HydroGEN Consortium: Advancements in Renewable Hydrogen Production

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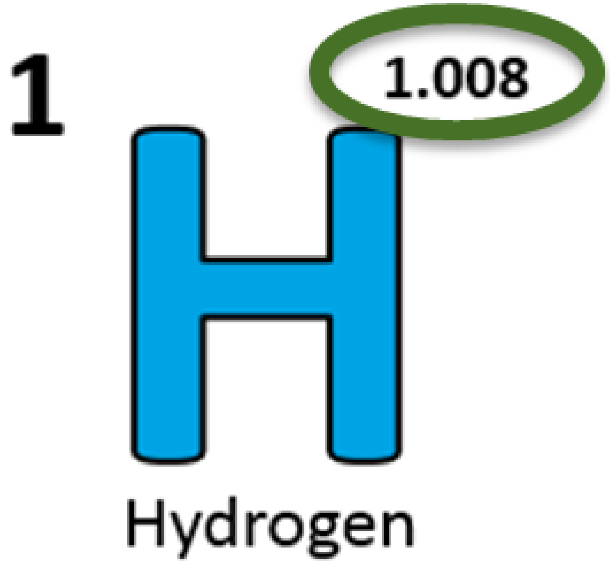
Director of HydroGEN, NREL

PRiME, Honolulu, HI
October 6, 2024
L04 – Solar Hydrogen Evolution Reaction or Water Reduction

When is hydrogen day?

Hydrogen and Fuel Cells Day
October 8

- Held on hydrogen’s very own atomic weight-day



Biden Administration Energy Goals

2035

Carbon-free U.S. electricity generation

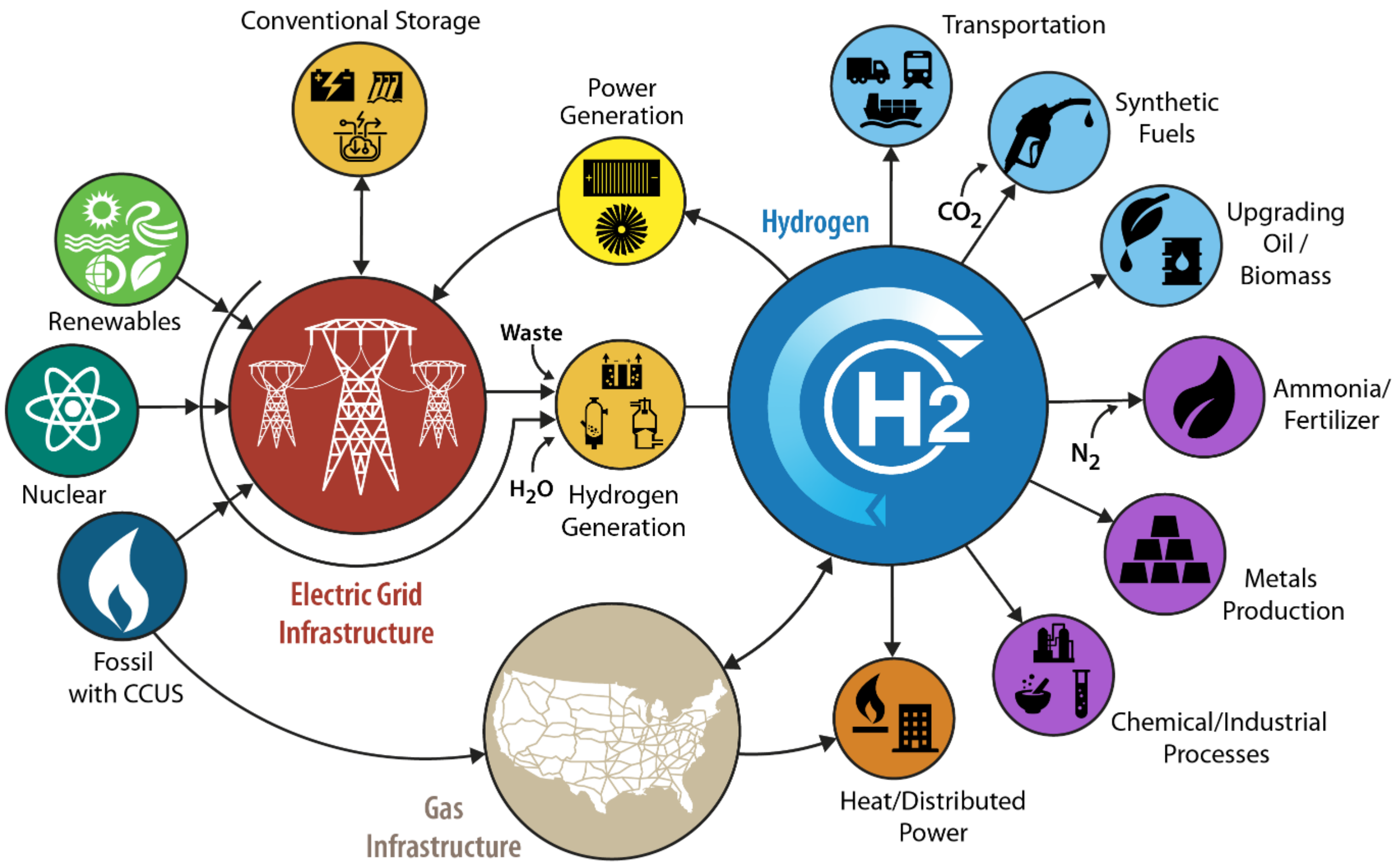
2050

Net zero greenhouse gas (GHG) emissions—including transportation, buildings, industry, and agriculture

Environmental Justice

Diversity, equity, and inclusion for energy jobs, manufacturing, and supply chain all over the United States

H2@Scale: Enabling Affordable, Reliable, Clean and Secure energy



Source: DOE Hydrogen and Fuel Cell Technologies Office, https://energy.gov/eere/fuelcells/h2-scale

Transportation and Beyond

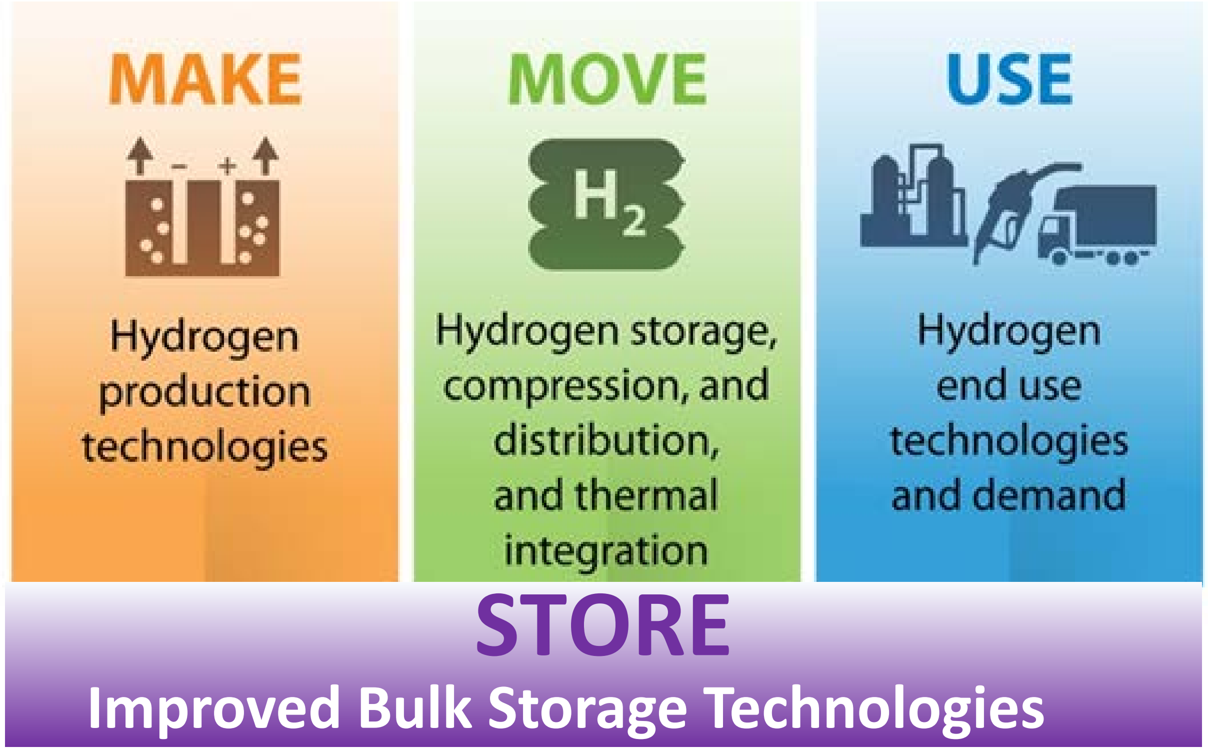
- Large-scale, low-cost hydrogen from diverse domestic resources enables an economically competitive and environmentally beneficial future energy system across sectors
- Hydrogen can address specific applications that are hard to decarbonize
- Today: 10 MMT H_2 in the US
- Economic potential: 2x to 4x more

Materials innovations are key to enhancing performance, durability, and reduce cost of hydrogen generation, storage, distribution, and utilization technologies key to H2@Scale

“Hydrogen at Scale (H_2@Scale): Key to a Clean, Economic, and Sustainable Energy System,” Bryan Pivovar, Neha Rustagi, Sunita Satyapal, Electrochem. Soc. Interface Spring 2018 27(1): 47-52; doi:10.1149/2.F04181if.

