Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Highly efficient solar water-splitting using 3D/2D hydrophobic perovskites with corrosion resistant barriers

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P193

Project Overview

Project Partners

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Project Vision

Achieve cost-effective solar water-splitting by combining high-efficiency, low-cost perovskite solar cells with HER and OER catalysts made from earth abundant materials

Project Impact

The development of a durable and efficient water splitting system for hydrogen production using low-cost, abundant materials is a game-changer for renewable solar energy storage and chemical transformations

Award #	DE-FOA-0002022
Start/End Date	01/01/20-01/01/23
Total Project Value* Cost Share %	$ 1M (DOE + Cost Share) 200K

** this amount does not cover support for HydroGEN resources leveraged by the project (which is provided separately by DOE)*

Approach: Summary

Project Motivation

Our team has published high-impact papers in optoelectronics, device integration, and perovskites, as well as catalyst material synthesis, corrosion chemistry, and catalyst optimization. Preliminary results show >1h device lifetime in aqueous media and 14% efficiency as a PV.

Barriers

Stability of perovskite solar cells in aqueous media – incorporate impermeable and passivating barrier materials

Develop multiple barriers without compromising efficiency – achieve charge transport across barrier systems

Key Impact

Metric	State of the Art	Expected Advance
Stability [h]	*150h*	*500h*
STH efficiency	*19.3%*	*20%*
Cost [$/m^2]	20K	$2/gge

Partnerships

LBNL, Toma: *Understanding degradation mechanisms in PECs through in-situ characterization techniques, PEC measurements and benchmarking, multiscale modeling of PECs*

NREL, Deutsch: Technoeconomic analysis of perovskite-based PEC system

Approach: Innovation

3D/2D perovskite solar cells:

Tunable band-gap

Composition determines band alignment

Record efficiency, promising stability to light/humidity

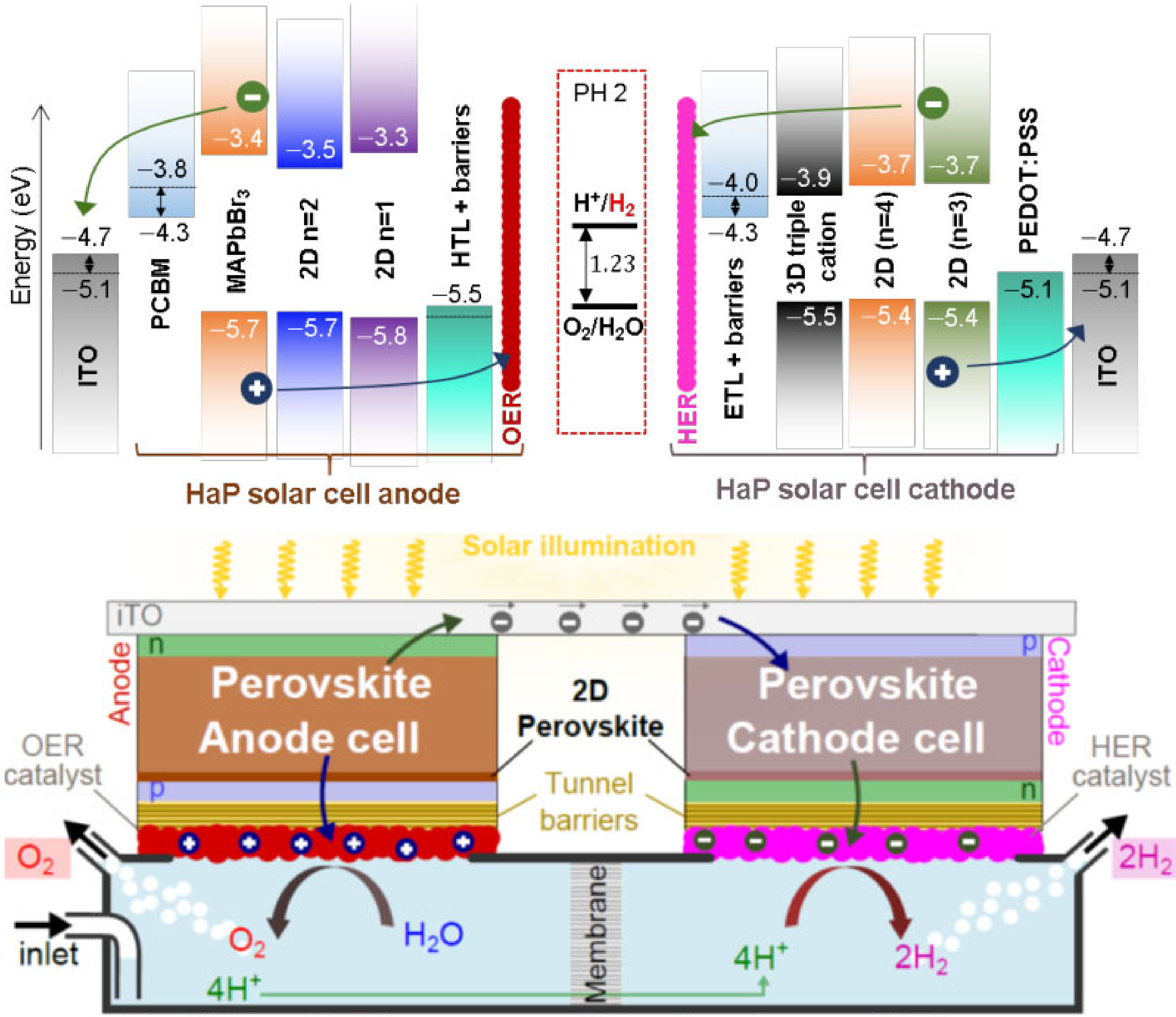
Barriers: hydrophobic polymers, carbons, ALD oxides (Al_2O_3, HFO_2)

