Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

HydroGEN: Photoelectrochemical (PEC) Hydrogen Production

Nemanja Danilovic, James Young, Todd Deutsch, Adam Z. Weber
April 30, 2020
Annual Merit Review

P148C

NREL National Renewable Energy Laboratory
Berkeley Lab
Sandia National Laboratories
INL Idaho National Laboratory
Lawrence Livermore National Laboratory
SRNL

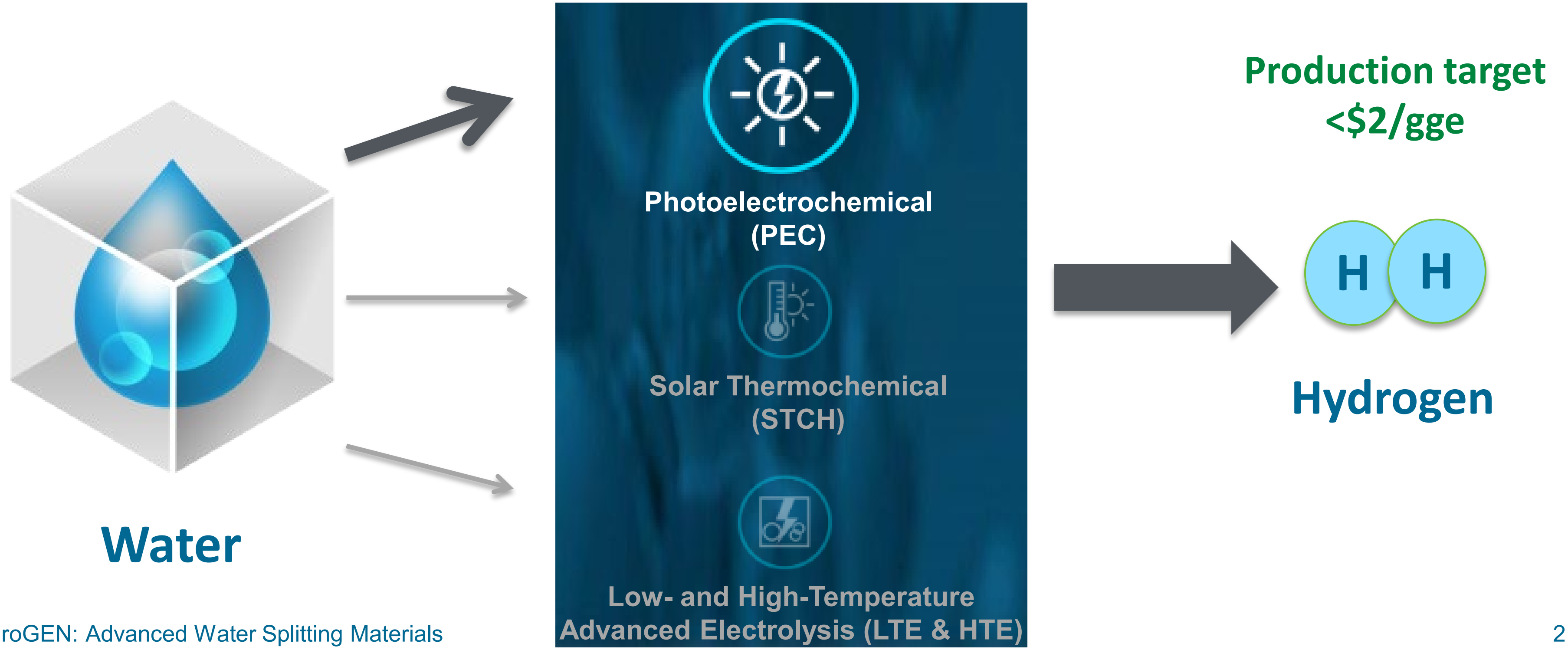
Advanced Water-Splitting Materials (AWSM)

Relevance

AWSM Consortium
6 Core Labs:

NREL
NATIONAL RENEWABLE ENERGY LABORATORY
BERKELEY LAB
Sandia National Laboratories
INL
Idaho National Laboratory
Lawrence Livermore National Laboratory
SRNL

Accelerating R&D of innovative materials critical to advanced water splitting technologies for clean, sustainable & low cost H_2 production, including:


Water

Photoelectrochemical (PEC)

Solar Thermochemical (STCH)

Low- and High-Temperature Advanced Electrolysis (LTE & HTE)

Production target <\$2/gge

Hydrogen

Approach

- Cost, durability, efficiency

- Benchmarking workshop
  - Device stability and scalability
    - Protocols
    - Scaling studies should also inform/guide materials processing pathways & component performance criteria.
  - Protocols relate to real world conditions, such as varying illumination, temperature and low concentrated sunlight conditions
  - Advanced spatially resolved techniques, such as pH imaging, are needed

- Internal lab work this year addresses those barriers above

Approach – EMN HydroGEN

PEC: Photoelectrochemical Electrolysis

Barriers
- Cost
- Efficiency
- Durability

PEC Node Labs

NREL
NATIONAL RENEWABLE ENERGY LABORATORY

BERKELEY LAB

Sandia National Laboratories

Lawrence Livermore National Laboratory

Support through:

Personnel

Equipment

Expertise

Capability

Materials

Data

PEC Projects

University of Hawai'i

RICE

THE STATE UNIVERSITY OF NEW JERSEY RUTGERS

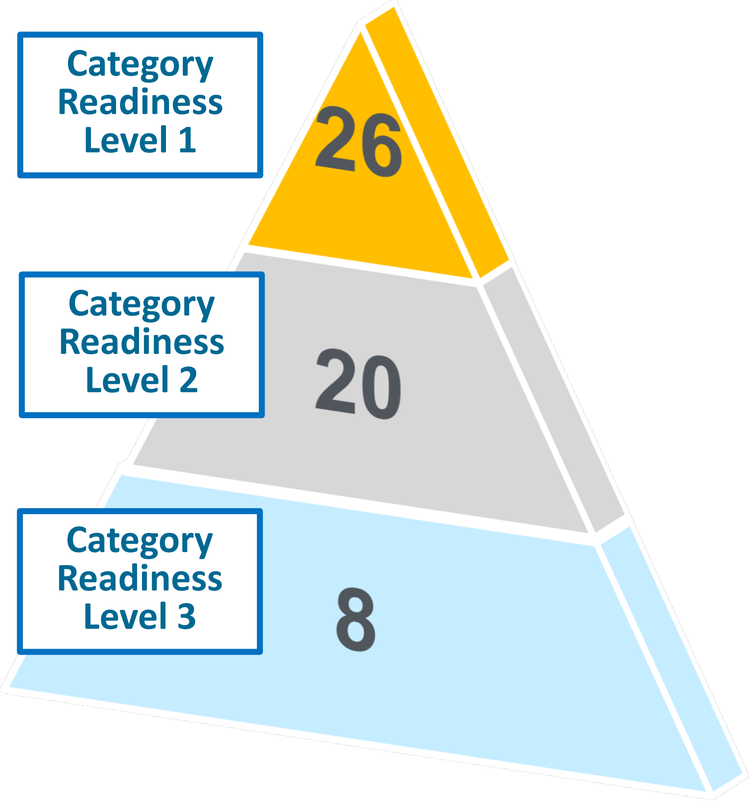
STANFORD UNIVERSITY

UNIVERSITY OF MICHIGAN

The University of California · Irvine

THE UNIVERSITY OF TOLEDO

Collaboration: 54 PEC Nodes, 2 Supernodes



Category Readiness Level 1

26

Analysis: 2
Computation: 8
Process and Scale up: 4
Integration: 2
Characterization: 14
Synthesis: 5
Benchmarking: 4

Category Readiness Level 2

20

Analysis: 2
Computation: 6
Process and Scale up: 4
Integration: 2
Characterization: 12
Synthesis: 5
Benchmarking: 6

Category Readiness Level 3

8

Analysis: 3
Computation: 3
Characterization: 3
Synthesis: 2

- Nodes comprise equipment and expertise including uniqueness
- Category refers to availability and readiness with 1 being most ready and available
- Many nodes span classification areas

22 (17 by FOA) Nodes utilized
22 Lab PIs engaged
100’s of files on Data Hub

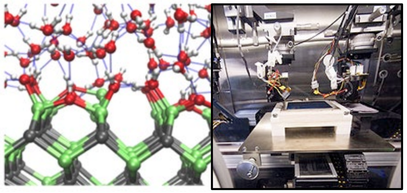
Collaboration: HydroGEN PEC Node Utilization

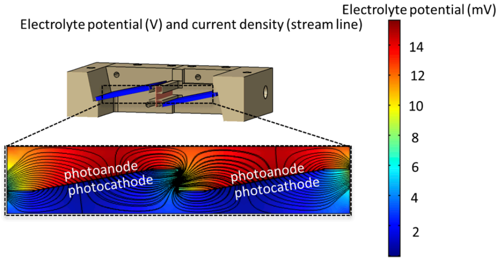
Lab	Node	Hawaii	Stanford	Rutgers	Michigan	Rice	Toledo	UCI	Super
LLNL	Material Design and Diagnostics	✓							
LLNL	Interface Modeling				✓			✓	✓
LBNL	Multiscale Modeling								✓
NREL	Structure Modeling								✓
NREL	First principles theory						✓		
NREL	MOVPE		✓	✓					✓
NREL	CIGS	✓							
NREL	Combi/High Throughput	✓		✓					
NREL	Surface Modifications				✓			✓	
NREL	Corrosion analysis	✓	✓					✓	✓
NREL	Surface Analysis Cluster Tool				✓				

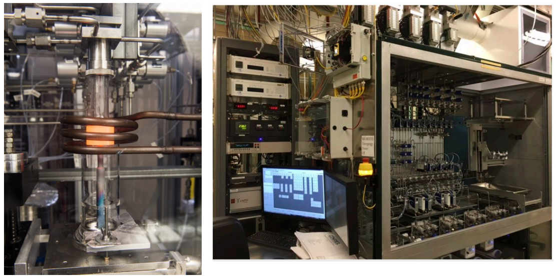
Computation

Material Synthesis

Characterization



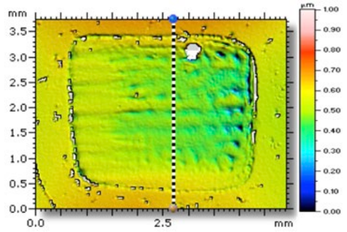


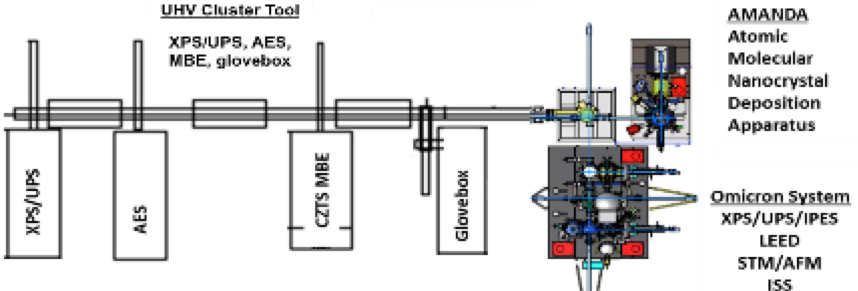


Collaboration: HydroGEN PEC Node Utilization

Lab	Node	Hawaii	Stanford	Rutgers	Michigan	Toledo	Rice	UCI	Super
NREL	PEC Characterizations		✓	✓					✓
NREL	On-Sun Efficiency Benchmarking	✓	✓	✓		✓	✓	✓	✓
NREL	RDE								✓
LBNL	Microelectrode								✓
LBNL	Probing and mitigation corr						✓		✓
LBNL	In situ and operando				✓		✓		✓
LBNL	Prototyping								✓
LBNL	Photophysical Characterization	✓	✓						
LBNL	On-Sun Testing						✓		✓
LBNL	In situ APXPS and XAS								✓
LLNL	In situ X-ray characterization					✓			

Characterization





NREL Surface Science Cluster Tool

Best-in-class Platinum Group Metal-free Catalyst Integrated Tandem Junction PEC Water Splitting Devices

Rutgers University PI: Garfunkel/Dismukes

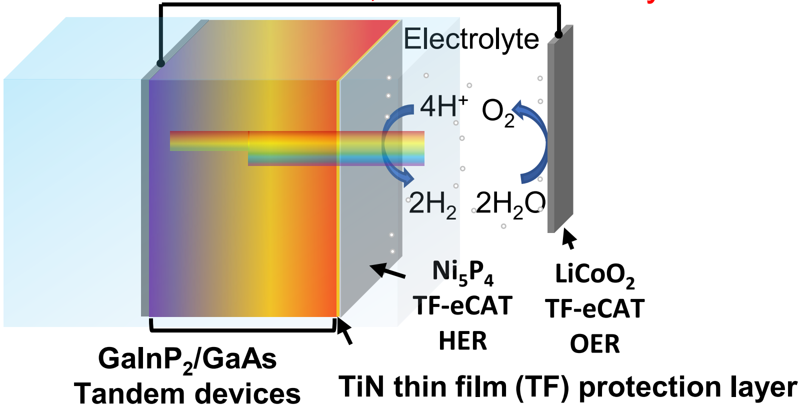
RUTGERS

#P160

Project Goals:

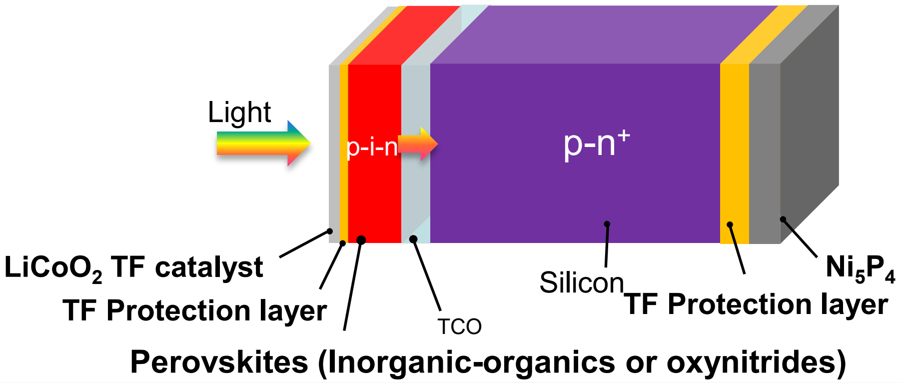
High-Performance (HP) device

Goal: >10% STH, > 100h durability



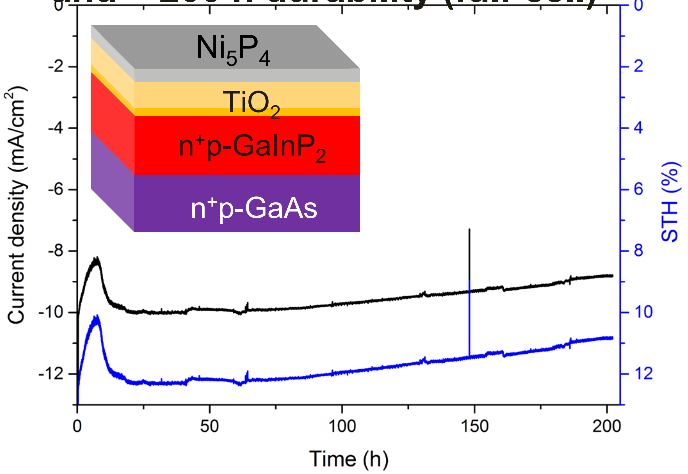
High-Value (HV) device

Goal: ~10% STH, > 24h durability

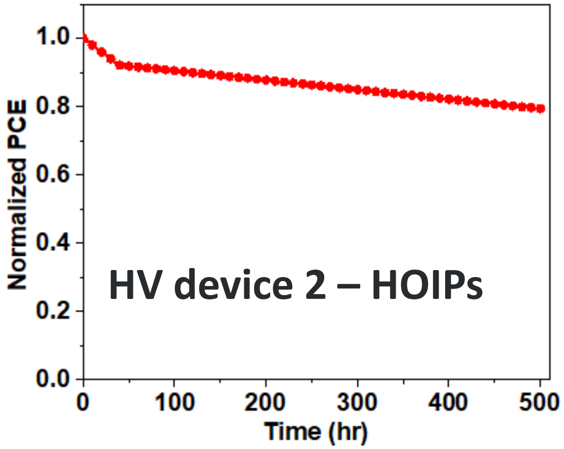


Achievements: Highlights

HP device achieves >12% STH and > 200 h durability (full-cell)



HV progress – Hybrid organic inorganic perovskite (HOIPs) wide bandgap (1.61 eV) n-i-p orientation achieves PCE > 20% and > 500 h



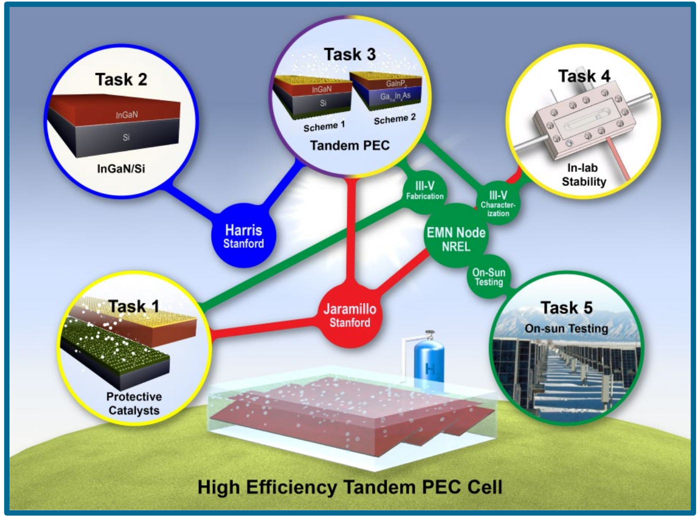
Protective Catalyst Systems on III-V and Si-based Semiconductors for Efficient, Durable Photoelectrochemical Water Splitting Devices

Stanford University PI: T. Jaramillo

#P161

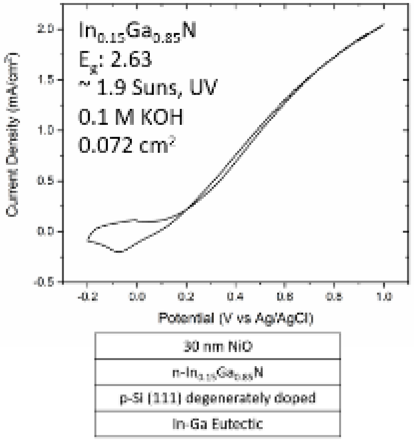
Goals:

- To develop unassisted water splitting devices that can achieve > 20% solar-to-hydrogen (STH) efficiency.
- Devices that can operate on-sun for at least 2 weeks.
- Devices that can provide a path toward electrodes that cost $200/m^2 by incorporating earth-abundant protective catalysts and novel epitaxial growth schemes.

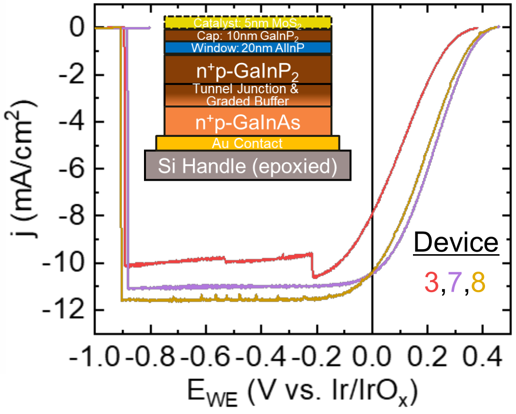


Highlights

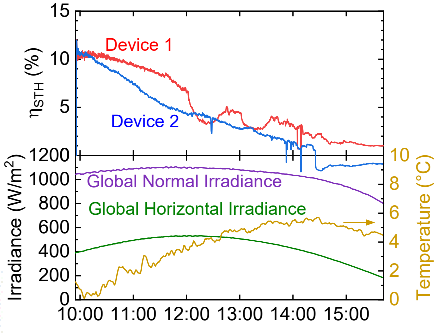
InGaN grown by MOCVD gives photoanode behavior

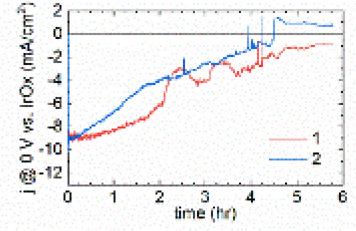


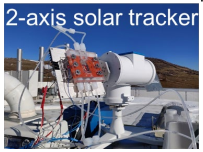
MoS$_2$-protected GaInP$_2$/GaInAs tandem yields 12.8% STH

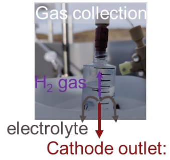


On-sun PEC testing of MoS$_2$/GaInP$_2$/GaAs. Generated 14.4 mL of H$_2$ on 1/15/20









Novel Chalcopyrites for Advanced Photoelectrochemical Water-Splitting

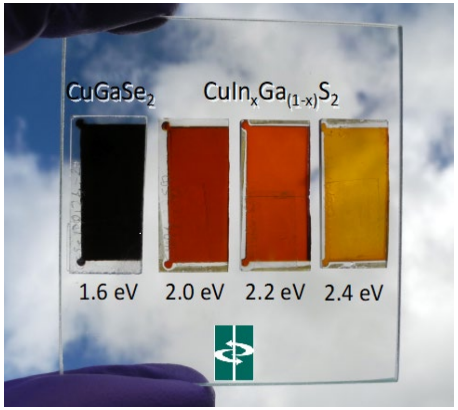
University of Hawaii PI: Gaillard

#P162

Project Goals

Strengthen **theory, synthesis and advanced characterization "feedback loop"** to accelerate the development of efficient materials for H_2 production.

Develop innovative technologies to synthesize and integrate chalcopyrites into efficient and low-cost PEC devices.

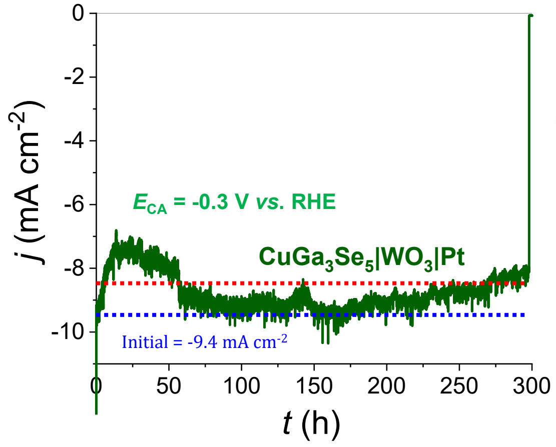


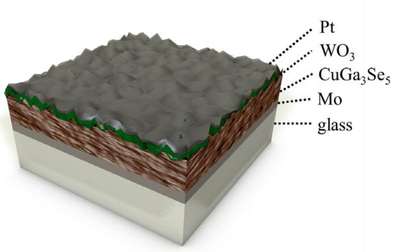
Addressing materials **efficiency**, **durability** & **integration** barriers through multi-disciplinary research.

N. Gaillard **(Device integration)**	**C. Heske** **(Spectroscopy)**	**T. Jaramillo** **(Catalysis/Corrosion)**
T. Ogitsu **(Theory)**	**J. Cooper** **(Carrier dynamics)**	**K. Zu (absorbers)** **A. Zakutayev (junctions)** **T. Deutsch (benchmarking)**

Highlights

1) Extending chalcopyrites durability with WO_3 ALD coatings

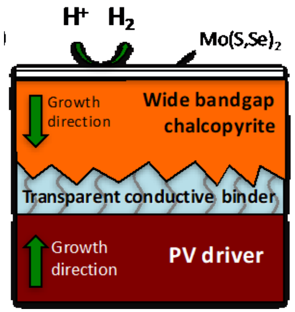


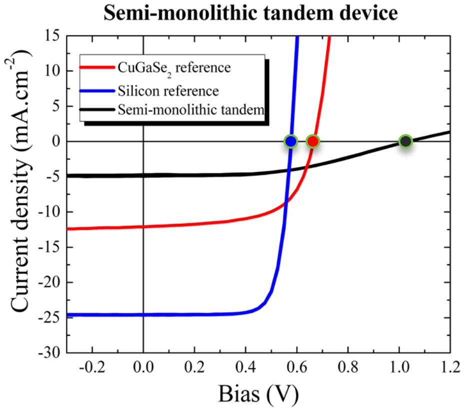


→ Retained > 90% of initial photocurrent density for more than 270 h of continuous testing

2) Semi-monolithic tandem devices

→ Solid-state devices created by exfoliating and bonding wide bandgap (1.7 eV) $CuGaSe_2$ onto narrow bandgap (1.1 eV) silicon.





→ Tandem device photovoltage (1,035 mV) represents over 80% than the sum of the individual sub cells.

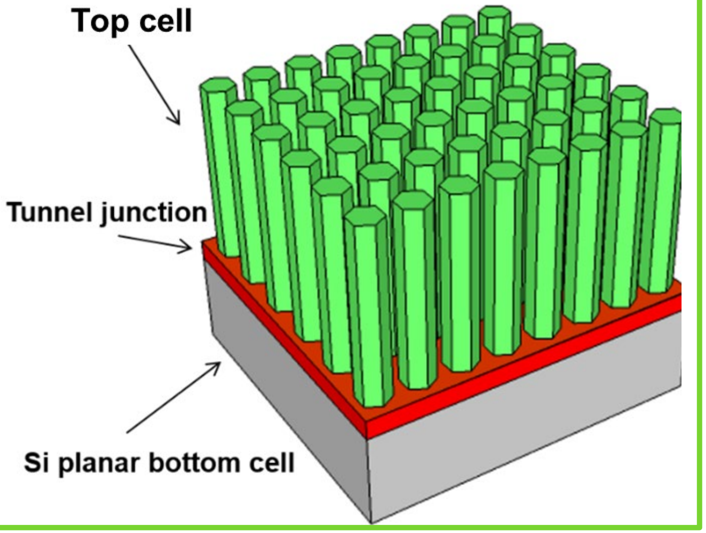
Monolithically Integrated Thin-Film/Si Tandem Photoelectrodes

University of Michigan PI: Z. Mi

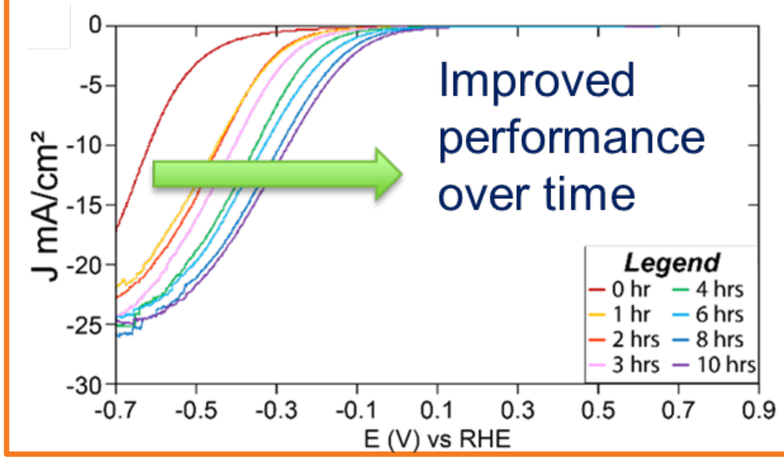
#P163

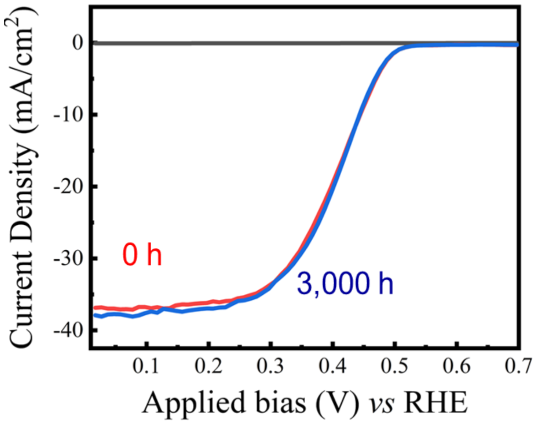
Project Goals: Develop Si-based low cost tandem photoelectrodes to achieve high efficiency (>15%) and stable (>1,000 hrs) water splitting systems

(i) The use of Si and GaN, the two most produced semiconductors, for scalable, low cost manufacturing; (ii) The incorporation of nanowire tunnel junction for high efficiency operation; (iii) The discovery of N-rich GaN surfaces to protect against photocorrosion and oxidation



Highlights Through combined theoretical and experimental studies, we have observed a unique self-healing process for N-terminated GaN photocathodes, which leads to stable water splitting without using any extra surface protection.





