HydroGEN
Advanced Water Splitting Materials

Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Breakout Session Supplemental Slides
Photoelectrochemical Water Splitting (PEC)

March 2 – 3, 2021

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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) Frances Houle (LBNL)
PEC-7	Standard Hardware for Bench-Scale and Sub-Scale Testing	James Young (NREL)

Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

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

Technology: PEC

Session ID: PEC-1
Session Chair: Todd Deutsch
Affiliation: NREL
Date: March 2, 2021

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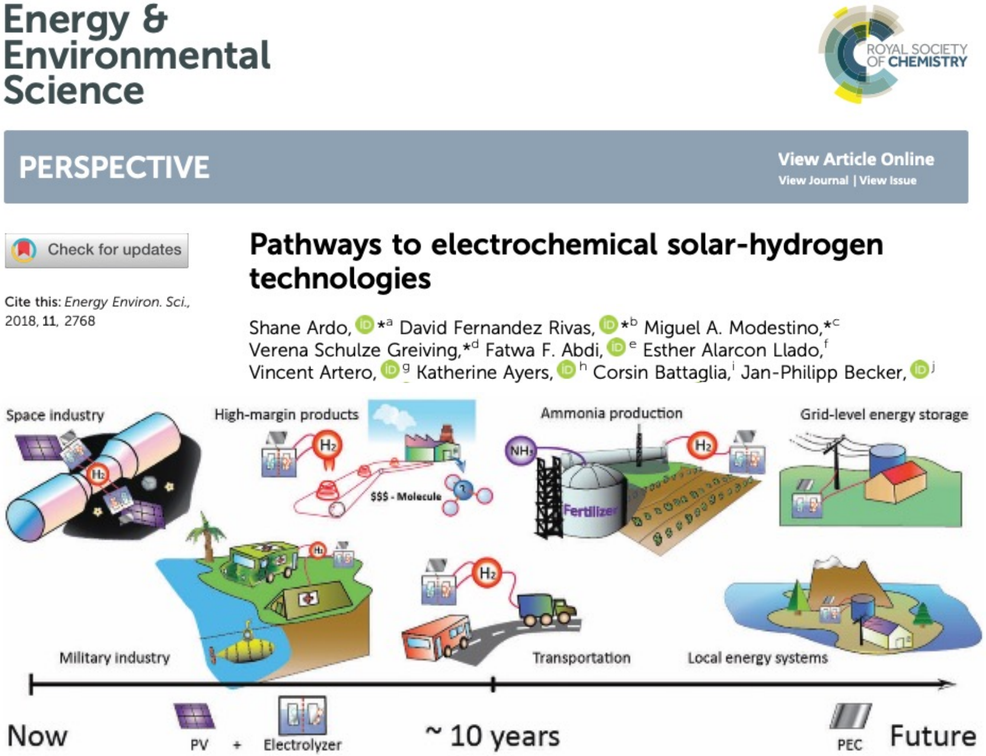
Session goals

- Brief introduction of the topic
  - Solar-generated H_2 is the most technologically advanced solar fuel but has stalled at deployment. This breakout session will examine a few case studies, with different degrees of photo-electrochemical integration, that show promising system-level solutions for efficient and stable solar water splitting. We will discuss how these approaches might offer a new value proposition for solar hydrogen in specific applications and identify opportunities for pilot-scale projects.
- Session Logistics
  - Session topic introduction (20 min),
  - Mural-facilitated discussion, 3 topics (45 min)
  - Summarize and discuss action items (10 min)
  - Rules for session: Mural- please add your name when signing in as visitor
  - Start with sticky notes, then discussion based on that input
  - Report out

Background and motivation

- Photo-electrochemical hydrogen: time to move from bench to pilot scale
  - 2016 workshop- Leiden, Netherlands
- Scaling will take time and effort
  - Manufacturing readiness level
  - Supply chain, distribution, market analysis
- Beyond the semiconductor-liquid junction – buried junction
  - Enabled higher efficiency and durability
- Expand value proposition – Look for niche applications where wet, lower pressure H_2 can be used and has value over PV-electrolysis
  - Biomethanation, steel making, separate step in CO_2 reduction process
  - PEC flow batteries



Energy & Environmental Science

ROYAL SOCIETY OF CHEMISTRY

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Cite this: *Energy Environ. Sci.*, 2018, **11**, 2768

Pathways to electrochemical solar-hydrogen technologies

Shane Ardo, *[a] David Fernandez Rivas, *[b] Miguel A. Modestino,*[c] Verena Schulze Greiving,*[d] Fatwa F. Abdi, [e] Esther Alarcon Llado,[f] Vincent Artero, [g] Katherine Ayers, [h] Corsin Battaglia,[i] Jan-Philipp Becker, [j]

PV-electrolysis facilities:

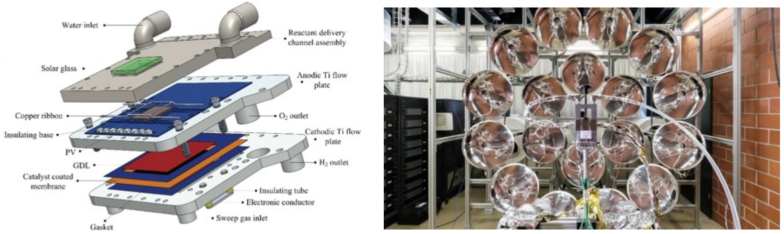
6MW Linz, Austria

10 MW electrolyzers + 20MW PV – Fukushima, Japan

Integrated concentrated PV-electrolysis

Sophia Haussener – EPFL

- III-V tandems with >15% STH efficiency
- Durability by encapsulation
- Concentration ~1000x to defray absorber cost
  - Membrane electrode assembly- high current without bubbles/scattering
- Thermal integration
  - PV cooling, electrolyzer heating
- Demonstration at scale
  - 7 m diameter dish
  - >1000x concentration



Small (~120W), ~0.8 g_{H2}/h, η_{STH}=17%, *t*=minutes, indoor, controlled

Commercialization

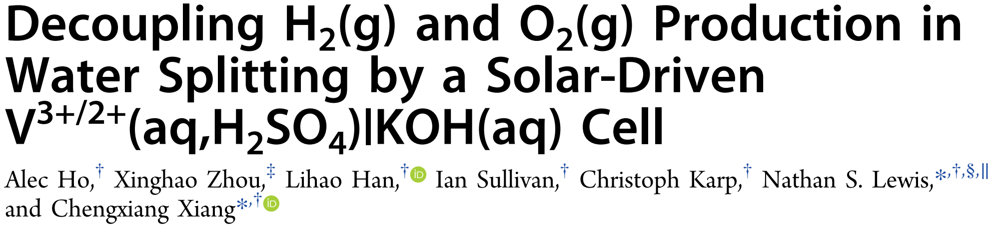
SoHHytec
Solar Fuel, the smarter way.

Scalable, large (~20kW_{peak}), co-generation, *t*>10 days, ~0.45 kg_{H2}/day (~20 bar),
(for average day in Lausanne)
$\eta_{STH,device}$=21%, outdoor, dynamic/fluctuations, live: https://solardish.epfl.ch

Solar water splitting to pressurized hydrogen

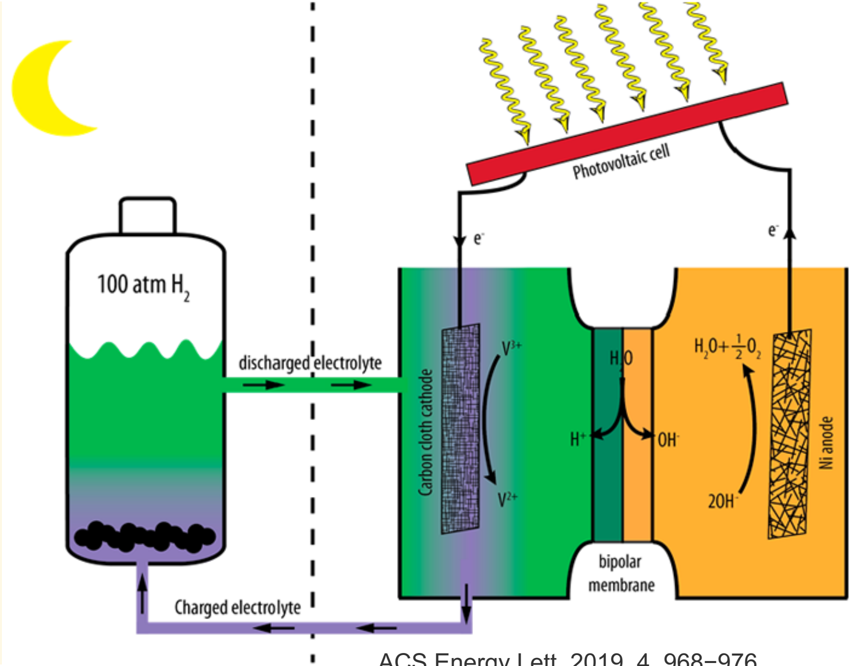
CX Xiang – Caltech

- Significant fraction of levelized cost of hydrogen production is purification and compression up to 300 psi
- Compression is costly, inefficient, and unreliable – especially if starting at 1 bar
- PV-Redox Flow Battery (RFB): more integrated than PV-electrolysis, less integrated than EPFL approach
- Good stability and efficiency
- H_2 produced up to 100 atm, on-demand (dark)
- DOE targets \$2/kg for H_2 production, another \$2/kg for **compression**, storage, delivery
- Advantage of pumping liquid vs. low pressure H_2 and centralized H_2 generation



Decoupling H_2(g) and O_2(g) Production in Water Splitting by a Solar-Driven $V^{3+/2+}$(aq,H_2SO_4)|KOH(aq) Cell

Alec Ho,[†] Xinghao Zhou,[‡] Lihao Han,[†] Ian Sullivan,[†] Christoph Karp,[†] Nathan S. Lewis,[*,†,§,||] and Chengxiang Xiang[*,†]



ACS Energy Lett. 2019, 4, 968−976

Solar water splitting to pressurized hydrogen

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- DOE targets $2/kg for H_2 production, another $2/kg for **compression**, storage, delivery
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20 bar → 700 bar

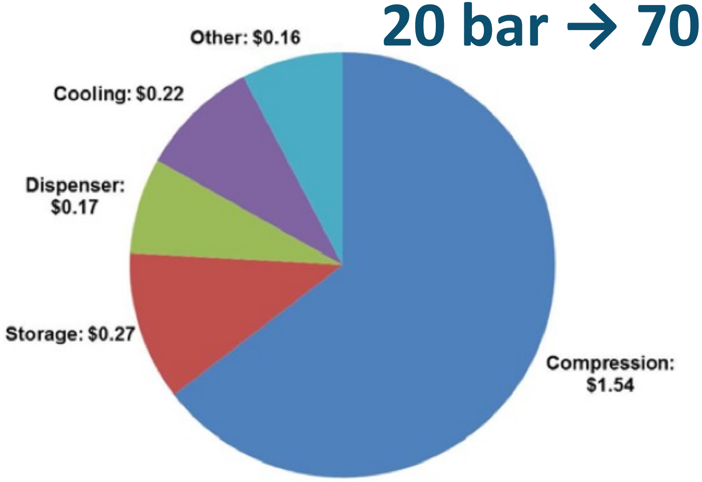


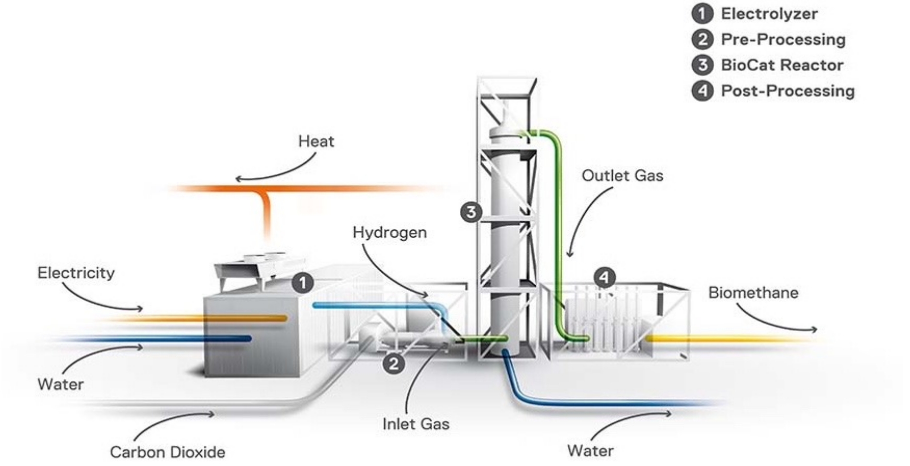
Figure ES-1. CSD cost breakdown for the pipeline scenario ($2.40/kg total)

Hydrogen Station Compression, Storage, and Dispensing (CSD)
Technical Status and Costs
Technical Report
NREL/BK-6A10-58564
May 2014

Pilot scale H_2 + CO_2 to renewable natural gas

Kevin Harrison, Nancy Dowe – NREL

- Renewable electrons electrolyze water to H_2 and O_2
- Optimized strain of methanogenic archaea perform methanation under industrial conditions
- 125 kW PEM electrolyzer feeds 2.5 kg H_2/h, continuously producing 4.1 scfm CH_4
  - Equivalent to 550 m^2 PEC system @ 15% STH
- Potential long-term storage strategy via PEC H_2 & CO_2 to CH_4
- Large market for natural gas and gas grid can absorb any H_2 produced
  - Site where gas grid accessible but electric delivery is difficult/costly
- Can be directly fed with low-pressure, wet hydrogen
- Low carbon fuel standard credit



BioCatProject
POWER-TO-GAS VIA BIOLOGICAL CATALYSIS

SoCalGas
A Sempra Energy utility

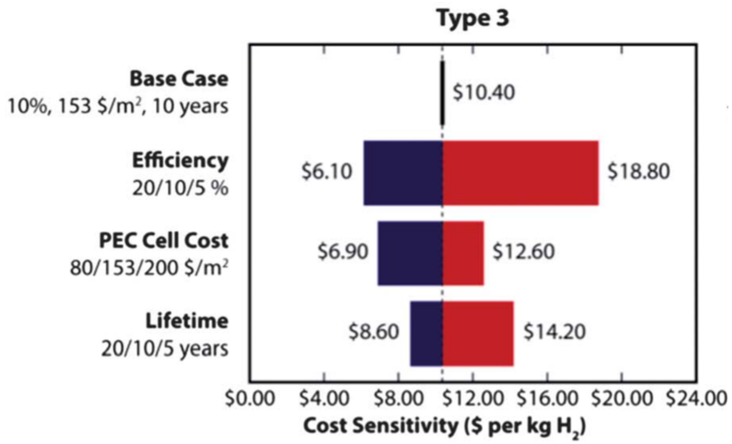
NREL
NATIONAL RENEWABLE ENERGY LABORATORY

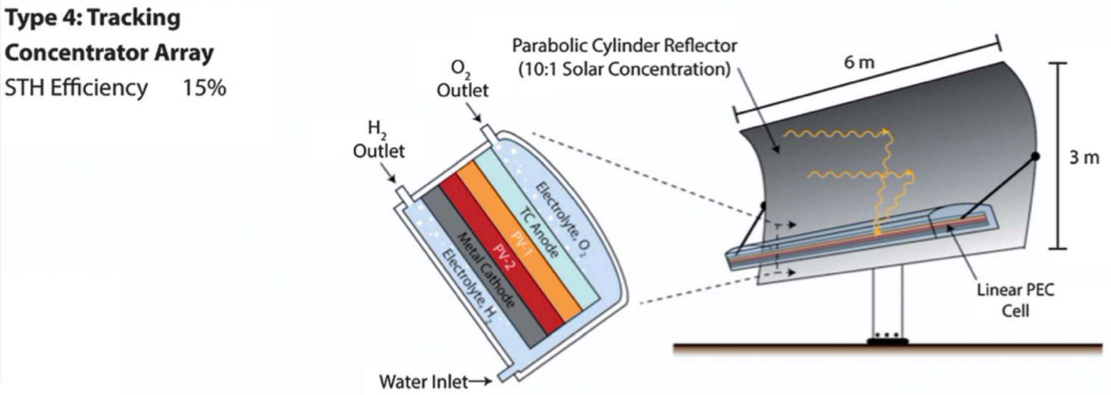
Electrochaea

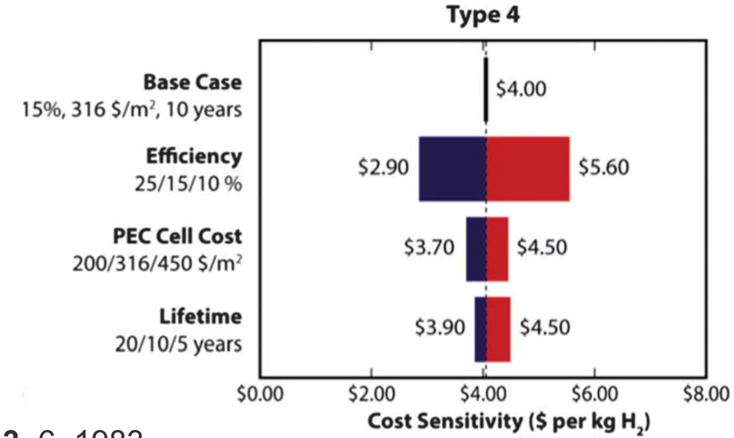
Research priorities guided by technoeconomic analysis

Technoeconomic analysis (TEA) from 2013

- 1-sun Type 3 flat panel will never be economical
- High cost of H_2 collection, drying, and compression
- Hard to hit $2/kg with 2013 Type 4 design
- H2A analysis tool can tell us what combinations of system performance metrics could be feasible…if our assumptions match the state of technology





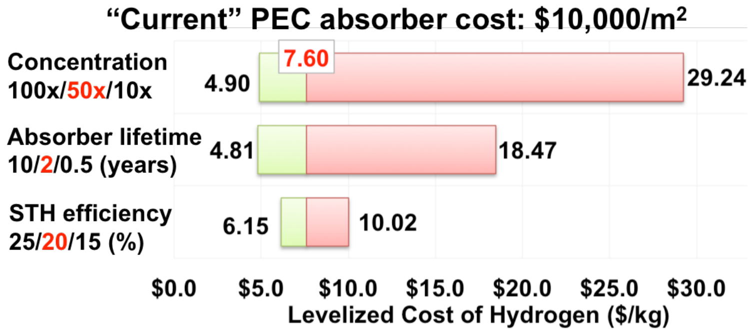


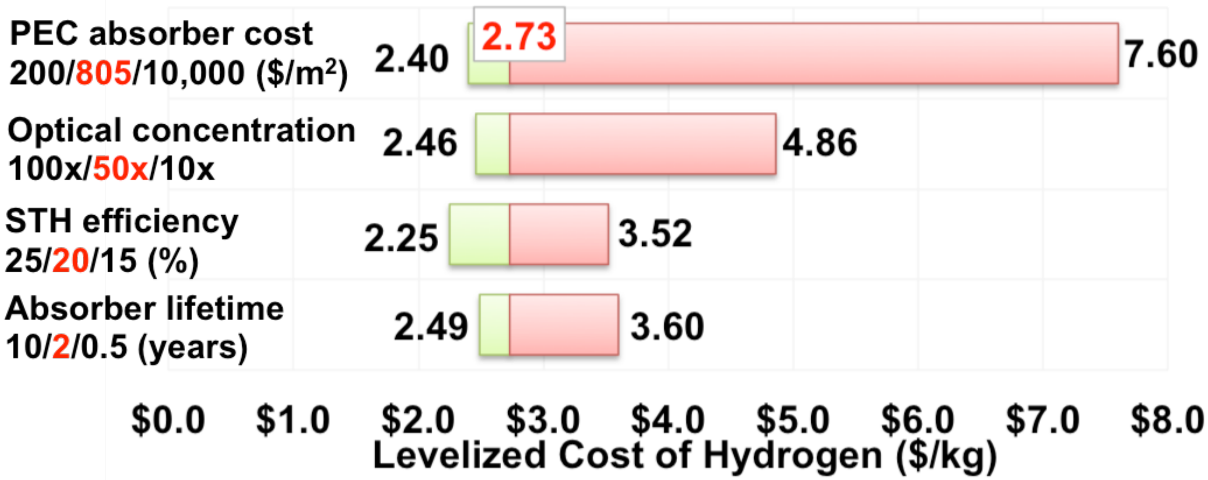
Energy Environ. Sci., **2013**, 6, 1983

Hydrogen analysis (H2A) tool

H2A modeling can inform policy makers and researchers on which metrics to target

- To date, most H2A models have very optimistic assumptions of absorber costs – most critical parameter
- Performed sensitivity analysis using more realistic "current" costs:





https://www.hydrogen.energy.gov/h2a_analysis.html

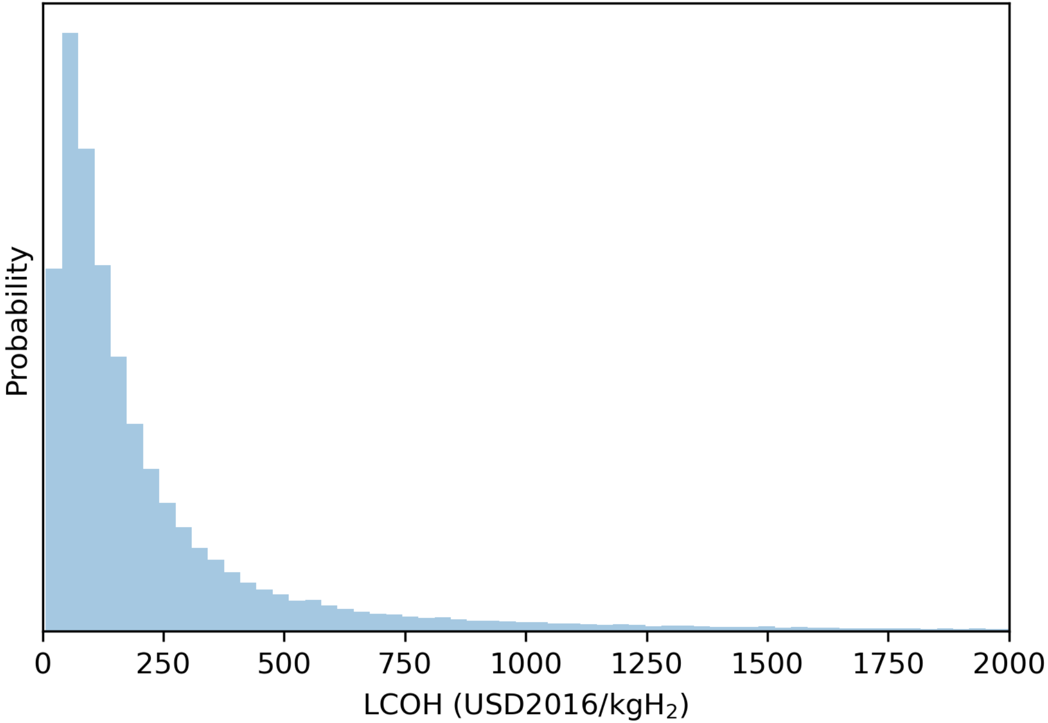
TEA targets

- William Xi (Mark Ruth’s group) – NREL
- Use H2A production model
- **Top-down, target-setting approach**
- Include more realistic PEC absorber costs and higher concentration ratios
- Monte Carlo simulations that vary key H2A parameters to identify opportunity windows
- Goal is to find the technology or parameter regime that allows us to meet the targets