Improving the economics of H2@Scale

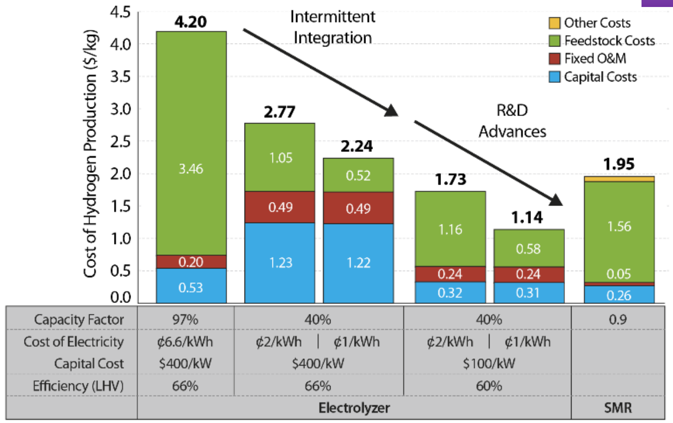
Early-stage research is required to evolve and de-risk the technologies.

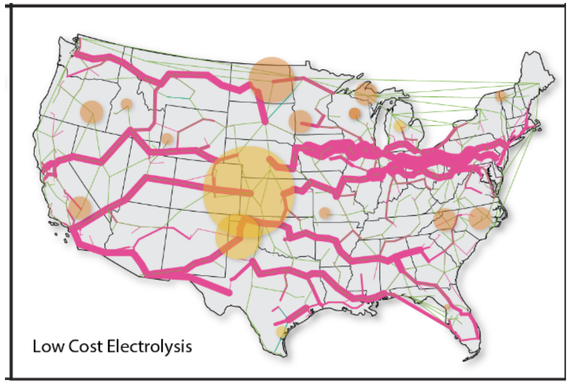


Preliminary

Use	Potential MMT/yr
Refineries & CPI	8
Metals	12
Ammonia	4
Synthetic Chemicals	14
Biofuels	1
Natural Gas	10
Light Duty Vehicles	57
Other Transport	17
Electricity Storage	28
Total	**151**

Decreasing cost of H_2 production





Optimizing H_2 storage and distribution

Leveraging of national laboratories' early-stage R&D capabilities needed to develop affordable technologies for production, delivery, and end use applications.

https://www.hydrogen.energy.gov/pdfs/review18/tv045_ruth_2018_o.pdf

What is Hydrogen Energy EarthShot?

ENERGY earthshots U.S. DEPARTMENT OF ENERGY | Hydrogen

Hydrogen Energy Earthshot

"Hydrogen Shot"

"1 1 1"
$1 for 1 kg clean hydrogen in 1 decade

Launched June 7, 2021
Summit Aug 31-Sept 1, 2021

S. Satyapal, et al., "Overview of DOE RFI Supporting Hydrogen Bipartisan Infrastructure Law Provisions, Environmental Justice, and Workforce Priorities, Feb. 24, 2022

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

U.S. National Clean Hydrogen Strategy and Roadmap

www.hydrogen.gov
Released June 5, 2023

Strategy

1. **Target strategic, high-impact end uses**
   Achieve 10 MMT/year of clean hydrogen by 2030
2. **Reduce the cost of clean hydrogen**
   Enable $2/kg by electrolysis by 2026 and $1/kg H_2 by 2031
3. **Focus on regional networks**
   Deploy regional clean hydrogen hubs and ramp up scale

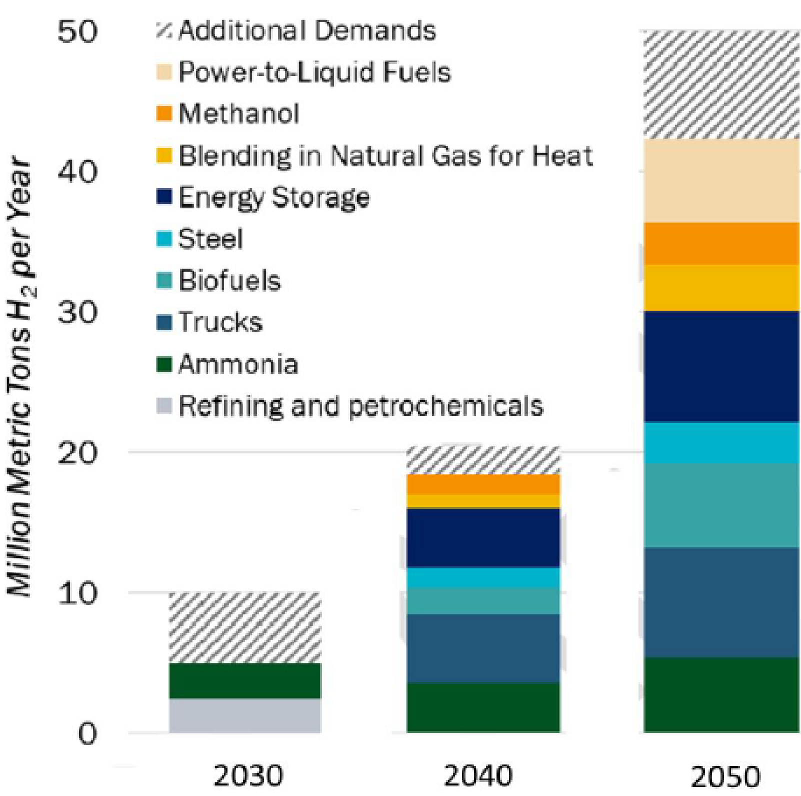
Vision:
Affordable clean hydrogen for a net-zero carbon future and a sustainable, resilient, and equitable economy