No performance degradation was observed for 3,000 hrs continuous solar water splitting for GaN/Si photocathode.

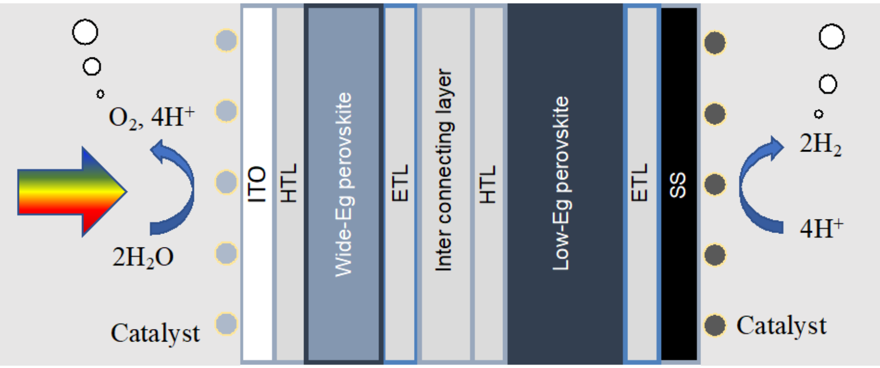
Perovskite/Perovskite Tandem Photoelectrodes for Low-Cost Unassisted Photoelectrochemical Water Splitting

University of Toledo PI: Y. Yan

#P191

Project Goals:

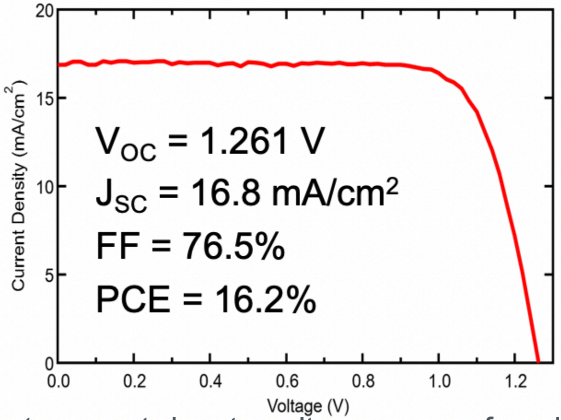
- Demonstrate perovskite/perovskite tandem photoelectrodes for wireless and unassisted water splitting.
- Develop water impermeable coating to protect tandem photoelectrodes during the operation in water.
- Demonstrate tandem photoelectrodes with a STH efficiency of up to 20%.



Schematic device structure and working principle of the proposed perovskite/perovskite tandem photoelectrode

Highlights or Approach for BP1

- Demonstrated efficient semitransparent n-i-p wide band-gap perovskite ($FA_{0.75}Cs_{0.2}MA_{0.05}Pb(Br_{0.3}I_{0.7})_3$) solar cells.
- Fabricated n-i-p low-bandgap mixed Sn-Pb perovskite solar cells.
- Discovered critical issues for fabricating efficient n-i-p low-bandgap mixed Sn-Pb perovskite solar cells.
- A plan is proposed to mitigate the critical issues, i.e., to increase the bandgap by increasing the Pb/Sn atomic ratio.



Photocurrent densty-voltage curve of a wide-bandgap perovskite solar cell in a n-i-p configuration, i.e., glass/ITO/SnO_2/C_{60}-SAM/$FA_{0.75}Cs_{0.2}MA_{0.05}Pb(Br_{0.3}I_{0.7})_3$/Spiro-OMeTAD/$MoO_x$/ITO.

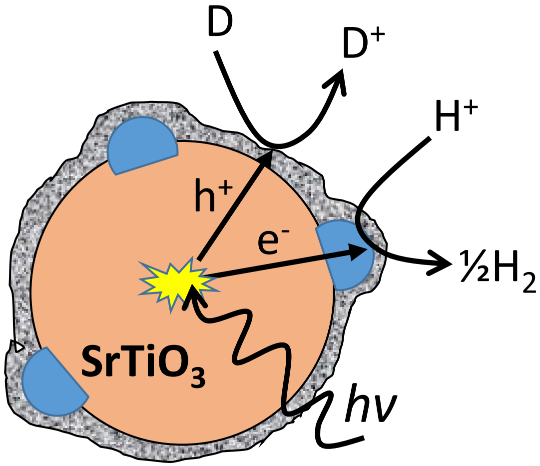
Development of Composite Photocatalyst Materials that are Highly Selective for Solar Hydrogen Production and their Evaluation in Z-Scheme Reactor Designs

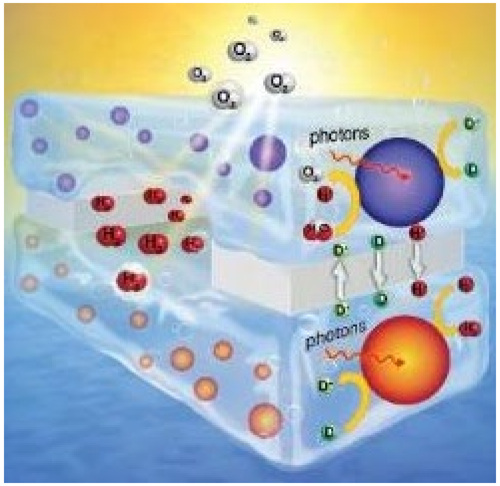
University of California-Irvine PI: S. Ardo

#P192

Project Goals

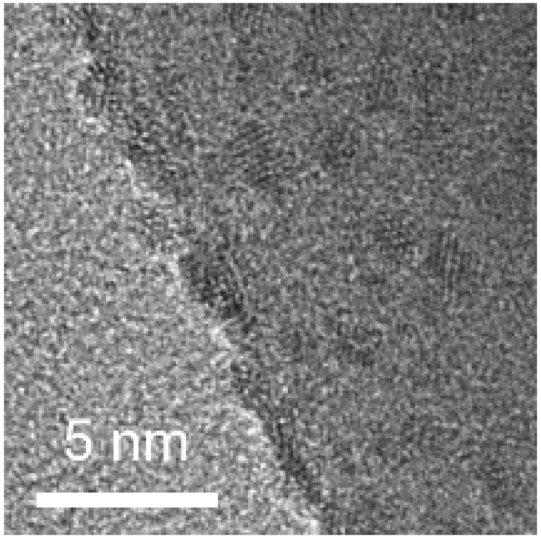
- Improve yield for H_2 evolution from doped $SrTiO_3$ photocatalyst particles illuminated with near-infrared light
- Engender selective H_2 evolution over redox shuttle reduction using coatings deposited on photocatalyst particles
- Develop detailed models to simulate particle-to-reactor-level processes





Highlights or Approach for BP1

- Ir-doped $SrTiO_3$ with Ir cocatalysts evolves H_2 using ≤650 nm light ***(BP1 Target: H_2 evolution using ≥750 nm light)***
- SiO_x-coated Pt electrodes attenuate undesired Fe(III) reduction, yet allow for partial desired Fe(II) oxidation and full desired H_2 evolution ***(BP1 Targets: deposit TiO_x coatings on electrodes; evaluate coated electrodes for selective O_2 evolution)***
- Our models can simulate processes operative in photocatalytic reactors, including undesired reactions ***(BP1 Target: include effects due to thermal gradients in the model)***



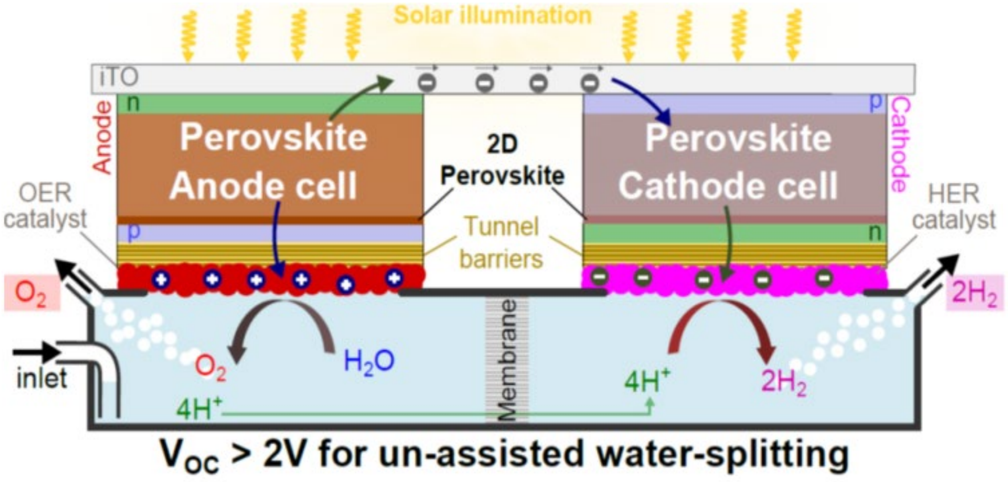
Highly Efficient Solar Water Splitting Using 3D/2D Hydrophobic Perovskites with Corrosion Resistant Barriers

Rice University PI: A. Mohite

#P193

Project Goals:

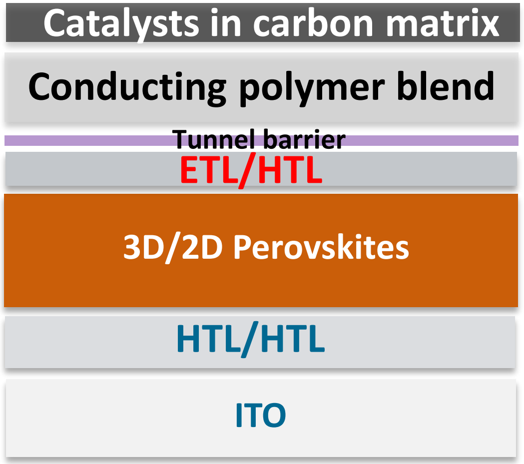
- **Develop high-efficiency heterostructure 3D/2D halide perovskite solar cells (PCE >20%) with hydrophobic termination**
- **Fabricate corrosion-resistant barriers, integrate HER/OER catalysts, test durability in electrolyte**
- **Understand degradation mechanisms in PEC and mitigate**
- Test, benchmark, optimize performance and stability of PEC
- Scale up to 5x5in^2