TEA targets

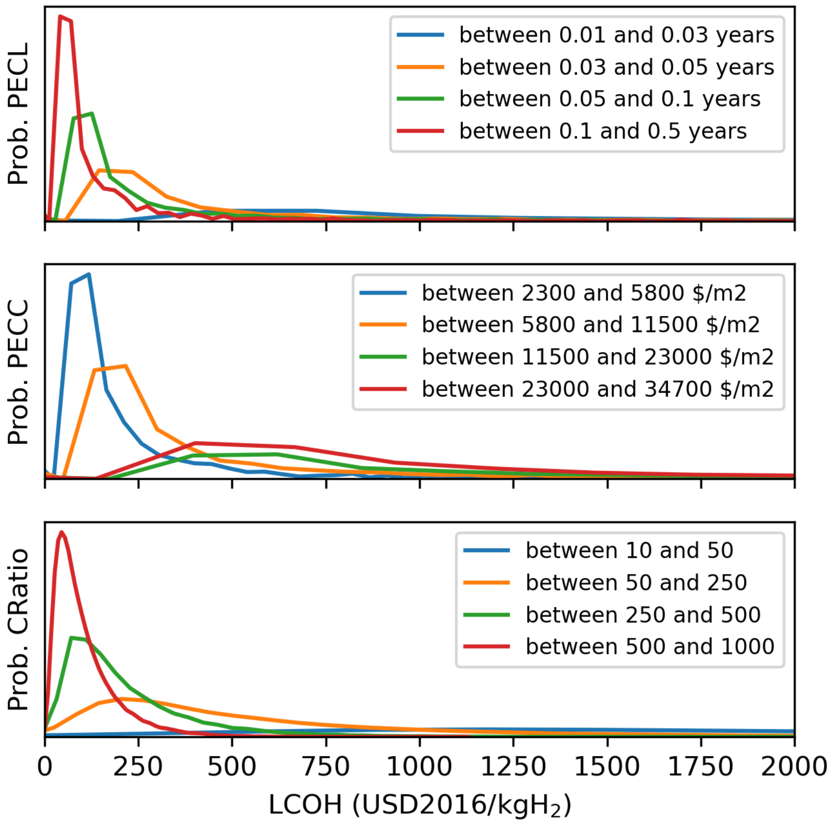
Parameter	Current Baseline	Current Variable Range	Future Baseline	Future Variable Range
Concentration Ratio	10	10 → 1000	10	10 → 1000
Collector System Cost $\$/m^2$ USD 2016	137	100 →200	70	65 → 137
PEC Absorber Cost $\$/m^2$ USD 2016	11,500	2,300 → 34,700	925	810 → 2300
PEC Absorber Lifetime (years)	150 hours	100h → 0.5	2	0.5 → 10
STH Efficiency (%)	10	5 →12.4	15	5 → 25
Operating Capacity (%)	90	90 →100	90	90 → 100

Probability distribution simulation results



Parameter	Variable Range
Concentration Ratio	10 → 1000
Collector System Cost (Parabolic Trough)	100→200 $/m^2$ USD 2016
PEC Absorber Cost	2,300→ 34,700 $/m^2$ USD 2016
PEC Lifetime	0.01→ 0.5 years
STH	5→12.4 %
Operating Capacity	90→100 %

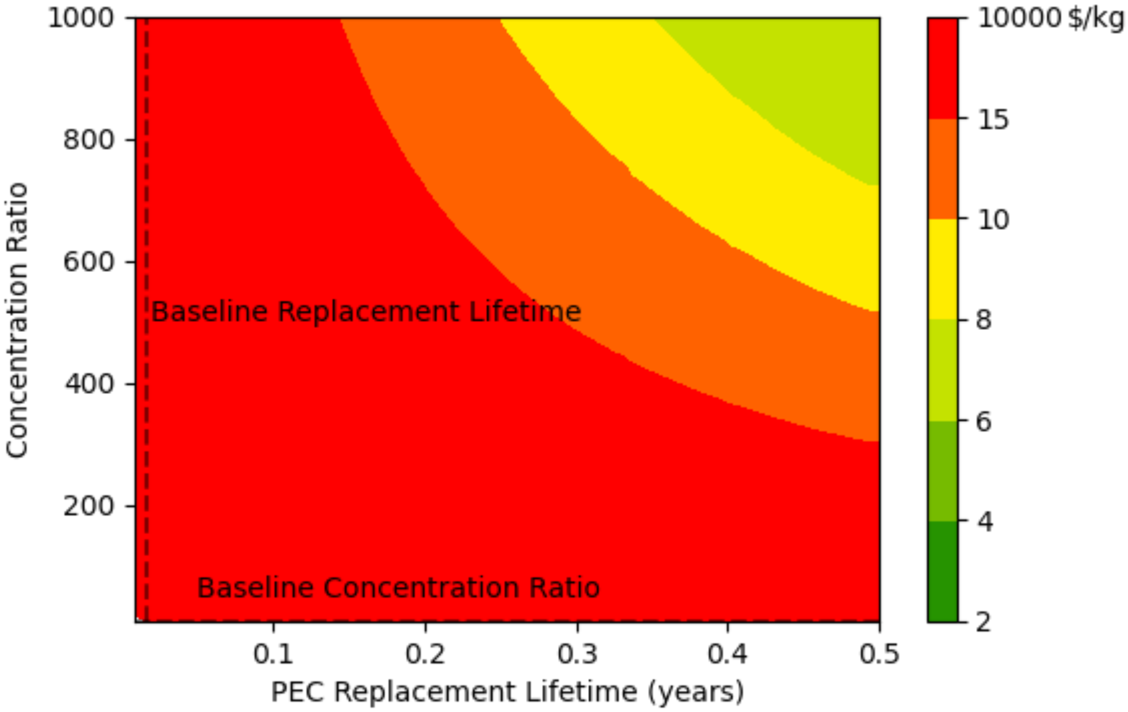
Varying lifetime, absorber cost, and concentration ratio



Parameter	Variable Range
Concentration Ratio (CRatio)	10 → 1000
Collector System Cost	100→200 $/m^2 USD 2016
PEC Absorber Cost (PECC)	2,300→ 34,700 $/m^2 USD 2016
PEC Absorber Lifetime (PECL)	0.01→ 0.5 years
STH Efficiency	5→12.4 %
Operating Capacity	90→100 %

TEA contour plots

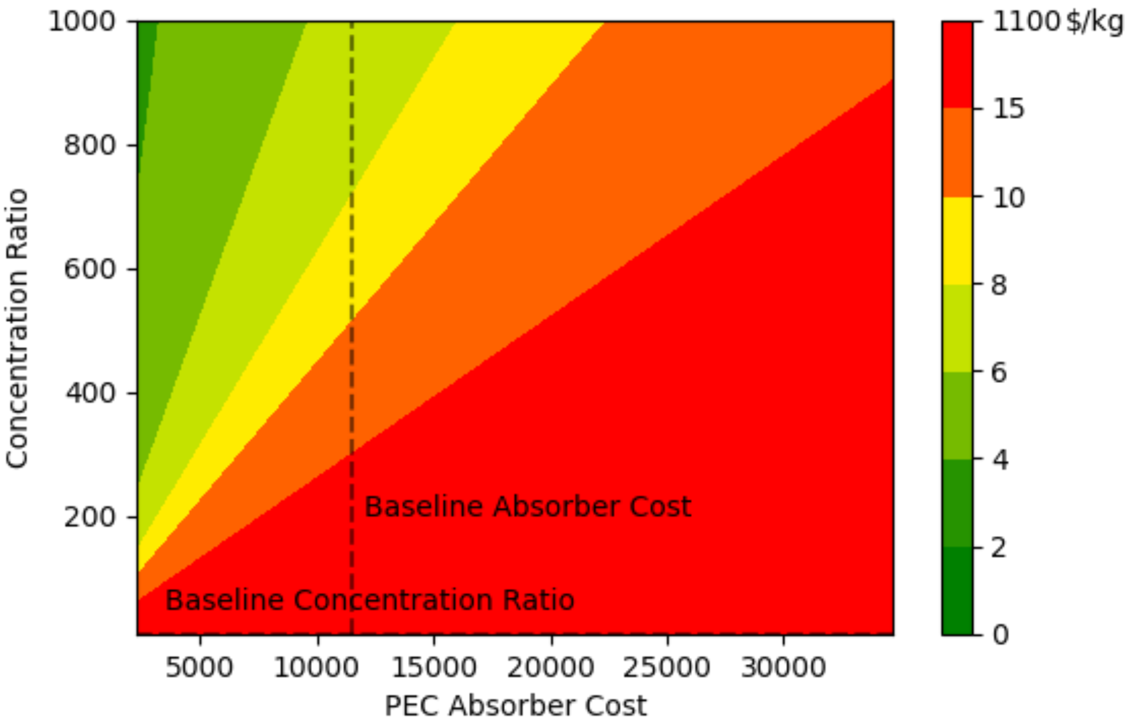
Solar concentration can’t compensate for poor durability with high absorber costs



Parameter	Value
Concentration Ratio	10-1000x (10)
Collector System Cost	137 \$/m^2
PEC Absorber Cost	**11,500 \$/m^2**
PEC Lifetime (years)	**0.01→0.5 (0.02)**
STH Efficiency	10%
Operating Capacity	90%

TEA contour plots

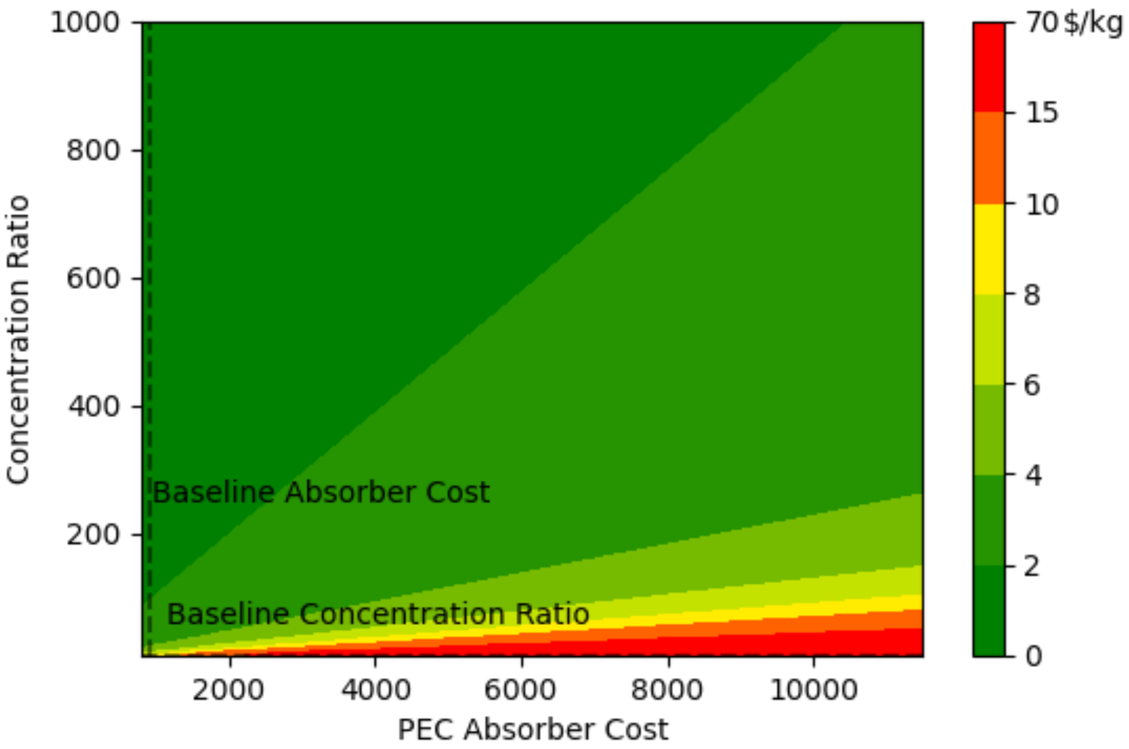
Solar concentration can compensate for poor durability at lower absorber costs



Parameter	Value
Concentration Ratio	10-1000x (10)
Collector System Cost	137 $/m^2
PEC Absorber Cost	**2,300 to 34,700 $/m^2 (11,500)**
PEC Lifetime	**0.5 years**
STH Efficiency	10%
Operating Capacity	90%

TEA contour plots

At 2-year lifetime, moderate solar concentration can compensate for high absorber costs



Parameter	Value
Concentration Ratio	10→1000x (10)
Collector System Cost	**70 $/m²**
PEC Absorber Cost	**810-11500 (925) $/m²**
PEC Lifetime	**2 years**
STH Efficiency	**15%**
Operating Capacity	90%

Combinations that achieve \$4/kg H_2 production

Parameter	Set 1	Set 2	Set 3	Set 4	Range (Baseline)
Concentration Ratio	10	54	100	500	10→1000 (10)
Collector System Cost (\$/m² USD 2016)	75	72	94	137	65→137 (70)
PEC Absorber Cost (\$/m² USD 2016)	1,003	1,049	1,926	2,300	810→2,300 (925)
PEC Lifetime (years)	5	1	2	2	0.5→10 (2)
STH Efficiency (%)	17	12	10	8	5→25 (15)
Operating Capacity (%)	98	98	94	94	90→100 (90)

Discussion topics

- **Topic 1**: Can we identify potential (niche) opportunities where existing PEC systems might have advantages over PV-electrolysis?
- **Topic 2**: What approaches might help us meet the requirements of the opportunities identified in discussion Topic 1?
- **Topic 3**: What are the most promising concepts– from discussion topics 1 & 2 or from the top-down TEA targets–to elevate to pilot scale? What research is needed (near and long-term) to accelerate deployment of the most promising configurations?

- **Questions:**
  - Does this change materials challenges?
  - What new tools or protocols need to be developed?
  - What markets, sectors, locations, adjacencies, incentives should be considered?
  - Are there alternative oxidation products that can add value? Do they scale?

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Advanced Water Splitting Materials

Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Techno-Economic Analysis Breakout Session
Photoelectrochemical (PEC)

Session ID: PEC-2
Session Chair: Brian James
Affiliation: Strategic Analysis Inc.
Date: March 2, 2021

STRATEGIC ANALYSIS INC

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Session Goals

- Session Goals
  - Briefly review TEA methodology & assumptions for latest case studies
  - Discuss where the analysis goes next
    - Provide feedback on validity of key parameters
    - Suggest other key parameters
    - Suggest alternative case study ideas
    - Suggest informative and useful sensitivity studies

- Session Logistics
  - Rules for session
  - Mural link
  - Attendance list

Overview of Techno-Economic Analysis Methodology

- The objective of techno-economic analysis (TEA) is to **evaluate** and **compare** competing technologies and **chart progress** on the basis of cost and technical performance
- **TEA Method Steps**
  - Define system: develop flow schematic and bill of materials
  - Perform system mass & heat balance modeling to identify critical design parameters
  - Enumerate H_2 production plant capital cost
  - Investigate and input technical and financial values into discounted cash flow analysis model H2A to evaluate the levelized cost of hydrogen ($/kg$H_2$)
- **Results and Post-Analysis**
  - Perform sensitivity analyses to identify components with greatest impact on cost
    - Tornados and Monte Carlo
  - Obtain external review and feedback
  - Use feedback to update models

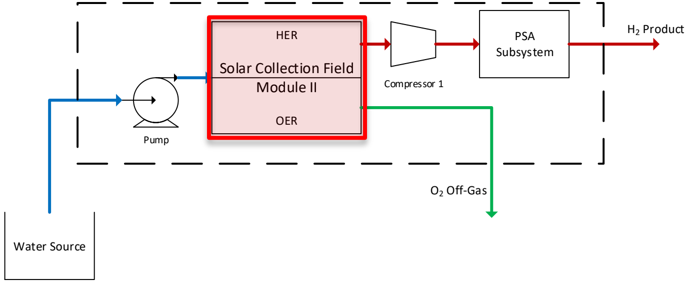
System Generally divided between Solar Conversion Module and BOP

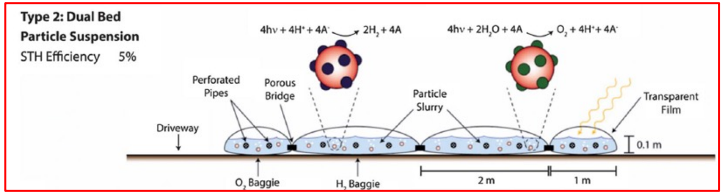
Generalized PEC Plant

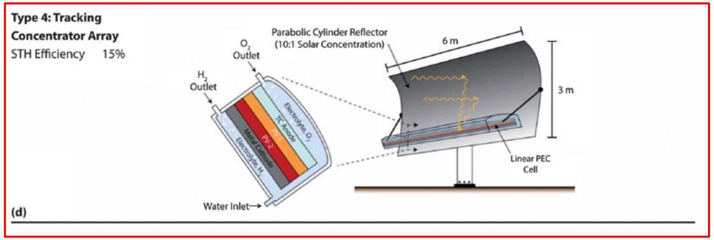
- Water management
- H_2 compression (if needed)
- H_2 management/purification

Solar Conversion Module

- H_2 generation
- H_2 compression (if needed)



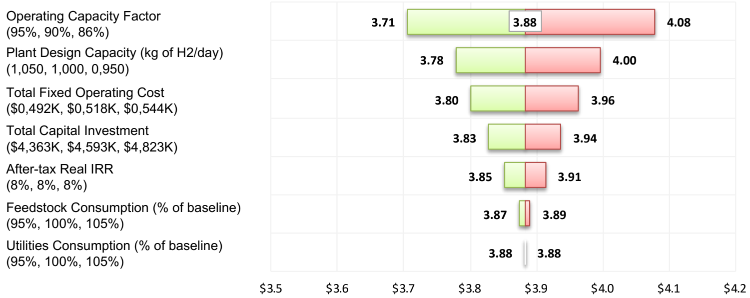


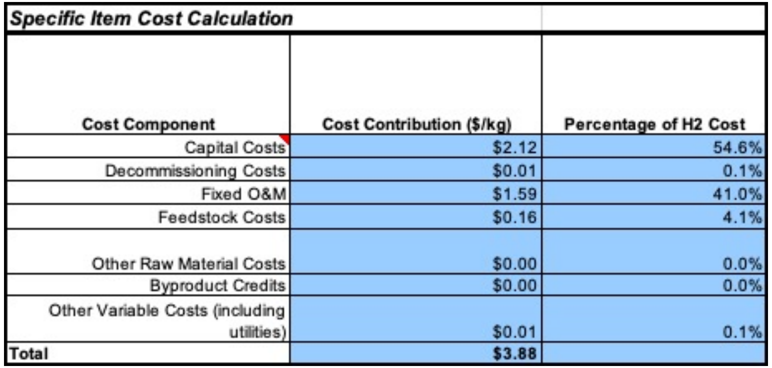


Blaise A. Pinaud et al., "Technical and Economic Feasibility of Centralized Facilities for Solar Hydrogen Production via Photocatalysis and Photoelectrochemistry," *Energy & Environmental Science* 6, no. 7 (2013): 1983, https://doi.org/10.1039/c3ee40831k.

Bottom-Up Technology Status: PEC Type 2

Base on old PEC H2A Case. In process of update.





Specific Item Cost Calculation

Cost Component	Cost Contribution ($/kg)	Percentage of H2 Cost
Capital Costs	$2.12	54.6%
Decommissioning Costs	$0.01	0.1%
Fixed O&M	$1.59	41.0%
Feedstock Costs	$0.16	4.1%
Other Raw Material Costs	$0.00	0.0%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.01	0.1%
Total	**$3.88**	

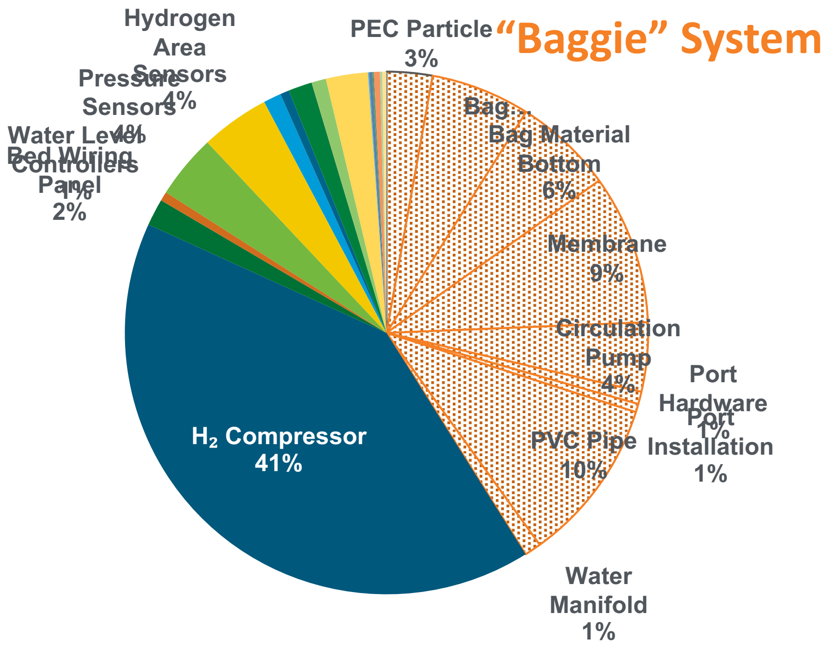
- Levelized Cost of Hydrogen: $3.88 / kg (2007$)
- Installed Equipment Cost: $3,200,000 (for 1 TPD module)
- Total Capital Investment: $4,600,000 (for 1 TPD module)
- **Capital Costs represent the majority of Hydrogen cost. (55%)**
- **O&M (41%) dominated by labor costs**

Type 2 Installed Equipment Cost Breakdown

- "Baggies" are 41% of total
  - Stacked baggies concept addresses this
- BOP cost is substantial
  - System simplification needed
  - Stack baggies concept addresses this
  - H_2 compressor is substantial
- PEC Particles <5%
  - Even at ~$300/kg and 5% conversion
- $/m² for baggies is convenient cost metric

Cost breakdown is from draft/updated analysis. Does not exactly match H2A Case.

"Baggie" System



Baggies ~$7/m²

Energy Feedstocks & Utilities: PEC Type 2

- Process Water (Utility)
  - Price in Startup Year: \$0.0018 / gal
  - Usage: 2.37 gal / kgH2
  - \$0.0018 / gal x 2.37 gal / kgH2 = <\$0.01 / kgH_2

Water cost is negligible.