Benefits:
Emissions reduction; job growth; energy security and resilience

Enablers

Work with other agencies to accelerate market lift off

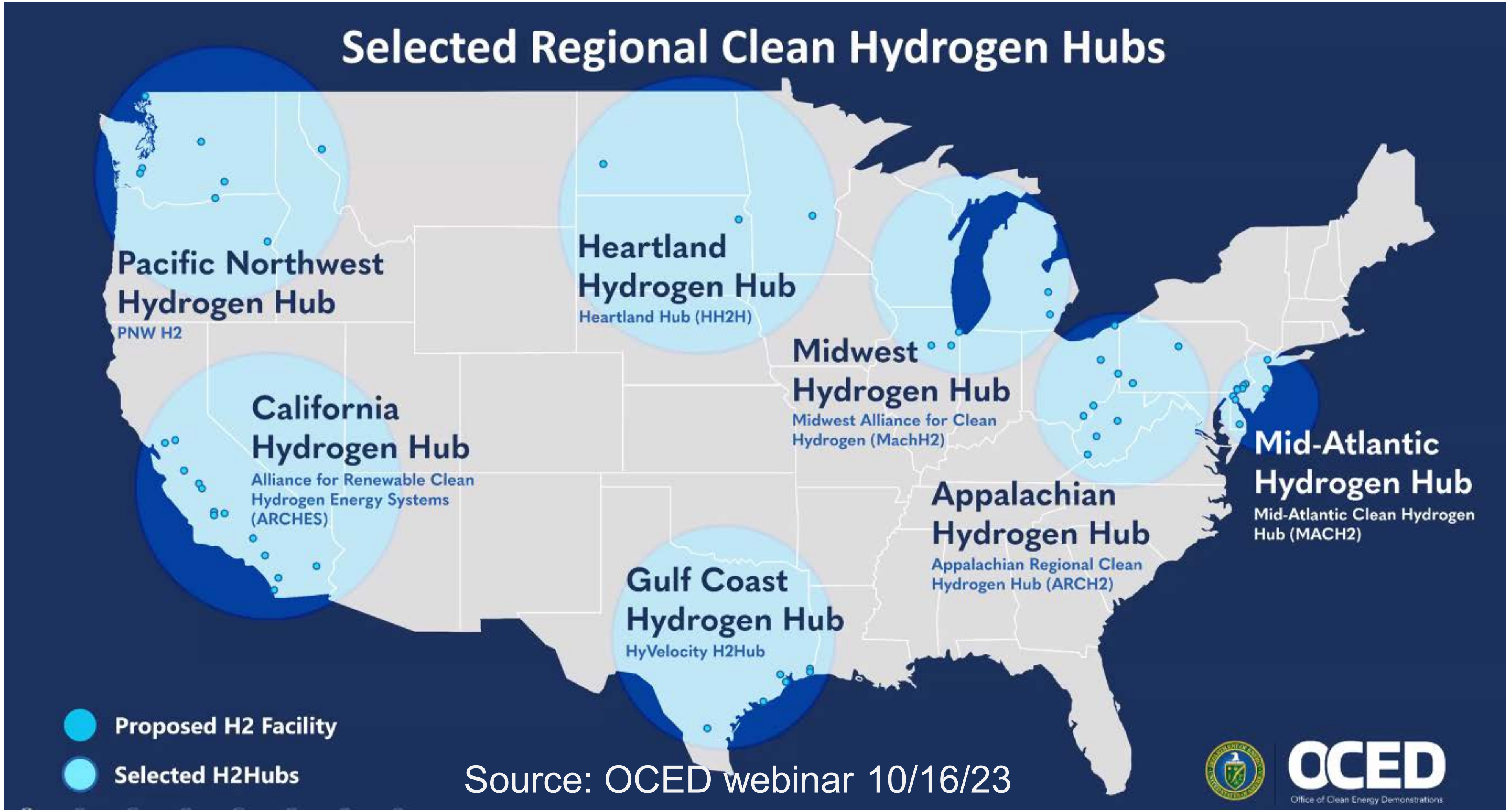
- Good Jobs and Workforce Development
- Safety, codes and standards
- Policies and incentives
- Stimulating private sector investment
- Energy and environmental justice



Opportunity: 10MMT/yr by 2030 → 20 MMT/yr by 2040 → 50 MMT/yr by 2050

~100K Jobs by 2030. ~10% Emissions Reduction by 2050.

$7B for 7 Hydrogen Hubs Announced October 13, 2023



DOE selects consortium to bridge demand for clean H_2 providing market certainty and unlock private capital Jan 2024

H2 Hubs managed by OCED: See https://www.energy.gov/oced/office-clean-energy-demonstrations

National Laboratory Collaboration is Critical for Success

H2NEW – Hydrogen from Next-generation Electrolyzers of Water (U.S. Department of Energy)

Hydrogen Production

NREL (Transforming ENERGY), INL (Idaho National Laboratory), Argonne National Laboratory, Pacific Northwest National Laboratory, Los Alamos National Laboratory, National Energy Technology Laboratory (NETL), Oak Ridge National Laboratory, Lawrence Livermore National Laboratory, Berkeley Lab (Bringing Science Solutions to the World)

ElectroCat – Electrocatalysis Consortium

Production & Fuel Cells

Los Alamos National Laboratory, Argonne National Laboratory, NREL (Transforming ENERGY), Oak Ridge National Laboratory

HydroGEN – Advanced Water Splitting Materials

Hydrogen Production

NREL (Transforming ENERGY), Berkeley Lab (Bringing Science Solutions to the World), INL (Idaho National Laboratory), Lawrence Livermore National Laboratory, Sandia National Laboratories

HyMARC – Hydrogen Materials Advanced Research Consortium

Hydrogen Storage

Sandia National Laboratories, NREL (Transforming ENERGY), Pacific Northwest National Laboratory, Lawrence Livermore National Laboratory, Berkeley Lab (Bringing Science Solutions to the World)

BioH2

Hydrogen Production

NREL (Transforming ENERGY), Berkeley Lab (Bringing Science Solutions to the World), Argonne National Laboratory, Pacific Northwest National Laboratory

M2FCT – Million Mile Fuel Cell Truck (U.S. Department of Energy)

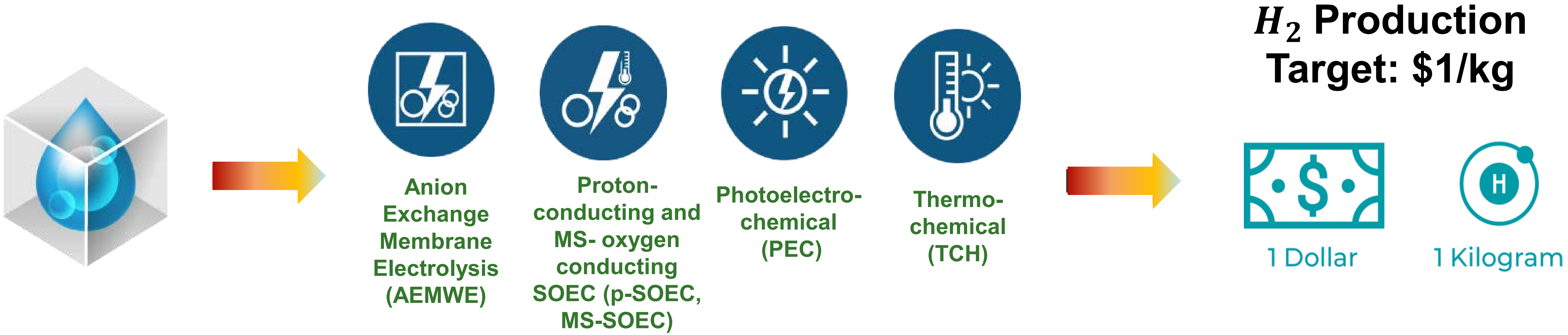
Fuel Cells

Berkeley Lab (Bringing Science Solutions to the World), Los Alamos National Laboratory, Argonne National Laboratory, NREL (Transforming ENERGY), Oak Ridge National Laboratory

HydroGEN: an AWSM Consortium

Website: https://www.h2awsm.org/

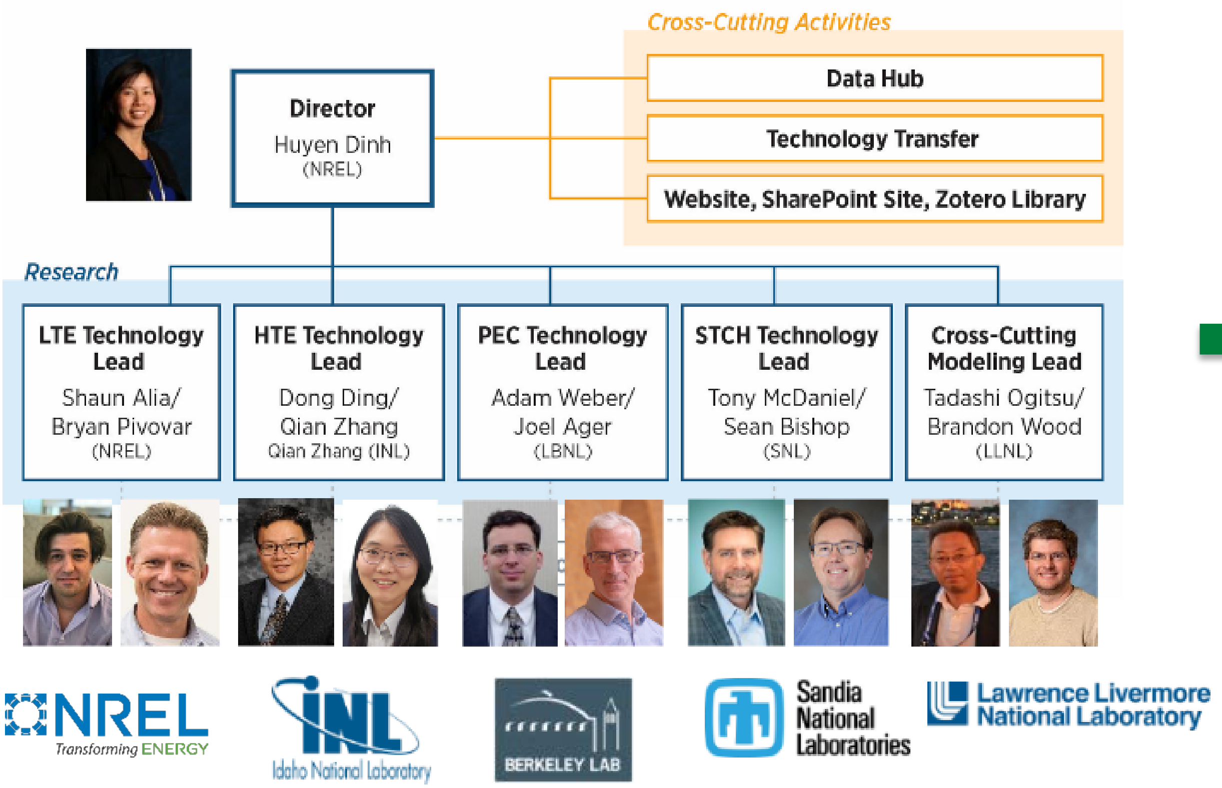
<u>Goal</u>: Accelerate foundational R&D of innovative materials for advanced water splitting (AWS) technologies to enable clean, sustainable, and low-cost ($1/kg H_2) hydrogen production.