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

Highlights or Approach for BP1

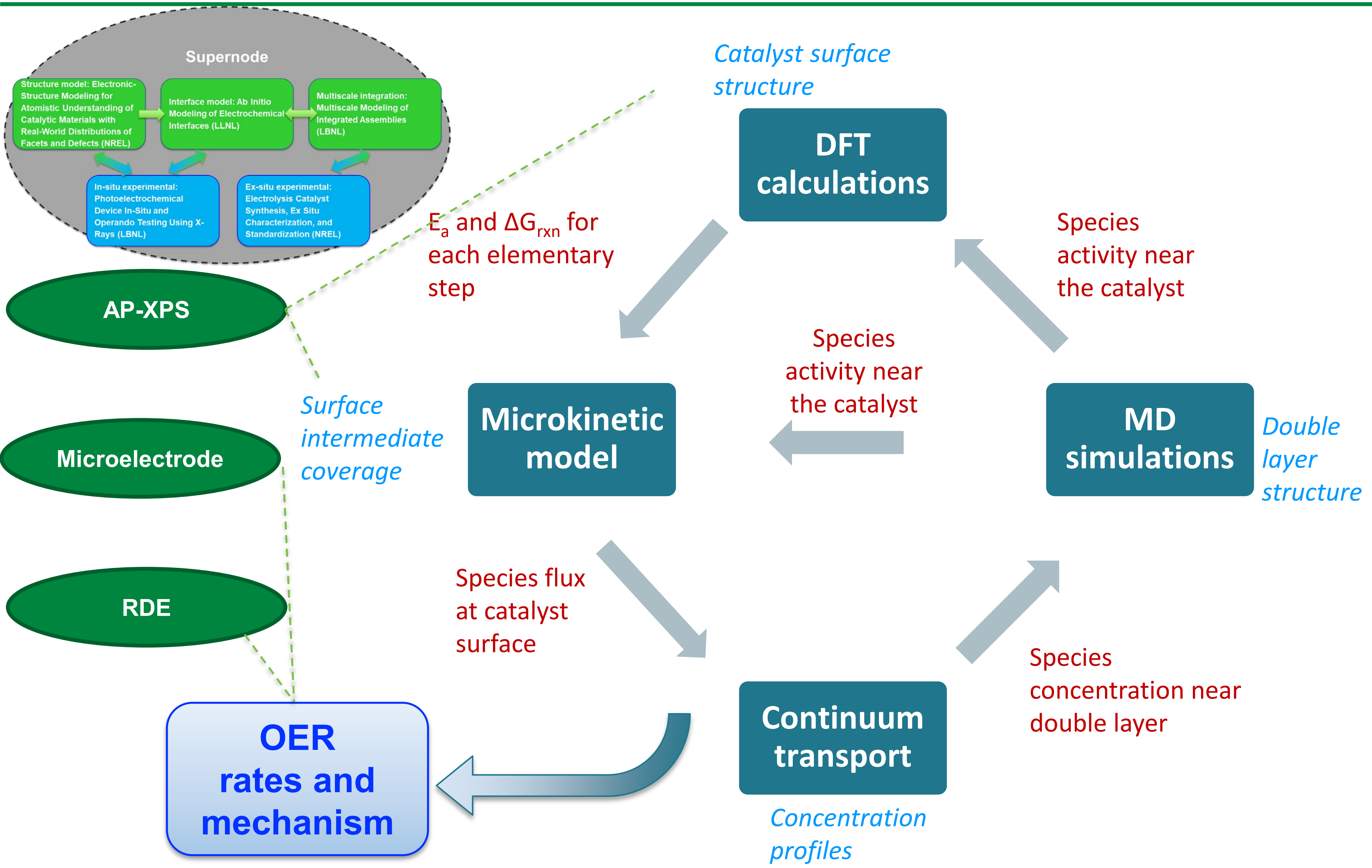
- Selection, fabrication, optimization of 3D/2D perovskites for efficiency and band alignment
- Demonstrate a 3D/2D PSC with ~20% PCE with 1000h stability, <10% voltage degradation over 100h in electrolyte with 1-Sun flux
- Demonstrate PEC with photocathode and photoanode as HaP-PEC with 5-10% STH efficiency for 1 hour
- **3D/2D perovskite solar cell with 20% PCE and well-aligned bands**
- **Over 1h anticorrosion performance in acidic electrolyte and initial device PV efficiency 15%**


Catalysts in carbon matrix
Conducting polymer blend
Tunnel barrier
ETL/HTL
3D/2D Perovskites
HTL/HTL
ITO

OER Modeling Supernode

- **Objective**
  - Utilize validated theory across length scales to understand the mechanism of oxygen evolution going from acid to neutral to alkaline pH
    - Develop new models and structures for the inherent “messy” real system
  - Apply multiscale theories for reaction mechanism analysis on IrO_2
    - Validate experimentally using both RDE and developed microelectrode setups and ambient-pressure XPS
  - Provide critical analysis for both LTE and PEC technologies
- **Knowledge gaps**
  - Develop and demonstrate rigorous continuum/DFT/microkinetic multiscale theoretical descriptions of electrochemical reactions in general, including structure and interfaces
  - Need to understand proton source and limiting pathways for OER
  - Need to explore spectator ion and related electrolyte effects
  - Explore how ionomer interactions differ from aqueous ones in terms of controlling kinetics
- Seedling projects not focused specifically on OER and not at such a fundamental level, can benefit from knowledge and new capabilities
- New nodes possibly developed and leveraged
  - Dynamic microelectrode

OER Modeling Approach: Multiscale Interactions



Supernode

Structure model: Electronic-Structure Modeling for Atomistic Understanding of Catalytic Materials with Real-World Distributions of Facets and Defects (NREL)

Interface model: Ab Initio Modeling of Electrochemical Interfaces (LLNL)

Multiscale integration: Multiscale Modeling of Integrated Assemblies (LBNL)

In-situ experimental: Photoelectrochemical Device In-Situ and Operando Testing Using X-Rays (LBNL)

Ex-situ experimental: Electrolysis Catalyst Synthesis, Ex Situ Characterization, and Standardization (NREL)

AP-XPS

Microelectrode

RDE

OER rates and mechanism

Catalyst surface structure

DFT calculations

E_a and ΔG_{rxn} for each elementary step

Species activity near the catalyst

Surface intermediate coverage

Microkinetic model

Species activity near the catalyst

MD simulations

Double layer structure

Species flux at catalyst surface

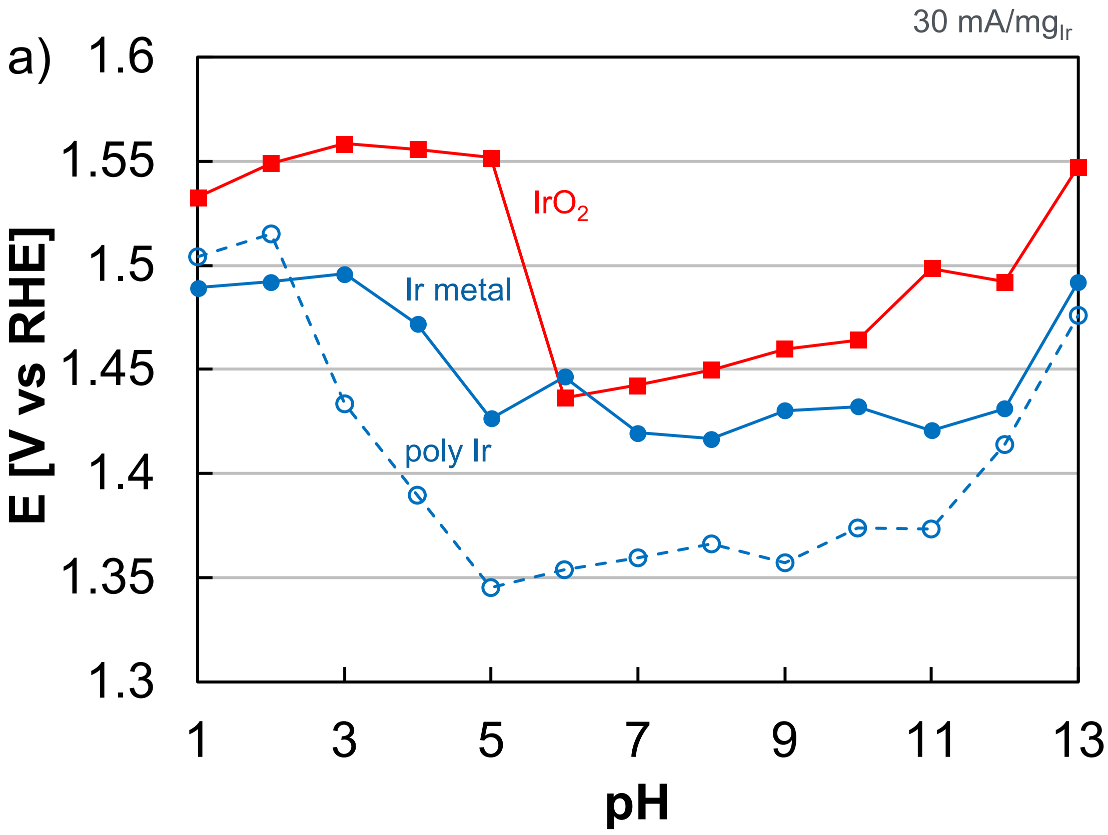
Species concentration near double layer

Continuum transport

Concentration profiles

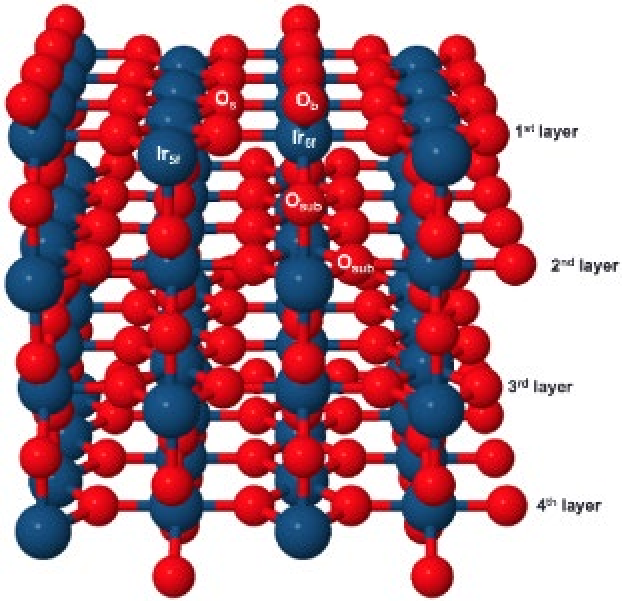
Metal/Oxide Data Comparisons

- Materials evaluated:
  - Ir oxide (Alfa Aesar), red
  - Ir metal (Johnson Matthey), blue solid
  - Polycrystalline Ir, blue dashed
- For metal, activity improvement extended into weakly basic pH
- Activity dropped at pH 0/14, may be due to contaminants at higher concentrations



Atomistic Modeling

- Two limiting cases to explore reaction mechanisms and how to determine barriers
  - Case 1: Bare Ir metal sites available and vacuum calculations to understand possible mechanisms
  - Case 2: Pourbaix-informed surface species and reaction mechanism in solution to feed into microkinetic modeling
- Bare IrO_2 (110) surface

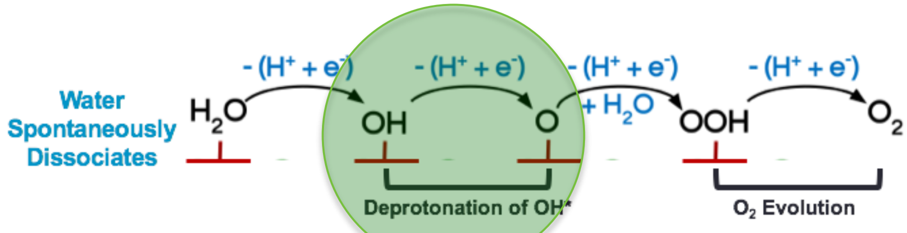


Active Sites	No.	Notes
O (O_s + O_b)	24	H* can adsorb on O_s or O_b or Ir_{5f} sites
Ir (Ir_{5f} only)	8	O*, OH*, OOH*, O_2* adsorb only on Ir_{5f} sites Ir_{6f} fully coordinated and typically unreactive (also blocked by O_b)

Lattice Vectors:
a = 12.73774 Å
b = 12.59768 Å
SA = a x b = 160.46 $Å^2$

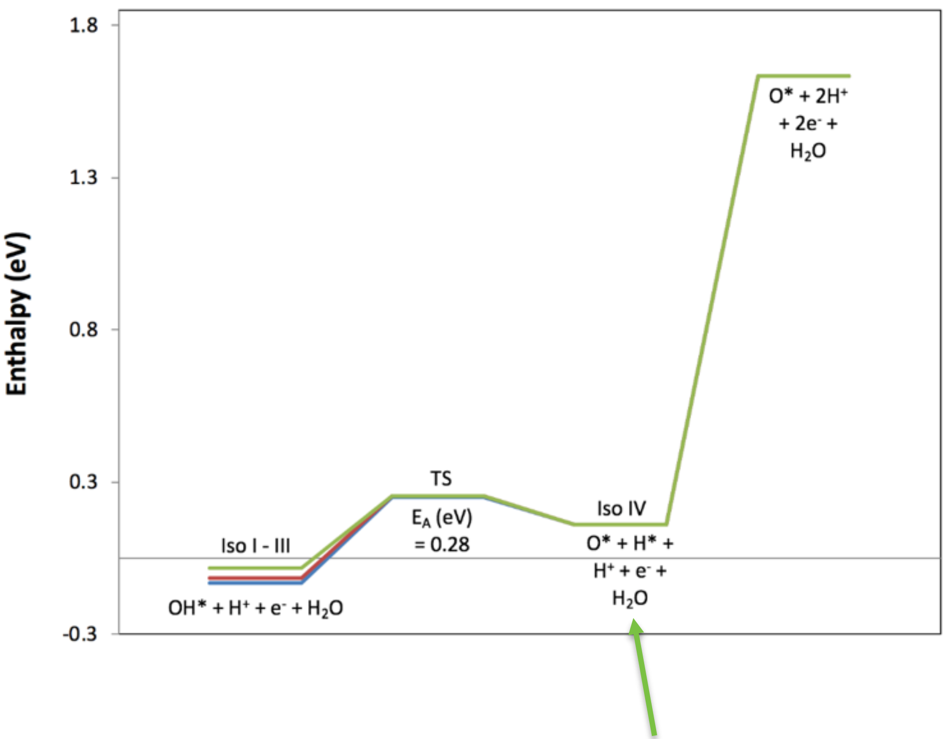
Case 1: Bare Ir Surface: searching for alternative reaction pathways

