **27.3%**

Some suggested glass cell, some suggested clear resin that's stable and durable.

3.) What chassis material should be used for benchmarking in basic solutions? (choose one)

Teflon: **53.1%**

Polycarbonate: **12.5%**

High density polyethylene: **12.5%**

Other: **21.9%**

Some suggested clear resin that's stable and durable.

4.) What chassis style would your lab like to work with?

Single unit louvered: **6.3%**

Planar cell: **21.9%**

Wired two electrode cell: **34.4%**

Other: **37.4%**

Some suggest that the chassis style is part of the research and should not be restricted. Some suggested multiple configurations.

5.) What maximum price range would you be willing to pay for a standard cell? Labs participating in HydroGEN should be provided cells as part of the initiative, but we would like to gauge whether these can be produced at a price that other labs could afford. (choose one)

Less than $10: **0%**

$10-$30: **5.9%**

$30-$50: **11.8%**

$50-$100: **14.7%**

More than $100: **17.6%**

Price is not the first consideration for us: **34.2%**

Other: **15.8%**

A ide range of costs were suggested. Performance and reliability are far more important factors, and worth extra cost.

6.) What is the price of the current cell your lab uses to test photoelectrochemical devices? It would be useful to consider designing cells that would be a competitively priced alternative that labs outside the initiative would purchase.one)

Many cells were custom made in researcher's group and a wide range of pricing from $25 to $1700 was suggested.

7.) Other things that you would like to know, please list.

Some suggested to have a standard and make standard PEC testing cells commercially available.

<u>Section 4:</u> Open Questions

1. What are the most pressing needs/challenges for PEC water splitting?
   Device stability: **82%**
   Lack of suitable light absorbers: **9%**
   Cost per kg of H_2: **9%**

2. What are the critical parameters to calculate and characterize for PEC?
   STH was the most common
   Stability was also a frequent answer
   Some were interested in J-V characteristics (including V_{OC}, photovoltage, FF)

3. How can we accelerate testing of device stability?
   Several responded that devices are not yet stable enough to worry about accelerating degradation, but that this concern should be tabled for future discussion.
   Answers among others varied, but mostly fell into either high-throughput testing or extreme testing conditions (higher illumination intensity, high/low temperatures)
   A few thought diurnal cycling was important at this stage.

4. What additional techniques/instruments/capabilities would be most useful for the HydroGEN consortium to develop (see existing capabilities at https://www.h2awsm.org/)?
   Most capabilities that were suggested seem to be included by at least one node in the consortium, so connecting labs to nodes with the right capabilities to assist them might be the challenge.
   Nodes equipped to study particle suspension reactors were suggested by a few.

5. What is the most immediate way to address the scale up challenge (elaborate a bit on the gaps)?
   Several suggested that it is premature to address this before some high efficiency and stable devices are demonstrated that compete with PV-electrolyzer.
   Some indicated that public demand is the critical limiting factor.
   Some suggested less expensive methods for deposition (especially of III-Vs) that are highly reproducible

6. Additional questions or comments regarding PEC water-splitting?
   Few people had additional questions, and most reiterated concerns about competitiveness with PV-electrolyzer technologies.

7. Would you like to get involved in developing the Test Framework for PEC water-splitting? and here is what the Test Framework might look like.

   Yes: **52.6%**
   No: **13.2%**
   Maybe: **34.2%**