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

PI: Thomas Jaramillo¹, co-PI: James Harris²

¹ Dept. of Chemical Engineering, Stanford University
² Dept. of Electrical Engineering, Stanford University

May 20th, 2020

2020 DOE Hydrogen and Fuel Cells Annual Merit Review

This presentation does not contain any proprietary, confidential, or otherwise restricted information
Project Overview

Project Partners
PI: Thomas Jaramillo, Stanford University
Co-PI, James Harris, Stanford University

Project Vision
We are developing unassisted water splitting devices based on III-V materials coupled with protective, non-precious metal catalyst coatings, creating pathways to improve efficiency, durability, and cost.

Project Impact
This research aims to develop unassisted water splitting devices that can achieve >20% solar-to-hydrogen (STH) efficiency, operate on-sun for at least 2 weeks, and provide a path toward electrodes that cost $200/m².

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

Project Motivation
We seek to combine the expertise in electrocatalysis and protective layer development of the Jaramillo group with the semiconductor growth capabilities of the Harris group and III-V fabrication knowledge at NREL. These synergies give a path towards efficient and durable III-V/III-V and III-V/Si PEC Devices.

Key Impact

<table>
<thead>
<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Expected Advance</th>
</tr>
</thead>
<tbody>
<tr>
<td>PEC STH (III-V)</td>
<td>19% Young, J. L. et al. Nat. Energy 2017, 2, 17028.</td>
<td>&gt;20%</td>
</tr>
<tr>
<td>PEC Stability (III-V)</td>
<td>100 h indoor – GaAs/GaInP Sun, K. et al. Adv Energy Mater 2016, 6(13), 1600379</td>
<td>2 weeks on-sun</td>
</tr>
<tr>
<td>Si/III-V Tandem</td>
<td>Si-InGaN nanowire synthesis Wang, Y. et al. Nano Energy, 2019, 57, 405-413.</td>
<td>epitaxial growth InGaN on Si</td>
</tr>
</tbody>
</table>

Partners

**Jaramillo Group**
Electrochemistry, catalysis, protective layer expertise (characterization, catalyst deposition)

**Harris Group**
Semiconductor expertise, particularly in novel synthesis, processing, and fabrication techniques (InGaN growth)

**NREL**
III-V fabrication (epitaxial growth) expertise, on-sun testing expertise, unassisted water splitting device expertise

**LBNL**
In Situ Photoelectrochemical Raman spectroscopy

---

**Barriers**

**AF – Materials Durability – Bulk and Interface**
Stabilization of unstable III-V surfaces in acid using MoS₂ and other non-precious metal protecting/catalytic layers

**AE – Materials Efficiency – Bulk and Interface**
Develop fabrication of crystalline InGaN on Si by MOCVD to lead to a high efficiency tandem absorber

**AK – Diurnal Operation Limitations**
Develop outdoor test setup and conduct on-sun testing of stabilized III-V unassisted water splitting devices

---


Approach: The team

- Prof. Jim Harris, Stanford
- Dr. Myles Steiner
- Dr. Daniel Friedman, NREL
- Dr. Reuben Britto
- Dr. Andrew Wong
- Dr. Ye Sheng Yee
- Dr. Laurie King
- Prof. Thomas Jaramillo, Stanford
- Micha Ben-Naim
- Dr. Adam Nielander
- Dave Palm
- Ben Reeves

HydroGEN: Advanced Water Splitting Materials
## Approach: Innovation

### Scheme 1

**III/V-III/V**

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom</td>
<td>GaInP</td>
<td>Robust fabrication, Prior success protecting in acid, Most direct pathway to high efficiency devices</td>
</tr>
<tr>
<td>Middle</td>
<td>GaAs</td>
<td></td>
</tr>
<tr>
<td>Top</td>
<td>GaInP</td>
<td></td>
</tr>
<tr>
<td>Middle</td>
<td>GaInAs</td>
<td></td>
</tr>
</tbody>
</table>

### Scheme 2

**III/V-Si**

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom</td>
<td>Si</td>
<td></td>
</tr>
<tr>
<td>Middle</td>
<td>InGaN</td>
<td>New fabrication approaches – growth of crystalline InGaN on Si is a challenge in the field, Pathway to cheaper fabrication, Prior success growing LEDs</td>
</tr>
</tbody>
</table>

### End of Project Goal #1

On-sun testing of unassisted water splitting devices for ≥ 2 weeks.