Approach

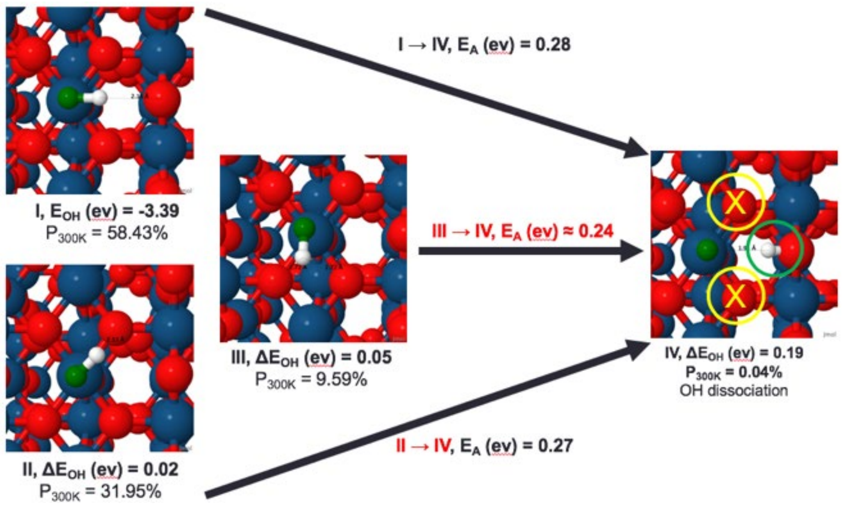


Completed
Running
ⓧ Spontaneous Reprotonation
○ Deprotonation

Reaction Profile of Deprotonation of OH*



O* and H* co-adsorbates



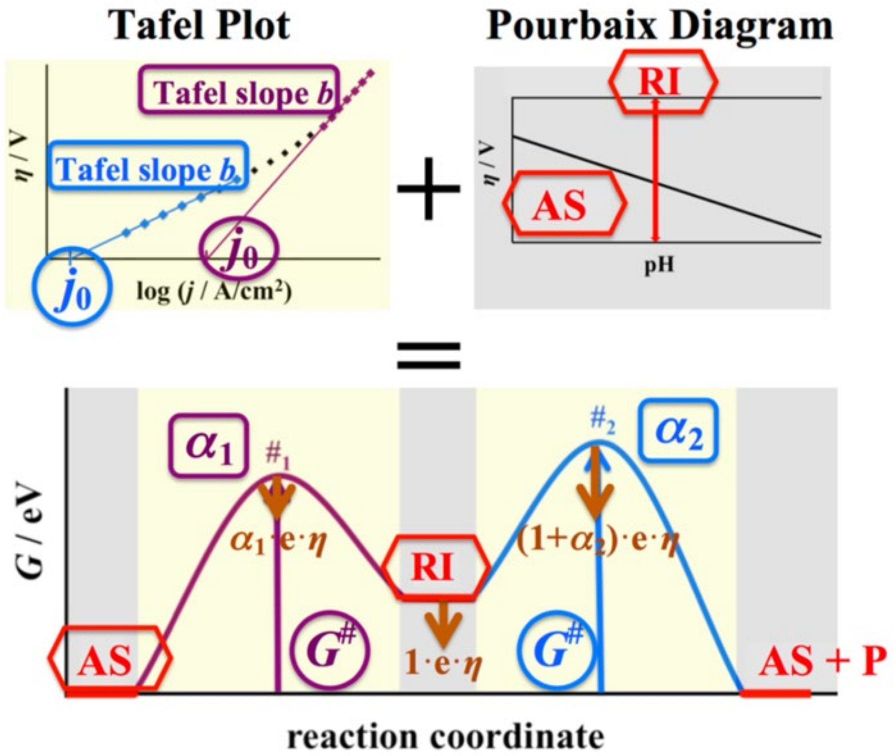
Rxn: $OH^* \rightarrow O^* + H^*$		
Isomer	E_A (ev) (TS)	Notes
I → IV	0.28	Main Pathway
II → IV	0.27	Iso II → Iso I → IV
III → IV	0.24	Iso III → Iso I → IV

Case 1: Key findings

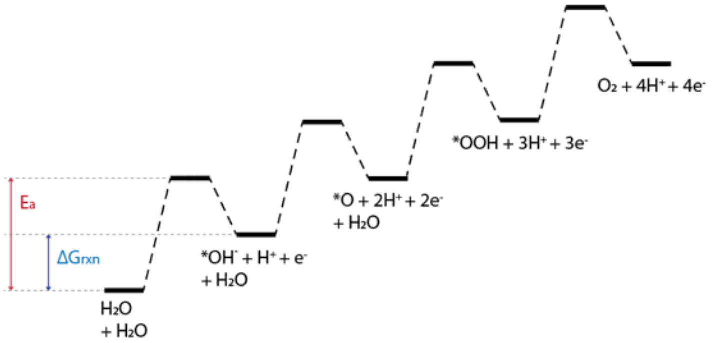
- Low O coverage limit
  - Multiple pathways of OH* deprotonation collapse to one
  - Characterization of a new, alternative mechanism utilizing co-adsorbed O* and OH* in proximity to each other in order to evolve O_2
    - Multiple pathways to deprotonation of O* + OH* -> O* + O* + H*

- High O coverage limit (thermodynamically favored): two adjacent O vacancies (active sites) for O* + OH* co-adsorption pathway may be possible at high reaction rate (or high potential)

Case 2: IrO_2 Surface from Pourbaix Analysis



Free Energy Landscape @η = 0 V

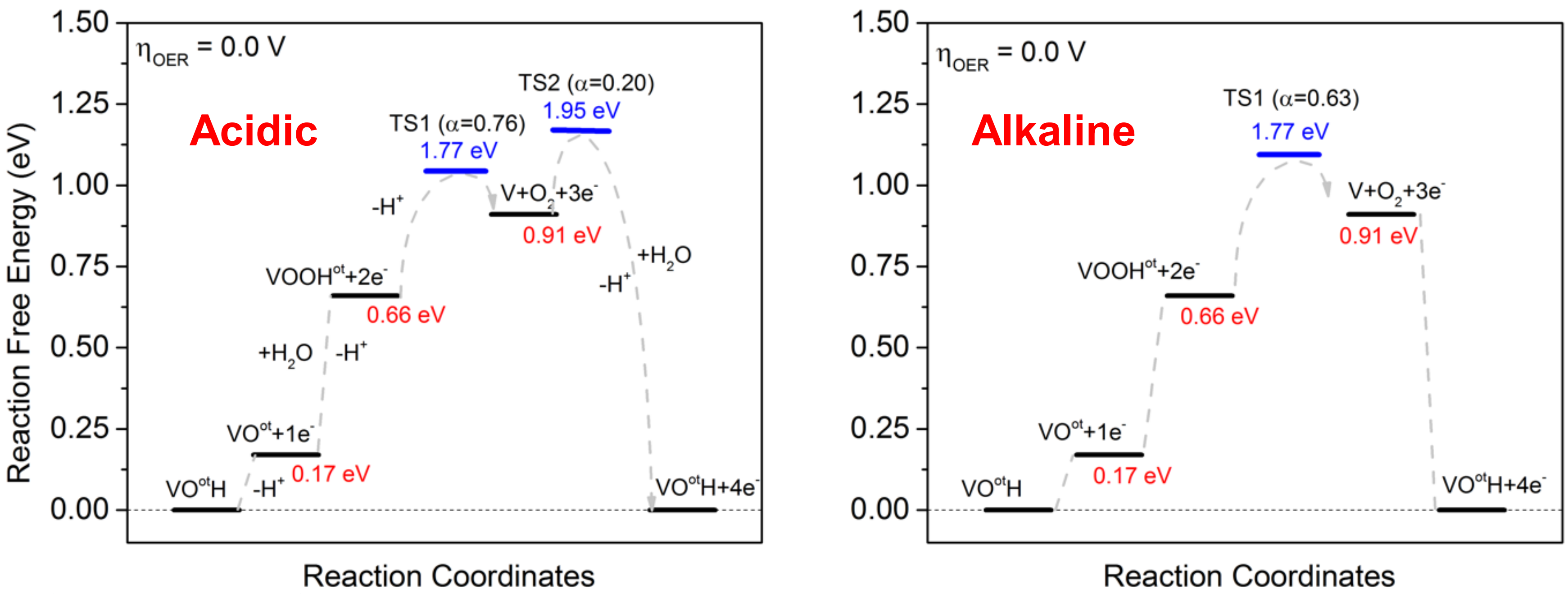


1. (We know the intermediate steps)
2. **Pourbaix diagram => initial step**
   - Sequence is determined
3. **Tafel Plot =>** E_a corresponding to j_o
4. Which TS is rate limiting?

Exner and Over, ACS Catalysis 9, 6755 (2019)

Case 2: Key Findings

- Established a way to determine intermediates, energetics and kinetics of OER based on Exnter and Over, ACS Cat. 9, 6755 (2019)
- Improved *ab-initio* Pourbaix diagram
- Refining transition states with *ab-initio* simulations
- Method to examine effects of solvation established

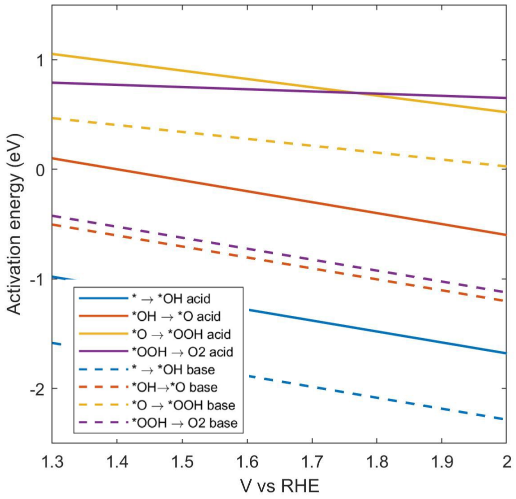


Approach

Microkinetic Modeling Framework

- Using DFT inputs to model OER rate and pathways including mass-transport effects

Potential-dependent free energies



$$K_i = \exp\left(-\frac{\Delta G^o_{rxn} - n_i eV}{k_B T}\right)$$

$$k_{fi} = A\exp\left(-\frac{E^o_a - \beta_i n_i eV}{k_B T}\right)$$

Alkaline and acidic elementary steps

$H_2O + * \leftrightarrow *OH + H^+ + e^-$ (1)

$*OH \leftrightarrow *O + H^+ + e^-$ (2)

$H_2O + *O \leftrightarrow *OOH + H^+ + e^-$ (3)

$*OOH \leftrightarrow * + O_2 + H^+ + e^-$ (4)

$OH^- + * \leftrightarrow *OH + e^-$ (5)

$OH^- + *OH \leftrightarrow *O + H_2O + e^-$ (6)

$OH^- + *O \leftrightarrow *OOH + e^-$ (7)

$OH^- + *OOH \leftrightarrow * + H_2O + O_2 + e^-$ (8)

$$r_1 = k_{f1} a_0 \theta_* - k_{r1} a_{H^+} \theta_{*OH}$$

$$r_2 = k_{f2} \theta_{*OH} - k_{r2} a_{H^+} \theta_{*O}$$

$$r_3 = k_{f3} a_0 \theta_{*O} - k_{r3} a_{H^+} \theta_{*OOH}$$

$$r_4 = k_{f4} \theta_{*OOH} - k_{r4} a_{H^+} a_{O_2} \theta_*$$

...

$$\frac{\partial \theta_*}{\partial t} = -r_1 + r_4 - r_5 + r_8$$

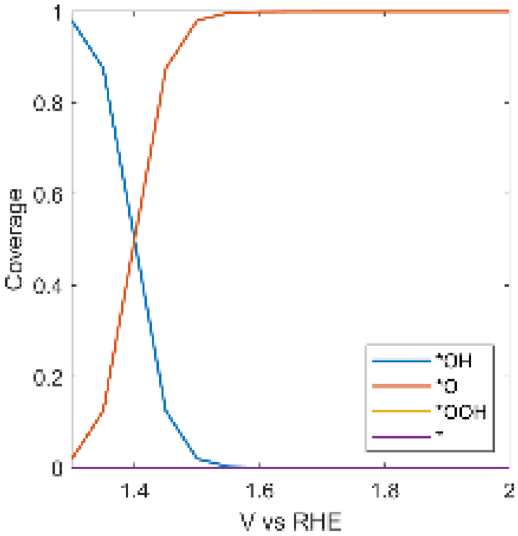
$$\frac{\partial \theta_{*OH}}{\partial t} = r_1 - r_2 + r_4 - r_5$$