Catalysts: HER TMDs (MoS_2, $Nb_{1.35}S_2$), OER metal oxides ($Fe\text{-}NiO_x$, CoO_2)

Current budget period scope:

Select and fabricate 3D/2D perovskites for efficiency, band alignment

Demonstrate 2D perovskite PV with >20% PCE, >100h electrolyte stability at 1 Sun



V_{OC} > 2V for un-assisted water-splitting

Relevance and Impact

- The proposed PEC technology is a high-risk/high-reward project in which expensive III-V based photoabsorbers are replaced with orders-of-magnitude cheaper, but still high-efficiency, halide perovskites, addressing longstanding unit cost issues in PECs
- The HydroGEN Consortium R&D model offers nodes to complement research programs by furnishing expertise and facilities; this project relies on LBNL (Toma) to facilitate PEC characterization and modeling, and NREL (Deutsch) to develop cost analysis for the proposed technology. These areas help to bridge the solar-to-electric and catalytic energy trasnformation expertise of the PI and co-PI
- The node utilization in this project facilitates introduction of the proposed technology into major centers of PEC research (NREL, LBNL). Due to lack of standardization in the field and particularly with novel materials like perovskites, developing familiarity in nodes will improve their capabilities and facilitate expansion of the current work by other collaborating groups in the future

Accomplishments

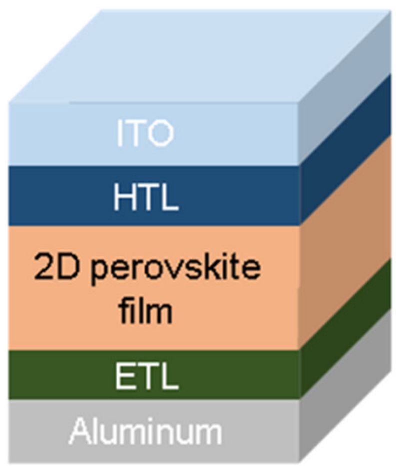
- The major tasks are (1) Design of photocathode/anode; (2) Development of anti-corrosion barriers, and (3) Optimization of halide perovskite PECs