- Industrial Electricity (Utility)
  - Price in Startup Year: \$0.064 \$ / kWh
  - Usage: 2.01 kWh / kgH2
  - \$0.064 / kWh x 2.01 kWh/ kgH2 = \$0.13 / kgH_2

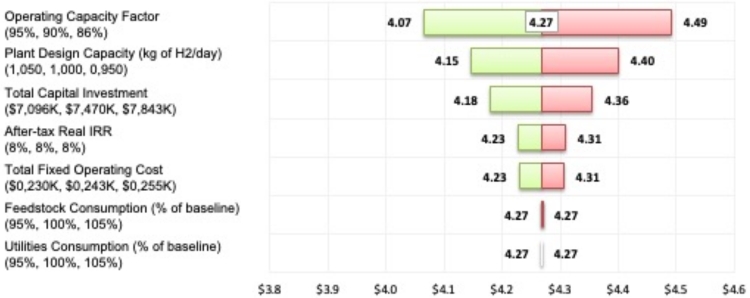
Electricity cost is modest.

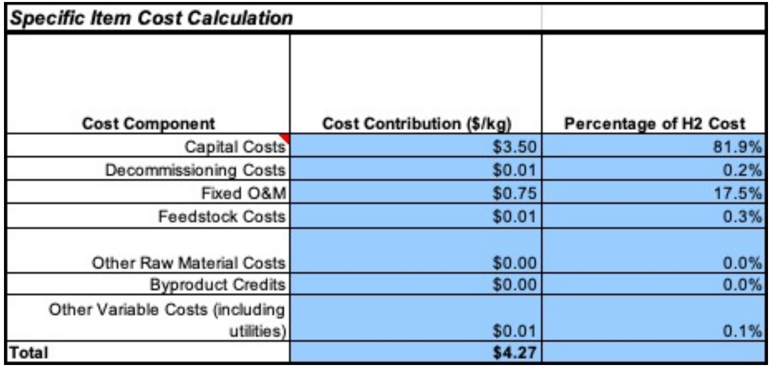
- Replacement Schedule
  - Unplanned Replacements: 0.5%/year of Total Deprec. Capital Cost
  - Planned Maint./Repair: 4%/ year of compressor cost
  - Planned Maint./Repair: 5%/year of total sys minus compr./films/nanoparticles
  - Replacement of pond films every 5 years
  - Replacement of nanoparticles every year

Annual catalyst replacement

Bottom-Up Technology Status: PEC Type 4

Base on old PEC H2A Case. In process of update.





Specific Item Cost Calculation

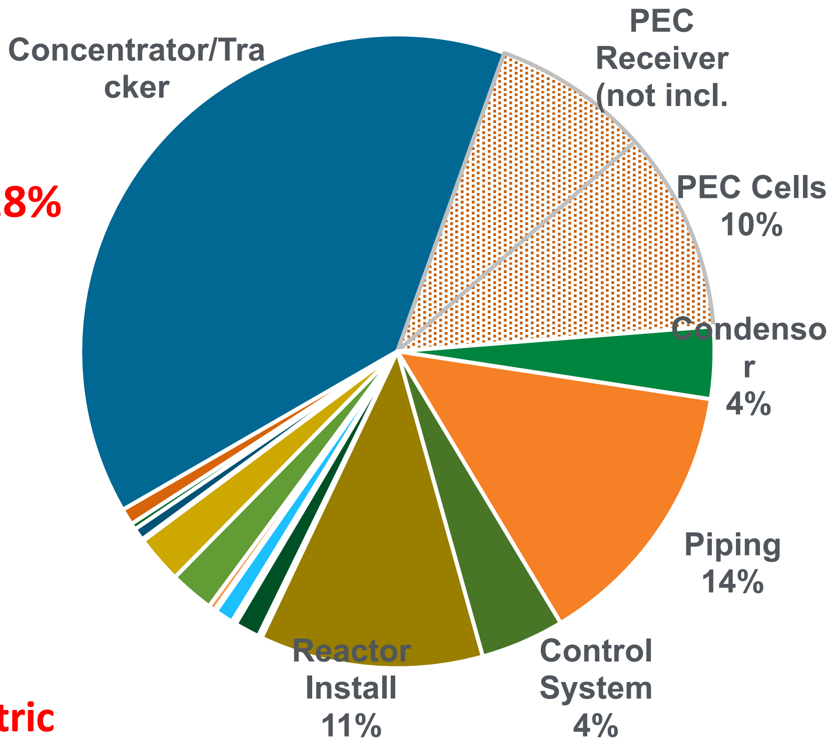
Cost Component	Cost Contribution ($/kg)	Percentage of H2 Cost
Capital Costs	$3.50	81.9%
Decommissioning Costs	$0.01	0.2%
Fixed O&M	$0.75	17.5%
Feedstock Costs	$0.01	0.3%
Other Raw Material Costs	$0.00	0.0%
Byproduct Credits	$0.00	0.0%
Other Variable Costs (including utilities)	$0.01	0.1%
Total	**$4.27**	

- Levelized Cost of Hydrogen: $4.27 / kg (2007$)
- Installed Equipment Cost: $5,400,000 (for 1 TPD module)
- Total Capital Investment: $7,500,000 (for 1 TPD module)
- **Capital Costs represent the majority of Hydrogen cost. (82%)**
- **Capital is dominated by the solar concentrator and H_2 containment module**
- **O&M (18%) dominated by labor costs**

Type 4 Installed Equipment Cost Breakdown

- Solar concentrator dominates capital cost 39%
- PEC electrodes & Receiver 18%
- Total BOP is 43%
  - Needs simplification
- $/m² for baggies and Solar Module is convenient cost metric

Cost breakdown is from draft/updated analysis. Does not exactly match H2A Case.



Concentrator ~$75/m² solar capture area

PEC Module= ($200 (electrode) + $155 (Rec.))/m² electrode area

PEC Discussion Topics

1. Provide feedback on validity of key parameters
   - What assumptions or values do you disagree or consider dubious? State basis and preferred value if possible.
   - What area could be improved that is not currently flagged as a cost driver?
2. What do you want to get out of TEA studies?
   - What cost sensitivities would aid you as researchers?
   - What do you have the biggest cost uncertainty about?
3. Intersection of stack design & (low-cost) manuf.: How to reduce PEC module cost?
   - Use stacked reactor beds to improve efficiency, reduce material and land cost
   - Alternative to expensive parabolic solar concentrator? Fresnel lens?
   - Explore Type 3 (non-concentrated) systems?
4. What big technology, component, or material advances do you see in the future? (and specify approx. year of achievement)
5. What alternative case studies should be modeled?

   (Alternative to Distr./Central with 24/7 constant-price electricity)

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Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Durability in Materials and Devices

Technology: PEC

Session ID: PEC-3
Session Chair: Francesca M. Toma
Co-moderator/note taker: Olivia Alley
Affiliation: LBNL
Date: March 2nd, 2021

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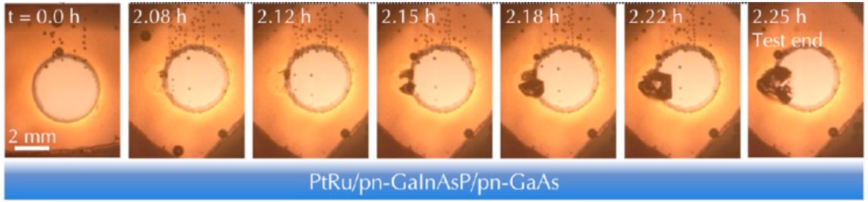
Background

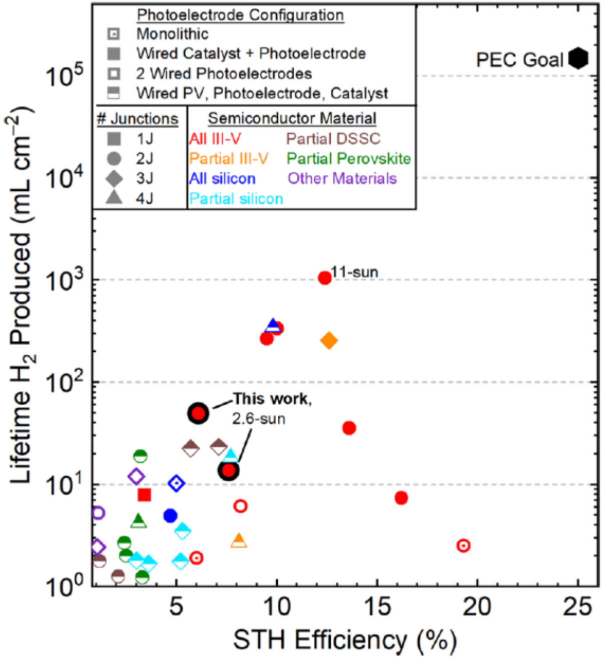
Durability as critical barrier to the deployment of PEC



ACS Energy Lett. 2020, 5. 2631-2640

Outcome of the 2019 HydroGEN Benchmarking Workshop, the PEC Technology focus will be on: “*the understanding of degradation mechanisms and stressors and the development of standardized protocols*”

HydroGEN 2.0 PEC Technology



Comparison of the solar to hydrogen efficiency (STH) and lifetime H_2 produced for unassisted water splitting devices. The "PEC Goal" point in the upper right was calculated assuming a 20% capacity factor over a 10 year lifetime

ACS Energy Lett. 2020, 5. 2631-2640

Session Goals

- Session Goals – Discuss Durability in PEC Materials/Devices
  - What are classes of materials we should focus on?
  - What are common failure mechanism in PEC materials and devices?
  - What should be the protocol(s) to characterize degradation?
  - How can theory and modeling help?
  - What accelerated testing, if any, may be useful in this context?
  - How can we share data (and failures) across the community?
  - ?
- Session Logistics
  - Session Chair Introduction
  - Our co-moderator/note taker is Olivia Alley (LBNL)
  - Fill out attendance list
  - Mural – ice breaker: please list your name, the material(s) you are working with and one (or more) major challenge(s)

Discussion Prompts

- What are classes of materials we should focus on?

Share your experience with materials stability and protection strategies

- What are common failure mechanism in PEC materials and devices?

- What should be the protocol(s) to characterize degradation?

Discussion Prompts

- How can theory and modeling help?

- What accelerated testing, if any, may be useful in this context?

- How can we share data (and failures) across the community?

- What else?

Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Photocatalyst (PC) and Particle Based Systems

Technology: PEC

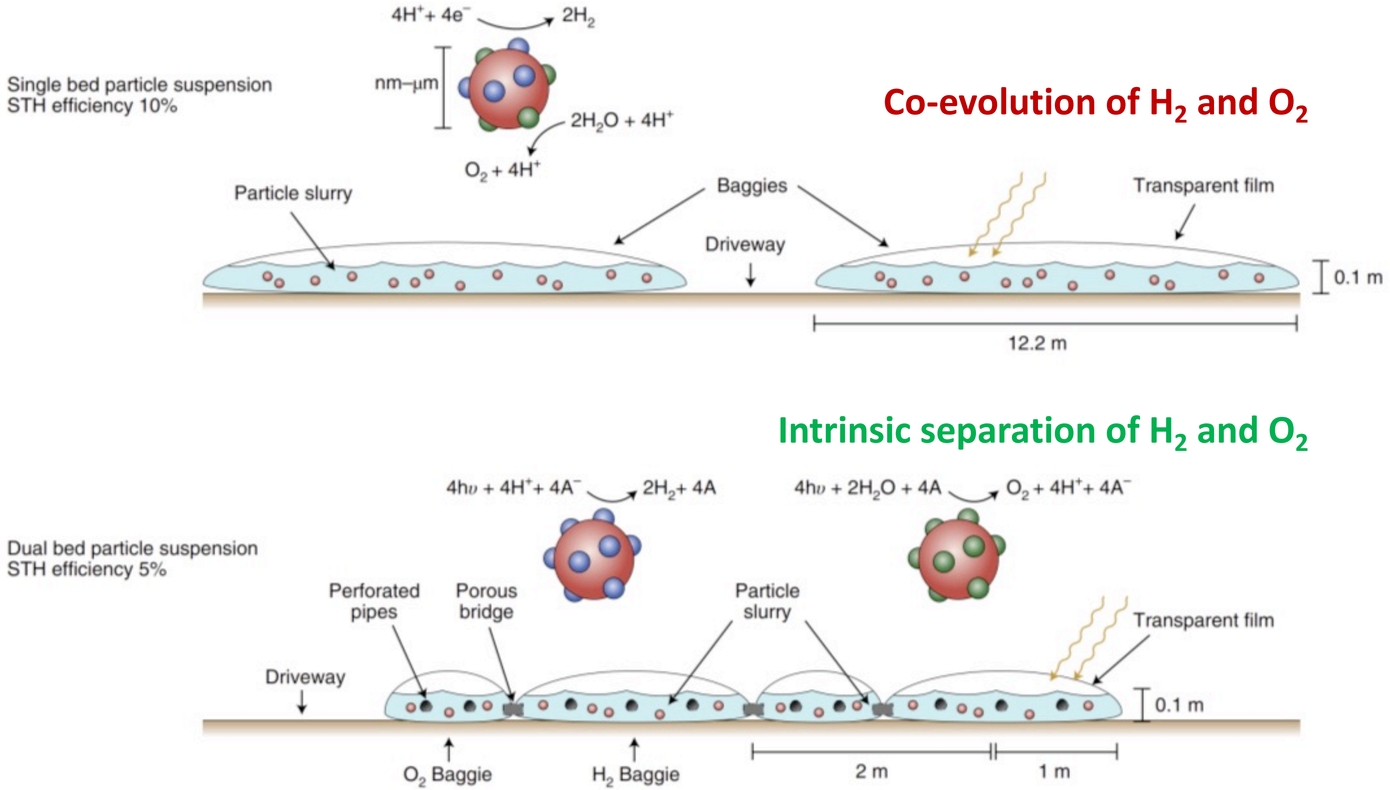
Session ID: PEC-4
Session Chairs: Shane Ardo, Zejie (Justin) Chen
Affiliations: UC Irvine
Date: March 2, 2021

Session Goals

- Session Goals
  - Review protocols written to date *in PEC*; **none in PC**
  - Discuss what **PC** protocols should be written next (first), if any???
  - Strategy for implementation of protocols

- Session Logistics
  - **2 min**: Intro & Rules (Chair: Prof. Shane Ardo; Co-Chair: Zejie (Justin) Chen (UCI))
  - **20 min**: Setting the Stage with Background and Overview (Ardo)
  - **2 min**: Logistics: Attendance (**You!**), Rules (Ardo), MURAL Instructions (Ardo)
  - **45 min**: Facilitated "MURAL Board" Discussion (All)
  - **5 min**: Summarize and Converge on Action Items (All)
  - Report Out (Ardo & Chen)

What is **PC (Photocatalysis)**? Think **Particles in Bags**!



Co-evolution of H_2 and O_2

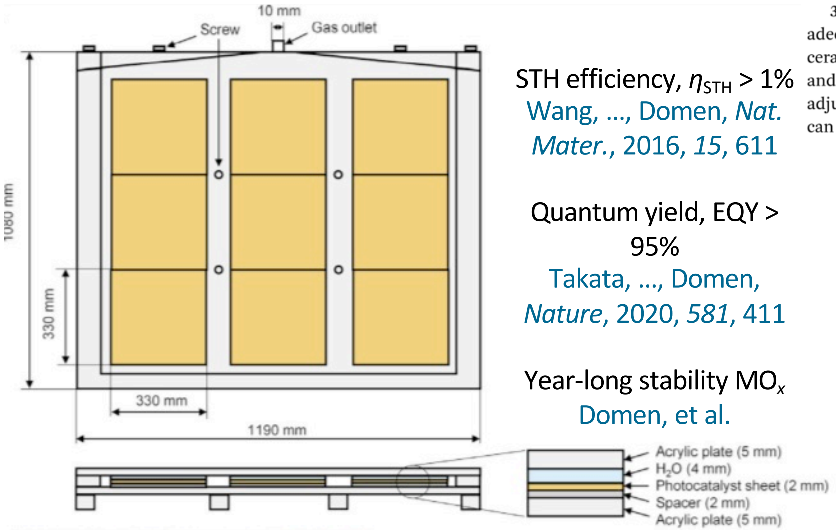
Intrinsic separation of H_2 and O_2

Pinaud, Benck, Seitz, Forman, Chen, Deutsch, James, Baum, Baum, Ardo, Wang, Miller & Jaramillo, *Energy Environ. Sci.*, 2013, *6*, 1983

Hisatomi & Domen, *Nat. Catal.*, 2019, *2*, 387

What is **PC (Photocatalysis)**? **Think Particles as Sheets**!

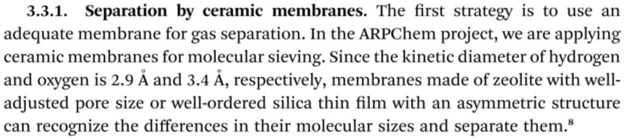
Setoyama, Takewaki, Domen & Tatsumi, *Faraday Disc.*, 2017, *198*, 509



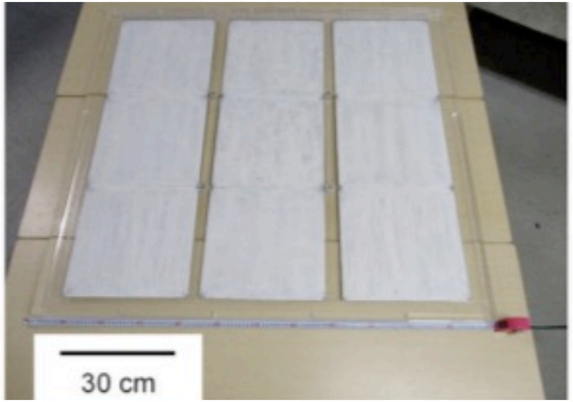
STH efficiency, η_{STH} > 1%
Wang, …, Domen, *Nat. Mater.*, 2016, *15*, 611

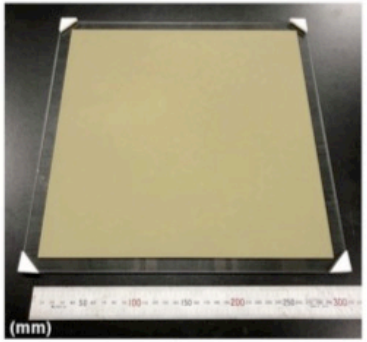
Quantum yield, EQY > 95%
Takata, …, Domen, *Nature*, 2020, *581*, 411

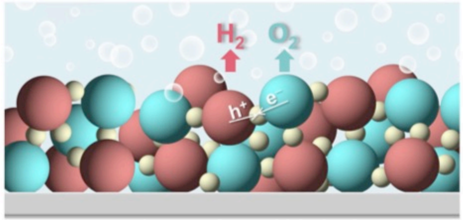
Year-long stability MO_x
Domen, et al.



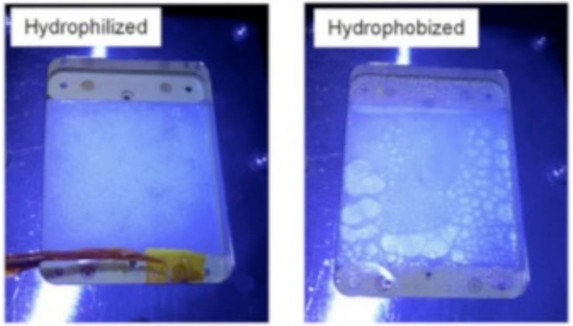
3.3.1. Separation by ceramic membranes. The first strategy is to use an adequate membrane for gas separation. In the ARPChem project, we are applying ceramic membranes for molecular sieving. Since the kinetic diameter of hydrogen and oxygen is 2.9 Å and 3.4 Å, respectively, membranes made of zeolite with well-adjusted pore size or well-ordered silica thin film with an asymmetric structure can recognize the differences in their molecular sizes and separate them.[8]





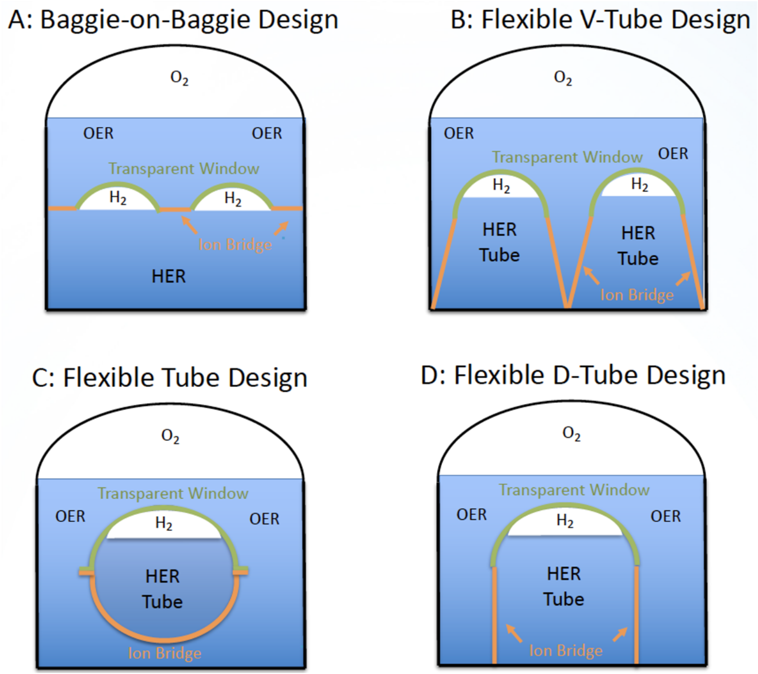


Wang, …, Domen, *Joule*, 2018, *2*, 2667

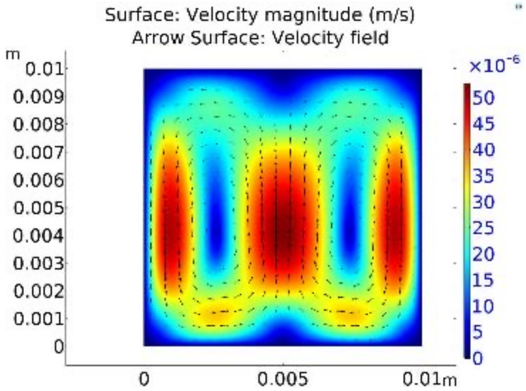


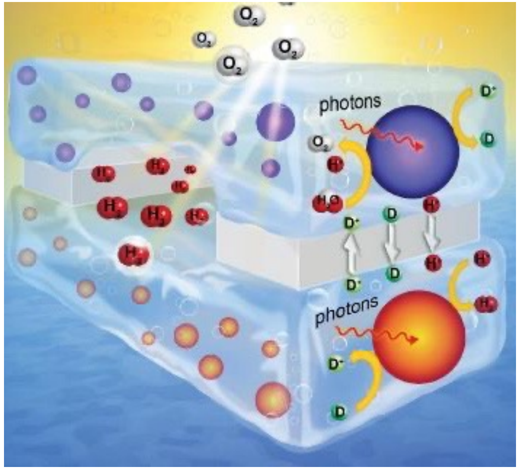
Goto, …, Domen, *Joule*, 2018, *2*, 509

What is **PC (Photocatalysis)**? Think **Particles in Bags**!