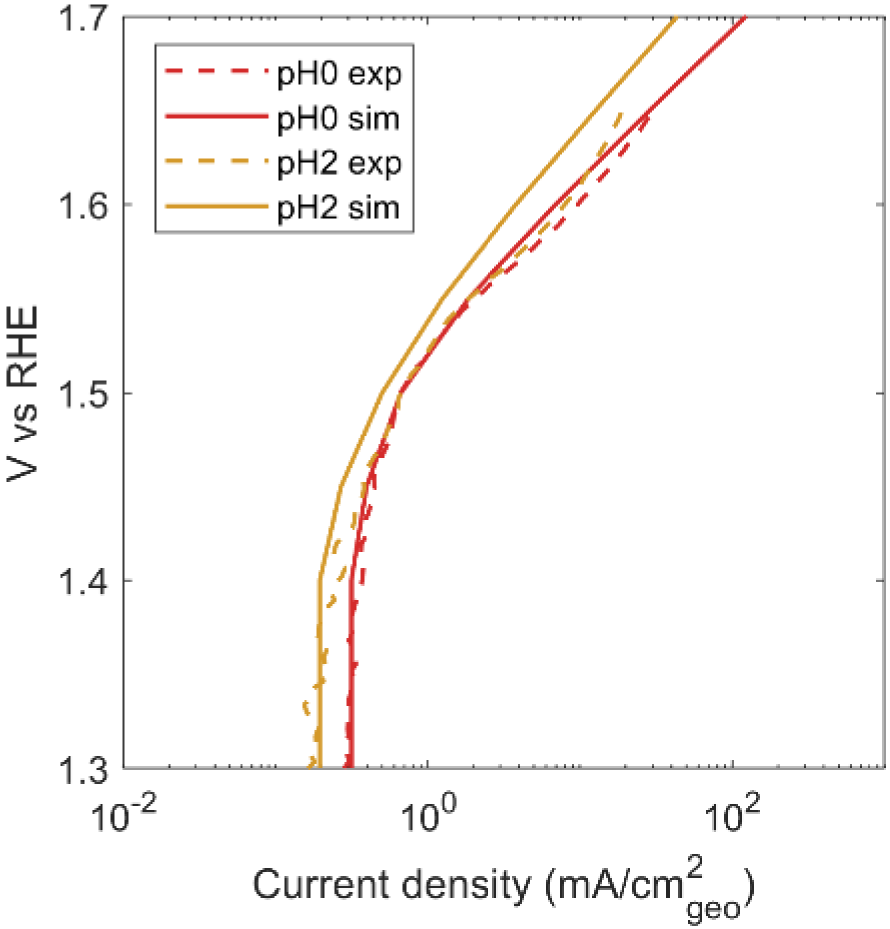
$$\frac{\partial \theta_{*O}}{\partial t} = r_2 - r_3 + r_6 - r_7$$

$$\theta_* + \theta_{*OH} + \theta_{*O} + \theta_{*OOH} = 1$$

Microkinetic Model Results

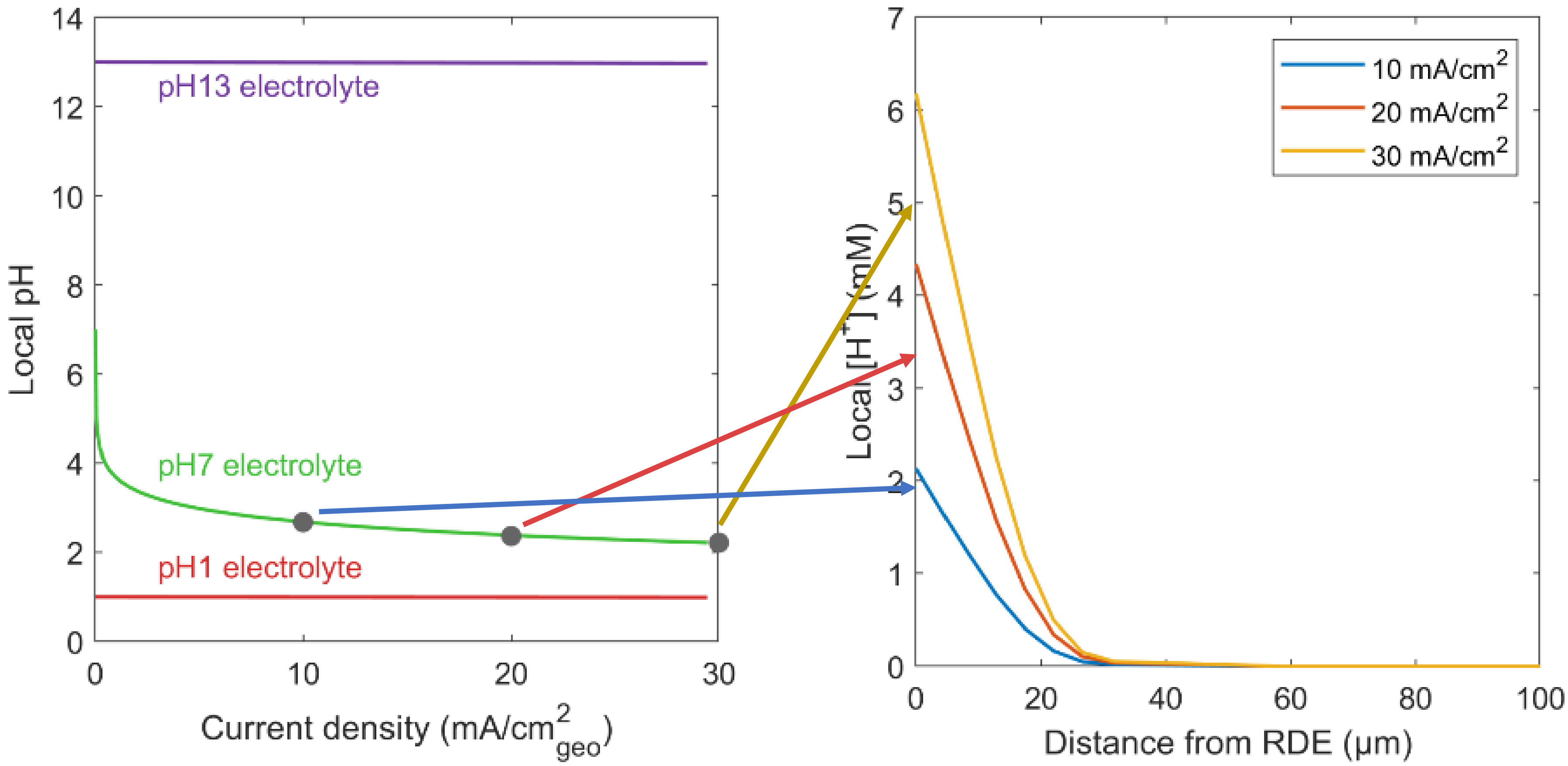
- Using only site density as a fitting parameter
  - Barriers from DFT & MD calculations
- Good agreement for low pH
  - Added a capacitive element for low current density
- Surface Coverages





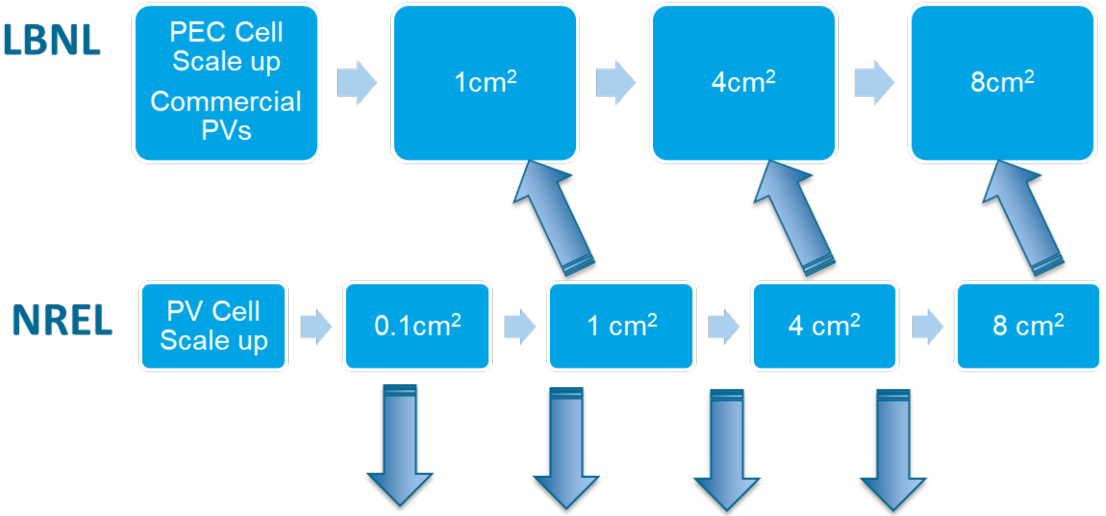
Mass-Transport Effects

- Concentration polarization effects are significant in neutral pH
  - Concentration boundary layer ~ 30 µm near the electrode



PEC Supernode Approach

***Goal**: Understand integration issues and emergent degradation mechanisms of PEC devices at relevant scale, and demonstrate an integrated and durable 50 cm^2 PEC panel.*



LBNL

PEC Cell Scale up

Commercial PVs

1cm^2

4cm^2

8cm^2

NREL

PV Cell Scale up

0.1cm^2

1 cm^2

4 cm^2

8 cm^2

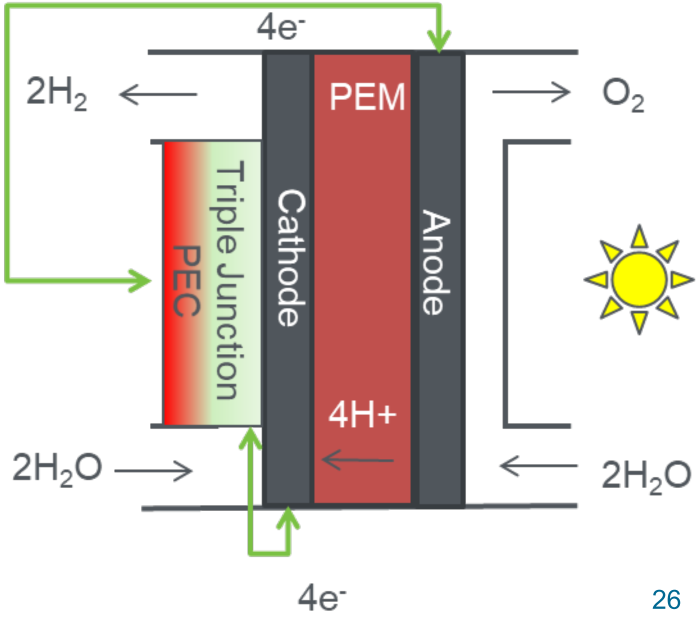
Benchmarking

In situ degradation and characterization

Emerging Degradation Pathways

Modeling

Integrated Photoelectrochemical



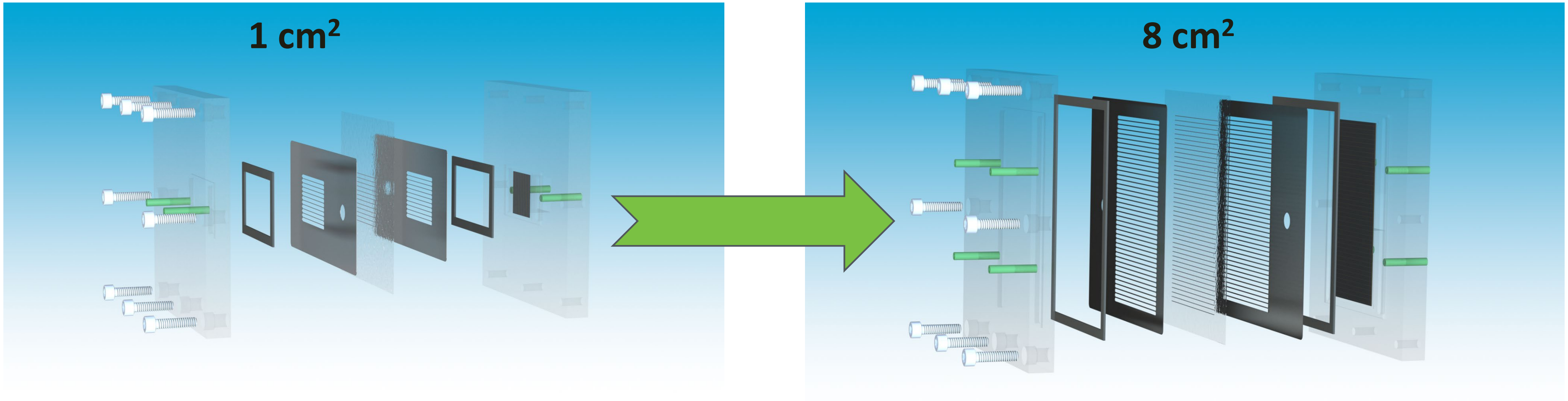
PEC Supernode

- Much of existing PEC work is on < 1cm^2 cells
  - Unclear what issues lie for larger cells
  - Need to scale up *and* improve durability to approach $2/kg
- The main focus of the PEC Supernode is to:
  - Develop understanding of integration issues and emergent degradation mechanisms of PECs at scales > 1 cm^2
  - Demonstrate fabrication of PEC cells at scale

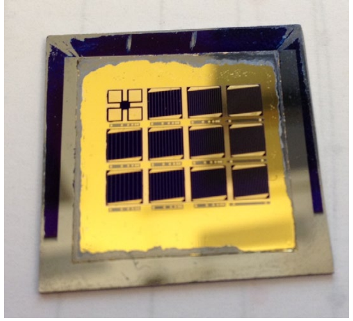
Identify looming issues with scale up

Tough for seedlings (resources, equipment)

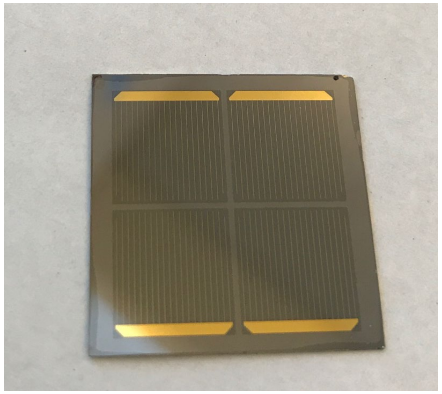
Supernode benefits seedlings and benchmarking