Milestone Summary Table					
Task no.	Title	M. no.	Milestone description	Verification Process	Quarter
1	**HaP screening**	**1.1**	**Selection of HaP materials**	**Characterization PI lab**	**Q1**
1	**Fabrication of PV**	**1.2**	**>20% cell efficiency, J, V, FF, 1000h**	**Solar test in PI lab**	**Q3**
2	**Understand corrosion**	**2.1**	**Understand the mechanisms at the origin of corrosion in HaP photocells**	**Electrochemical test and model**	**Q4**
3	**HaP-PEC completed**	**3.1**	**Integration of all components in proof-of-concept HaP-PEC device**	**Photoelectrochemical tests**	**Q4**

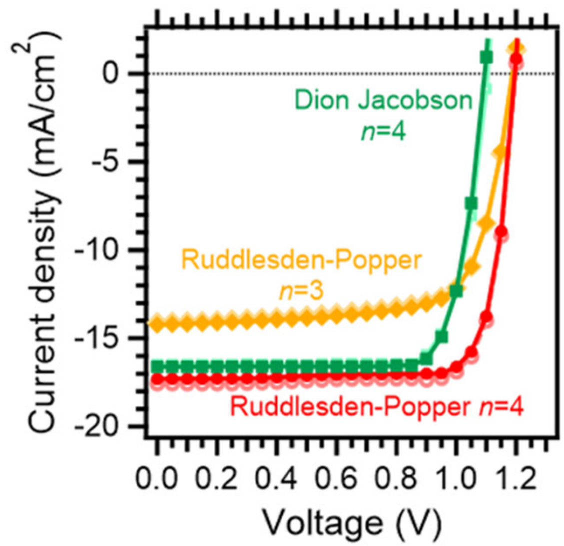
- Success in above-listed BP1 milestones results in a unique water-splitting technology leveraging novel halide perovskite materials and serves as proof-of-concept for the entire project

Highly-efficient and stable hydrophobic 2D HaP photoabsorbers for photovoltaics

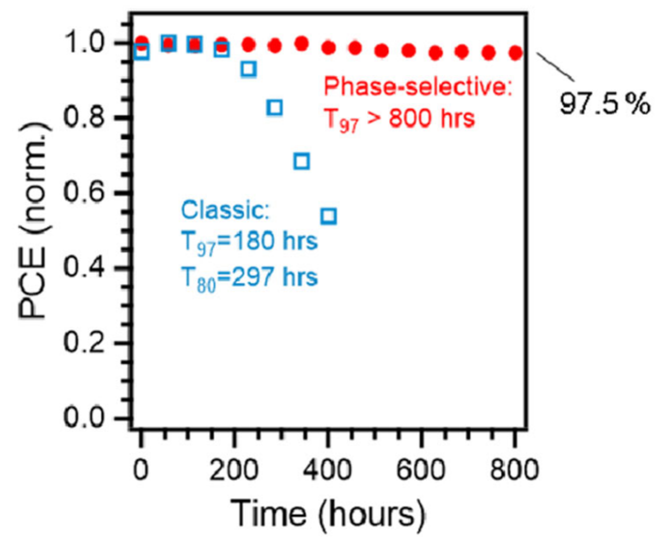
Device architecture



J-V Characteristics



Photostability in RH 65%



Novel approach: control crystal seeds in precursor spin-coating solution to achieve phase-pure 2D HaP (higher efficiency, stability)