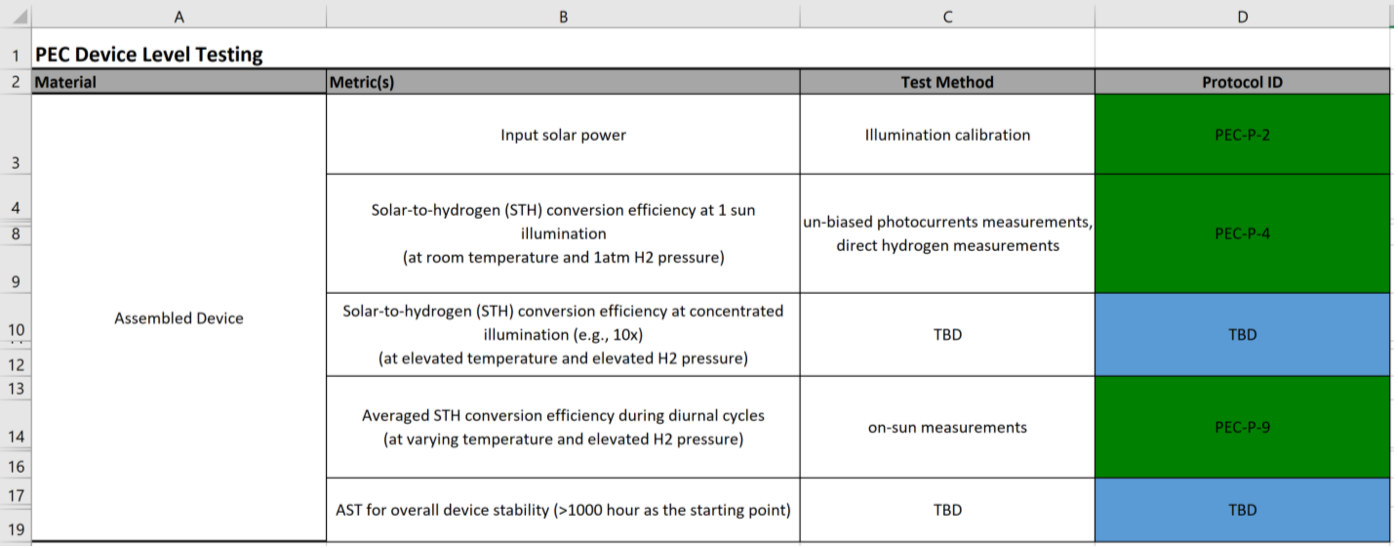
STRATEGIC ANALYSIS INC





Bala Chandran, Breen, Shao, Ardo & Weber, *Energy Environ. Sci.*, 2018, *11*, 115

PEC Benchmarking/Protocols: Device Level

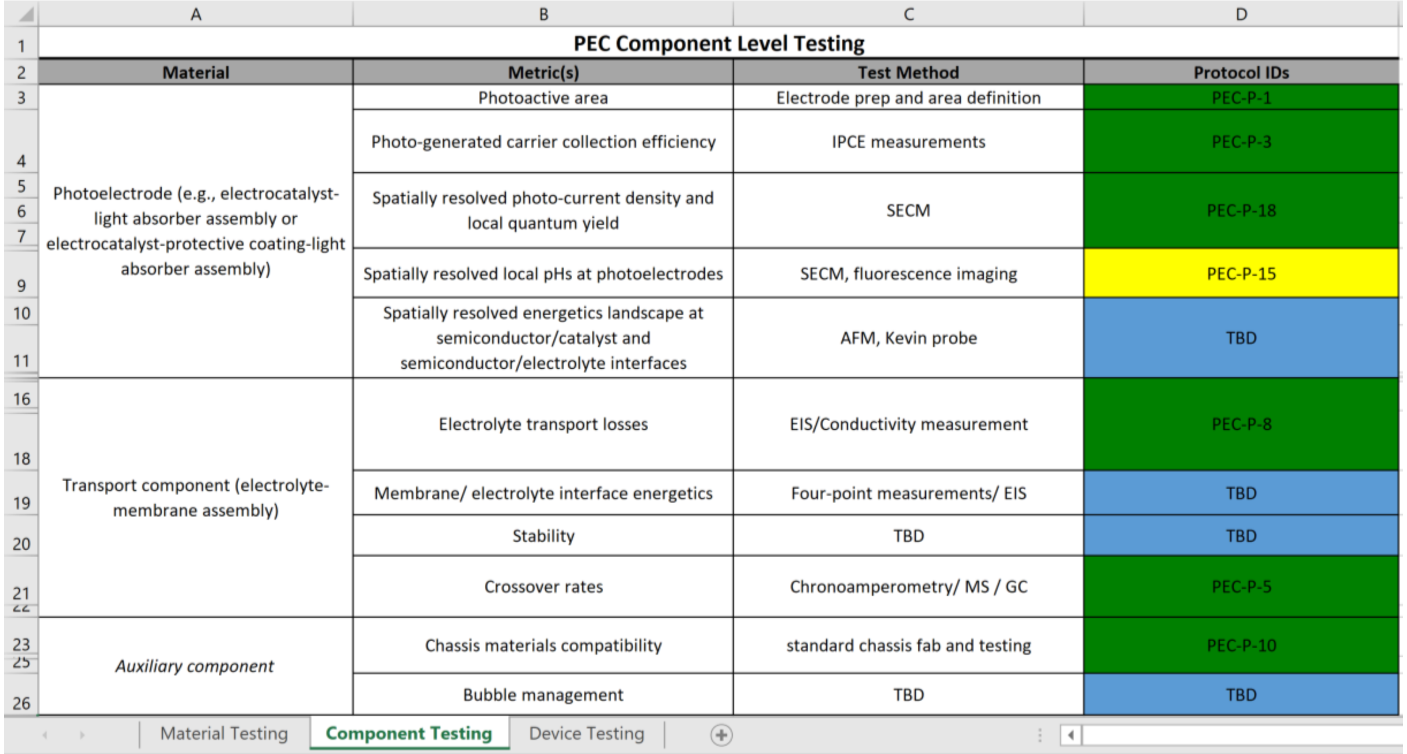


PEC Device Level Testing

Material	Metric(s)	Test Method	Protocol ID
Assembled Device	Input solar power	Illumination calibration	PEC-P-2
	Solar-to-hydrogen (STH) conversion efficiency at 1 sun illumination (at room temperature and 1atm H2 pressure)	un-biased photocurrents measurements, direct hydrogen measurements	PEC-P-4
	Solar-to-hydrogen (STH) conversion efficiency at concentrated illumination (e.g., 10x) (at elevated temperature and elevated H2 pressure)	TBD	TBD
	Averaged STH conversion efficiency during diurnal cycles (at varying temperature and elevated H2 pressure)	on-sun measurements	PEC-P-9
	AST for overall device stability (>1000 hour as the starting point)	TBD	TBD

Status Key	Draft Complete
	Draft in Process
	Draft not Started

PEC Benchmarking/Protocols: Component Level

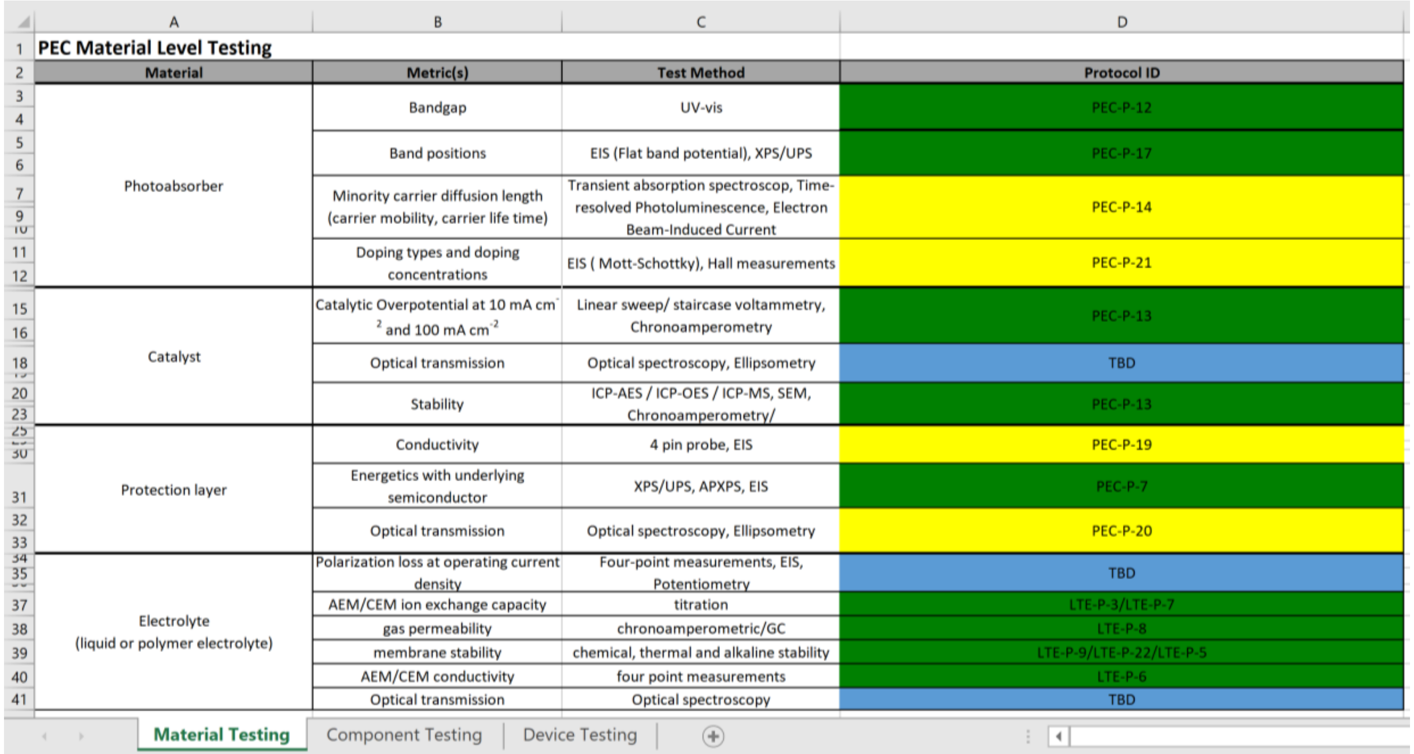


PEC Component Level Testing

Material	Metric(s)	Test Method	Protocol IDs
Photoelectrode (e.g., electrocatalyst-light absorber assembly or electrocatalyst-protective coating-light absorber assembly)	Photoactive area	Electrode prep and area definition	PEC-P-1
	Photo-generated carrier collection efficiency	IPCE measurements	PEC-P-3
	Spatially resolved photo-current density and local quantum yield	SECM	PEC-P-18
	Spatially resolved local pHs at photoelectrodes	SECM, fluorescence imaging	PEC-P-15
	Spatially resolved energetics landscape at semiconductor/catalyst and semiconductor/electrolyte interfaces	AFM, Kevin probe	TBD
Transport component (electrolyte-membrane assembly)	Electrolyte transport losses	EIS/Conductivity measurement	PEC-P-8
	Membrane/ electrolyte interface energetics	Four-point measurements/ EIS	TBD
	Stability	TBD	TBD
	Crossover rates	Chronoamperometry/ MS / GC	PEC-P-5
Auxiliary component	Chassis materials compatibility	standard chassis fab and testing	PEC-P-10
	Bubble management	TBD	TBD

Status Key	Draft Complete
	Draft in Process
	Draft not Started

PEC Benchmarking/Protocols: Material Level

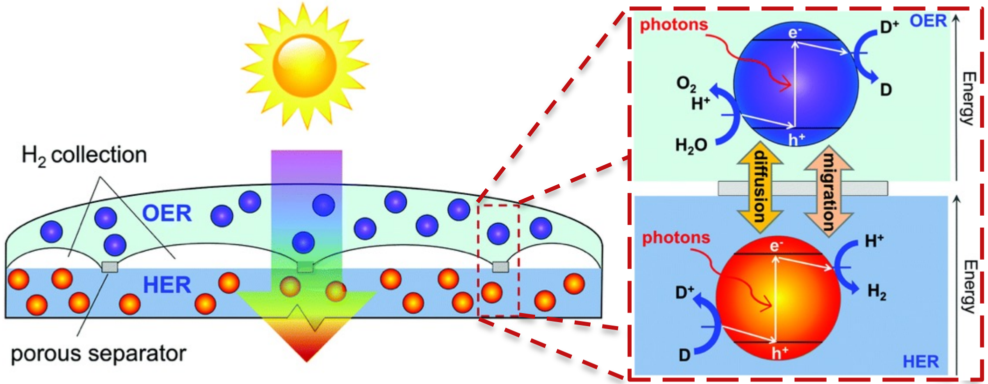


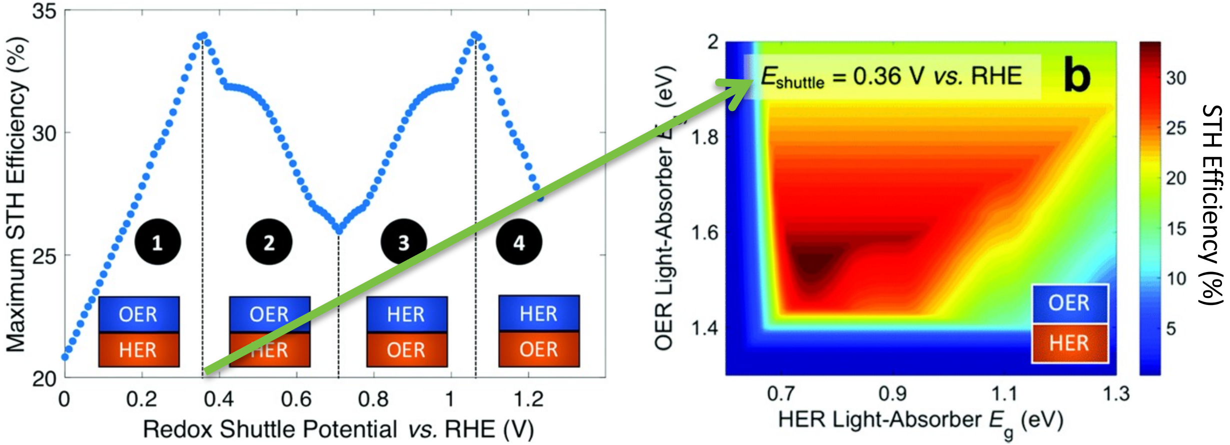
PEC Material Level Testing

Material	Metric(s)	Test Method	Protocol ID
Photoabsorber	Bandgap	UV-vis	🟩 PEC-P-12
	Band positions	EIS (Flat band potential), XPS/UPS	🟩 PEC-P-17
	Minority carrier diffusion length (carrier mobility, carrier life time)	Transient absorption spectroscop, Time-resolved Photoluminescence, Electron Beam-Induced Current	🟨 PEC-P-14
	Doping types and doping concentrations	EIS (Mott-Schottky), Hall measurements	🟨 PEC-P-21
Catalyst	Catalytic Overpotential at 10 mA cm^{-2} and 100 mA cm^{-2}	Linear sweep/ staircase voltammetry, Chronoamperometry	🟩 PEC-P-13
	Optical transmission	Optical spectroscopy, Ellipsometry	🟦 TBD
	Stability	ICP-AES / ICP-OES / ICP-MS, SEM, Chronoamperometry/	🟩 PEC-P-13
Protection layer	Conductivity	4 pin probe, EIS	🟨 PEC-P-19
	Energetics with underlying semiconductor	XPS/UPS, APXPS, EIS	🟩 PEC-P-7
	Optical transmission	Optical spectroscopy, Ellipsometry	🟨 PEC-P-20
Electrolyte (liquid or polymer electrolyte)	Polarization loss at operating current density	Four-point measurements, EIS, Potentiometry	🟦 TBD
	AEM/CEM ion exchange capacity	titration	🟩 LTE-P-3/LTE-P-7
	gas permeability	chronoamperometric/GC	🟩 LTE-P-8
	membrane stability	chemical, thermal and alkaline stability	🟩 LTE-P-9/LTE-P-22/LTE-P-5
	AEM/CEM conductivity	four point measurements	🟩 LTE-P-6
	Optical transmission	Optical spectroscopy	🟦 TBD

Status Key	
	🟩 Draft Complete
	🟨 Draft in Process
	🟦 Draft not Started

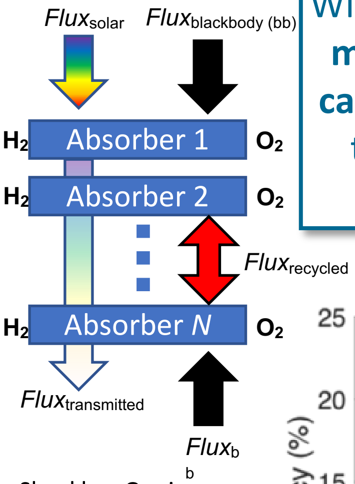
Critical Insight from **PC** Theoretical STH Efficiency





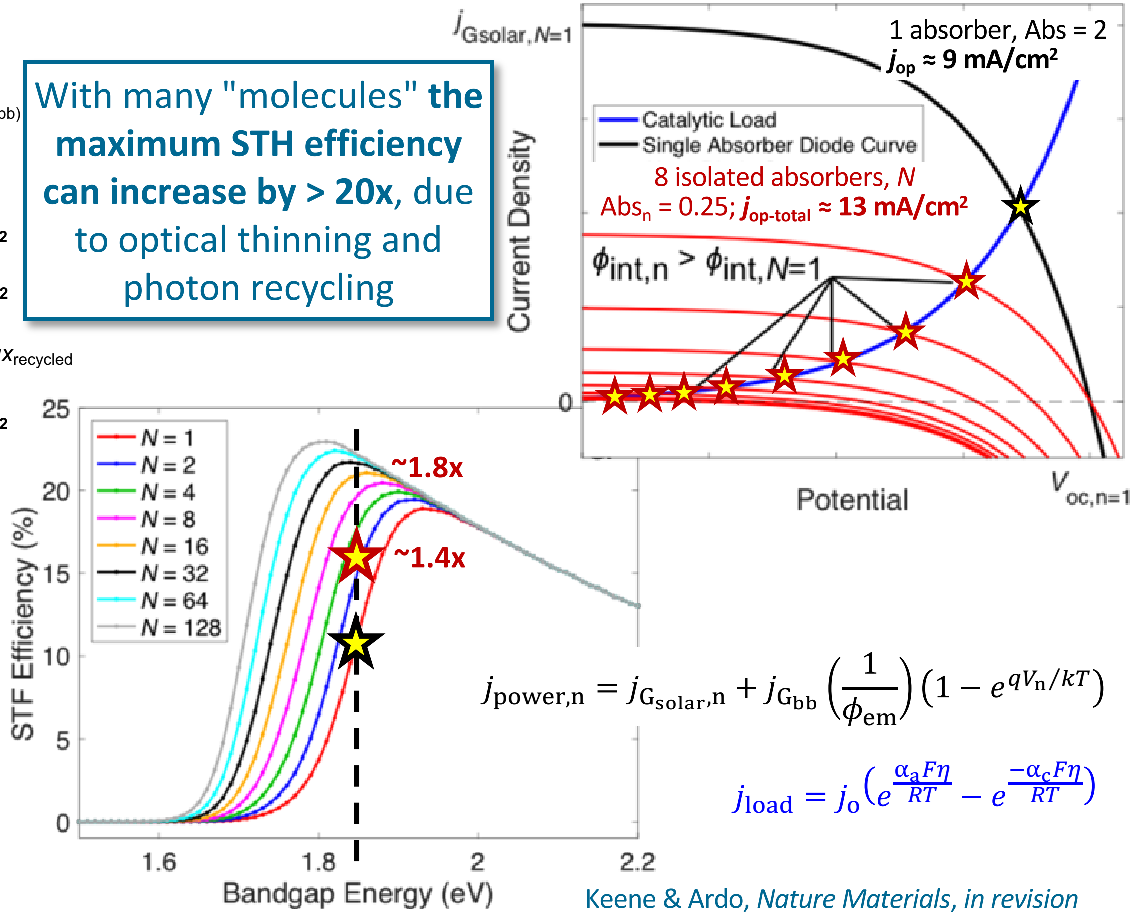
Keene, Bala Chandran & Ardo, *Energy Environ. Sci.*, 2019, *12*, 261

Critical Insight from **PC** Theoretical STH Efficiency



Shockley, Queisser, Henry, De Vos, Pauwels, Wurfel, Ross, Hsiao, et al.