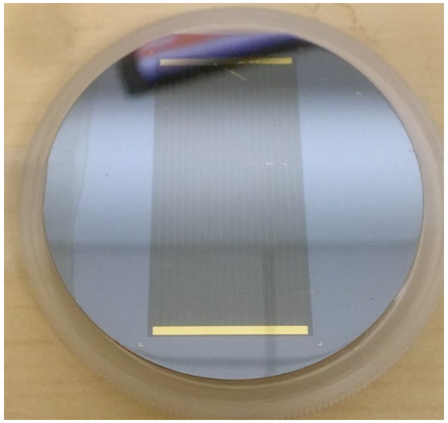
NREL PEC Fabrication: GaInP/GaAs cells with 0.1-8 cm^2



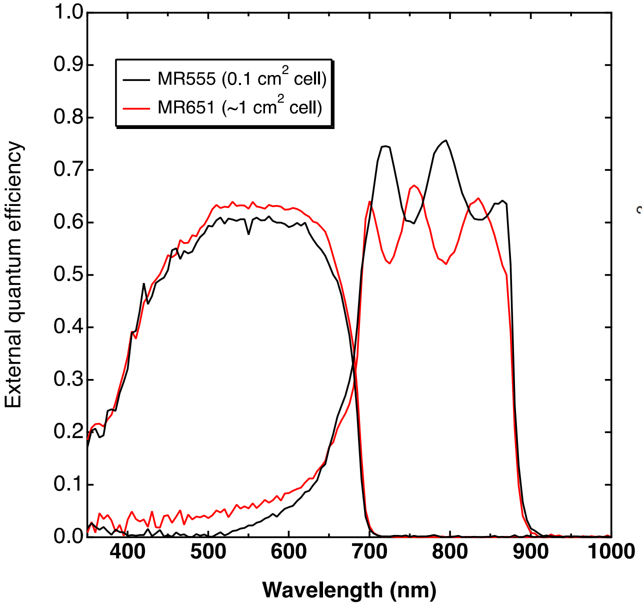
11 PV cells, ~0.1 cm^2

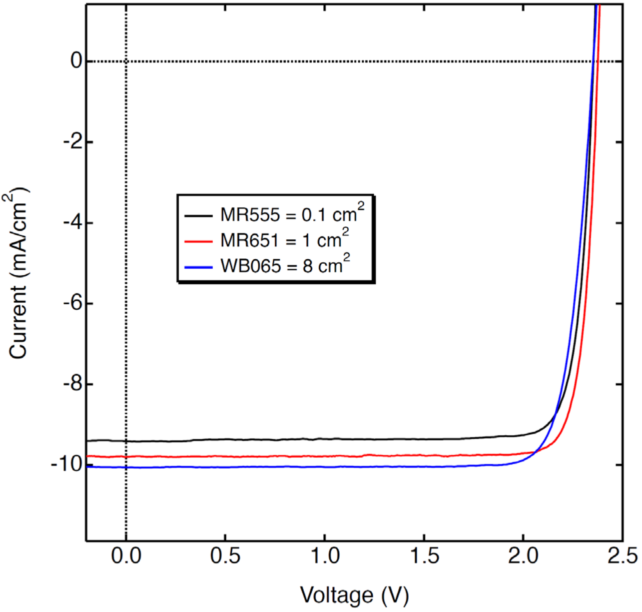


4 PV cells, ~1 cm^2



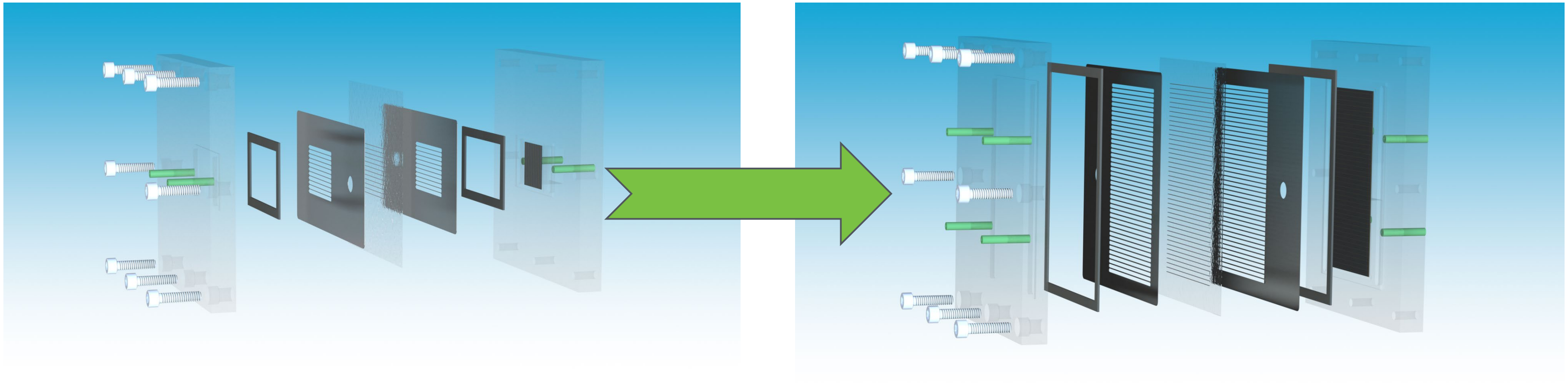
1 PV cell, 8 cm^2





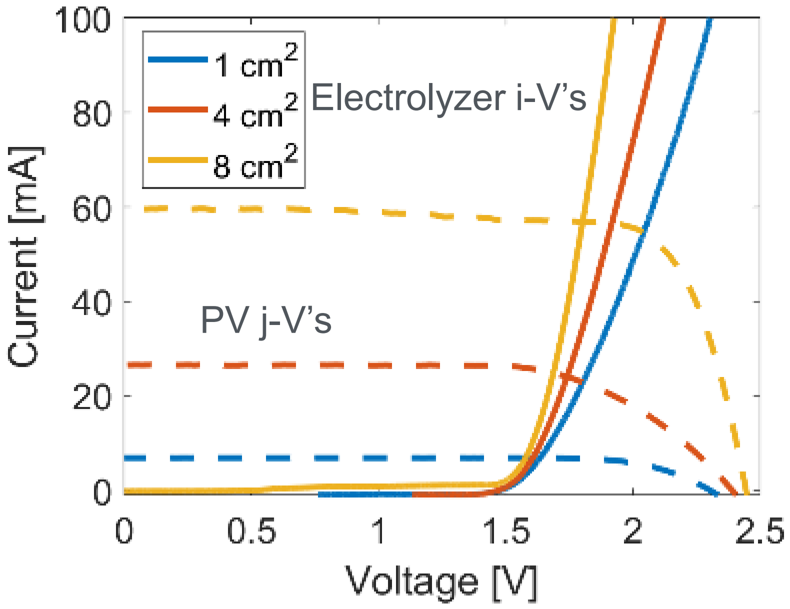
- Successful growth of a large area tandem cells on our 2" MOVPE reactor.
- Significant effort toward developing growth recipes for uniform and high-quality GaInP
- ***These are the largest area III-V cells made at NREL, and enable larger area PEC studies.***

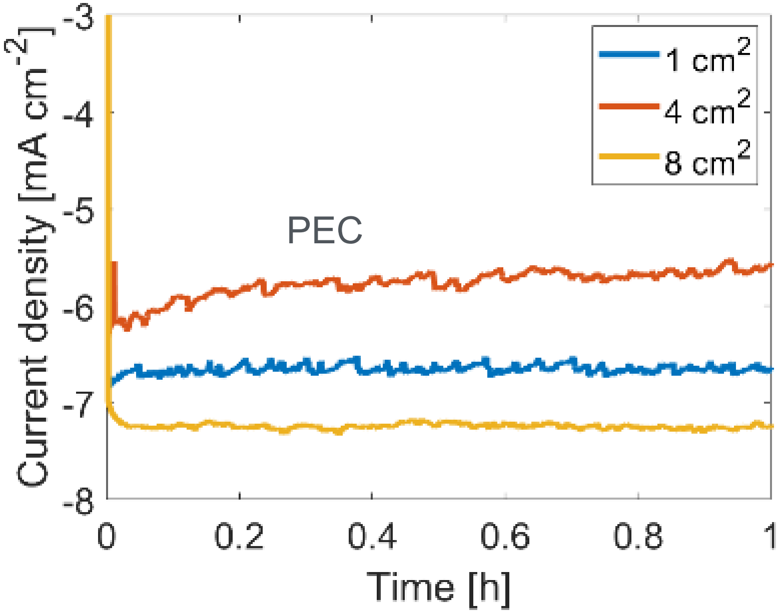
Scale Up Towards 8cm² Illuminated Area



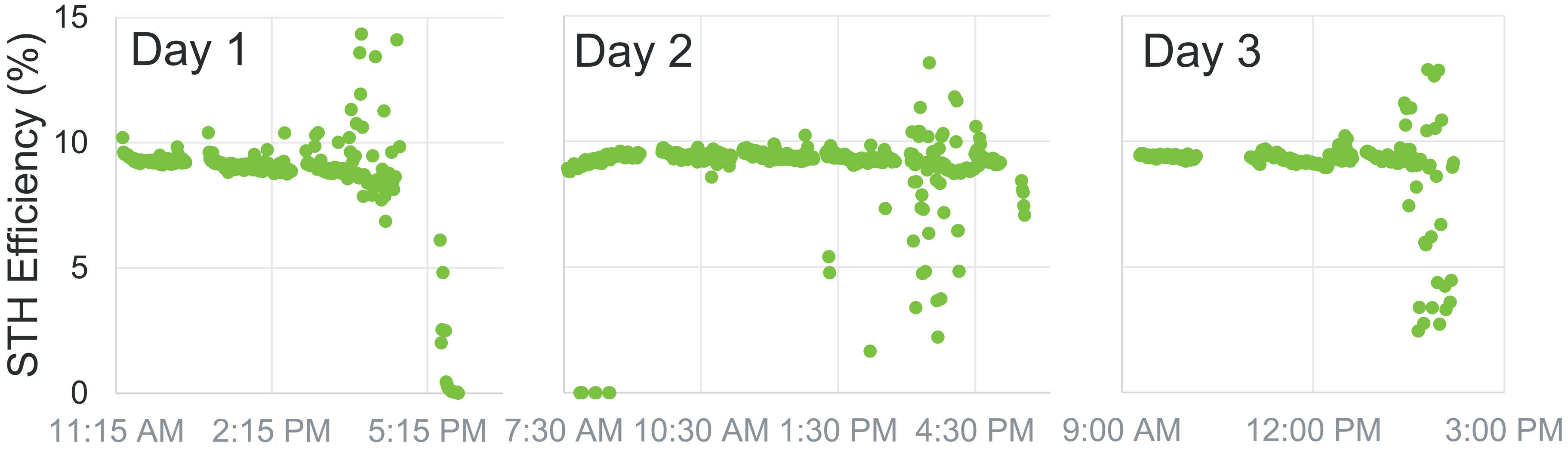
1 cm²

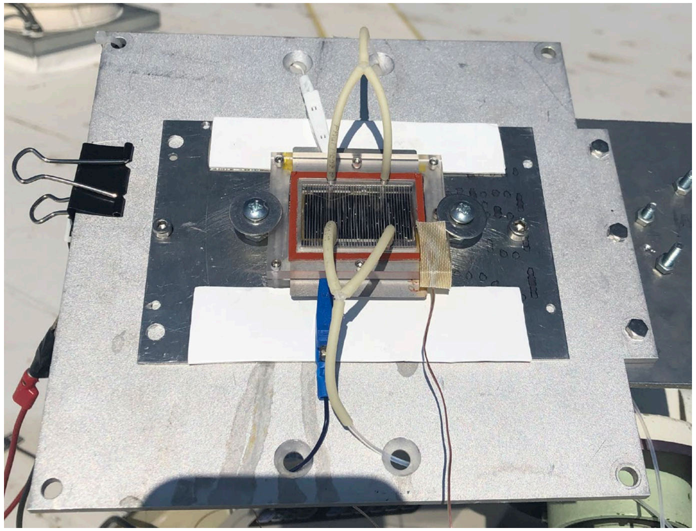
8 cm²





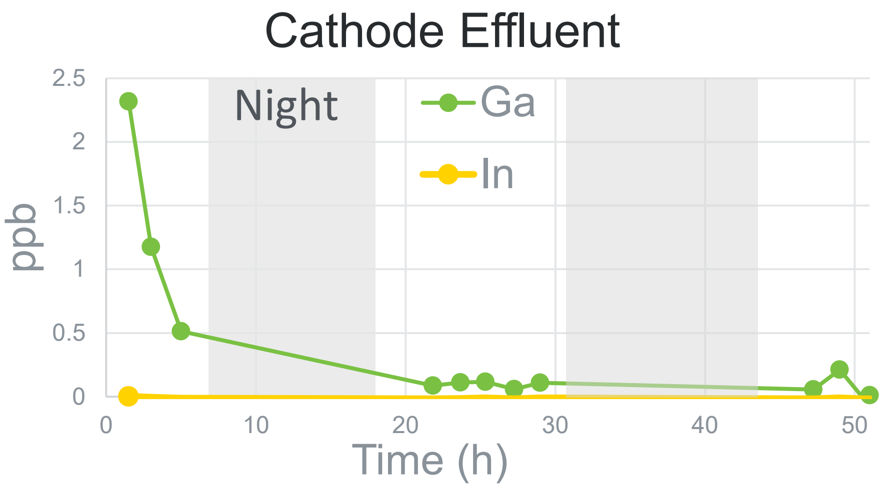
8-cm^2 Cell Testing at NREL: On Sun Durability