J_{sc} = 17.6mA/cm^2

V_{oc} = 1.20V

FF ~ 0.81

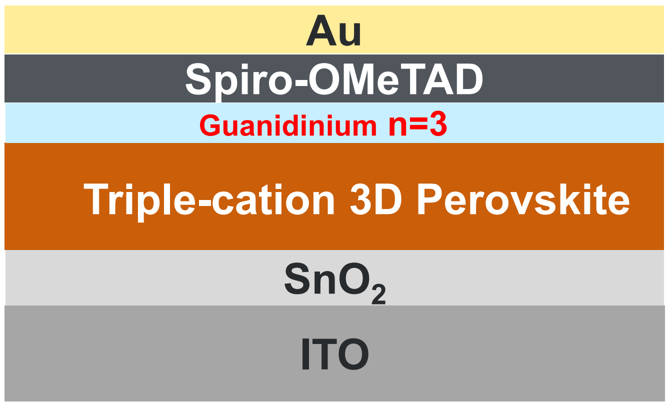
Overall **>800h** stability as PV, **17.1% PCE**

This addresses a long-standing bottleneck for realizing stable, highly-efficient 2D HaP solar cells and will be adapted to 3D/2D architecture with HER, OER catalysts for the PEC device (M. no. 1.1 – materials selection, M. no. 1.2 – 1000h lifetime PV)