With many "molecules" **the maximum STH efficiency can increase by > 20x**, due to optical thinning and photon recycling

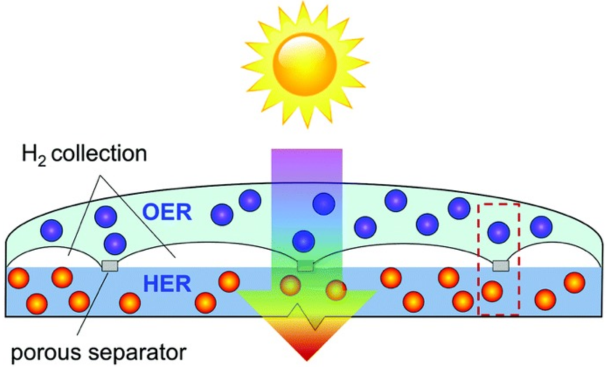


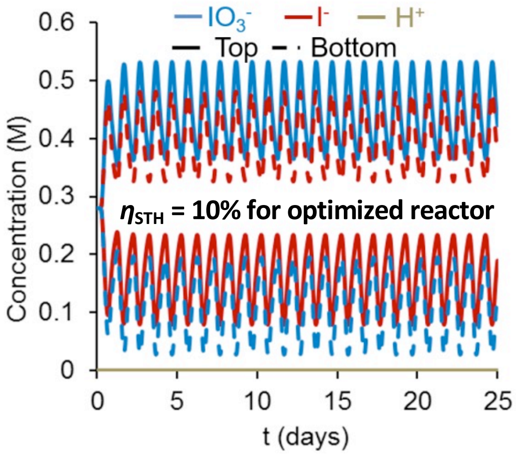
$$j_{\mathrm{power,n}} = j_{\mathrm{G_{solar},n}} + j_{\mathrm{G_{bb}}}\left(\frac{1}{\phi_{\mathrm{em}}}\right)\left(1 - e^{qV_{\mathrm{n}}/kT}\right)$$

$$j_{\mathrm{load}} = j_{\mathrm{o}}\left(e^{\frac{\alpha_{\mathrm{a}}F\eta}{RT}} - e^{\frac{-\alpha_{\mathrm{c}}F\eta}{RT}}\right)$$

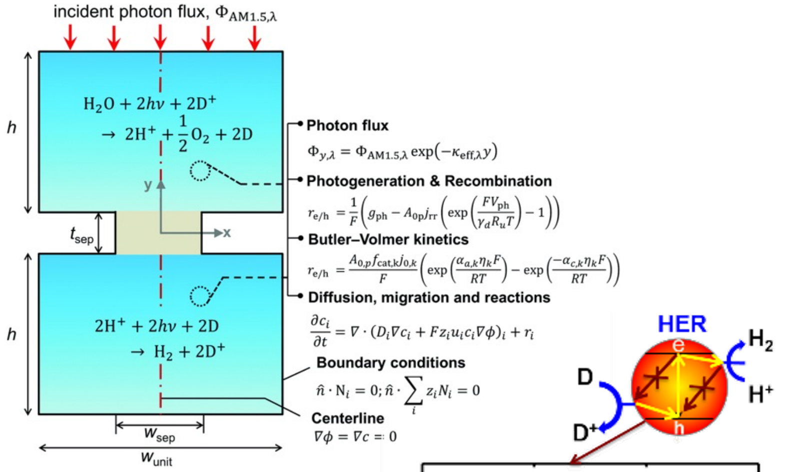
Keene & Ardo, *Nature Materials*, *in revision*

Critical Insight from **PC** Theoretical STH Efficiency

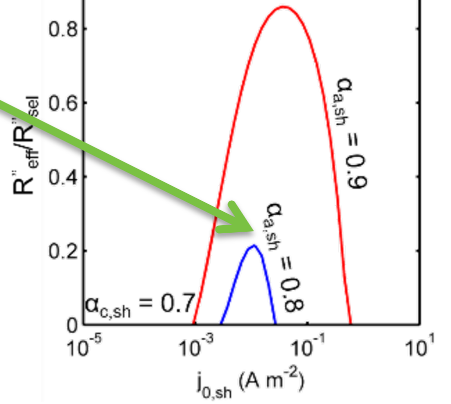




η_{STH} = 10% for optimized reactor

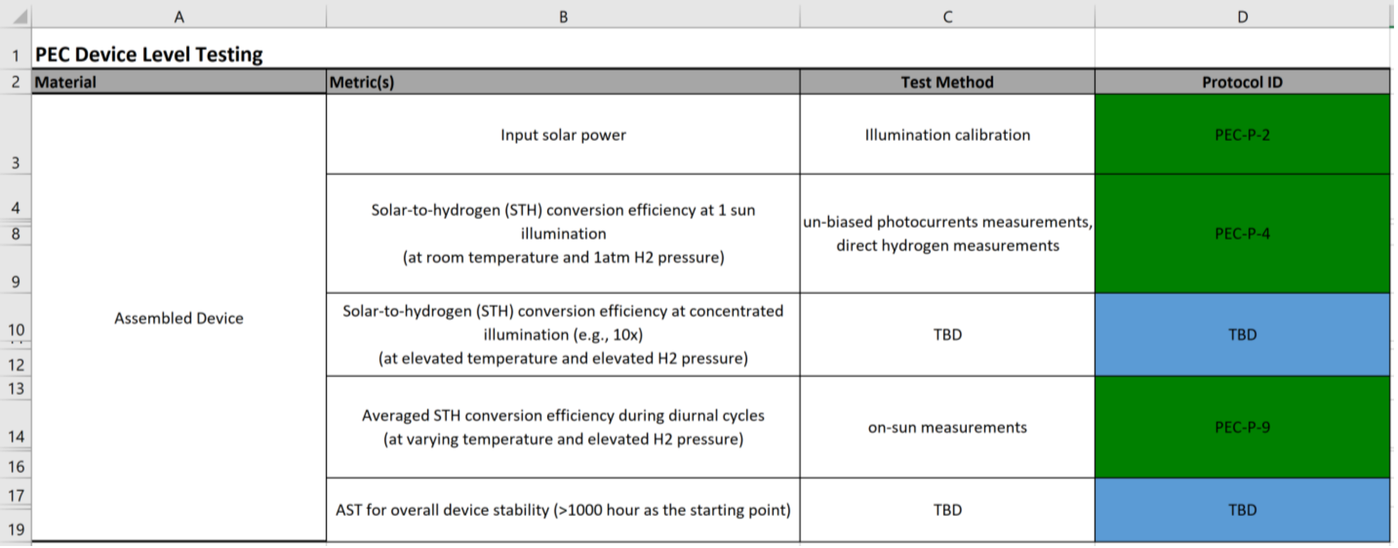


The rate of non-selective HER (R''_{eff}), relative to the rate of selective HER (R''_{sel}), depends greatly on redox selectivity ($\alpha_{a,sh}$)



Bala Chandran, Breen, Shao, Ardo & Weber, *Energy Environ. Sci.*, 2018, *11*, 115

PEC Benchmarking/Protocols: Device Level



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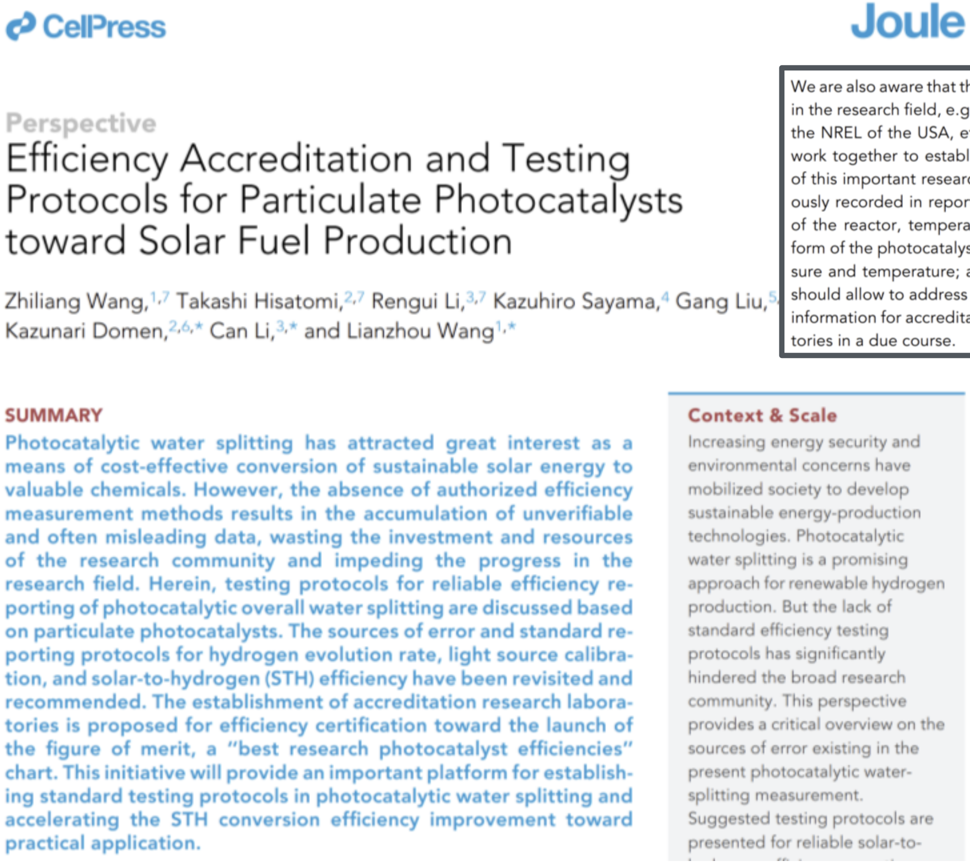
	Solar-to-hydrogen (STH) conversion efficiency at concentrated illumination (e.g., 10x) (at elevated temperature and elevated H2 pressure)	TBD	TBD
	Averaged STH conversion efficiency during diurnal cycles (at varying temperature and elevated H2 pressure)	on-sun measurements	PEC-P-9
	AST for overall device stability (>1000 hour as the starting point)	TBD	TBD

Status Key	Draft Complete
	Draft in Process
	Draft not Started

PC *(not PEC!)* Benchmarking and Protocols



CellPress

Joule

Perspective

Efficiency Accreditation and Testing Protocols for Particulate Photocatalysts toward Solar Fuel Production

Zhiliang Wang,[1,7] Takashi Hisatomi,[2,7] Rengui Li,[3,7] Kazuhiro Sayama,[4] Gang Liu,[5
Kazunari Domen,[2,6,*] Can Li,[3,*] and Lianzhou Wang[1,*]

SUMMARY

Photocatalytic water splitting has attracted great interest as a means of cost-effective conversion of sustainable solar energy to valuable chemicals. However, the absence of authorized efficiency measurement methods results in the accumulation of unverifiable and often misleading data, wasting the investment and resources of the research community and impeding the progress in the research field. Herein, testing protocols for reliable efficiency reporting of photocatalytic overall water splitting are discussed based on particulate photocatalysts. The sources of error and standard reporting protocols for hydrogen evolution rate, light source calibration, and solar-to-hydrogen (STH) efficiency have been revisited and recommended. The establishment of accreditation research laboratories is proposed for efficiency certification toward the launch of the figure of merit, a "best research photocatalyst efficiencies" chart. This initiative will provide an important platform for establishing standard testing protocols in photocatalytic water splitting and accelerating the STH conversion efficiency improvement toward practical application.

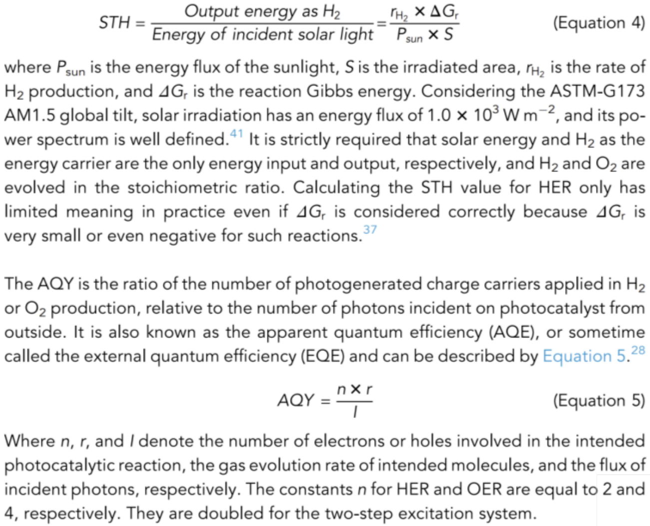
Context & Scale

Increasing energy security and environmental concerns have mobilized society to develop sustainable energy-production technologies. Photocatalytic water splitting is a promising approach for renewable hydrogen production. But the lack of standard efficiency testing protocols has significantly hindered the broad research community. This perspective provides a critical overview on the sources of error existing in the present photocatalytic water-splitting measurement. Suggested testing protocols are presented for reliable solar-to-

> We are also aware that there are many other leading labs/institutes around the world in the research field, e.g., the Solar Fuel Testing Facility at Helmholtz Centre Berlin, the NREL of the USA, etc. It is our hope that the leading research institutions can work together to establish the unified testing standards to promote the progress of this important research field. All the experimental conditions will be unambiguously recorded in reporting the STH efficiency including the size and atmosphere of the reactor, temperature, volume, and pH of the reaction solution; mass and form of the photocatalyst; intensity and spectrum of the light source; ambient pressure and temperature; and gas product detection method; and etc. This practice should allow to address the major concerns about the reproducibility. The relevant information for accreditation will become available on the websites of these laboratories in a due course.

Wang, …, Liu, Domen, Li & Wang, *Joule*, **Feb 2021**, *5*, 344 (Australia, China, Japan)

PC Benchmarking/Protocols: Device/Component Level



$$STH = \frac{\text{Output energy as } H_2}{\text{Energy of incident solar light}} = \frac{r_{H_2} \times \Delta G_r}{P_{sun} \times S} \qquad \text{(Equation 4)}$$

where P_{sun} is the energy flux of the sunlight, S is the irradiated area, r_{H_2} is the rate of H_2 production, and ΔG_r is the reaction Gibbs energy. Considering the ASTM-G173 AM1.5 global tilt, solar irradiation has an energy flux of 1.0×10^3 W m^{-2}, and its power spectrum is well defined.[41] It is strictly required that solar energy and H_2 as the energy carrier are the only energy input and output, respectively, and H_2 and O_2 are evolved in the stoichiometric ratio. Calculating the STH value for HER only has limited meaning in practice even if ΔG_r is considered correctly because ΔG_r is very small or even negative for such reactions.[37]

The AQY is the ratio of the number of photogenerated charge carriers applied in H_2 or O_2 production, relative to the number of photons incident on photocatalyst from outside. It is also known as the apparent quantum efficiency (AQE), or sometime called the external quantum efficiency (EQE) and can be described by Equation 5.[28]

$$AQY = \frac{n \times r}{I} \qquad \text{(Equation 5)}$$

Where n, r, and I denote the number of electrons or holes involved in the intended photocatalytic reaction, the gas evolution rate of intended molecules, and the flux of incident photons, respectively. The constants n for HER and OER are equal to 2 and 4, respectively. They are doubled for the two-step excitation system.

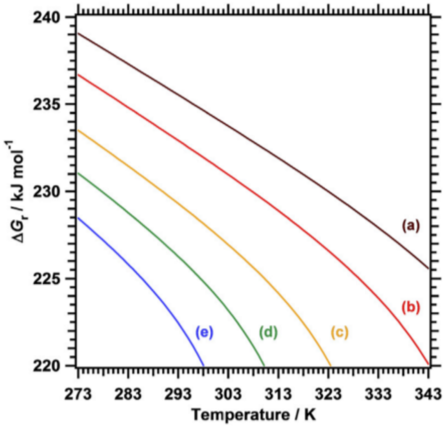
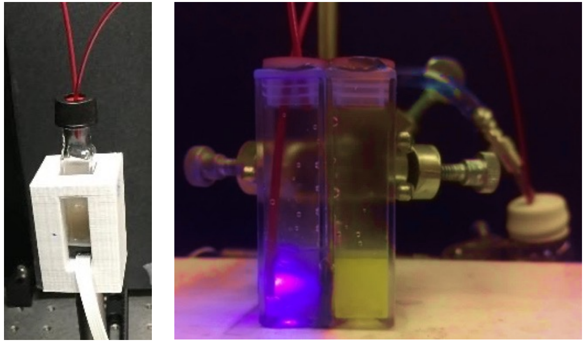


Figure 5. The Change of Gibbs Free Energy of Water Splitting along with the Change of Balance Temperature

(A–E) The dependence of the reaction Gibbs energy ΔG_r of OWS at different total pressure of (A) 1, (B) 0.5, (C) 0.2, (D) 0.1, and (E) 0.05 bar as a function of the temperature.



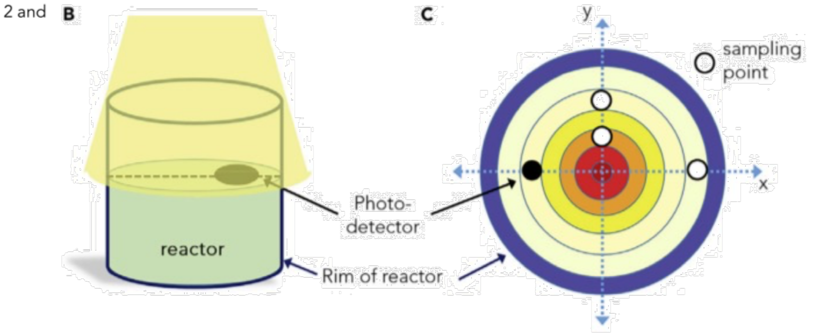
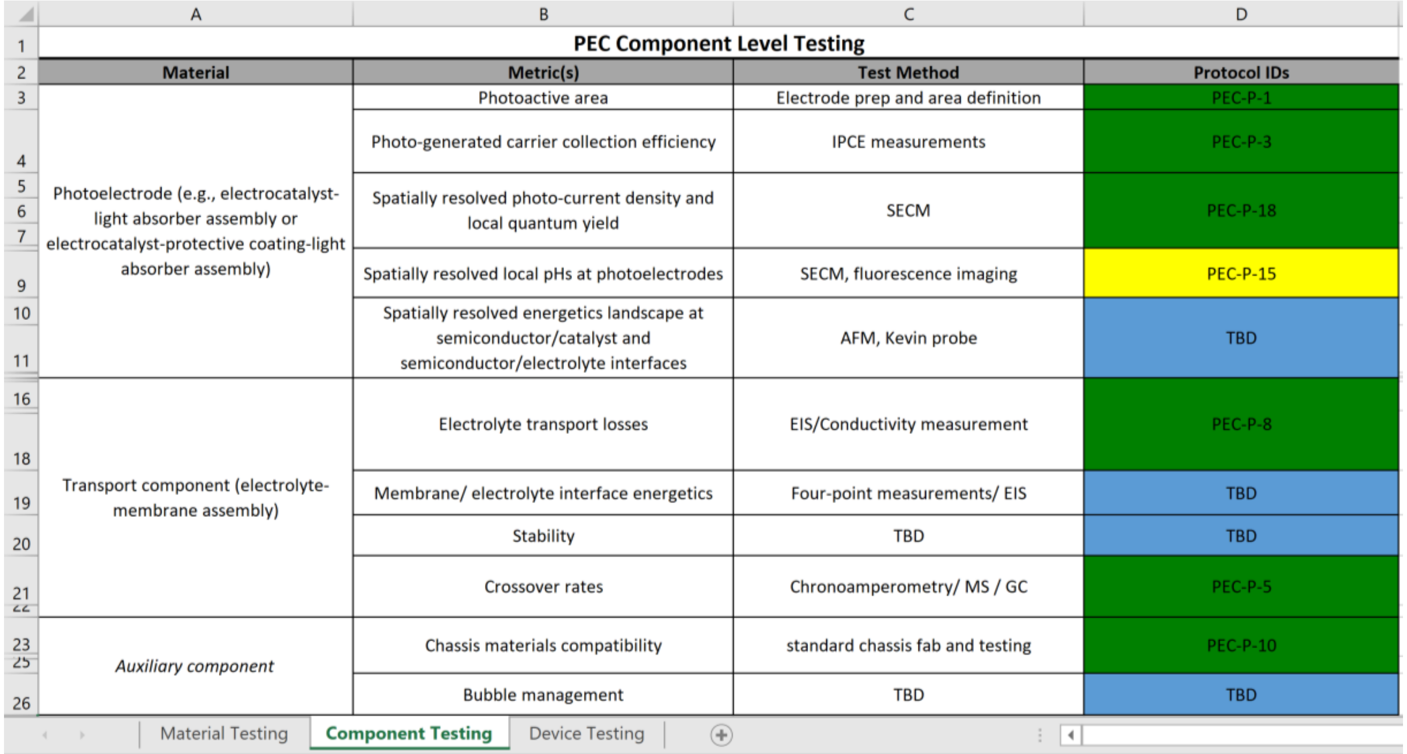


Figure 4. The Spectrum of Different Light Sources and the Method for Measuring Integral Incident Light Intensity

Wang, …, Liu, Domen, Li & Wang, *Joule*, **Feb 2021**, *5*, 344 (Australia, China, Japan)

PEC Benchmarking/Protocols: Component Level



PEC Component Level Testing

Material	Metric(s)	Test Method	Protocol IDs
Photoelectrode (e.g., electrocatalyst-light absorber assembly or electrocatalyst-protective coating-light absorber assembly)	Photoactive area	Electrode prep and area definition	🟩 PEC-P-1
	Photo-generated carrier collection efficiency	IPCE measurements	🟩 PEC-P-3
	Spatially resolved photo-current density and local quantum yield	SECM	🟩 PEC-P-18
	Spatially resolved local pHs at photoelectrodes	SECM, fluorescence imaging	🟨 PEC-P-15
	Spatially resolved energetics landscape at semiconductor/catalyst and semiconductor/electrolyte interfaces	AFM, Kevin probe	🟦 TBD
Transport component (electrolyte-membrane assembly)	Electrolyte transport losses	EIS/Conductivity measurement	🟩 PEC-P-8
	Membrane/ electrolyte interface energetics	Four-point measurements/ EIS	🟦 TBD
	Stability	TBD	🟦 TBD
	Crossover rates	Chronoamperometry/ MS / GC	🟩 PEC-P-5
Auxiliary component	Chassis materials compatibility	standard chassis fab and testing	🟩 PEC-P-10
	Bubble management	TBD	🟦 TBD

Status Key	🟩 Draft Complete
	🟨 Draft in Process
	🟦 Draft not Started

PC Benchmarking/Protocols: Device/Component Level

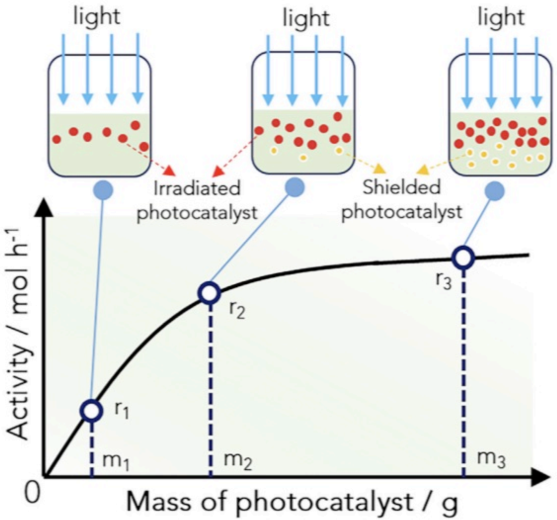
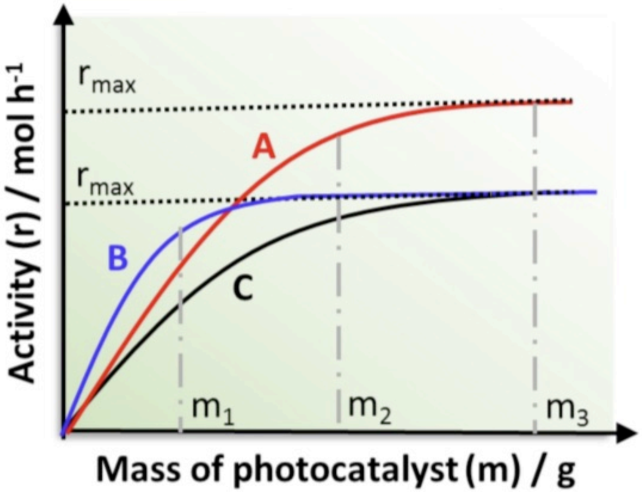


Figure 3. The Gas Evolution Rate Changes along with the Mass of Photocatalyst

The light -shielding effect of photocatalysts system with increased mass of photocatalyst are schematically illustrated. When the photocatalysts amount increases from m_1 to electron-consuming process, the shielding effect becomes significant. And the gas evolution rate reaches a peak reaction rate.

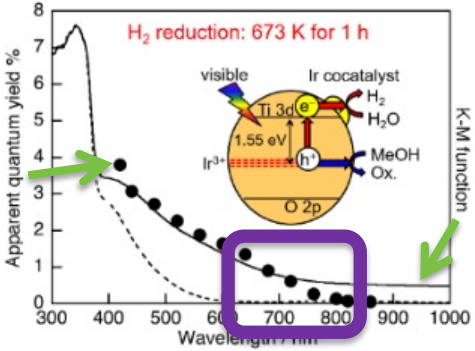
indicated in Figure 3. [40,14] With high mass concentration of photocatalyst in the reaction system, numerous particles cannot engage in light absorption and the subsequent photocatalytic reaction due to the limited light penetration depth. It is recommended to provide the *r-m* curve when an improvement in the efficiency (i.e., *r*, H_2 evolution rate) is claimed. Meanwhile, the maximum photocatalytic activity (r_{max}) should be used as a benchmark of H_2 evolution rate as discussed in Figure S2, under which condition the photon absorption is maximized. In addition, normalization of the reaction rate by the surface area (area-specific rate) or active site density also lacks validity because photocatalysis is governed not only by surface catalytic reactions but also by bulk physical processes including charge generation and charge separation.

