

HydroGEN PEC Benchmarking Questionnaire

This survey is designed to collect feedback about best practices for screening and benchmarking of materials, component and devices for PEC water-splitting from the research community. The survey begins with three multiple choice sections that address 1) conditions used during the benchmarking of PEC devices, 2) standard PEC materials, and 3) standard chassis materials/designs. These questions will help develop guidelines for the best practices to use in benchmarking PEC device performance and enable effective comparison of devices across research groups. At the end of the survey, we have also included open questions on critical areas that need further development and how collaboration with national labs can best advance this technology.

After the survey, we would like know whether you would be interested in participating in the development of a Test Framework for PEC water-splitting. If you would like to get involved, we will send out a follow-up email that includes a draft Test Framework and ask for your edits/comments /suggestions. By drawing from the experience of our experts in photoelectrochemistry, we hope to streamline data collection and foster a collaborative environment that leads to new breakthroughs in PEC water-splitting.

* Required

1. Email address *

2. Please list your name: *

3. Please list your affiliation *

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.

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

Mark only one oval.

Yes

No

5. If no, please explain:

6. 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)

Mark only one oval.

- A minimum size is unnecessary
- 0.1 cm²
- 0.5 cm²
- 1.0 cm²
- Option 5
- Other: _____

7. 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)

Check all that apply.

- 0
- 7
- 14
- Other: _____

8. If no, please explain:

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

Check all that apply.

- H₂SO₄
- HClO₄
- HCl
- Other: _____

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

Check all that apply.

- Phosphate buffer solution
- Borate buffer solution
- Un-buffered KCl or NaCl solution
- Other: _____

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

Check all that apply.

- NaOH
- KOH
- Other: _____

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

Check all that apply.

- A standard illumination is necessary
- 0.1 Sun
- 1 Sun
- 10 Sun
- Other: _____

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

Mark only one oval.

- Diurnal cycling is unnecessary (please explain below)
- 1
- 2
- 4
- 20
- 40
- Other: _____

14. If you think diurnal cycling is unnecessary, please explain:

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

Check all that apply.

- ~30 C (room temperature)
- ~70 C (elevated temperature)
- Other: _____

16. If you don't think we need to benchmark operating temperature, please explain:

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

Check all that apply.

- None, STH is sufficient
- Total hydrogen produced in kg
- Faradaic Efficiency for HER and OER
- Spectral responses
- Other: _____

18. 11.) Comments and/or questions that we missed regarding benchmarking conditions?

Skip to question 18.

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.

19. **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?**

Mark only one oval.

- Triple junction amorphous silicon? (e.g., $V(OC)=2.2$ V, $J(SC)=7$ mA/cm², $FF=0.57$) (J.Jin et al., Energy Environ. Sci., 2014, 7, 3371-3380 and SY Reece et al., Science, 2011, 334, 645-648)
- Tandem junction III-V (e.g., $V(OC)=2.4$ V, $J(SC)=7.6$ mA/cm², $FF=0.76$) (E. Verlage et al., Energy Environ. Sci., 2015, 8, 3166-3172)
- Triple junction III-V from Spectrolab Inc.? (e.g., $V(OC)=2.55$ V, $J(SC)=14.85$ mA/cm², $FF=0.7$) (K. Walczak et al., Adv. Energy Mater., 2017, 7, 1602791)
- Custom tandem III-V ($V(OC)>2.0$ V, $J(SC)=11.5$ mA/cm²) (JL Young et al., Nature Energy, 2017, 2, 17028)
- Not useful
- Other: _____

20. **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 characteristics for the referenced electrodes are shown below)**

Mark only one oval.

- n-p+-Si photoanode ($V(OC)=0.55$ V, $J(SC)=33.6$ mA/cm², $FF=0.29$) (see S.Hu et al., Science, 2014, 344, 1005-1009)
- p-n+-Si ($n(D)=$ not reported, $V(OC)=0.58$ V, $J(SC)=30$ mA/cm², $FF=0.58$) (see M. Kast et al., ACS Appl. Mater. & Inter., 2014, 6, 22830-22837)
- p-Si ($V(OC)=0.37$ V, $J(SC)=22.7$ mA/cm², $FF=0.58$) (see E.L. Warren et al., J. Phys. Chem. C, 2011, 115, 594-598)
- n-Si ($n(D)=1 \times 10^{19}$ cm⁻³), $V(OC)=0.55$ V, $J(SC)=34.7$ mA/cm², $FF=0.29$) (see S.Hu et al., Science, 2014, 344, 1005-1009)
- np+-GaAs ($n(D)=5 \times 10^{17}$ cm⁻³), $V(OC)=0.77$ V, $J(SC)=33.6$ mA/cm², $FF=0.86$) (see S. Hu et al., Science, 2014, 344, 1005-1009)
- p-GaAs ($n(D)=1 \times 10^{17}$ cm⁻³), $V(OC)=0.7$ V, $J(SC)=22$ mA/cm², $FF=$ not reported) (see JL Young et al., J. Mater. Chem. A, 2016, 4, 2831-2836)
- n-GaAs ($n(D)=5.5 \times 10^{16}$ cm⁻³), $V(OC)=0.7$ V, $J(SC)=20$ mA/cm², $FF=0.6$) (see F.Yang et al., J. Phys. Chem. C., 2016, 120, 6989-6995)
- Not Useful
- Other: _____

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

Mark only one oval.