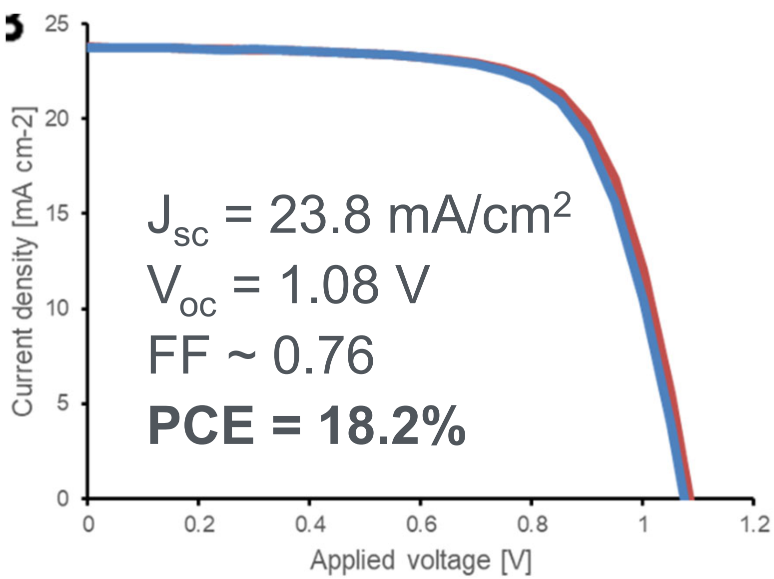
Submitted to Science

Fabrication of high-efficiency and stable 3D/2D HaP solar cells

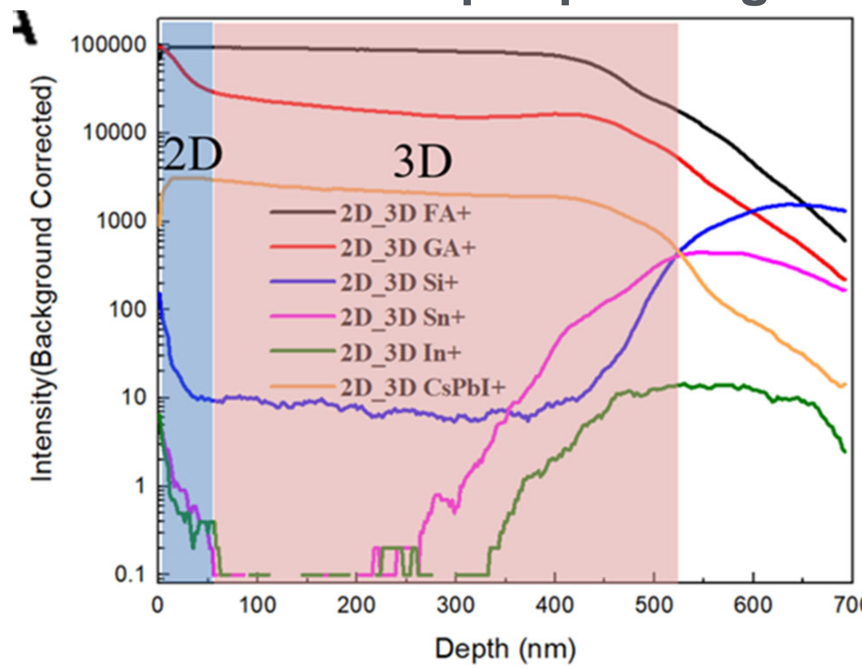
Device architecture



J-V curve in 1 sun Illumination



TOF-SIMS depth profiling

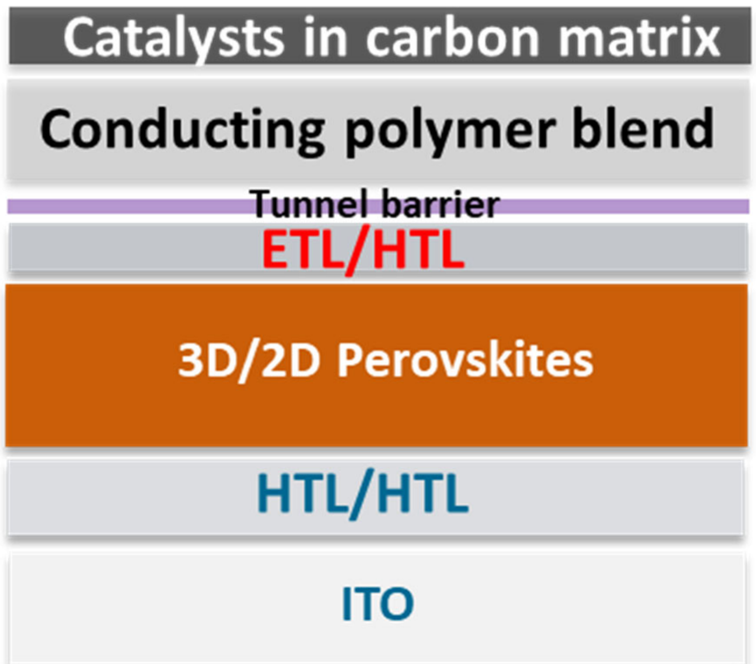


3D layer capped by 2D HaP will passivate the device from electrolyte when used as a photoelectrochemical cell

(M. no. 1.2 – 20% PCE PV)

Integrate charge transport layers as barriers for stability in electrolytes

HaP Photoelectrode Device Architecture



- Substantial materials screening completed (**M. no. 1.1**)
- Conducting polymer blend using classical hydrophobic polymethylmethacrylate (PMMA) and semiconducting particles (PCBM, P3HT)
- Tunnel barriers such as lead oxy-salts [1], evaporated PTFE, etc. to passivate device surfaces

Initial results are promising: Over 1h of anticorrosion performance in acidic media and initial device PCE 14%

Observed unexpected proportionality of stability and ionic strength of solutions (M. no. 2.1 – understand corrosion, M. no. 3.1 proof-of-concept photocathode)

[1] Yang et al., Science 365, 473–478 (2019)

Accomplishments

- Substantial progress in all three early tasks
- On track for completion of year 1 tasks on schedule

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- Expect complete proof-of-concept HaP-PEC during BP1 and initial results on optimization and system integration for efficient, stable device