HydroGEN is focused on early-stage R&D in H_2 production and fosters cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production

HydroGEN Lab R&D + Lab Capability Support

Lab R&D
Early-Stage Materials R&D Projects



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Lab Support
Lab capabilities + experts support early-stage materials R&D projects

HydroGEN Materials Capability Network
55 Lab- and FOA-awarded Projects

LTE Node Labs
NREL
BERKELEY LAB
Sandia National Laboratories
Lawrence Livermore National Laboratory

Support through:
Personnel
Equipment
Expertise
Capability
Materials
Data

LTE FOA Projects
BERKELEY LAB
nel
Lawrence Livermore National Laboratory
ecolectro
Georgia Tech Research Corporation

Lab Capability Support of 24 New "Seedling" Projects

5 AEME projects: 3 FOA-awarded projects & 2 Lab-call awarded projects

LTE Node Labs
- NREL (National Renewable Energy Laboratory)
- Berkeley Lab
- Sandia National Laboratories
- Lawrence Livermore National Laboratory

Support through: Personnel, Equipment, Expertise, Capability, Materials, Data

LTE FOA Projects
- Berkeley Lab
- nel
- Lawrence Livermore National Laboratory
- ecolectro
- Georgia Tech
- Research Corporation

6 p-SOEC projects : 4 FOA-awarded projects & 2 Lab-call awarded projects

HTE Node Labs
- INL (Idaho National Laboratory)
- NREL (Transforming ENERGY)
- Sandia National Laboratories
- Berkeley Lab
- Lawrence Livermore National Laboratory

Support through: Personnel, Equipment, Expertise, Capability, Materials, Data

Interactive HTE Projects
- Raytheon Technologies
- West Virginia University
- Georgia Institute of Technology
- Colorado School of Mines
- The University of Oklahoma
- Lawrence Livermore National Laboratory

6 PEC FOA-awarded projects

PEC Node Labs
- NREL (National Renewable Energy Laboratory)
- Berkeley Lab
- Lawrence Livermore National Laboratory

Support through: Personnel, Equipment, Expertise/Protocols, Capability, Materials/cells, Data

Interactive PEC projects
- Rice
- Yale
- California Institute of Technology
- The University of Toledo
- University of Michigan
- University of Hawai'i

5 TCH FOA-awarded projects

STCH Node Labs
- Sandia National Laboratories
- INL (Idaho National Laboratory)
- Lawrence Livermore National Laboratory
- NREL (National Renewable Energy Laboratory)

Support through: Personnel, Equipment, Expertise, Capability, Materials, Data

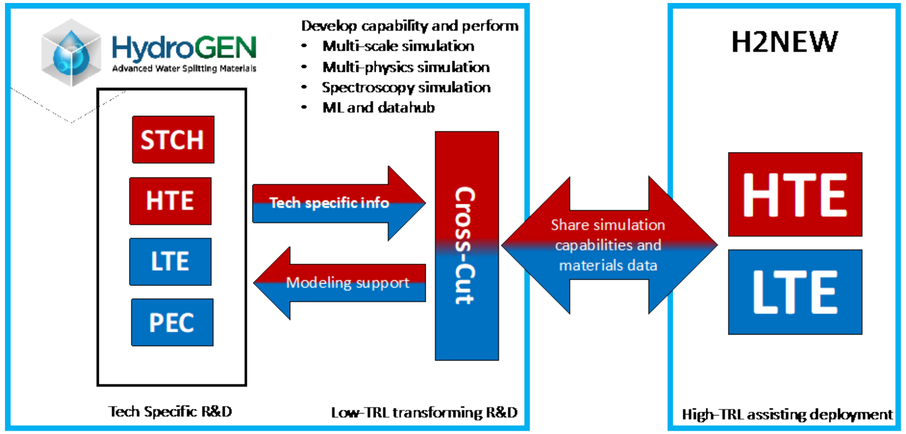
Interactive STCH Projects
- Arizona State University
- University of Colorado Boulder
- Massachusetts Institute of Technology
- Washington University in St. Louis
- Saint-Gobain

6 PEC and 5 STCH FOA-awarded projects have AMR presentations (https://www.hydrogen.energy.gov/amr-presentation-database.html). Some project technical accomplishments are highlighted in this presentation.

Science Challenges for Impactful HydroGEN Lab R&D:

- ***LTE***: improve AEM electrolysis performance and durability
- ***HTE***:
  - **MS-SOEC**: improve performance and durability with a scaled-up cell
  - **p-SOEC**: understand the proton conduction and electronic leakage mechanisms of electrolyte materials in proton-conducting SOEC
- ***PEC***: materials stability and device durability
- ***STCH***: identify and understand how structural features, composition, and defect dynamics engender high capacity–high yield behavior in materials

Cross-Cutting Modeling: theory-guided design to analyze performance and durability of materials under simulated operating conditions



HydroGEN PEC Lab R&D Goal and Approach

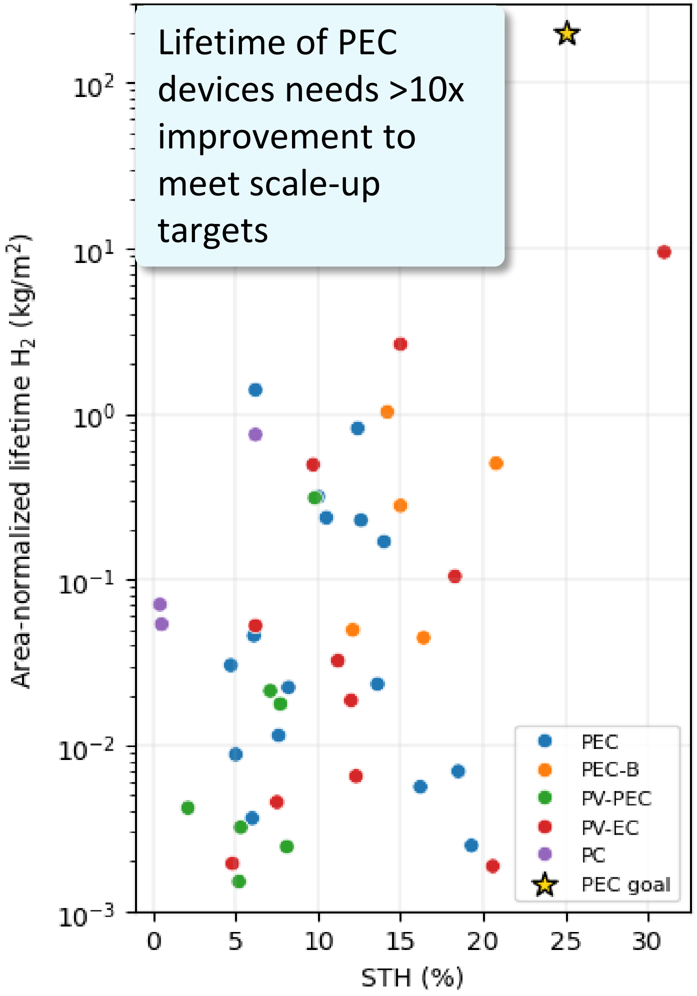
(Lead: Joel Ager, LBNL)

STH efficiency has improved but durability has not and is limiting PEC advancement

Goal: Elucidate the degradation mechanism(s) and improve the durability of PEC materials and devices.