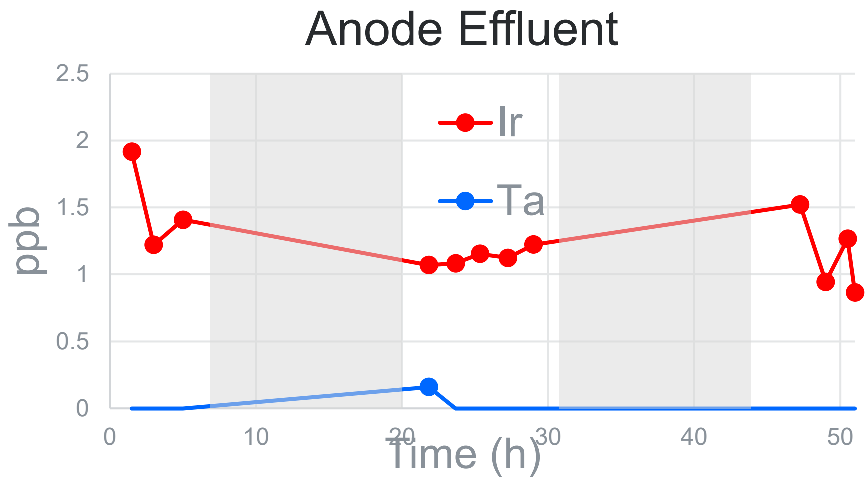




- ***Test Duration:*** **2 days, 2 hours, and 50 minutes**
- Global Normal insolation (Kipp & Zonen CMP22) was measured using data collected at the Solar Radiation Research Laboratory (SRRL)
- Data spikes in afternoon of each day are due to intermittent cloud coverage (data collection offset between device and insolation measurements)
- Steady-state STH efficiency was **9.2%**

8cm² PEC Testing at NREL: ICP-MS Results





Cathode Effluent

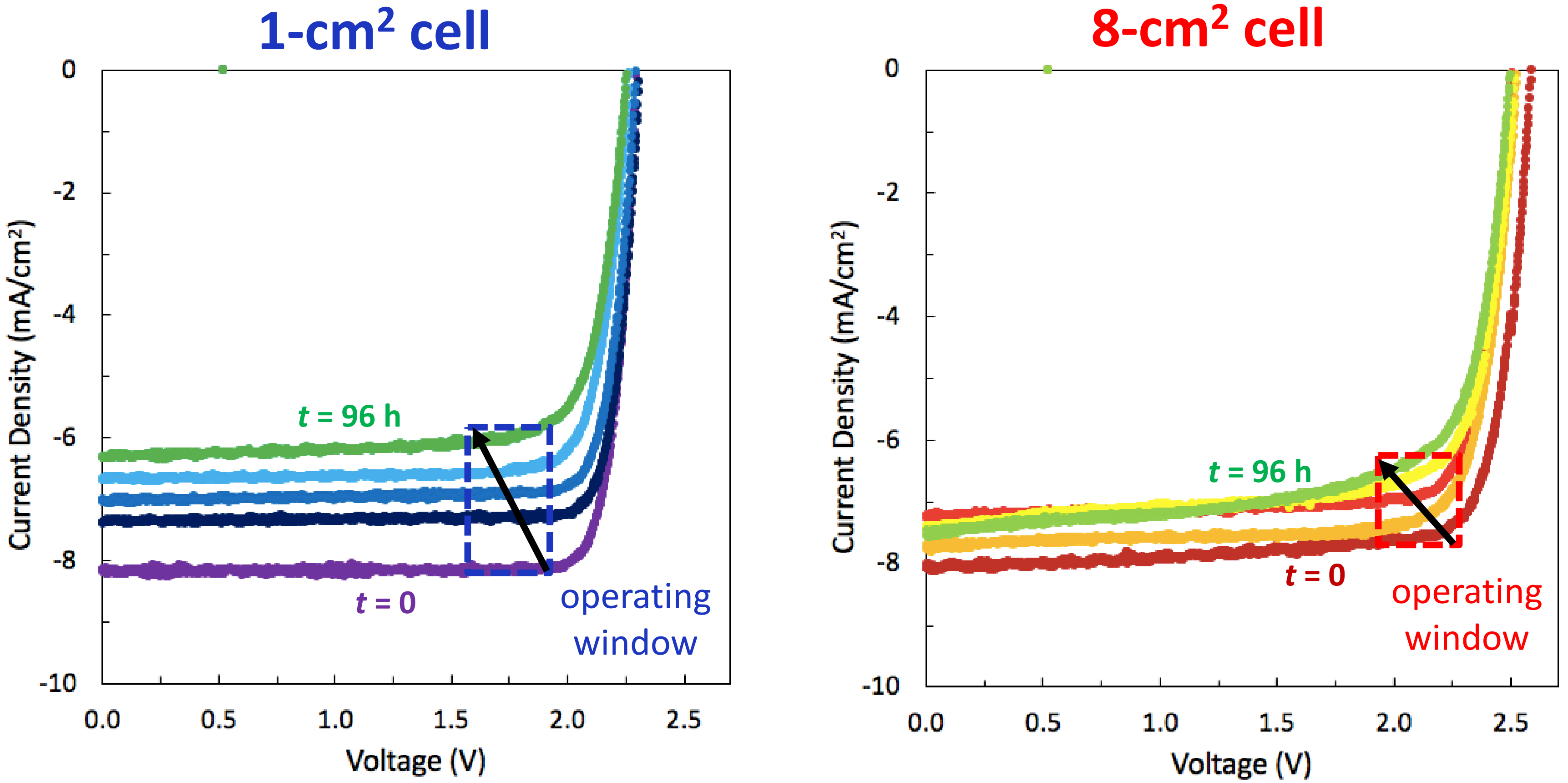
- Gallium content in electrolyte was initially high but dropped off by Day 2
- Indium was not detected

Anode Effluent

- Approximately 1-2 ppb of iridium was found in every aliquot
- Little to no tantalum was detected

Durability: 1-cm^2 and 8-cm^2 cells

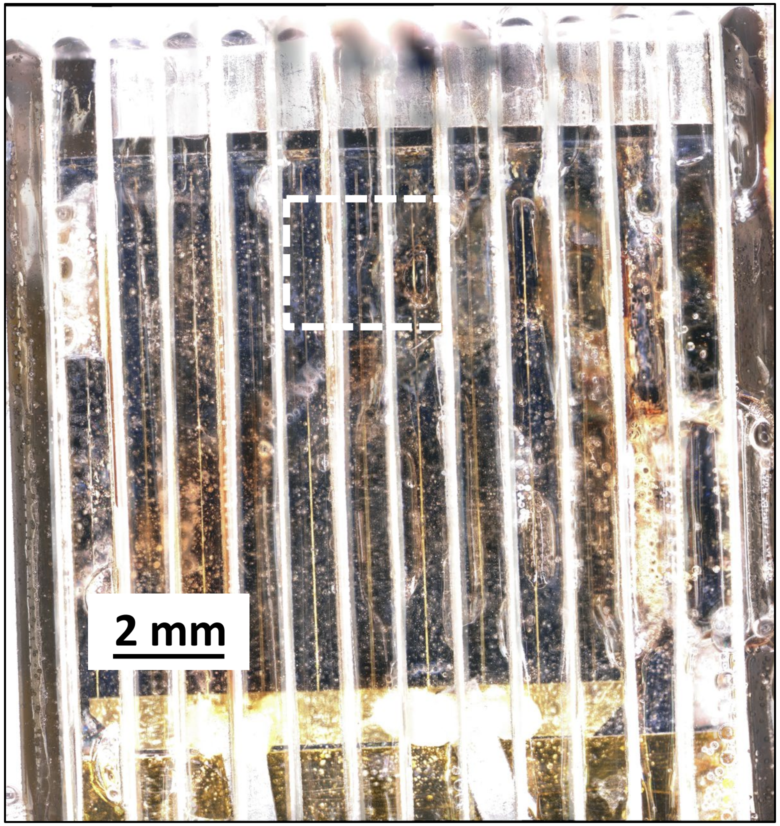
- **PV** performance vs. time

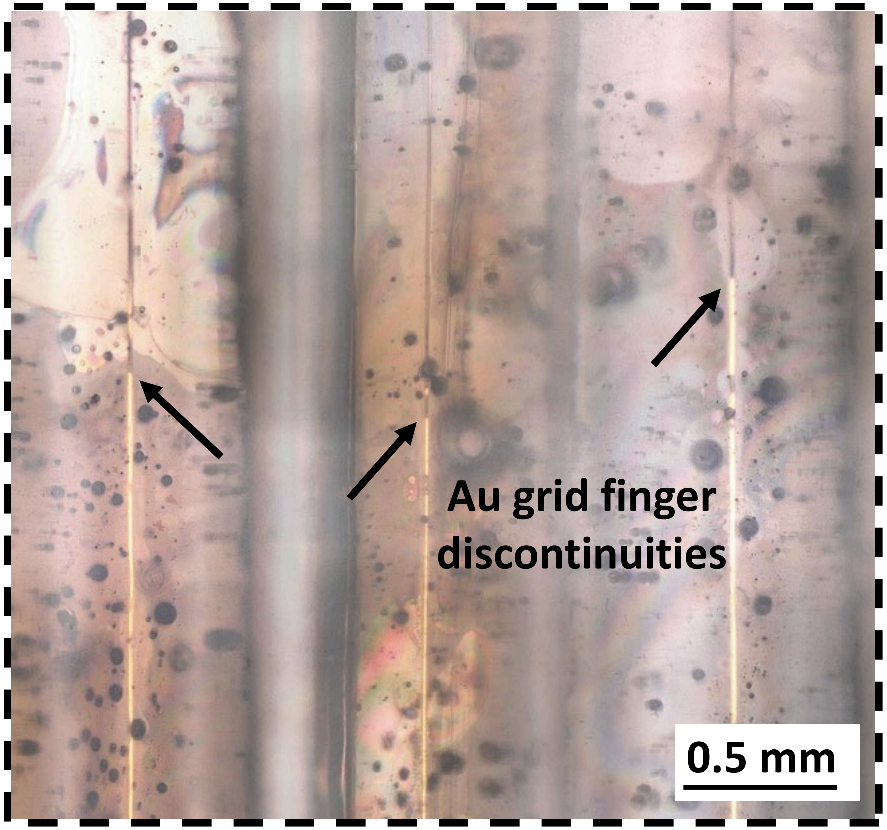


Both cells show light-limited photocurrent decrease vs. time, while the 8-cm^2 cell also shows significant photocurrent losses due to shunting (slope at short-circuit)

Durability: 1-cm^2 and 8-cm^2 cells

- Stereoscopy after durability testing





Indicates failure of the epoxy to resist a combination of water or ion permeation to the PV anti reflection coating and current collectors

Degradation Modes

- Water permeates epoxy
- Gold grid finger delamination
  - Epoxy swelling and pulling up on gold and/or
  - Photo-anodic corrosion of underlying n-GaAs contact layer
- Anti-reflective coating dissolution
  - Consistent with photocurrent decline without photovoltage decline
  - For Al_2O_3, slight acidity would cause it to dissolve (Pourbaix)
- Bubbles in epoxy – more light scattering
  - Heat/light-driven degassing of epoxy and/or
  - H_2 permeation
- Blistering

Future Work

- **OER Supernode**
- Refine DFT mechanism gaps, especially under neutral and alkaline
  - Examine relevant pathways and mechanisms
    - Subsurface oxygen delivery
    - Complete coverage dependent reaction pathway study
    - Evaluate Tafel curve calculated based on our parameter
  - Determine reaction mechanisms at neutral pH and impact of local effects
  - Include solvation and potential effects in the simulation of transition states
- Build further pipelines and linkages across the modeling scales
  - Include additional pathways (i.e. co-adsorption) into microkinetic model
  - Couple mass transport, bubble transport, and microkinetics to simulate full polarization curve across different pHs
- Increased validation
  - Gas-phase using microelectrodes
  - Validate the surface coverages using ambient pressure XPS
- **PEC Supernode**
- Durability parametric and round-robin studies to establish the influence of test conditions and their relevance to actual operation
  - 2-electrode vs 3-electrode PEC and integrated PEC cells
  - Tandem: dependencies on current limiting junction & light source
  - Intermittent/diurnal vs. constant illumination
  - Electrolyte (pH, surfactant, anion/cation species and concentration)
  - Statistics – understanding intrinsic variability on a common photoelectrode across multiple labs (GaInP/GaAs with Pt cocatalyst)

Any proposed future work is subject to change based on funding levels

Summary

- Supporting 7 FOA projects with 22 nodes and 22 PIs
  - Synthesis, benchmarking, modeling, characterization
  - 100’s of files on the data hub and numerous exchanged samples
  - Personnel exchange of postdocs, students, and PIs to the labs
- Working closely with the project participants to advance knowledge and utilize capabilities and the data hub and move the technology forward
  - Seedling projects demonstrate improvements in durable, less expensive materials with high performance and improved durability
- Water and/or solid electrolyte contact with PV are detrimental to durability
  - Barrier layer helps prevent PV corrosion, but may fail upon stress tests
- Successful scale up to 8 cm^2 cells
- Brought together various modeling nodes to work to determine different OER reaction pathways
  - Going from *ab-initio* calculations to macroscale microkinetic and transport ones
  - Demonstrated different OER reactions pathways and ways to refine model predictions
- Future work
  - Examine durability issues under both 2-electrode and 3-electrode cells and real-world conditions
  - Validate predicted surface coverages and refine multiscale models

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HydroGEN
Advanced Water Splitting Materials

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SRNL

Response to reviewers

- This project was not reviewed last year