Collaboration: Effectiveness

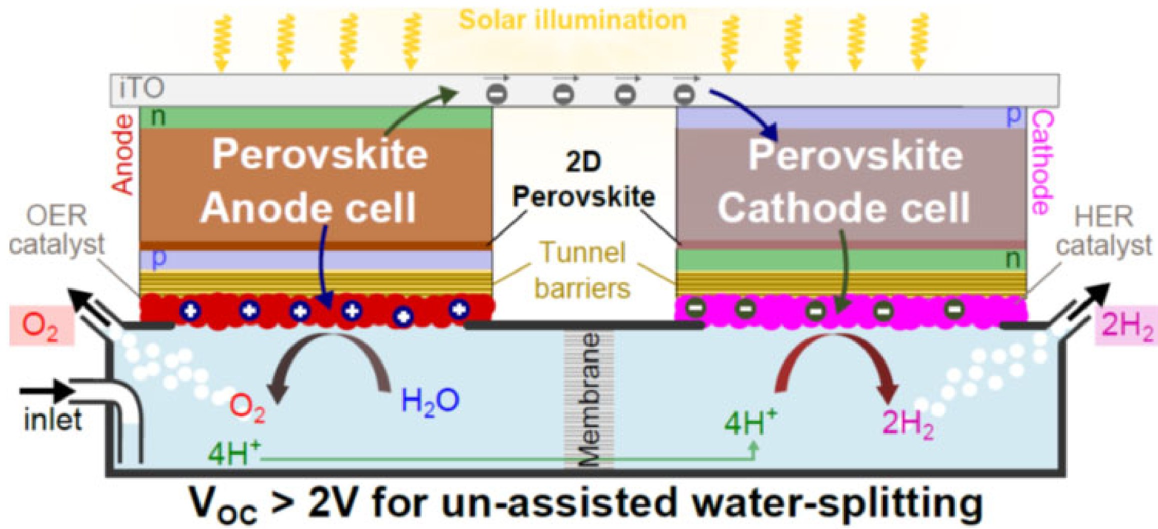
- **Lawrence Berkeley National Laboratory** – Francesca Toma
  - Probing and mitigating chemical and photochemical corrosion of device assemblies
  - In-situ and operando nanoscale characterization for PEC materials and integrated assemblies
  - Testing PEC devices
  - Multiscale modeling of PEC devices
  - Contacted through conference calls and planned visits of team members in Mar 2020 (postponed due to COVID-19)
- PI, co-PI, and team members attended kickoff meeting and participated in breakouts for developing standards and protocols for PEC device evaluation

Proposed Future Work

- The project will continue to pursue a >20% STH, >500h lifetime halide perovskite PEC, which is transformational for the solar fuels field
- The rest of BP1 will focus on achieving target metrics in PV devices and complete proof-of-concept PEC devices; BP2 will complete target metrics in PVs and focus on integrating tandem systems (>15% STH, >100h); and BP3 will focus on converting learnings on corrosion and current loss mechanisms into improved systems (>20% STH, >500h stability) with cost analysis for translation to industrial practice
- Estimated budget

Project Summary

The goal of this project is a low-cost, efficient, stable halide perovskite PEC system with >20% STH, >500h stability.



- In BP1, the go/no-go is a proof-of-concept halide perovskite PEC
- So far, we have shown:
  - Ultrastable, high-efficiency 2D halide perovskite PVs
  - High-efficiency 3D/2D PVs
  - A protective barrier system for >1h stability in aqueous media and 14% efficiency as a PV

Publications and Presentations

Water-Stable 1D Hybrid Tin(II) Iodide Emits Broad Light with 36%Photoluminescence Quantum Efficiency *Ioannis Spanopoulos, Ido Hadar, Weijun Ke, Peijun Guo, Siraj Sidhik, Mikaël Kepenekian, Jacky Even,Aditya D. Mohite, Richard D. Schaller, and Mercouri G. Kanatzidis* ***JACS 2020***

Interfacial Electromechanics Predicts Phase Behavior of 2D Hybrid Halide Perovskites

Christopher C. Price, Jean-Christophe Blancon, Aditya D. Mohite and Vivek B. Shenoy* ACS Nano 2020, 14, 3, 3353–3364

Memory seeds control the crystal phase in 2D perovskite thin-films for high-efficiency photovoltaics, Siraj Sidhik, Wenbin Li, Mohammad Samani, Hao Zhang, Yafei Wang, Justin Hoffman, Austin Fehr, Claudine Katan, Jacky Even, Amanda B. Marciel, Mercouri G. Kanatzidis, Jean-Christophe Blancon, Aditya D. Mohite. In review