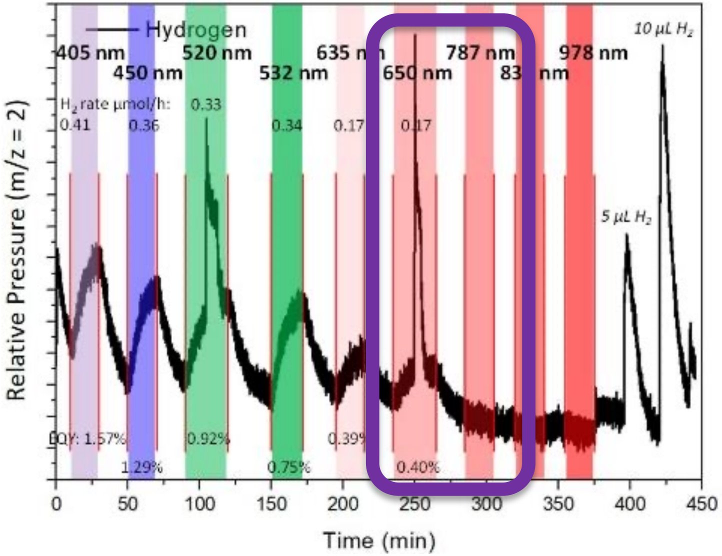


Wang, …, Liu, Domen, Li & Wang, *Joule*, **Feb 2021**, *5*, 344 (Australia, China, Japan)

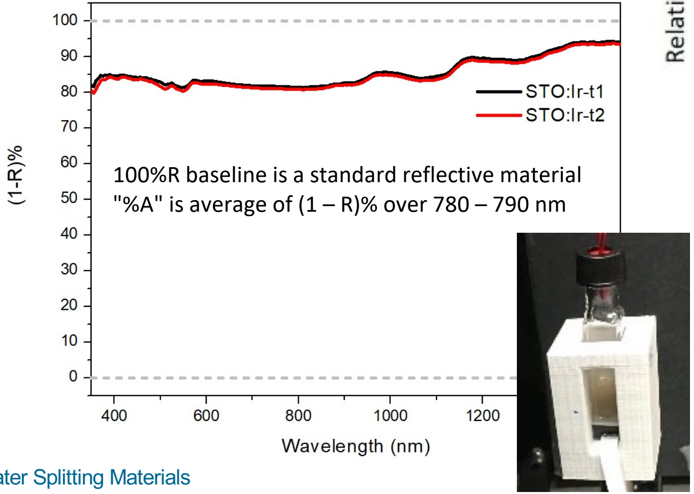
PC Benchmarking/Protocols: Component Level

Motivation: Suzuki, Matsumoto, Iwase & Kudo, *Chem. Comm.*, 2018, *54*, 10606





Ir/SrTiO$_3$:Ir (ID16) (1.0 mg/mL) with 0.3wt% Ir cocatalyst (impregnated @ 673 K for 2 h, H_2 anneal @ 673 K for 1 h) in aq 10 vol% CH_3OH under 785 nm LED illumination

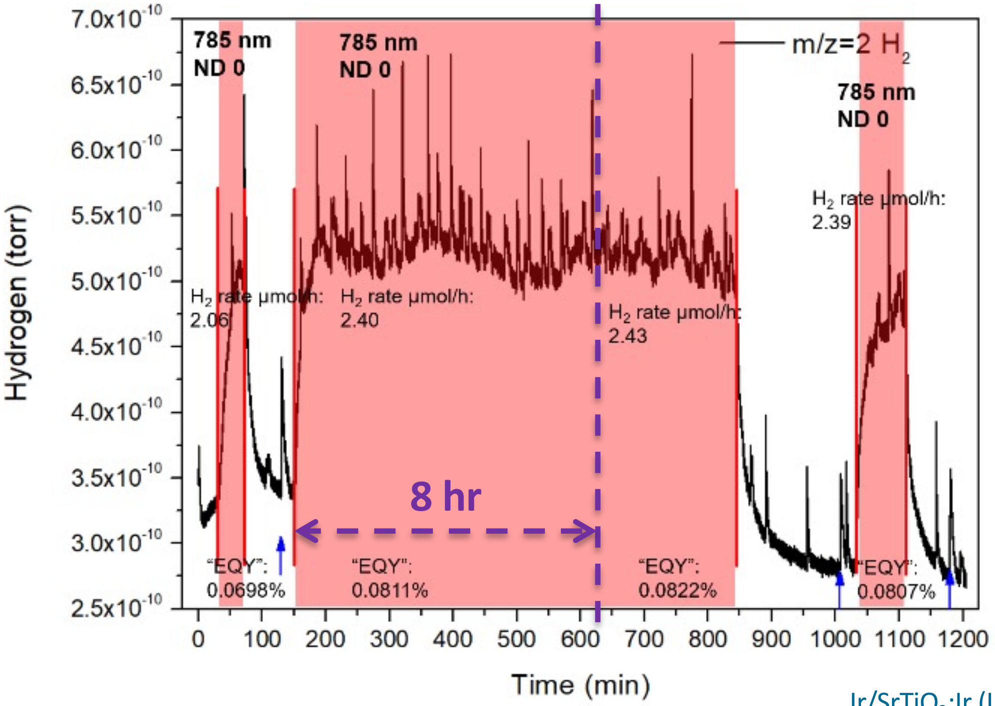


100%R baseline is a standard reflective material
"%A" is average of (1 – R)% over 780 – 790 nm

Absorptance + **R**eflectance + **T**ransmittance = 1

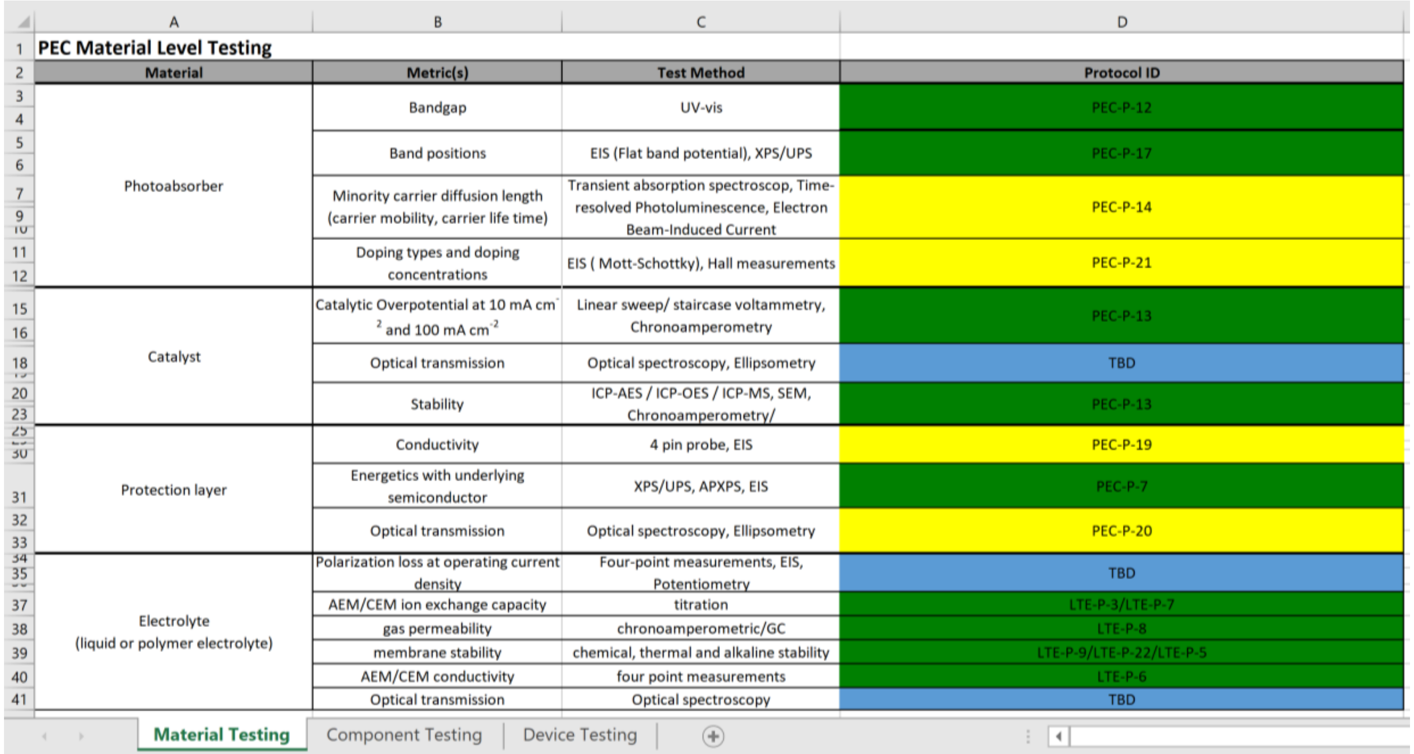
… Absorptance = 1 – Reflectance

PC Benchmarking/Protocols: Component Level



Ir/SrTiO$_3$:Ir (ID22) (1.8 mg/mL) with 0.3wt% Ir cocatalyst in aq 10 vol% CH$_3$OH under 785 nm LED illumination

PEC Benchmarking/Protocols: Material Level



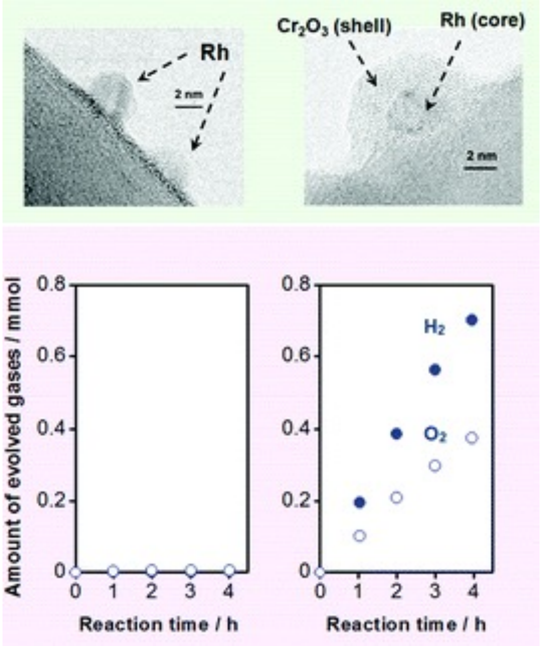
PEC Material Level Testing

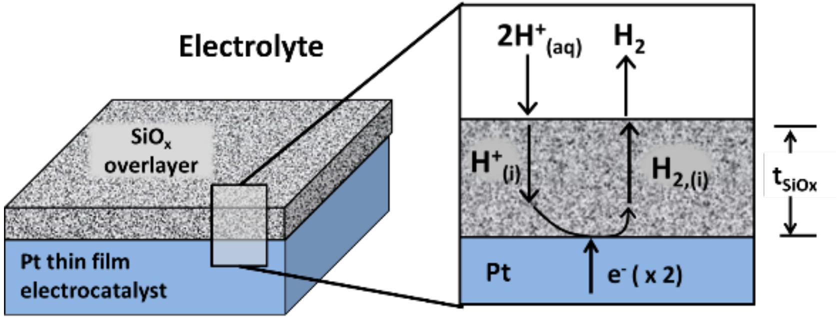
Material	Metric(s)	Test Method	Protocol ID
Photoabsorber	Bandgap	UV-vis	PEC-P-12
	Band positions	EIS (Flat band potential), XPS/UPS	PEC-P-17
	Minority carrier diffusion length (carrier mobility, carrier life time)	Transient absorption spectroscop, Time-resolved Photoluminescence, Electron Beam-Induced Current	PEC-P-14
	Doping types and doping concentrations	EIS (Mott-Schottky), Hall measurements	PEC-P-21
Catalyst	Catalytic Overpotential at 10 mA cm^{-2} and 100 mA cm^{-2}	Linear sweep/ staircase voltammetry, Chronoamperometry	PEC-P-13
	Optical transmission	Optical spectroscopy, Ellipsometry	TBD
	Stability	ICP-AES / ICP-OES / ICP-MS, SEM, Chronoamperometry/	PEC-P-13
Protection layer	Conductivity	4 pin probe, EIS	PEC-P-19
	Energetics with underlying semiconductor	XPS/UPS, APXPS, EIS	PEC-P-7
	Optical transmission	Optical spectroscopy, Ellipsometry	PEC-P-20
Electrolyte (liquid or polymer electrolyte)	Polarization loss at operating current density	Four-point measurements, EIS, Potentiometry	TBD
	AEM/CEM ion exchange capacity	titration	LTE-P-3/LTE-P-7
	gas permeability	chronoamperometric/GC	LTE-P-8
	membrane stability	chemical, thermal and alkaline stability	LTE-P-9/LTE-P-22/LTE-P-5
	AEM/CEM conductivity	four point measurements	LTE-P-6
	Optical transmission	Optical spectroscopy	TBD

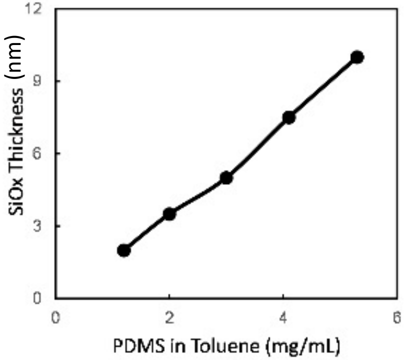
Status Key	
	Draft Complete
	Draft in Process
	Draft not Started

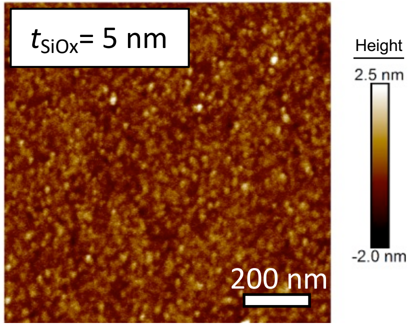
PC Benchmarking/Protocols: Material Level

Motivation: Maeda & Domen, *J. Phys. Chem. Lett.*, 2010, *1*, 2655





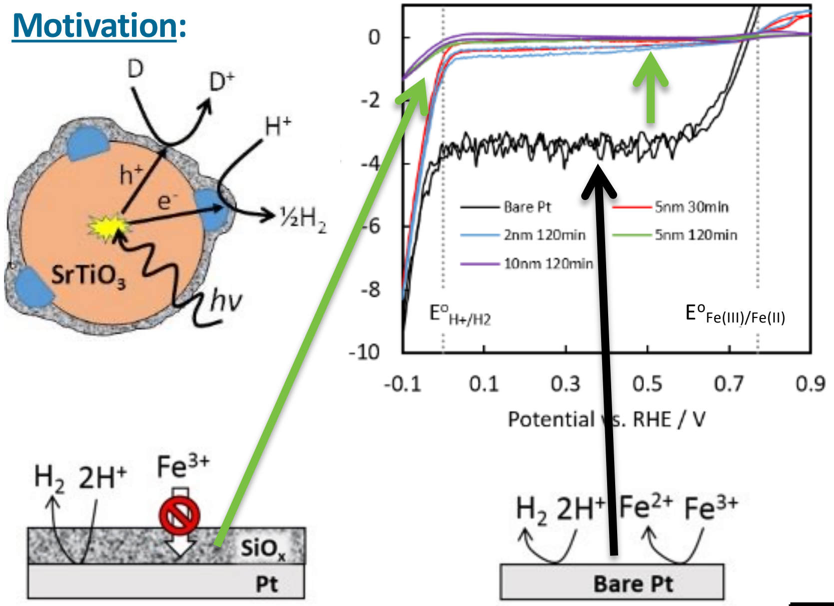




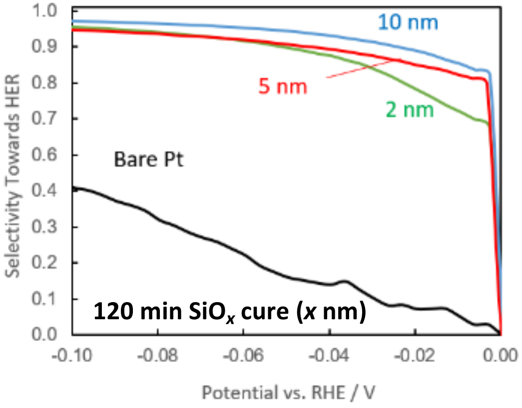
rms roughness
Pt|Ti|Si: ~0.3 nm
SiO_x|Pt|Ti|Si: ~0.3 nm

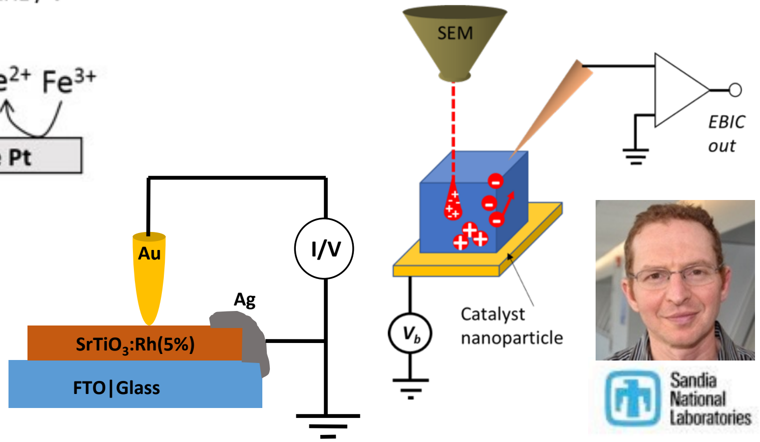
PC Benchmarking/Protocols: Material Level

Motivation:



CVs (20 mV/s) at Pt electrodes immersed in pH 1.5 aqueous Na_2SO_4(100 mM)–$Fe(SO_4)_n$(25 mM, 1:1 Fe(II):Fe(III))





Discussion Topics

Given that fundamental differences between **PC** and *PEC* are

(i) Incomplete per-particle above-bandgap light absorption, and

(ii) Selectivity toward less thermodynamically favored reactions,

does this warrant new, or simply updated:

1. **PC** (*PEC*) Device Protocols?
2. **PC** (*PEC*) Component Protocols?
3. **PC** (*PEC*) Material Protocols?

<u>Critical Question</u>: What new techniques and/or considerations should be taken into consideration, for both **PC** and *PEC*?

HydroGEN
Advanced Water Splitting Materials

Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Roadmap review and discussion

Technology: PEC

Session ID: PEC-5
Session Chair: Dan Esposito and Frances Houle
Notetakers: Will Stinson and Robert Stinson
Affiliation: DE: Columbia U, FH: LBNL
Date: March 3, 2021

nel number one by nature™ ASU Arizona State University Caltech PNNL

Session Goals

- Session Goals
  - Outline roadmap structure for materials and devices for future PEC H_2 technologies
  - Connect roadmap to protocols
  - Timelines

- Session Logistics
  - Session chair + note taker introductions (5 min.)
  - Fill out attendance list (1 min.)
  - Introductory slides (15 min.)
  - Discussion, populate MURAL (48 min)
  - Wrap-up - final chance to add to Mural, discussion (6 min.)
  - Report out on 3/8

Performance targets to reach low cost PEC H_2

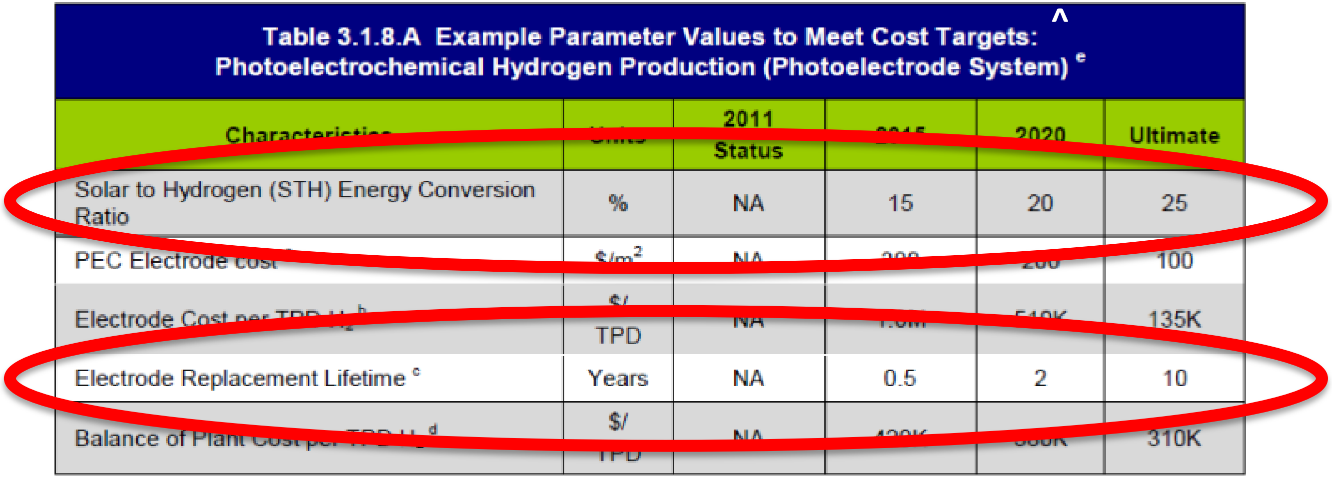


Table 3.1.8.A Example Parameter Values to Meet Cost Targets: ^ Photoelectrochemical Hydrogen Production (Photoelectrode System) [e]

Characteristics	Units	2011 Status	2015	2020	Ultimate
Solar to Hydrogen (STH) Energy Conversion Ratio	%	NA	15	20	25
PEC Electrode cost [a]	$\$/m^2$	NA	300	200	100
Electrode Cost per TPD H_2 [b]	$/ TPD	NA	1.0M	510K	135K
Electrode Replacement Lifetime [c]	Years	NA	0.5	2	10
Balance of Plant Cost per TPD H_2 [d]	$/ TPD	NA	430K	380K	310K

^Cost target: 2.10 $/kg H_2.

Note: Hydrogen cost represents the complete system hydrogen production cost for purified, 300 psi compressed gas. System level losses and expenses due to solar collection/concentration, window transmittance/refraction, replacement parts, operation, and maintenance are included in the cost calculations.

Note: Similar table available for dual bed photocatalyst reactor system.

Source: DOE EERE *Fuel Cell Technologies Program Multi-Year Research, Development, and Demonstration Plan (MYRD&D Plan), Planned program activities for 2011-2020. pp. 3.1-22.*

What is a Roadmap?