Approach:

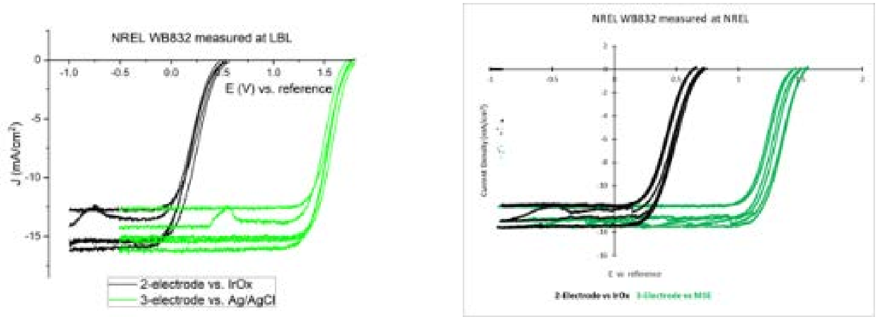
- Prioritize durability stressors and establish PEC device durability protocol
- Use density functional theory (DFT) and microkinetic modeling to describe the local environment at the electrode/electrolyte interface under operation
- Provide mechanistic understanding of PEC device degradation guided by theory and in operando characterization



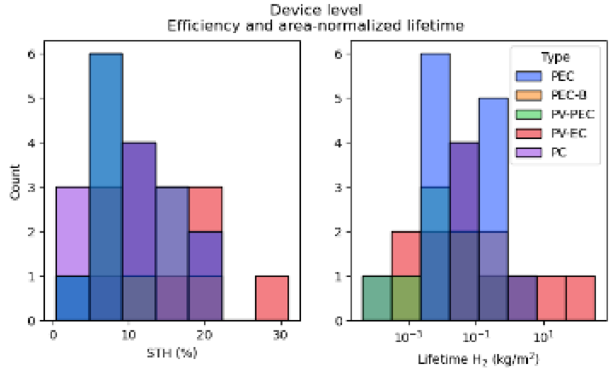
Comparison of the solar to hydrogen efficiency (STH) and lifetime H2 produced for unassisted water splitting devices. The "PEC Goal" point in the upper right. Data sourced with permission from Cheng et al. in 2022 Solar Fuels Roadmap, *J. Phys. D. Appl. Phys*. **2022**, 55 323003. PEC goal from Ben-Naim et al., *ACS Energy Lett.* **2020**, 5, 2631–2640.

HydroGEN PEC Lab R&D Relevance and *Potential Impact*

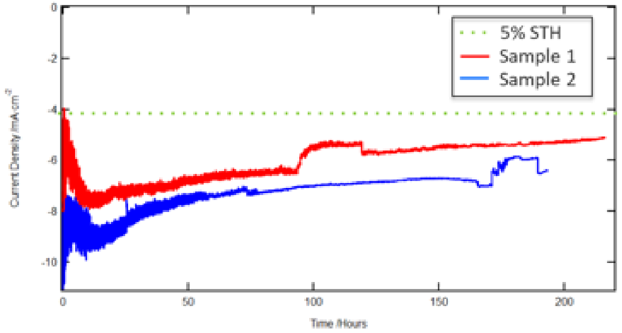
- Develop standardized PEC device measurement techniques
  Improves reproducibility between labs



- Develop device and system-level performance metrics
  Clearly define improvements needed for economic viability

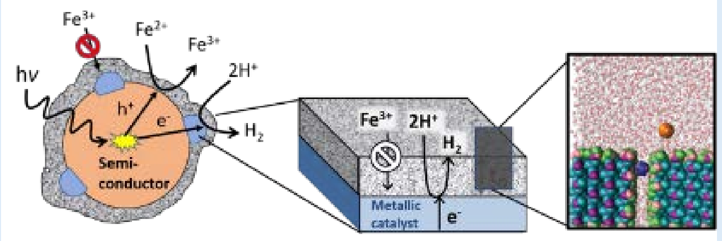


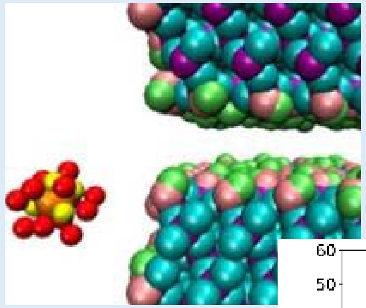
- Develop reliability science needed for closing the durability gap
  New materials for durable PEC water-splitting devices
  Accelerated wear protocols to quantify progress



PEC/LTE: Atomistic insights into transport, OER activities, stability

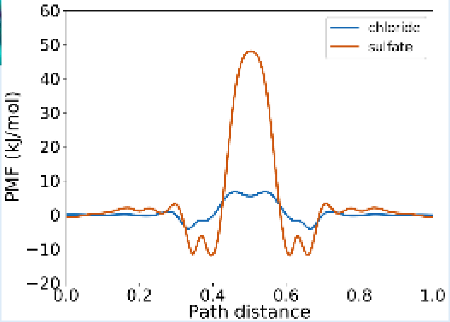
PEC: Protective layers





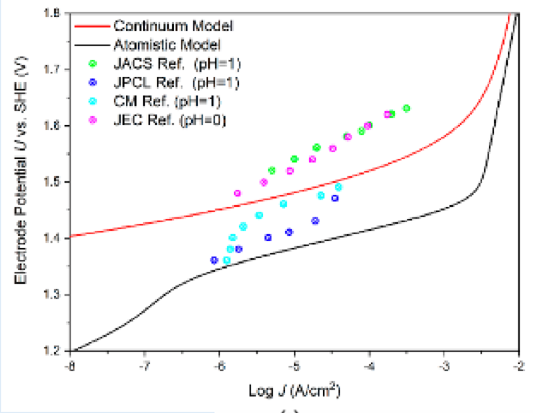
Oxide overlayer for selective transport

Aydin et al., EES Catalyst (Submitted)



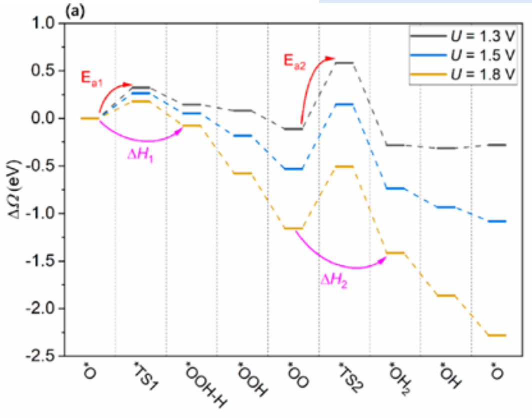
Developed **design principles** for optimizing protective layers

PEC: OER Activity



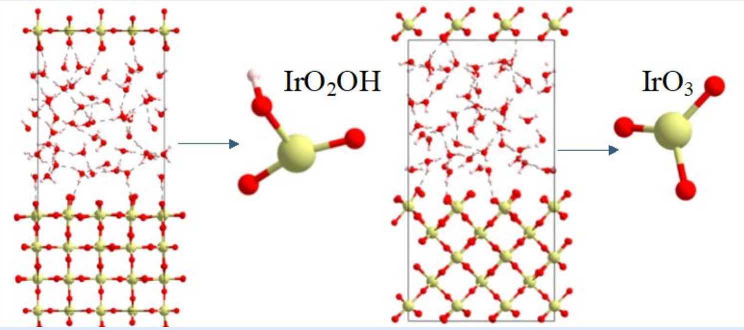
Developed models for predicting reaction kinetics

Reaction kinetics as a function of applied potentials



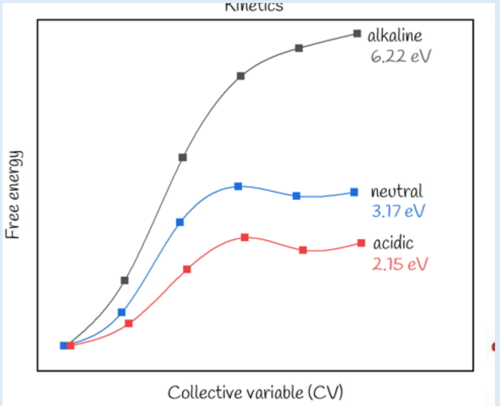
Deconvoluted impacts of operating conditions on activity

LTE: Catalyst Stability



Deconvolute impacts of **surface morphology**

Predict how **pH** influences dissolution kinetics



Identified **most important factors** controlling catalyst durability

Zhou et al., ACS Appl. Energy. Mater (2023)

Zagalskaya et al., (in preparation)

Proposed PEC device- and system-level performance metrics

Device-level metrics

- Solar to hydrogen conversion efficiency
  STH (%)
- Area-normalized lifetime production of H_2
  kg/m^2
  normalized to PV area for concentrators

System-level metrics

- Area
  m^2
  receiver area for concentrators
- Lifetime
  hours
  as reported by source
- System H_2 production rate
  kg/hr

Parkinson, B. *Acc. Chem. Res.* **1984**, *17*, 431–437

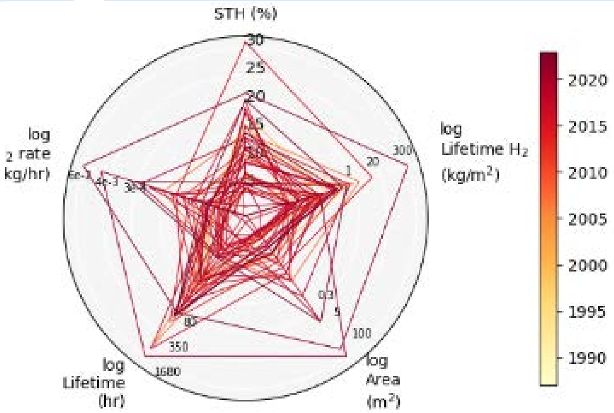
Pinaud et al, Energy Env. Sci. **2013**.