### End of Project Goal #2

Demonstration of an unassisted water splitting device with ≥ 20% STH efficiency.
Approach: Innovation

➤ Stabilization of III-V surfaces in acid
   - **Innovation**: Use MoS$_2$ and other non-precious protective catalysts that are stable in acid, conductive, and active for HER. Developing an understanding of fundamental degradation mechanisms through *in situ* studies and leverage those insights into better protective catalysts
     • **Task 1**: Translatable, thin-film catalyst and protection layer development
     • **Task 3**: III-V fabrication and PEC device development for tandem III-V and InGaN/Si
     • **Task 4**: In-situ stability studies
   - **EMN Nodes**: i) Characterization of Semiconductor Bulk and Interfacial Properties (Todd Deutsch, NREL), ii) Corrosion Analysis of Materials (Todd Deutsch, NREL), and iii) III-V Semiconductor Epi-structure and Device Design and Fabrication (Daniel Friedman, NREL).

➤ Fabrication scheme for high-quality InGaN growth on Si
   - **Innovation**: First demonstration of direct nucleation and growth of InGaN on monocrystalline Si by MOCVD in this field.
     • **Task 2**: Tandem InGaN/Si fabrication

➤ Collecting on-sun data at the weeks time-scale
   - **Innovation**: By stabilizing III-V unassisted water splitting devices for 100’s of hours, we can test them outside for weeks
     • **Task 5**: On-sun testing at NREL
   - **EMN Nodes**: On-Sun Solar-to-Hydrogen Benchmarking (Todd Deutsch, NREL)
## Approach: Budget Period 2 Milestones

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0</td>
<td>Task 2: Tandem InGaN/Si fabrication</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.4</td>
<td>Demonstrate working tandem InGaN/Si solar cell device</td>
<td>5/31/19</td>
<td>70%</td>
<td>Working InGaN solar cell</td>
</tr>
<tr>
<td>2.5</td>
<td>Demonstrate a tandem InGaN/Si solar cell with power conversion efficiencies of &gt;10%</td>
<td>12/31/19</td>
<td>30%</td>
<td>InGaN/Si solar cell with Si photovoltaic material</td>
</tr>
<tr>
<td>3.0</td>
<td>Task 3: III-V fabrication and PEC device development for tandem III-V and InGaN/Si</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3.2</td>
<td>Demonstrate InGaN/Si tandem absorbers that produce hydrogen during light-driven, unassisted water splitting</td>
<td>9/30/19</td>
<td>40%</td>
<td>Photoanode behavior by MOCVD-grown InGaN with NiO hole-transport layer</td>
</tr>
</tbody>
</table>
| 3.3       | 3.3.1: Demonstrate InGaN/Si as a photoelectrode for unassisted water splitting with >1% STH  
3.3.2: Design and implement improved dual III-V tandem absorbers which achieve STH efficiency >15% | 3/31/20 | 0% | 12.8% STH with IMM tandem GaInP$_2$/GaInAs |
| 3.4       | 3.4.1: Demonstrate unassisted water splitting device with >20% STH efficiency that maintains at least 10% STH efficiency for >100 h.  
3.4.2: Demonstrate unassisted water splitting using InGaN/Si with >2% initial STH that continues to produce hydrogen after >100 hrs of continuous illumination | 9/30/20 | 0% | 0% |
| 4.0       | Task 4: In-Lab Stability Studies |                 |                 |                |
| 4.2       | Utilize the flow cell for analyzing the degradation mechanisms of the III-V based tandem PEC devices. | 9/30/20 | 25% | PEC testing in flow cell and ex-situ Raman spectroscopy |
| 5.0       | Task 5: On-sun testing |                 |                 |                |
| 5.1       | 5.1.1: Finalize the outdoor PEC cell setup, design and protocols to enable on-sun data collection for >24 hours  
5.1.12: Collect >10 mL of hydrogen from an unassisted water splitting device in an on-sun testing in one day | 12/31/19 | 100% | Generated 14.4 mL of hydrogen during on-sun test on 1/15/20 |
| 5.2       | Demonstrate photode electrode that generates hydrogen under diurnal conditions on-sun for greater than or equal to 2 weeks | 9/30/20 | 0% |                |
| **End of Project Goal** | On-sun testing of Scheme 1 and 2 unassisted water splitting devices for >2 weeks. Demonstration of an unassisted water splitting device with an average greater than 20% STH efficiency. | 9/30/20 | 20% 30% | One-day of on-sun testing 12.8% STH with IMM tandem |
Relevance & Impact

