



Demonstration of a Robust, Compact Photoelectrochemical (PEC) Hydrogen Generator

PI: Joel A. Haber

Co-PIs: Harry Atwater, Chengxiang (CX) Xiang, John M. Gregoire

California Institute of Technology

August 21, 2023













Project Objectives

- End of Project Objectives
 - On ≥0.25 cm² area-matched devices demonstrate ≥15% STH efficiency for 1000 h under continuous AM1.5 illumination (FOA)
 - Demonstrate 0.1 g/h H₂ generation under diurnal cycle for 2 weeks at NREL PEC outdoor test facility (FOA)
- Additional Project Objectives
 - On ≥0.25 cm² area-matched devices demonstrate ≥25% STH efficiency for 0.5 h under continuous AM1.5 illumination
 - Area-match the electrochemical components to the light-absorbing components to demonstrate a tileable, deployable design



- Dual junction organo-halide perovskite (1.7 eV) and silicon heterojunction (SHJ) PV architectures
 - Collaborate with NREL's Hybrid Organic Inorganic Perovskite (HOIP) node (Kai Zhu) for the dual junction devices
 - Lowest cost dual junction capable of high efficiency and large-scale deployment
 - Concern about durability
- Portfolio of device integration levels to provide diagnostic insight into interface impacts on performance and degradation
 - Caltech-based PEC and pre- and post-mortem materials characterization
 - Collaborate with LBNL's (Photo)electrochemical-SPM node (Francesca Toma) for in situ and postmortem nano-characterization of degradation and failure modes
 - Collaborate with LBNL's Multiphysics Modeling of PEC Devices node (Adam Weber) to incorporate experimental measurements with device modeling to understand degradation/improve durability



Degrees of Integration

- a. Minimum integration, maximum flexibility in water-splitting approach
- b. 2-terminal monolithically integrated PVSK/Si PV—probe integration and durability
- c. 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





- In Project Month 18 begin Scale-up tasks
- Using the most promising small-area architectures, scale-up device components to large-area while retaining high performance and compatibility
- Design large-area hydrogen generator device including reactant feeds and product collection using experimental measurements and multiphysics modeling
- Design module interconnecting multiple large area devices to produce 0.1 g/h $\rm H_2$ during on-sun testing
 - Collaborate with the NREL On-Sun PEC Solar-to-Hydrogen node (Todd Deutsch) to devise reactant distribution and product collection and analysis capabilities



Project Schedule



Task 1: Maximize efficiency of ≥ 0.25 cm² devices via material and property characterization of differently integrated devices

Task 2: Evaluate degradation mechanisms and improve durability

Task 3: Scale-up subcomponents to \geq 25 cm²

Task 4: Design large-area PEC H₂ devices using experiments coupled with multi-physics modeling

Task 5: Tile multiple large-area devices into a module for on-sun production of 0.1 g/h H₂

Demonstration of a Robust, Compact Photoelectrochemical (PEC) Hydrogen Generator

Joel A. Haber/California Institute of Technology

Technology Summary

In this project, we will utilize holistic photoelectrochemical device design to enable water-splitting electrolysis at potentials that maximize photocurrent from two-terminal, dual junction Si/organohalide Perovskite photovoltaics. Design of the electrolysis components will minimize electrocatalytic overpotentials, electrolyte polarization, membrane resistance, and flow inhomogeneities, enabling operation below 1.7 V photopotential. This approach will enable us to drive the device performance to 25% solar-to-hydrogen (STH) efficiency and extend durability to 15% STH for over 1000 hours.

Holistic Design of Efficient, Durable, Cost-effective H₂ Generation.



Key Personnel

Prof. Harry A. **Atwater**; Res. Prof. John M. **Gregoire**; Res. Prof. Chengxiang **Xiang** (All at the California Institute of Technology)

Program Summary Period of performance: 36 months Federal funds: \$1,000,000 Cost-share: \$250,000 Total budget: \$1,250,000

	Key Milestones and Deliverables
Year 1	on \geq 0.25 cm ² demonstrate device efficiency \geq 15% under AM1.5
Year 2	on ≥ 0.25 cm ² demonstrate device STH efficiency $\ge 15\%$ for 100 h
Year 3	Demonstrate \geq 15% STH unassisted efficiency in \geq 25 cm ² device Demonstrate device STH efficiency of \geq 25% Demonstrate durability with STH efficiency \geq 15% for \geq 1000 h Demonstrate 0.1 g/h H ₂ generation for 2 weeks diurnal cycling

Technology Impact

A viable Photoelectrochemical hydrogen generator technology will require five things: high STH efficiency, durability, low-cost materials and components, product separation, and a compact tileable design. This proposal addresses all of these requirements using a total system design, modeling, testing, diagnosis and improvement cycle.





Thanks!

HydroGEN: Advanced Water Splitting Materials