Ager, J. W.; Shaner, M. R.; Walczak, K. A.; Sharp, I. D.; Ardo, S. *Energy Environ. Sci.* **2015**

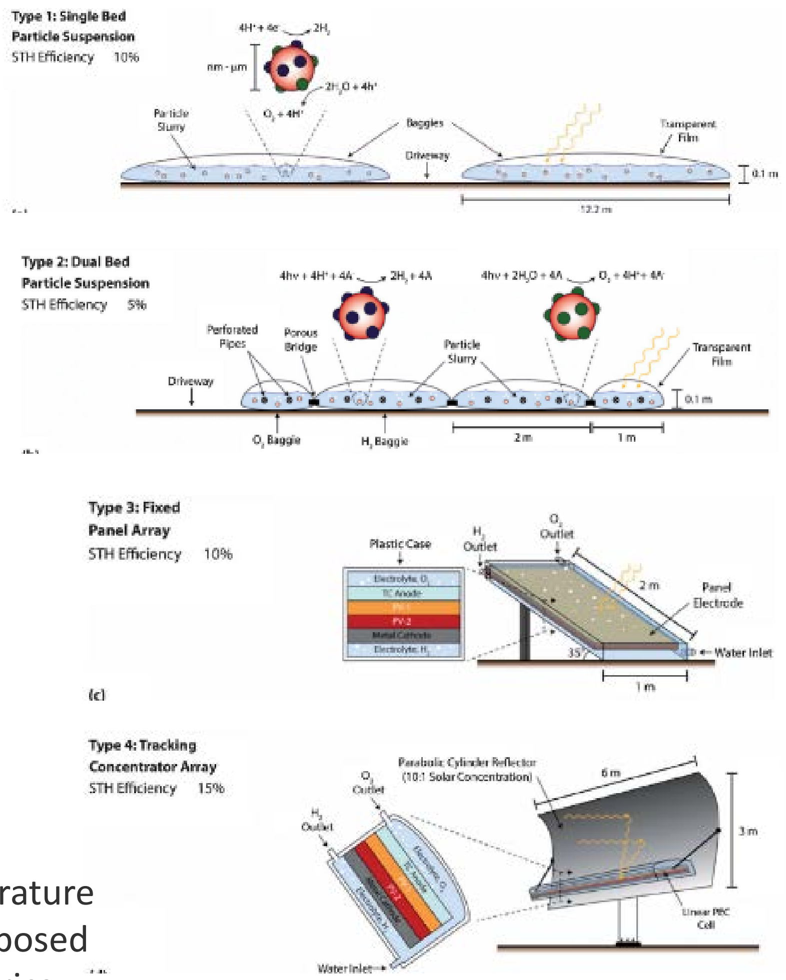
Ben-Naim, M.; Britto, R. J.; Aldridge, C. W.; Mow, R.; Steiner, M. A.; Nielander, A. C.; King, L. A.; Friedman, D. J.; Deutsch, T. G.; Young, J. L.; Jaramillo, T. F. *ACS Energy Lett.* **2020**,

Cheng, W.-H., Deutsch, T. G., Xiang, X. in 2022 Solar Fuels Roadmap, *J. Phys. D. Appl. Phys.* 2022

Holmes-Gentle, I.; Tembhurne, S.; Suter, C.; Haussener, S. *Nat. Energy* **2023**



Analysis of 44 literature reports using proposed performance metrics



HydroGEN PEC Seedling Projects & Lab Collaboration

PEC Node Labs

NREL Transforming ENERGY

BERKELEY LAB

Lawrence Livermore National Laboratory

Support through:

Personnel

Equipment

Expertise/Protocols

Capability

Materials/cells

Data

Interactive PEC projects

RICE

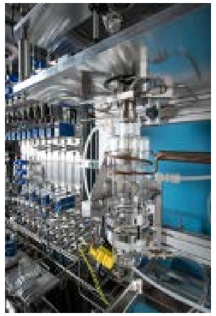
Y

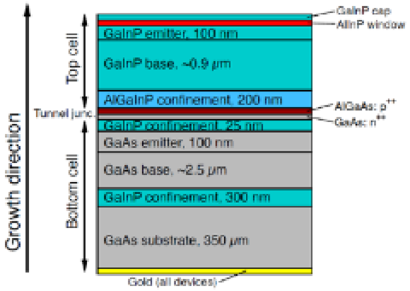
California Institute of Technology 1891

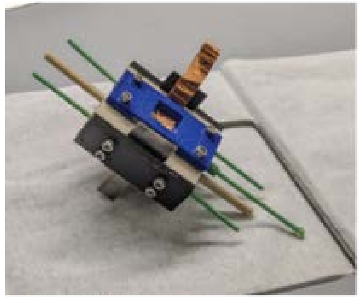
The University of Toledo

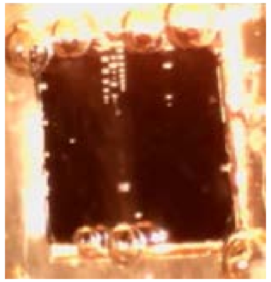
University of Michigan

University of Hawai'i 1907







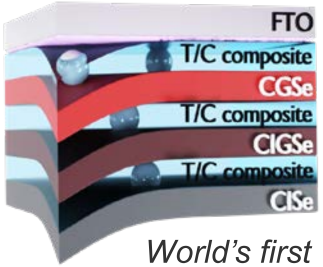


Semi-Monolithic Devices for Photoelectrochemical Hydrogen Production - Nicolas Gaillard (PI), University of Hawaii

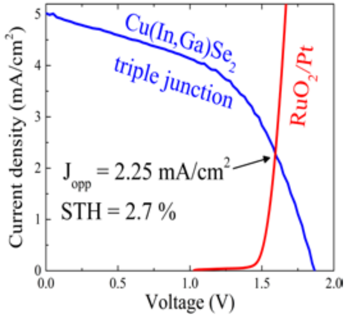
Project Vision: Develop innovative technologies to combine dissimilar material classes, such as **chalcopyrites** and **perovskites**, into multi-junction (MJ) devices for efficient, low-cost and durable PEC water splitting.

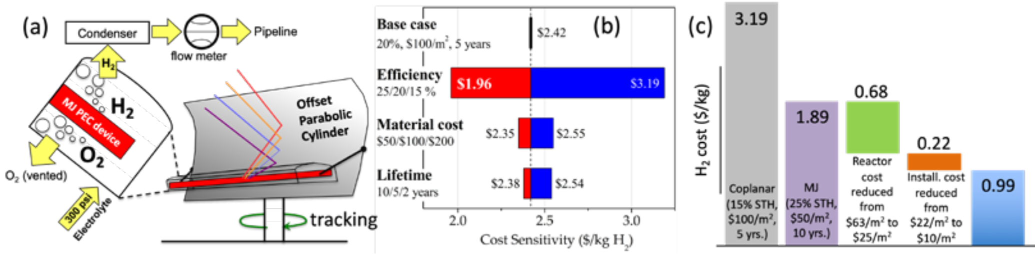
- **Task 1 - Perovskite-Chalcopyrite PEC devices**
  - Combine high efficiency wide bandgap perovskite (PCE record = 21.05% with 1.7 eV absorber) and high efficiency narrow bandgap chalcopyrite (PCE record = 23.3% with 1.1 eV absorber) single junction cells into standalone water splitting MJ devices
- **Task 2 - All-Chalcopyrite PEC devices**
  - Develop efficient wide bandgap chalcopyrites (e.g., $CuGaSe_2$, $CuGa_3Se_5$, $CuInGaS_2$)
- **Task 3 - Durable PEC devices**
  - Develop unique organic (polymer-based) and inorganic (non-precious catalysts) coating strategies to extend durability of PEC MJ devices
  - Superstrate MJ structure: photo-absorbers are sandwiched between an FTO-coated glass substrate and a thick stable OER catalyst layer, which shields the solar absorbers from the electrolyte, ensuring long-term operation.