- None, these are readily available.
- Ni/NO_x for pH=14
- IrO₂ for pH=0
- RuO₂
- NiFeO_x
- Other: _____

22. **4.) Would you find any of these catalysts useful as a standard dark cathode for HER to test photoanodes?**

Mark only one oval.

- None, these are readily available
- Pt
- Pd
- Ni/NiO_x
- Other: _____

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

What sort of standard chassis would be the most useful?

Background and motivations: 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.

24. **1.) Would a standardized chassis design be useful?**

Mark only one oval.

- Yes
- No
- Other: _____

25. If no, please explain:

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

Mark only one oval.

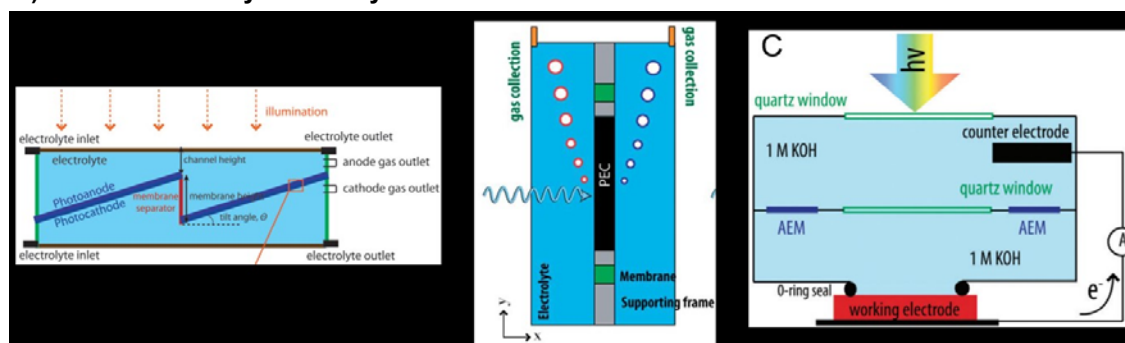
- Teflon
- Acrylic
- Polycarbonate
- High density polyethylene
- Other: _____

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

Mark only one oval.

- Teflon
- Acrylic
- Polycarbonate
- High density polyethylene
- Other: _____

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



Mark only one oval.

- Single unit louvered (K. Walczak, et al., ChemSusChem, 2015, 8, 544-551)
- Planar cell (J. Jin et al., Energy Environ. Sci., 2014, 7, 3371-3380)
- Wired two electrode cell (E. Verlag et al., Energy Environ. Sci., 2015, 8, 3166-3172)
- Other: _____

29. **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)**

Mark only one oval.

- Less than \$10
- \$10-\$30
- \$30-\$50
- \$50-\$100
- More than \$100
- Price is not the first consideration for us
- Other: _____

30. **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.**

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

OPEN QUESTIONS

32. **1.) What are the most pressing needs/challenges for PEC water splitting?**

Mark only one oval.

- Lack of suitable abundant materials
- Device stability
- STH efficiency
- Cost per kg of H₂
- Other: _____

33. 2.) What are the critical parameters to calculate and characterize for PEC?

34. 3.) How can we accelerate testing of device stability?

35. 4.) What additional techniques/instruments/capabilities would be most useful for the HydroGEN consortium to develop (see existing capabilities at <https://www.h2awsm.org/>)?

36. 5.) What is the most immediate way to address the scale up challenge (elaborate a bit on the gaps)?

37. 6.) Additional questions or comments regarding PEC water-splitting?

Feedback on Test Framework

38. 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. *

Material properties

Class of Material	Key Parameters	Standard	Techniques	References	Notes/Limitations	
Photo-absorber	Bandgap	Si: 1.1eV^1	UV-vis	2,3	-Subjective analysis -Bulk band gap may differ from surface	
			PL	4	-Shows optimum performance	
	Band positions (valence band/conduction band)	n-Si (111): $E_{\text{gap}}^{\text{Si}} = 0.88\text{ eV}^5$ p-Si (111): $E_{\text{gap}}^{\text{Si}} = 0.27\text{ eV}^5$		EIS (Flat band potential)	7	-Surface heterogeneity -Impacted by surface states -No spatial resolution
				XPS/UPS	6,7	-Ex situ
	Minority carrier diffusion length (carrier mobility, carrier life time)	p-Si (B-doped, $n_D = 6 \times 10^{15}\text{ cm}^{-3}$): 250 μm n-Si (P-doped, $n_D = 5 \times 10^{16}\text{ cm}^{-3}$): 168 μm^8		Transient absorption spectroscopy	9	-Measures lifetime only
				Time-resolved Photoluminescence	10	-Cryogenic temperatures -Non-radiative sources of decay may contribute
				Electron Beam-Induced Current	11	-Typically qualitative -Damages organic materials -Ex situ
				Chopped photocurrent-time	12	-Low precision
	Doping types and doping concentrations	p-Si: B, $6 \times 10^{15}\text{ cm}^{-3}$ n-Si: P, $5 \times 10^{16}\text{ cm}^{-3}$ ⁸		EIS (Mott-Schottky)	2,9,13	-Amorphous structures -Surface states
				Hall measurements		-Low mobility -High polycrystallinity -Multiple carrier species
Photo-generated carrier collection efficiency			EQE	2,9,13,15	-Sensitive to lamp calibration	
			IQE		-Determination of absorbed photons difficult	

Mark only one oval.

- Yes
- No
- Maybe

A copy of your responses will be emailed to the address you provided

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