This project advances towards <$2/kg hydrogen by:

• Improving efficiency and durability of state-of-the-art photoelectrodes using earth-abundant protection layers towards > 20% solar-to-hydrogen (STH) efficiency with long-term, on-sun operation

Leveraging EMN Resource Nodes:

• NREL EMN Node: Characterization of Semiconductor Bulk and Interfacial Properties, Todd Deutsch,
  – Characterization of fundamental semiconductor properties and growth defects before and after testing
• NREL EMN Node: Corrosion Analysis of Materials, Todd Deutsch,
  – Pre- and post- failure analysis and improved understanding of catalyst corrosion and interface energetics
• NREL EMN Node: III-V Semiconductor Epi-structure and Device Design and Fabrication, Daniel Friedman,
  – Fabrication of III-V materials and systems and improved understanding of growth defects
• NREL EMN Node: On-Sun Solar-to-Hydrogen Benchmarking, Todd Deutsch,
  – Testing station for collection of on-sun data for unassisted water splitting devices
• LBNL EMN Node: Photophysical Characterization of Photoelectrochemical Materials and Assemblies, Jason Cooper
  – In Situ Photoelectrochemical Raman spectroscopy to identify degradation pathways

Jaramillo group has worked with multiple EMN nodes to successfully protect III-V photocathodes in acid with collaboration track record spanning the last 6 years, resulting in published work and improved node capabilities
Accomplishments for Task 2: InGaN/Si Fabrication

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.4</td>
<td>Demonstrate working tandem InGaN/Si solar cell device</td>
<td>5/31/19</td>
<td>70%</td>
<td>Working InGaN solar cell</td>
</tr>
<tr>
<td>2.5</td>
<td>Demonstrate a tandem InGaN/Si solar cell with power conversion efficiencies of &gt; 10%</td>
<td>12/31/19</td>
<td>30%</td>
<td>InGaN/Si solar cell with Si photovoltaic material</td>
</tr>
</tbody>
</table>

Device structure with InGaN, a NiO hole transport layer and Au top contact.

InGaN with a NiO hole transport layer acts as a functioning photovoltaic, producing up to 0.3 mA/cm² of photocurrent.
Accomplishments for Task 3: Stable Unassisted Water Splitting

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.2</td>
<td>Demonstrate InGaN/Si tandem absorbers that produce hydrogen during light-driven, unassisted water splitting</td>
<td>9/30/19</td>
<td>40%</td>
<td>Photoanode behavior by MOCVD-grown InGaN with NiO hole-transport layer</td>
</tr>
</tbody>
</table>

- Open circuit potential in the dark and light showing a photoanode response
- Illuminated JV Characteristic under 2 sun illumination
- Dark JV characteristic showing minimal dark current

Device structure with InGaN and NiO hole transport layer: 30 nm NiO, n-InGa0.15Ga0.85N, p-Si (111) degenerately doped, In-Ga Eutectic

InGaN with a NiO hole transport layer acts as a photoanode, with up to 1.8 mA cm⁻² of photocurrent under 2 suns illumination in KOH electrolyte

Chronoamperometry over 2 hours at 1.23 V vs. RHE
### Accomplishments for Task 3: Stable Unassisted Water Splitting

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.3</td>
<td>3.3.2: Design and implement improved dual III-V tandem absorbers which achieve STH efficiency &gt;15%</td>
<td>3/31/20</td>
<td>75%</td>
<td>12.8% STH with IMM tandem GaInP₂/GaInAs</td>
</tr>
</tbody>
</table>

**Milestone 3.3.2:** Design and implement improved dual III-V tandem absorbers which achieve STH efficiency >15%

#### Device Structure

Catalyst: 5nm MoS₂
Cap: 10nm GaInP₂
Window: 20nm AlInP
n⁺ GaInP₂
p⁺ GaInP₂
Tunnel junction & graded buffer
n⁺ GaInAs
p⁺ GaInAs
Au Contact
Epoxy/Si handle

An Inverted Metamorphic Multijunction (IMM) tandem of GaInP₂ and GaInAs (1.8/1.18 eV) demonstrated an STH efficiency of 12.8%

9 devices were made from the same growth. Two-electrode LSV are shown for one lower-performance device (3) and the two highest-performance cells (7,8).