Metric	State of the Art	Expected Advance
STH	*3-5%*	*>15%*
Durability	*250-500 hrs.*	*> 1,000 hrs.*



World's first triple junction CIGSe cell

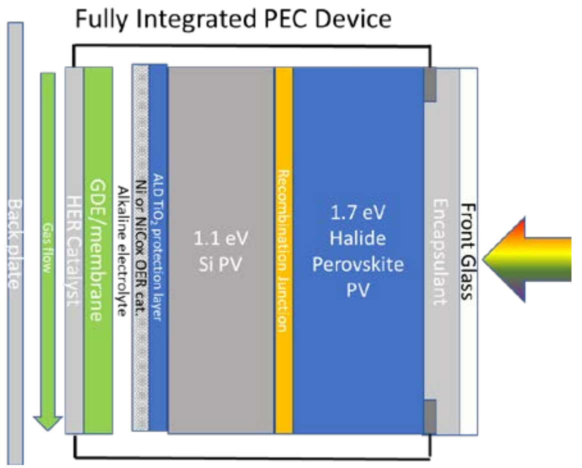




Demonstration of a Robust, Compact Photoelectrochemical (PEC) Hydrogen Generator – Joel A. Haber (PI), Caltech

Project Vision: Holistic PEC device design to enable water-splitting electrolysis at potentials that maximize photocurrent from two-terminal, dual junction Si/organohalide perovskite photovoltaics. Design electrolysis components that minimizes electrocatalytic overpotentials, electrolyte polarization, membrane resistance, and flow inhomogeneities, enabling operation below 1.7 V photopotential.

Holistic Design of Efficient, Durable, Cost-effective H_2 Generation.



Project Impact

- On ≥0.25 cm^2 area-matched devices demonstrate ≥15% STH efficiency for 1000 h under continuous AM1.5 illumination
- Demonstrate 0.1 g/h H_2 generation under diurnal cycle for 2 weeks at NREL PEC outdoor test facility

Project Approach

- Dual junction organo-halide perovskite (1.7 eV) and silicon heterojunction (SHJ) PV architectures
- Device integration levels to provide diagnostic insight into interface impacts on performance and degradation
  - 2-terminal monolithically integrated PVSK/Si PV—probe integration and durability
  - Ni activated ALD-TiO2 protected Si PV for OER
  - Fully integrated device, minimum shadowing from contacts, minimum charge carrier and ionic transport distances—highest potential efficiency
- Scale up: Design large-area hydrogen generator device, including reactant feeds and product collection using experimental measurements and multiphysics modeling.

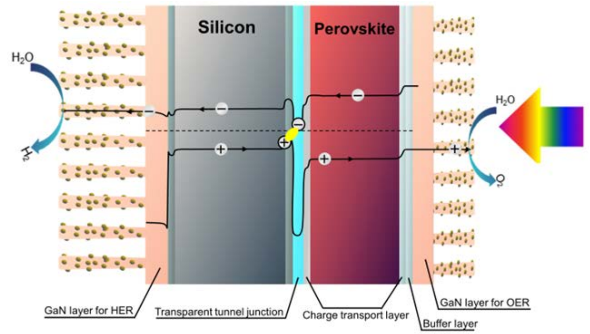
Gallium Nitride (GaN) Protected Tandem Photoelectrodes for High Efficiency, Low Cost, and Stable Solar Water Splitting – Zetian Mi (PI) University of Michigan, Ann Arbor

Project Vision: Develop GaN-protected multi-junction tandem photoelectrodes to achieve both high efficiency (STH >20%) and long-term stable (1,000 h) spontaneous water splitting systems.

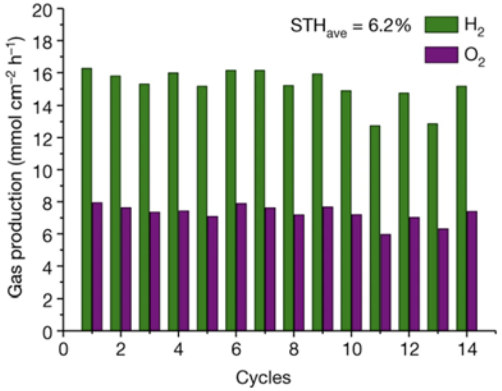
Metric	State of the Art	Expected Advance
STH Efficiency	*10-20%*	*15-20%*
Stability	*<200 h*	*>1,000 h*

Project Approach

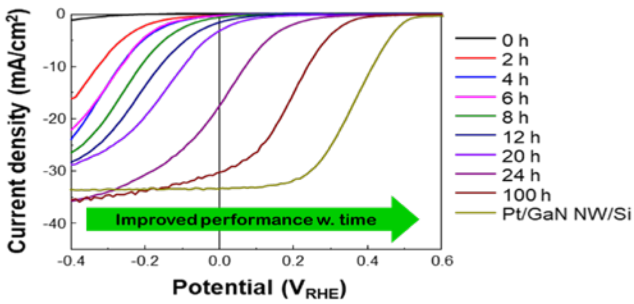
- Integrate GaN with high efficiency perovskite and III-V photoelectrodes to achieve stable operation
  - Have demonstrated the formation of GaON layer from GaN leads to self-improved performance and long-term stability (3,000 h).
- Address the processing incompatibility between III-V (or perovskites) with GaN by utilizing a low-temperature epitaxial growth process and nanoscale engineering to achieve high quality GaN surface protection.
- Use concentrated sunlight to significantly reduce the amount of photocatalyst and therefore the overall system cost.
  - With the use of GaN-based nanostructures, we have recently demonstrated direct solar water splitting with STH of 6.2% under 160x concentrated sunlight.

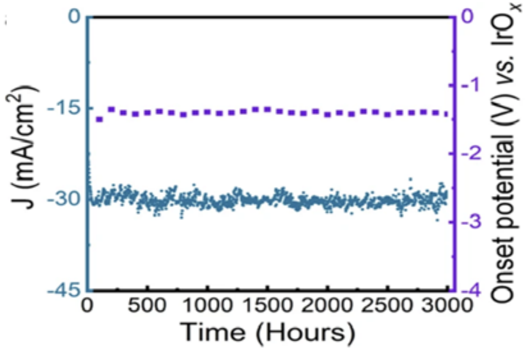


A wireless Si/perovskite photoelectrode protected by GaN.



Nat. Commun. **2023**, *14*, 2047.





Scalable halide perovskite photoelectrochemical cell modules with 20% solar-to-hydrogen efficiency and 1000 hours of diurnal durability – Aditya Mohite (PI) Rice University

Project Vision: Develop halide-perovskite based tandem PEC module with an area of 200 cm^2, with an unassisted STH efficiency of 20%, with 1000 hours of diurnal operation .

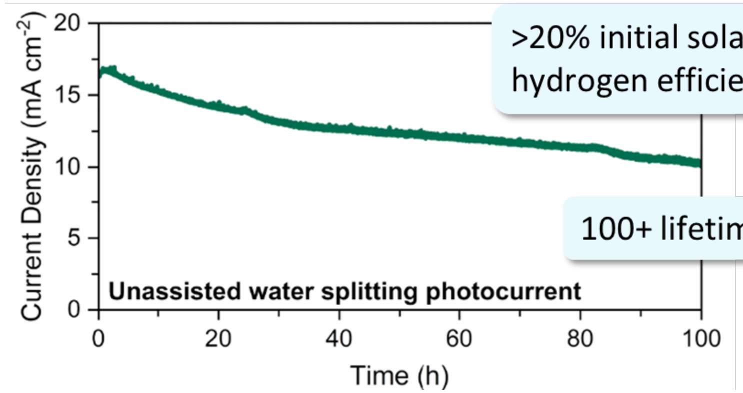
Metric	State of the Art	Expected Advance
STH Efficiency	*20.7*	*> 24.5%*
Stability	*100 h*	*250 h diurnal stability*
Scale	*1 cm^2 (BP1)*	*25 cm^2 (BP2)*

Project Approach

High-efficiency PVs: Exploit 3D/2D perovskite solar cells and Si-Perovskite tandem solar cells and minimodules with Voc > 1.9 V and Jmpp > 18 mA cm^{-2}

Barriers: Conductive Adhesive Barrier (CAB) design for protection and efficient electron/hole transport to catalysts