We are here

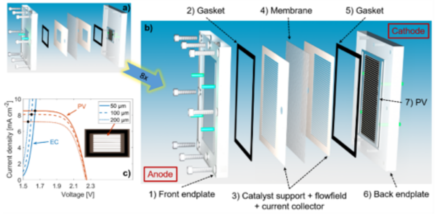
Materials strategy

Integration strategy

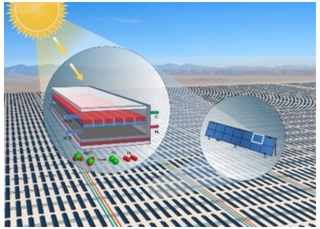
Performance strategy

Scale-up strategy

We need to be here



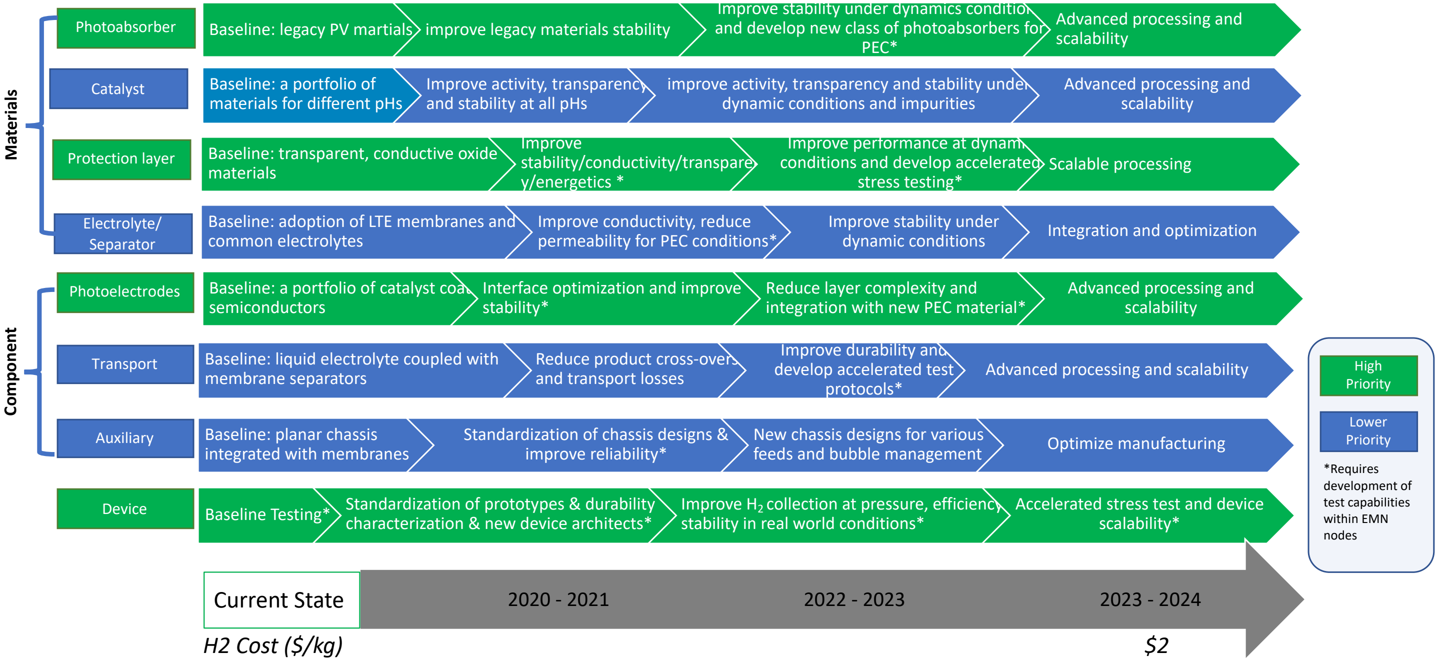
Kistler et al, Adv Energy Mater 2020
DOI: 10.1002/aenm.202002706



Sathre et al, Energy Env Sci 2014
DOI: 10.1039/c4ee01019a

PEC Roadmap, Fall 2019

What should the timeline look like for each strategy?



		Current State	2020 - 2021	2022 - 2023	2023 - 2024
Materials	🟩 Photoabsorber	Baseline: legacy PV martials	improve legacy materials stability	Improve stability under dynamics conditio and develop new class of photoabsorbers for PEC*	Advanced processing and scalability
	🟦 Catalyst	Baseline: a portfolio of materials for different pHs	Improve activity, transparenc and stability at all pHs	improve activity, transparency and stability under dynamic conditions and impurities	Advanced processing and scalability
	🟩 Protection layer	Baseline: transparent, conductive oxide materials	Improve stability/conductivity/transpare y/energetics *	Improve performance at dynam conditions and develop accelerated stress testing*	Scalable processing
	🟦 Electrolyte/ Separator	Baseline: adoption of LTE membranes and common electrolytes	Improve conductivity, reduce permeability for PEC conditions*	Improve stability under dynamic conditions	Integration and optimization
Component	🟩 Photoelectrodes	Baseline: a portfolio of catalyst coa semiconductors	Interface optimization and improve stability*	Reduce layer complexity and integration with new PEC material*	Advanced processing and scalability
	🟦 Transport	Baseline: liquid electrolyte coupled with membrane separators	Reduce product cross-over and transport losses	Improve durability an develop accelerated test protocols*	Advanced processing and scalability
	🟦 Auxiliary	Baseline: planar chassis integrated with membranes	Standardization of chassis designs & improve reliability*	New chassis designs for various feeds and bubble management	Optimize manufacturing
	🟩 Device	Baseline Testing*	Standardization of prototypes & durability characterization & new device architects*	Improve H_2 collection at pressure, efficienc stability in real world conditions*	Accelerated stress test and device scalability*
		H2 Cost ($/kg)			$2

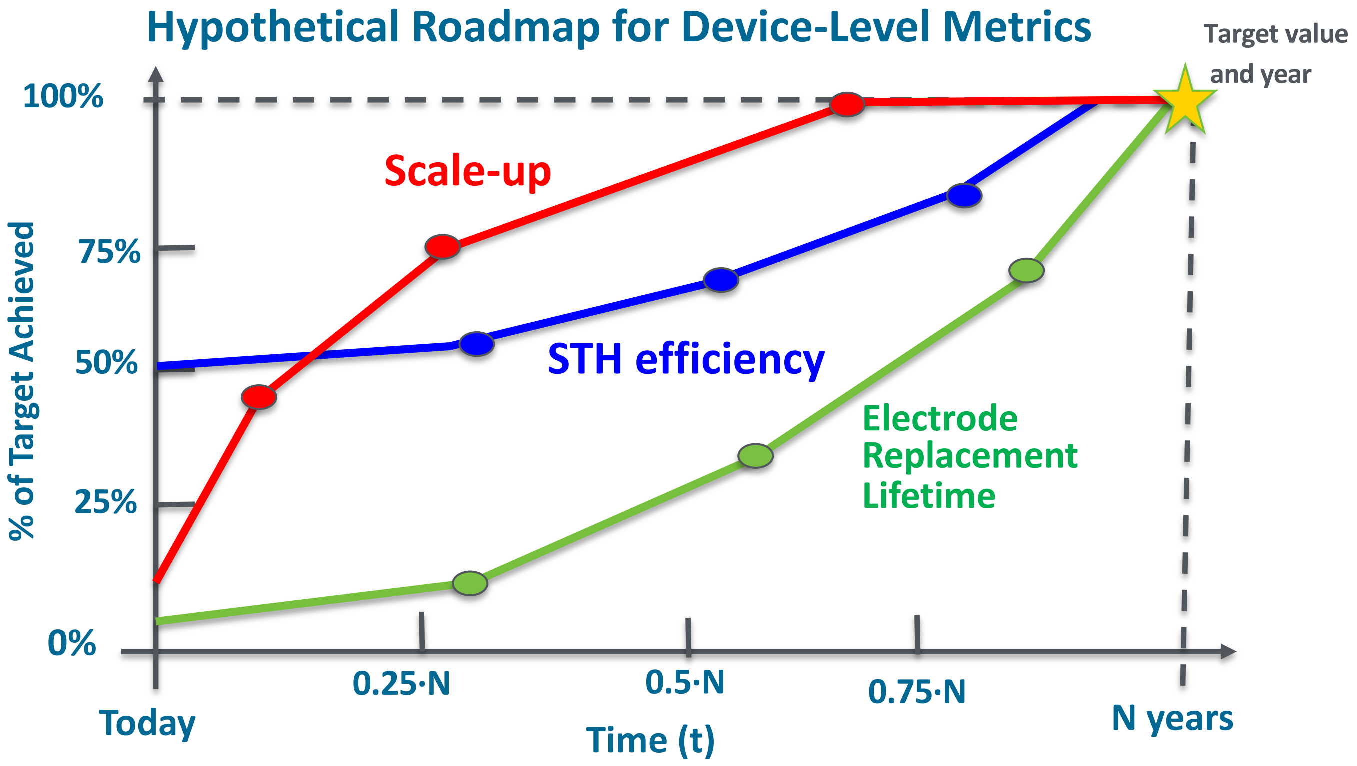
🟩 High Priority

🟦 Lower Priority

*Requires development of test capabilities within EMN nodes

Today's goal – revisit this scheme

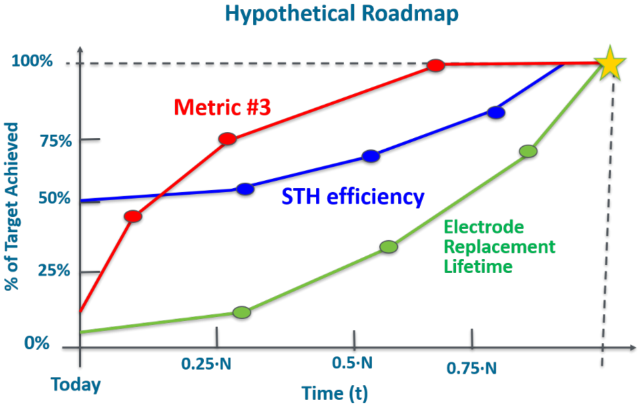
Roadmap basics



Note: there are many possible roadmaps, which will vary for different PEC technologies.

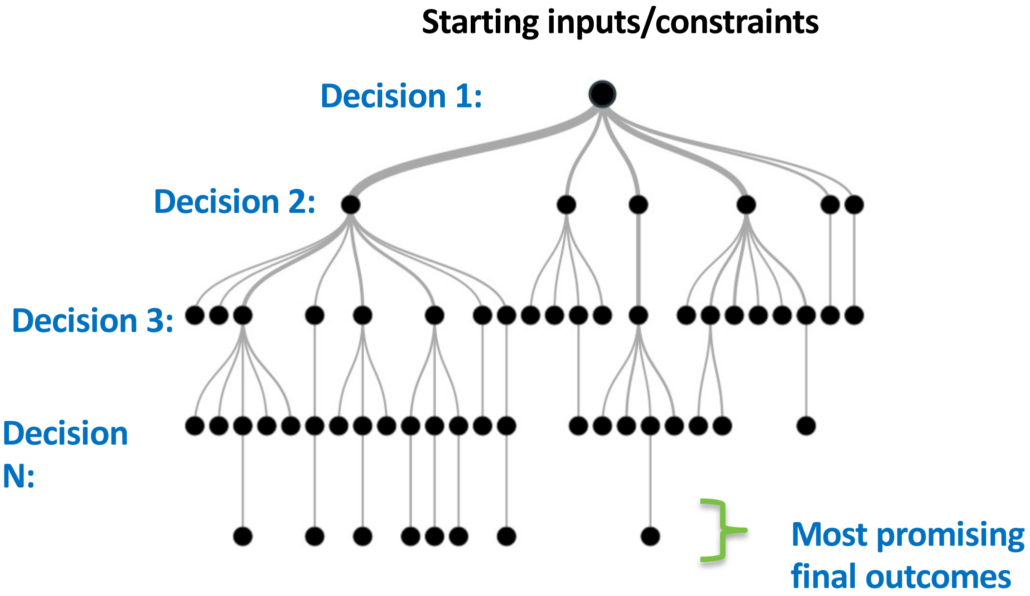
Questions to Consider when setting up a Roadmap

1. **What are the key system elements that most strongly influence LCOH, and what are their target performances? (discussed in PEC session #1)**
2. **What are the bottlenecks along the critical path for each element to achieve the technology target?**
3. **What are the dependencies* for the critical paths?**
4. **What is the timeline for the technology path?**
5. **What protocols are needed to accurately track progress?**



***Dependencies means interdependencies between critical paths: progress/delays on one can affect the others**

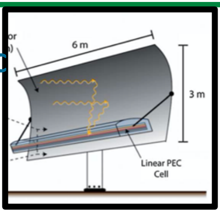
Decision Tree: a useful Tool for Formulating a PEC Target and Identifying Key Bottlenecks



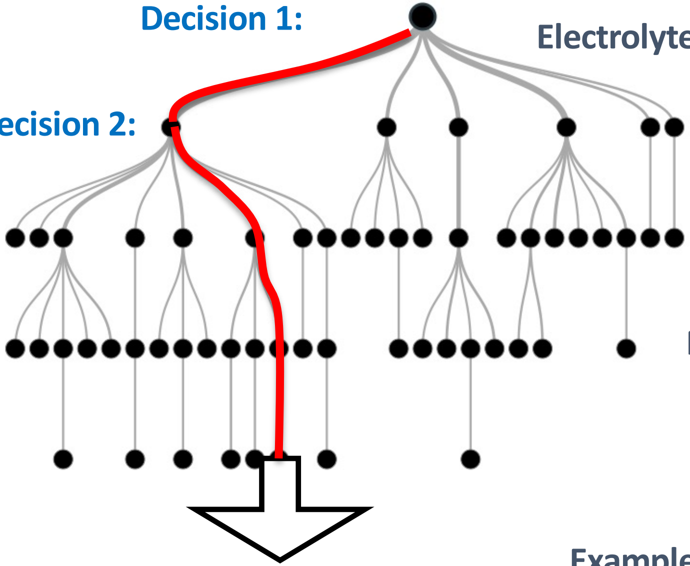
Decision Tree: a useful Tool for Formulating a PEC Target and Identifying Key Bottlenecks

Hypothetical decision tree:

Example: Concentrator PEC design



Starting inputs/constraints



Decision 1: Electrolyte type

Decision 2: Photoabsorber(s)/coatings

Decision 3: Electrocatalysts

Decision N: Membrane/divider

Most promising outcomes:

List of target specifications for material/component/system

Example: encapsulated III-V absorber with alkaline electrolyte, HE-membrane, and Ni-based OER & HER electrocatalysts.

How Does One use Outputs from a Decision Tree to Build a Roadmap?

1. **Understand how the properties/performance of each component impacts device-level target. (Modeling is key!)**
2. **Assess state-of-the-art performance for candidate components in comparison to that expected to be necessary to meet device-level target metrics.**
3. **What are the key bottlenecks for each component, and how difficult do we expect it will be to overcome them?**

Simple G/Y/R classification of bottlenecks:

🟩 **G: Likely to be easily overcome based on current R&D trajectory**

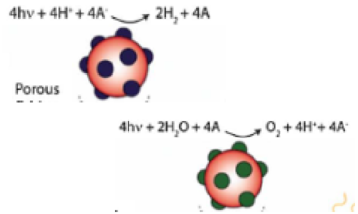
🟨 **Y: Likely to be overcome with substantial additional effort & resources.**

🟥 **R: "Red brick wall". At least an order of magnitude increase in effort & resources is likely needed to substantially alter current R&D trajectory. Success not guaranteed.**

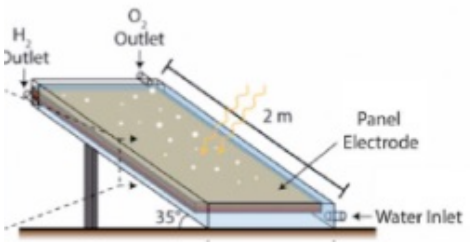
Today’s discussion topics

1. **What are key remaining bottlenecks and promising strategies for advancing the following PEC elements?:**
    1. **Photoabsorbers (12 min.)**
    2. **Electrocatalysts (12 min.)**
    3. **Membranes (12 min.)**
    4. **Devices & systems (12 min.)**
2. **What testing protocols should be in place to verify progress for materials and systems?**
3. **What is the timeline for overcoming key bottlenecks for each of three commonly considered PEC pathways?**

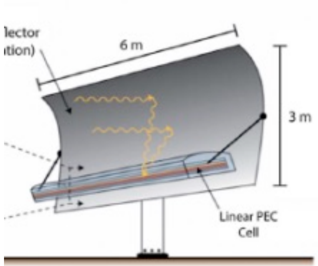
Type 2: Dual bed photocatalyst particle suspensions



Type 3: Fixed Panel Array
(No or limited solar concentration)

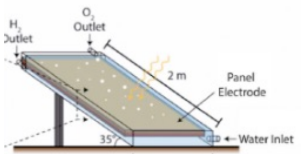
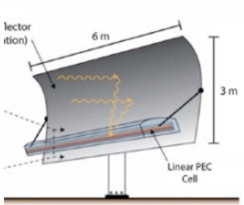
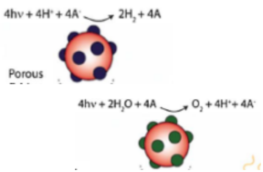


Type 4: Concentrator Array



General Targets^ to Consider for Discussion

Common Target for all: the ability to scale to GW- TW level cost effectively.

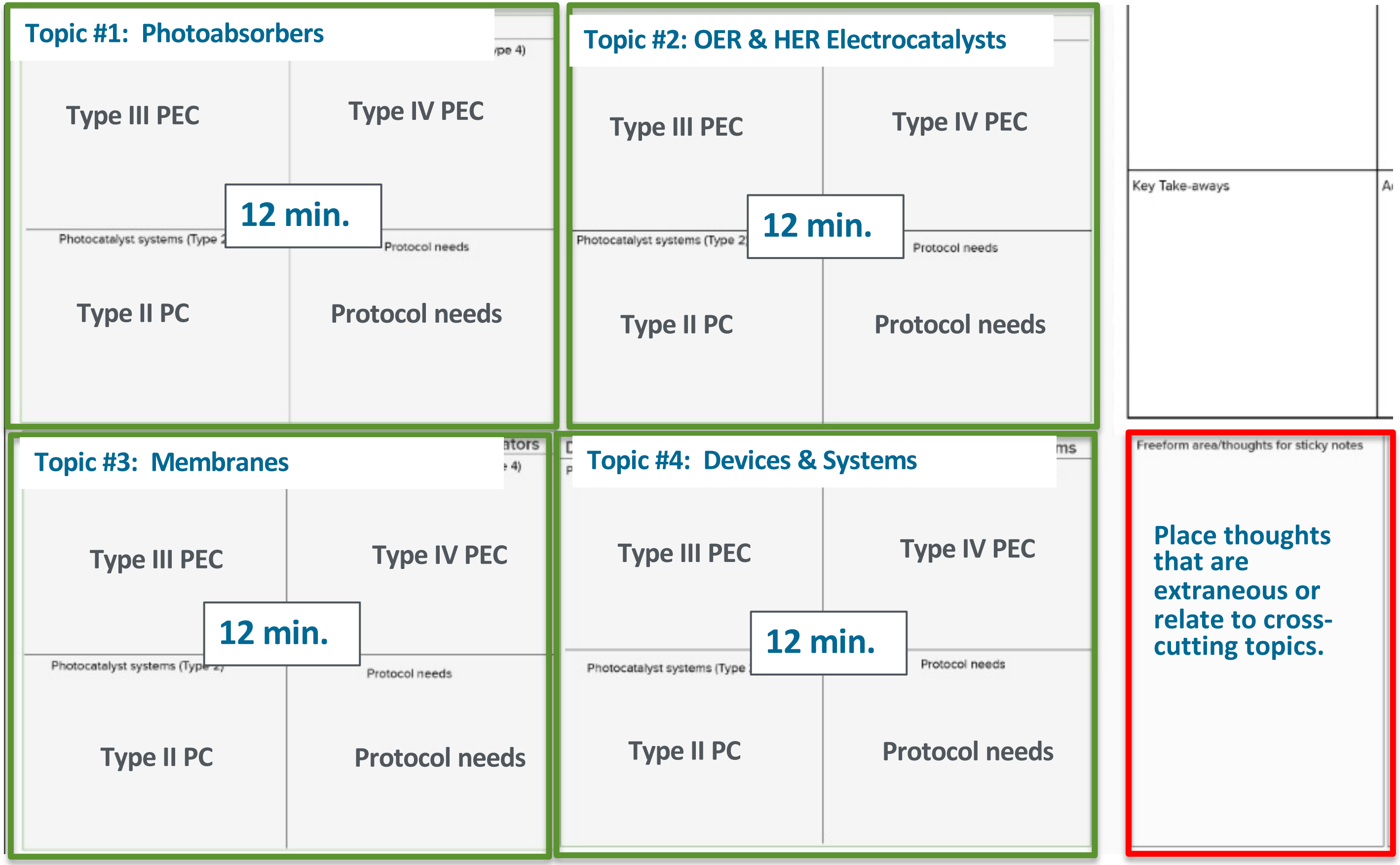
PEC Technology Path or "Type"	STH Efficiency	Replacement Lifetime
Fixed Panel Array (No or limited solar concentration) ("Type 3" from [1])  	15-25%	10-15 yrs.
Tracking Concentrator Arrays ("Type 4" from [1])  	15-25%	5-10 yrs.
Dual bed photocatalyst particle suspensions ("Type 2" from [1])  	8-12%	3-7 yrs.

[1.] Pinaud, et al., Energy & Environ. Sci., 6, 1983-2002 (2013).

^Targets include "ultimate" targets from 2015 FCTO's MYRD&D Production Section 3.1 to achieve LCOH $2.1/kg

MURAL Board for this Session

*Please sign in with your name so we can follow up w/ Questions if needed



Topic #1: Photoabsorbers

ype 4)

Type III PEC

Type IV PEC

12 min.

Photocatalyst systems (Type 2

Protocol needs

Type II PC

Protocol needs

Topic #2: OER & HER Electrocatalysts

Type III PEC

Type IV PEC

12 min.

Photocatalyst systems (Type 2)

Protocol needs

Type II PC

Protocol needs

Key Take-aways

A

Topic #3: Membranes

ators

e 4)

Type III PEC

Type IV PEC

12 min.

Photocatalyst systems (Type 2)

Protocol needs

Type II PC

Protocol needs

Topic #4: Devices & Systems

ms

Type III PEC

Type IV PEC

12 min.