**Nodes Utilized:**
Characterization of Semiconductor Bulk and Interfacial Properties
III-V Semiconductor Epi-structure and Device Design and Fabrication
Corrosion Analysis of Materials
Accomplishments for Task 5: On-sun Stability Studies

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>5.1.1: Finalize the outdoor PEC cell setup, design and protocols to enable on-sun data collection for &gt;24 hours</td>
<td>12/31/19</td>
<td>100%</td>
<td>Developed photoreactor and testing protocol</td>
</tr>
</tbody>
</table>

In collaboration with the On-sun EMN node at NREL, we developed a cell and protocol for outdoor testing on the NREL ESIF rooftop.

Stanford PhD student Micha Ben-Naim travelled to NREL in Dec 2019 to conduct on-sun testing.

Nodes Utilized:
On-Sun Solar to Hydrogen Benchmarking
## Accomplishments for Task 5: On-sun Stability Studies

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>5.1.12: Collect &gt;10 mL of hydrogen from an unassisted water splitting device in an on-sun testing in one day</td>
<td>12/31/19</td>
<td>100%</td>
<td>Generated 14.4 mL of hydrogen during on-sun test</td>
</tr>
</tbody>
</table>

2 electrode LSV measured on-sun showing unassisted water-splitting capability

Chronoamperometry measured on-sun over 6 hours at short circuit

On-sun testing of a GaInP$_2$/GaAs tandem (1.8/1.4 eV) protected by MoS$_2$ generated 14.4 mL of hydrogen on 1/15/20

Nodes Utilized:
On-Sun Solar to Hydrogen Benchmarking
Accomplishments: Outlook for future and End of Project Goals

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>End of Project Goal</td>
<td>On-sun testing of Scheme 1 and 2 unassisted water splitting devices for &gt;2 weeks.</td>
<td>9/30/20</td>
<td>20%</td>
<td>14.4 mL hydrogen generated in 1 day on-sun</td>
</tr>
<tr>
<td></td>
<td>Demonstration of an unassisted water splitting device with an average greater than 20% STH efficiency.</td>
<td></td>
<td>30%</td>
<td>Unassisted water-splitting</td>
</tr>
</tbody>
</table>

These end of project goals would push both the stability and efficiency records in the field of PEC water-splitting. Outdoor testing would provide new insights into real-world operating conditions.

We are excited to demonstrate on-sun testing at the weeks timescale as a demonstration of stable PEC hydrogen production.
Collaboration: EMN

<table>
<thead>
<tr>
<th>NREL: Characterization of Semiconductor Bulk and Interfacial Properties, Todd Deutsch</th>
<th>Worked with to analyze our photoelectrodes before and after testing to determine failure mechanisms and strategies for improvement.</th>
</tr>
</thead>
<tbody>
<tr>
<td>NREL: Corrosion Analysis of Materials, Judith Vidal, Todd Deutsch, James Young</td>
<td>Worked with to fabricate high-quality absorbers compatible with our catalytic protection layers.</td>
</tr>
<tr>
<td>‣ Pre- and post- characterization and failure analysis of photocathodes and unassisted water splitting devices</td>
<td></td>
</tr>
<tr>
<td>NREL: III-V Semiconductor Epi-structure and Device Design and Fabrication, Daniel Friedman</td>
<td>Worked with to design our electrodes to be compatible with NREL's on-sun testing setup. Stanford student was on-site in December 2019 to perform on-sun testing, with future experiments planned.</td>
</tr>
<tr>
<td>‣ Design and fabrication of III-V materials and systems</td>
<td></td>
</tr>
<tr>
<td>NREL: On-Sun Solar-to-Hydrogen Benchmarking, Todd Deutsch</td>
<td>Worked with to conduct in-lab stability studies</td>
</tr>
<tr>
<td>‣ Testing station for collection of on-sun data for unassisted water splitting devices</td>
<td></td>
</tr>
<tr>
<td>LBNL: Photophysical Characterization of Photoelectrochemical Materials and Assemblies, Jason Cooper</td>
<td></td>
</tr>
<tr>
<td>‣ In Situ photoelectrochemical Raman Spectroscopy</td>
<td></td>
</tr>
</tbody>
</table>
Collaboration: EMN and beyond