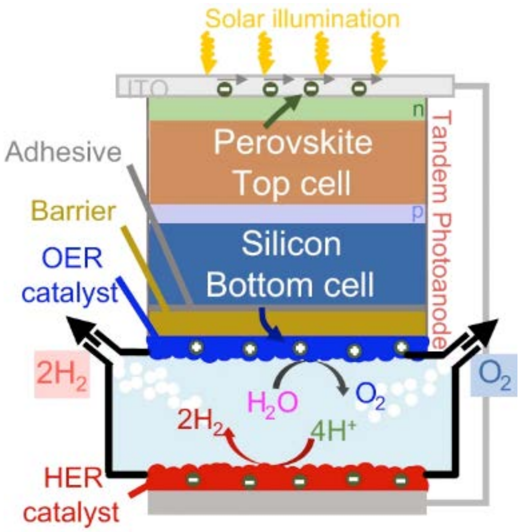
Integration of catalysts: Reactor design to integrate HER and OER catalysts with CAB in low-gap configuration e.g. PEMs or AWE reactors



>20% initial solar to hydrogen efficiency

100+ lifetime

Integrated PEC-PEM reactor design



Integrated PEC-PEM design: Monolithic Perovskite/Si photoanode with conductive adhesive barrier

All-Perovskite Tandem Photoelectrodes for Low-Cost Solar Hydrogen Fuel Production from Water Splitting – Yanfa Yan (PI), University of Toledo

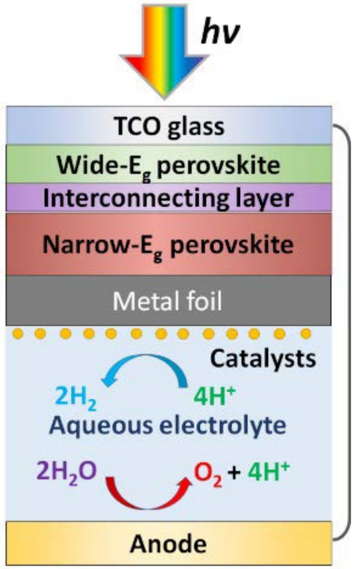
Project Vision: Design, fabricate, and test all-perovskite tandem photoelectrodes and panels to achieve low-cost, high solar-to-hydrogen efficiency as well as long-term stable, unassisted photoelectrochemical (PEC) water splitting systems.

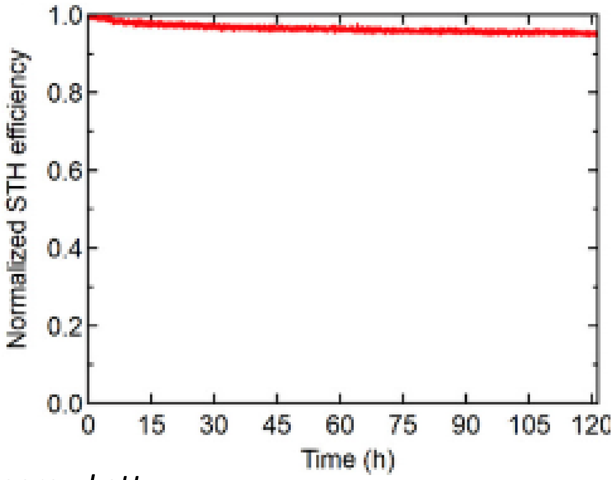
Project Approach

- **Wide-bandgap (1.7 - 1.8 eV) perovskite top absorbers**
  - Suppress halide segregation by reducing defect density
  - Use mixed 2D/3D and all-inorganic perovskites
- **Narrow-bandgap (1.2 - 1.5 eV) perovskite bottom absorbers**
  - Develop a single-crystal-synthesis route
  - Avoid catalytic interface erosion
- **Scaling-up production of tandem photoelectrode panels**
  - All-perovskite tandem photoelectrodes promise theoretical STH efficiencies of more than 22%.
- **Understand material properties and intrinsic stability**
- **On-sun PCE testing**

Achieved continuous operation in water for >120 h at 1 sun

Metric	State of the Art	Expected Advance
STH Efficiency	*15-18%*	*> 20%*
Stability	*100 - 500 h*	*> 1000 h*
Scale	*0.1 - 1 cm^2*	*> 25 cm^2*





ACS Energy Lett. **2023**, *8*, 2611.

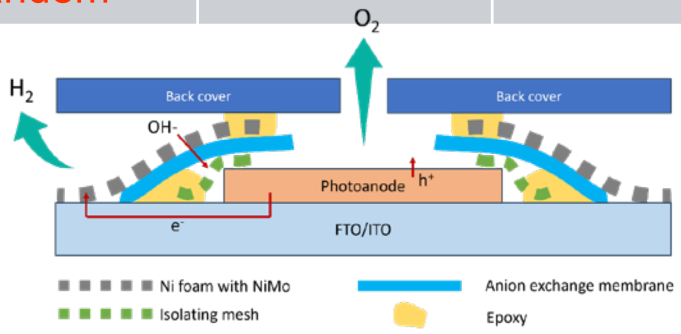
>200 cm^2 Type-3 PEC Water Splitting Prototype Using Bandgap-Tunable Perovskite Tandem and Molecular-Scale Designer Coatings – Shu Hu (PI), Yale University

Project Vision: Develop a Type-3 PEC water splitting system, combining low-cost hybrid organic-inorganic perovskite (HOIP) with molecularly-engineered ALD-grown coatings of protective, conductive, and catalytic multi-functionalities

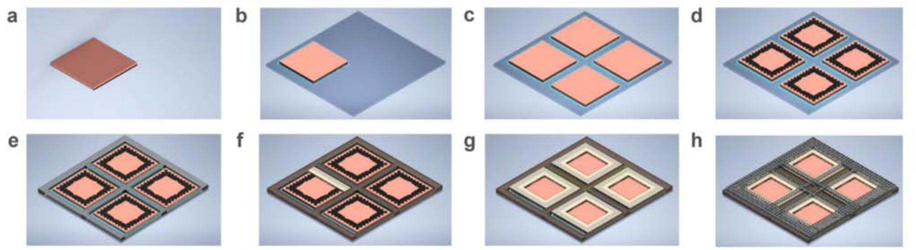
Project Impact & Approach:

- High efficiency (>18%), high purity (>99.999 vol% H_2), stability (>2-week diurnal), and 0.12 gram H_2 per hour throughput;
- Discovery of <1.15 eV bandgap new hybrid perovskite materials
  - Fabrication of thin films of a new Pb-free perovskite-like material ($Cs_4CuSb_2Cl_{12}$). Potentially more stable to light, temperature and water and can be mass-produced.
- Develop low-temperature protective coating ($TiAlO_x$)
  - 100 nm TiAlOx film grown at 85°C show good protection
- Advanced manufacturing approach
  - Quality control large scale fabrication by computer numerical control (CNC) machine
  - For each unit cell, the O2 and H2 can be generated and collected separately. Therefore, when assembled into the large-area device, no extra effort is needed to separate O_2 and H_2.

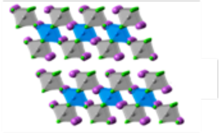
Metric	State of the Art	Expected Advance
Low-T coating	*150 °C*	*85 °C*
Bandgap	*1.2-1.8 eV*	*<1.15 eV*
HOIP tandem	1.8/1.2 eV	1.7/1.1 eV



Large-area device

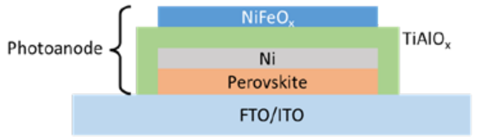


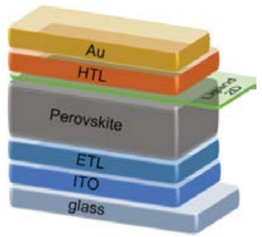
$Cs_4CuSb_2Cl_{12}$ (Copper-Antimony perovskite)



J. Am. Chem. Soc. **2017**, *139*, 27, 9116-9119

Coating integration (photoanode or PEC device)





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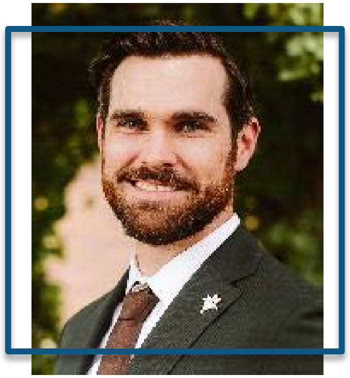

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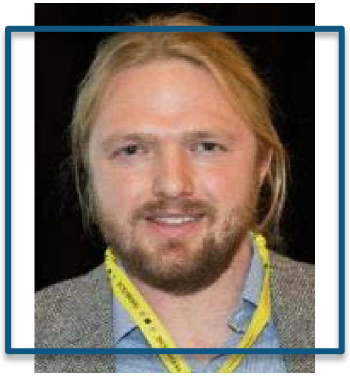

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Thank You

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