Photocatalyst systems (Type

Protocol needs

Type II PC

Protocol needs

Freeform area/thoughts for sticky notes

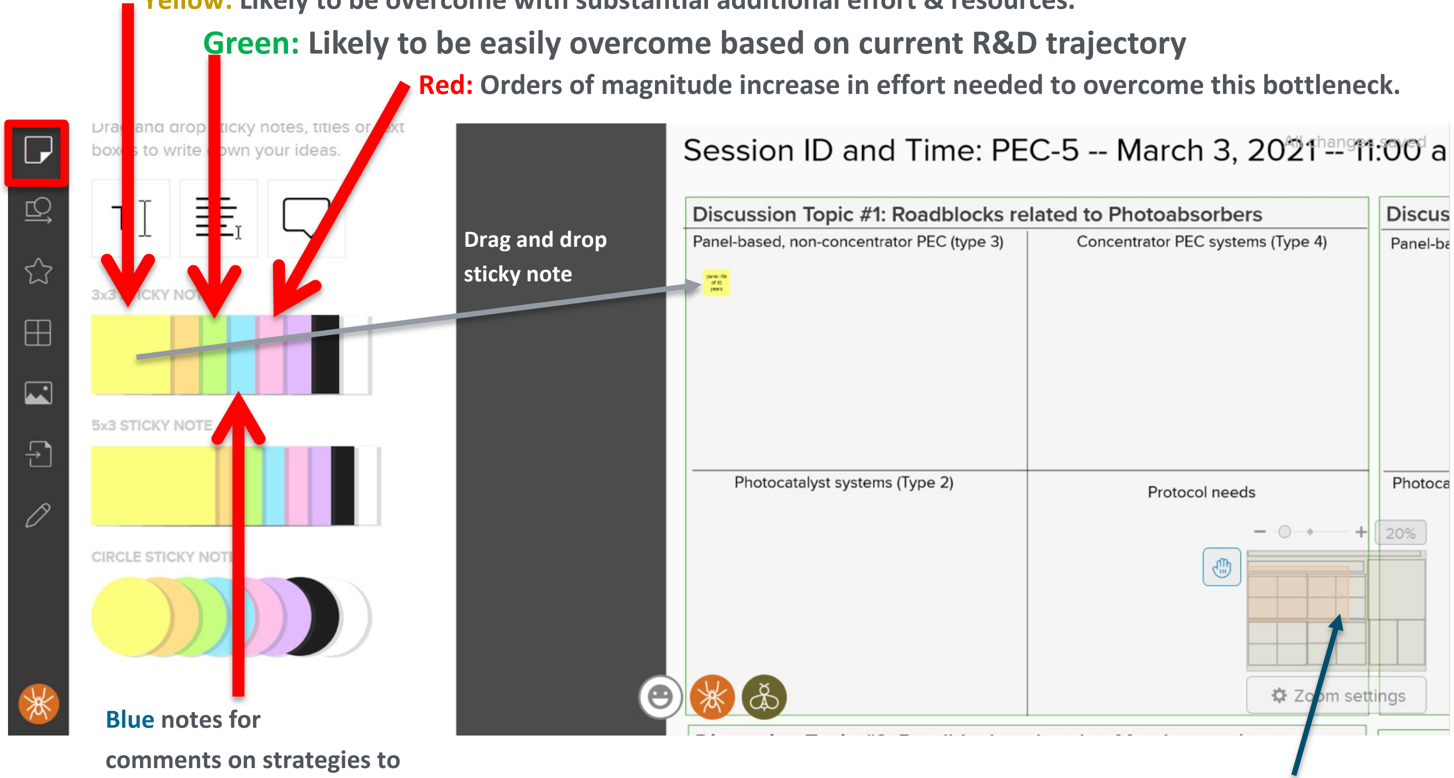
Place thoughts that are extraneous or relate to cross-cutting topics.

MURAL Board: Color-Coding for Sticky Notes

Yellow: Likely to be overcome with substantial additional effort & resources.

Green: Likely to be easily overcome based on current R&D trajectory

Red: Orders of magnitude increase in effort needed to overcome this bottleneck.



Session ID and Time: PEC-5 -- March 3, 2021 -- 11:00 a

Discussion Topic #1: Roadblocks related to Photoabsorbers

Blue notes for comments on strategies to overcome bottlenecks

Note: Zoom feature in lower right corner

PEC Roadmap Breakout Poll

Google Form Poll (Link provided in zoom chat box):

-Contains 4 sections (1 or each topic) with 6 questions each:

- **(3) G/Y/R voting questions** for each of 3 PEC technology pathways.
- **(3) timeline questions:** how long do you think it will take for the element of interest to advance to where it can enable commercialization?
- **(1) comment box**: comment on needed protocols for topic, elaborate on an answer, state a caveat, suggest a key strategy.

-Answer each set of 6 questions after completion of each of the 10-12 minute long topic-based discussions, then click “Next”.

Example: for the 12 minute section on photoabsorbers:

1. Is **photoabsorber** development G/Y/R for **Type III PEC (non-concentrator panel designs)**?
2. What is the expected timeline in years to achieve desired performance metrics?
3. **photoabsorber** development G/Y/R for **Type IV PEC (concentrator designs)**?
4. What is the expected timeline in years to achieve desired performance metrics?
5. Is **photoabsorber** development G/Y/R for **Type II PEC (dual bed photocatalyst designs)**?
6. What is the expected timeline in years to achieve desired performance metrics?

Topic 1 - Photoabsorbers

Targets: stable, sufficient photovoltage, high photocurrent

What are key remaining bottlenecks and promising strategies?

What testing protocols should be in place to verify progress for these materials?

What is the timeline for overcoming key bottlenecks for each of three commonly considered PEC pathways?

Topic 2 - Electrocatalysts

Targets: minimized overpotential for OER and HER, stable, compatible with photoabsorber and electrolyte

What are key remaining bottlenecks and promising strategies?

What testing protocols should be in place to verify progress for these materials?

What is the timeline for overcoming key bottlenecks for each of three commonly considered PEC pathways?

Topic 3 - Membranes/Separators

Targets: low resistance, zero product crossover, stable

What are key remaining bottlenecks and promising strategies?

What testing protocols should be in place to verify progress for these materials?

What is the timeline for overcoming key bottlenecks for each of three commonly considered PEC pathways?

Topic 4 - PEC Devices & Systems

Targets: high STH efficiency, long lifetime, safety, high energy return on energy invested (ERoEI)

What are key remaining bottlenecks and promising strategies?

What testing protocols should be in place to verify progress for these materials?

What is the timeline for overcoming key bottlenecks for each of three commonly considered PEC pathways?

Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

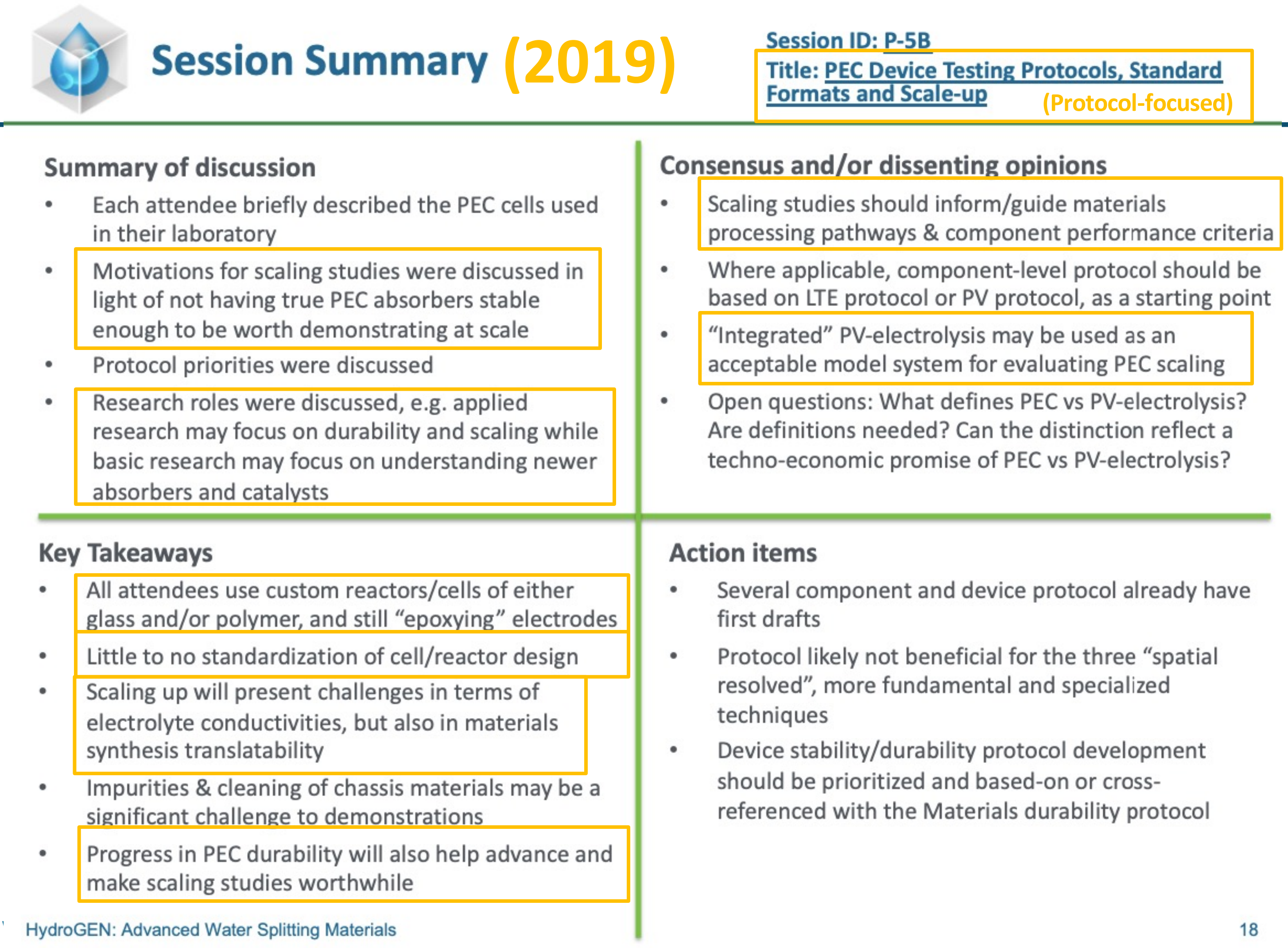
PEC-Standard hardware for bench and sub-scale testing
Technology: PEC

Session ID: PEC-7
Session Chair: James L. Young
Affiliation: NREL
Date: March 3, 2021

nel number one by nature™ · ASU Arizona State University · Caltech · PNNL

Session goals

- Session Logistics
  - Session topic introduction (10-15 min),
  - Mural facilitated discussion, 3-4 topics (45+ min)
  - Facility/capability needs for subscale testing (10 min)
  - Rules for session: Mural- please add your name when signing in as visitor
  - Start with sticky notes, priority voting (CX moderator), then comment and discuss
- Brief introduction of the topic
  - 2019 workshop session summary review
  - Overview of 2021 discussion topics
  - HydroGEN hardware examples designed to facilitate standardization
    - Bench scale: HydroGEN 2.0 common PEC cell version 1.0 (in 3D!)
    - Bench to subscale: NREL photoreactor platform (in motion picture!)



Session Summary (2019)

Session ID: P-5B

Title: PEC Device Testing Protocols, Standard Formats and Scale-up (Protocol-focused)

Summary of discussion

- Each attendee briefly described the PEC cells used in their laboratory
- Motivations for scaling studies were discussed in light of not having true PEC absorbers stable enough to be worth demonstrating at scale
- Protocol priorities were discussed
- Research roles were discussed, e.g. applied research may focus on durability and scaling while basic research may focus on understanding newer absorbers and catalysts

Consensus and/or dissenting opinions

- Scaling studies should inform/guide materials processing pathways & component performance criteria
- Where applicable, component-level protocol should be based on LTE protocol or PV protocol, as a starting point
- “Integrated” PV-electrolysis may be used as an acceptable model system for evaluating PEC scaling
- Open questions: What defines PEC vs PV-electrolysis? Are definitions needed? Can the distinction reflect a techno-economic promise of PEC vs PV-electrolysis?

Key Takeaways

- All attendees use custom reactors/cells of either glass and/or polymer, and still “epoxying” electrodes
- Little to no standardization of cell/reactor design
- Scaling up will present challenges in terms of electrolyte conductivities, but also in materials synthesis translatability
- Impurities & cleaning of chassis materials may be a significant challenge to demonstrations
- Progress in PEC durability will also help advance and make scaling studies worthwhile

Action items

- Several component and device protocol already have first drafts
- Protocol likely not beneficial for the three “spatial resolved”, more fundamental and specialized techniques
- Device stability/durability protocol development should be prioritized and based-on or cross-referenced with the Materials durability protocol

Overview of Discussion Topics

- Q0) Should bench- and sub-scale each be one word, two words, or hyphenated?
- Q1) How should PEC define **bench scale**?
  - Q2) Design features needed in standard **bench scale** PEC testing hardware
- Q3) How should PEC define **subscale**?
  - Q4) Design features needed in standard **subscale** PEC testing hardware
- Q5) What **subscale** targets should the field strive to demonstrate within 5 years? (add sticky notes then vote)
- Q6) What barriers are most critical to address in meeting these targets?

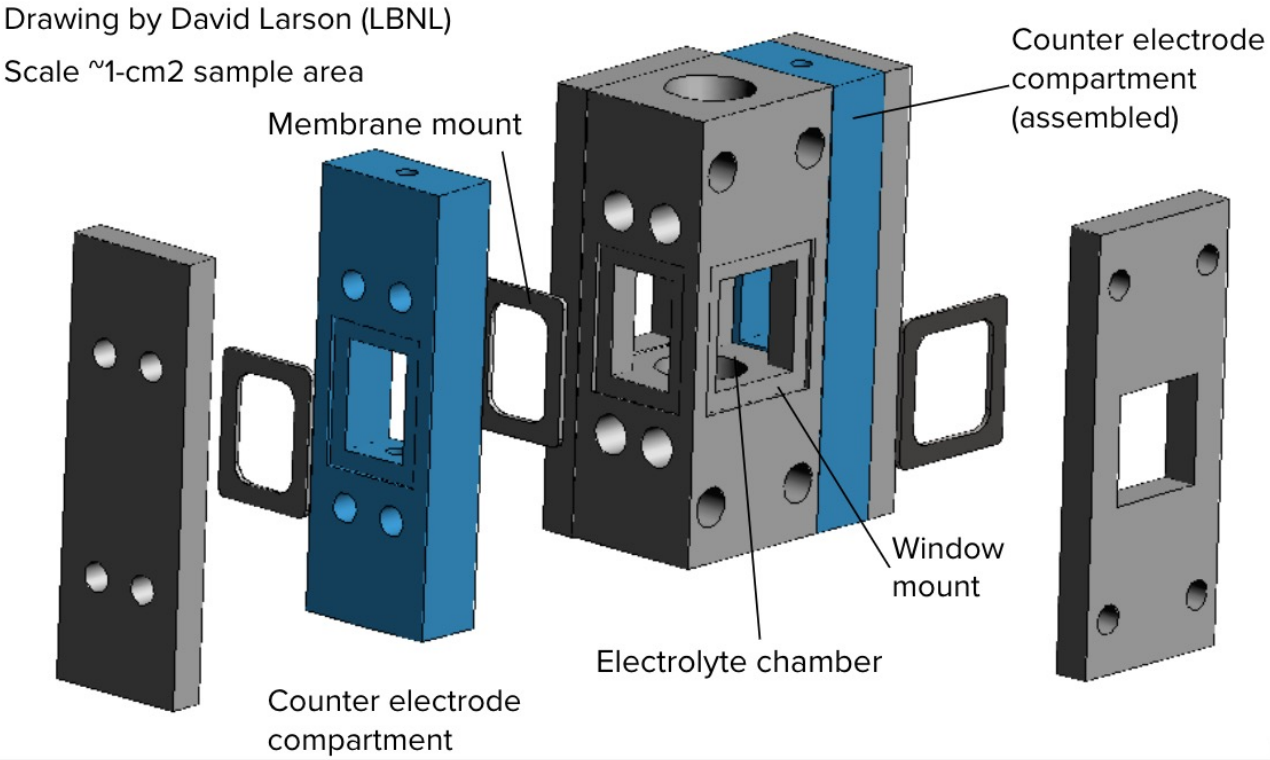
PEC Hardware Examples

Examples: Hardware designed to help facilitate testing in standard configuration(s)

- Ex. 1) HydroGEN PEC 2.0
  - Current initial work is establishing a common bench-scale hardware for PEC testing
- Ex. 2) NREL photoreactor platform
  - A flexible platform for bench- or sub-scale PEC testing

HydroGEN PEC 2.0

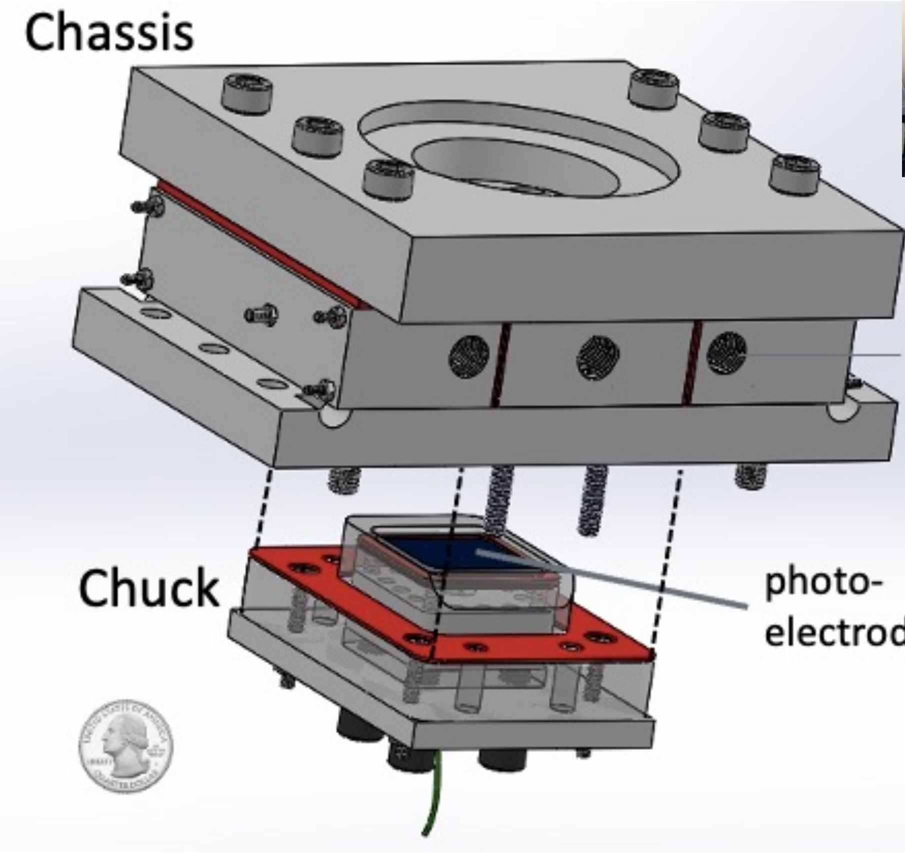
- Current initial work is establishing a common bench scale hardware for PEC testing

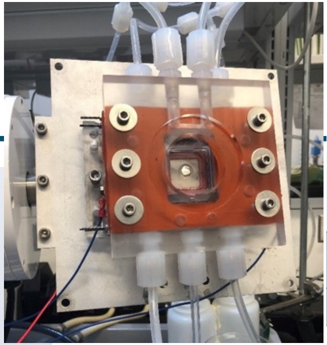


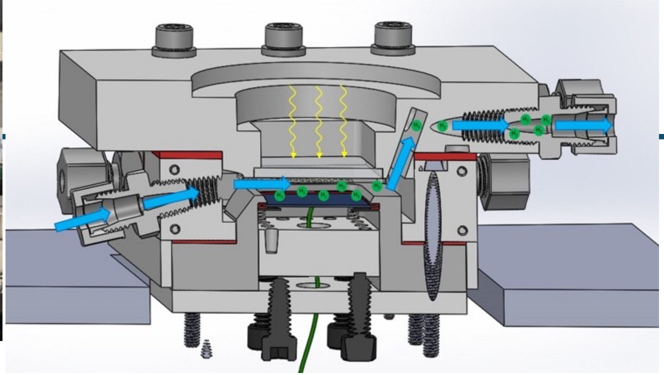
Drawing by David Larson (LBNL)

Scale ~1-cm2 sample area

NREL photoreactor platform





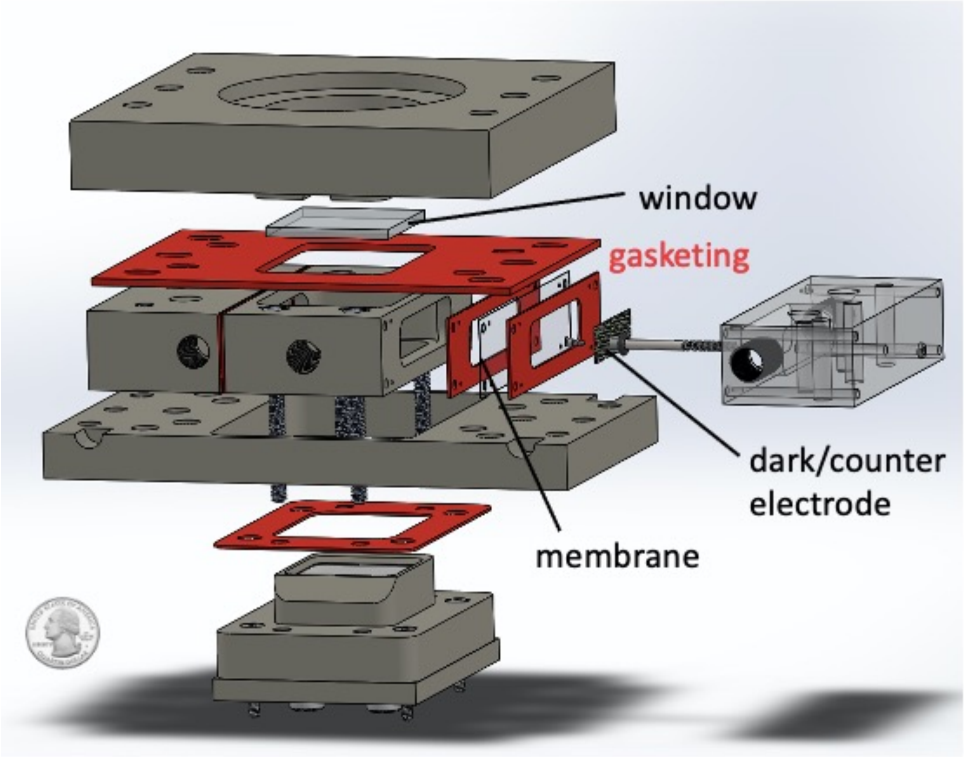


A flexible PEC testing platform

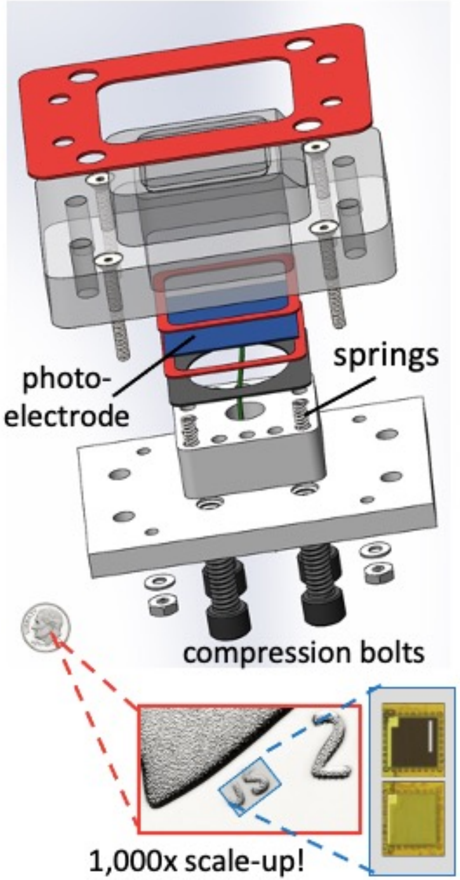
- Chassis-chuck two-part design
  - Quick slide in/out of pre-mounted samples
  - Customizable sample mounting
- Fresnel lens and collimating tube attachments
- Minimizes electrode separation, electrolyte resistance
- Flow pattern for bubble removal
- Separable anode compartments

NREL photoreactor platform

Chassis



Chuck



GaAs micro-cells

NREL photoreactor platform