• **EMN Collaboration**
  – Weekly videochats between Stanford (Micha Ben-Naim) and NREL (James Young, Chase Aldridge, Myles Steiner)
  – Weekly exchange of samples fabricated at NREL and further processed at Stanford
  – Parallel photoelectrochemical testing and characterization of samples at Stanford and NREL to ensure accuracy and accelerate research progress
  – Weeklong site visit to NREL (Micha Ben-Naim) for on-sun testing in December 2019

• **Positive interactions with the broad HydroGEN community**
  – Kickoff meeting in November 2017 at NREL provided an opportunity to engage with the community, learn about the plethora of available tools, methods, and expertise.
  – PEC community meeting at ECS in Seattle in May 2018 to discuss HydroGEN, benchmarking, and related activities.
  – HydroGEN EMN Advanced Water Splitting Technology Pathways Benchmarking & Protocols Workshop, Tempe, AZ in October 2018 and 2019
  – Presentation to Hydrogen Production Tech Team (HPTT) in February 2019.

• **Incorporating project data onto the HydroGEN data hub**
  – We learned how to use the H2awsm tools at the kickoff meeting to upload our data for the broader community.
  – All of our photocathode stability data and linear sweep voltammetry data will be uploaded.
  – We hope this will help accelerate the stability benchmarking effort.

• **Collaboration with LBNL: EMN node and Molecular Foundry**
  – Started working with Dr. Jason Cooper and the photophysical characterization node for in-lab stability efforts.
  – Worked with Dr. Jason Cooper at LBNL to write a successful Molecular Foundry user proposal to use ALD to deposit MoS$_2$ on III-V materials for improved PEC stability.
Proposed Future Work

Scheme 1
III/V-III/V

a. Upright Tandem

- GaInP
- GaAs

- High durability to allow for additional on-sun testing

b. IMM/High Efficiency Tandem

- GaInP
- GaInAs

- Target high efficiency systems

- Continue fabrication and regular sample exchanges between Stanford & NREL, coat with MoS$_2$
- Additional on-sun testing planned

Scheme 2
III/V-Si

- InGaN
- Si

- Continue to develop InGaN/Si growth by MOCVD
- Build upon photoanode behavior to develop tandem PEC systems

End of Project Goal #1

On-sun testing of unassisted water splitting devices for ≥ 2 weeks.

Proposed Budget: $53k

End of Project Goal #2

Demonstration of an unassisted water splitting device with ≥ 20% STH efficiency.

Any proposed future work is subject to change based on funding levels
**Proposed Future Work**

### In Situ Spectroscopy
- Work with the Photophysical Characterization of Photoelectrochemical Materials and Assemblies node at LBNL for *in situ* Raman studies
- Characterize degradation pathways to improve device longevity

### Improved MoS$_2$ Layers
- Utilize ALD + H$_2$S anneal to deposit thinner and more uniform layers of MoS$_2$
- Collaborate with Molecular Foundry at LBNL
- Improve device stability to enable testing outside for ≥ 2 weeks

Kastl, C. et al., *2D Mater.* 2017, 4, 021024

### InGaN Fabrication
- Reduce GaInN crystalline defects using different epitaxial growth techniques
- MOCVD on oxide/nitride-patterned Si (111) templates
- Molecular beam epitaxy on lattice-matched transition metal dichalcogenides

Proposed Budget: $53k

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

Task 2 – High Quality InGaN on Si
• Photovoltaic characteristics by In_{0.45}Ga_{0.55}N on Si (111) using MOCVD

Task 3 – Stable Unassisted Water Splitting
• IMM tandem (GaInP_2/GaInAs) protected with MoS_2 generated 12.8% STH

Task 5 – On-sun Stability Studies
• Successful on-sun hydrogen generation on 12/7/19, 12/20/19, and 1/15/20, generating up to 14.4 mL H_2 in a day

We have demonstrated on-sun hydrogen generation from an unassisted water-splitting device with >10% STH.
Publications and Manuscripts in preparation


- *Epitaxial Growth of InGaN Directly on Si (111) via MOCVD: Properties and Junction Characteristics*. Andrew B. Wong*, Yesheng Yee*, Laurie King, Muyu Xue, Thomas F. Jaramillo, James S. Harris. *In Prep*

- *Photovoltaic Properties of InGaN/Si Heterojunction Tandem Cells*. Andrew B. Wong, Yesheng Yee, Laurie King, Muyu Xue, Thomas F. Jaramillo, James S. Harris. *In Prep*

Presentations


- (Invited) Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX. “Catalyst design and development for sustainable fuels and chemicals,” T.F. Jaramillo, October 2019.

- (Invited) 236th Meeting of The Electrochemical Society (ECS), Atlanta, GA. “Materials Discovery and Development for the Sustainable Production of Fuels and Chemicals,” T.F. Jaramillo, October 2019.

Technical Backup Slides
Backup Slide 1: New semiconductor architecture accomplishments

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.3</td>
<td>3.3.2: Design and implement improved dual III-V tandem absorbers which achieve STH efficiency &gt;15%</td>
<td>3/31/20</td>
<td>75%</td>
<td>12.8% STH with IMM tandem GaInP$_2$/GaInAs</td>
</tr>
</tbody>
</table>

Device stacks tested with window and capping layers on pn-GaInP$_2$

J-V characteristics of three photocathodes

Post-test XPS showing that the window layer alone is unstable

The addition of a window and capping layer improve photocathode efficiency and stability. This architecture was translated to the top cell of scheme 1 tandems.
Backup Slide 2: On-sun Testing Accomplishments

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>5.1.1: Finalize the outdoor PEC cell setup, design and protocols to enable on-sun data collection for &gt;24 hours</td>
<td>12/31/19</td>
<td>100%</td>
<td>Developed photoreactor and testing protocol</td>
</tr>
</tbody>
</table>

**SRRL Instrumentation**

Solar Research Radiation Laboratory (SRRL) at NREL provides > 80 environmental and irradiance monitoring equipment 0.5 mi from PEC test setup.

Dashboard with real-time data collected by SRRL: [https://midcdmz.nrel.gov/apps/gdisplay.pl?BMS](https://midcdmz.nrel.gov/apps/gdisplay.pl?BMS)

Nodes Utilized:
On-Sun Solar to Hydrogen Benchmarking

---

HydroGEN: Advanced Water Splitting Materials
Backup Slide 3: On-sun Testing Accomplishments 12/7/19

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>5.1.12: Collect &gt;10 mL of hydrogen from an unassisted water splitting device in an on-sun testing in one day</td>
<td>12/31/19</td>
<td>100%</td>
<td>Generated 14.4 mL of hydrogen during on-sun test</td>
</tr>
</tbody>
</table>

On-sun testing of a GaInP₂/GaAs tandem (1.8/1.4 eV) protected by MoS₂ generated 1.8 mL of hydrogen on 12/7/19, but electrodes had degraded from previous day.

Sunlight profile during partially cloudy day on 12/7/19

Gas collection tank at the end of testing

2 electrode LSV measured on-sun showing unassisted water-splitting capability

Chronoamperometry measured on-sun over 2 hours at short circuit

Nodes Utilized:
On-Sun Solar to Hydrogen Benchmarking
Backup Slide 4: On-sun Testing Accomplishments 12/20/19

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>5.1.12: Collect &gt;10 mL of hydrogen from an unassisted water splitting device in an on-sun testing in one day</td>
<td>12/31/19</td>
<td>100%</td>
<td>Generated 14.4 mL of hydrogen during on-sun test</td>
</tr>
</tbody>
</table>

2 electrode LSV measured on-sun showing unassisted water-splitting capability

Chronoamperometry measured on-sun over 6 hours at short circuit

On-sun testing of a GaInP$_2$/GaAs tandem (1.8/1.4 eV) protected by MoS$_2$ generated 11.3 mL of hydrogen on 12/20/19

- 76 C cathodic current = 11.3 mL H$_2$
- Collected 10.2 mL gas (10.0 mL subtracting out water vapor pressure)
## Backup Slide 5: On-sun Testing Accomplishments

<table>
<thead>
<tr>
<th>Milestone</th>
<th>Project Milestones</th>
<th>Completion Date</th>
<th>Percent Complete</th>
<th>Progress Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>5.1.12: Collect &gt;10 mL of hydrogen from an unassisted water splitting device in an on-sun testing in one day</td>
<td>12/31/19</td>
<td>100%</td>
<td>Generated 14.4 mL of hydrogen during on-sun test</td>
</tr>
</tbody>
</table>

**Thermal IR camera image of photoreactor during testing on 1/20/20. $T_{air} \sim 4 \, ^{\circ}C$**

**Photoreactor platform allows for a variety of supplementary datasets**

**Photoreactor chuck showing two devices run in parallel**

**Timelapse pictures of solar tracker at beginning, middle, and end of test (top, middle, bottom, respectively)**

---

HydroGEN: Advanced Water Splitting Materials