Photoelectrochemical Hydrogen Production

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This presentation does not contain any proprietary or confidential information

PDP37

Overview

Timeline

- Project start date: TBD
- Project end date: TBD
- 0% complete

Barriers

AP. Materials Efficiency

AQ. Materials Durability

AR. Bulk Materials Synthesis

AS. Device Configuration Design

AT. Systems Design and Evaluation

Budget

- Total project funding: $4,090,172
  - DOE share $3,271,630
  - Cost share $818,542
- Funding received in FY04: $0
- Funding for FY05: $0

Partners

- Hawaii Natural Energy Institute (University of Hawaii)
- Intematix Corporation
- UC Santa Barbara
- Southwest Research Institute
- Duquesne University
- NREL

Objectives

(1) The demonstration of a multi-junction photoelectrochemical solar-powered hydrogen production system with 7.5% solar-to-hydrogen (STH) conversion efficiency and 1,000 hours operational life

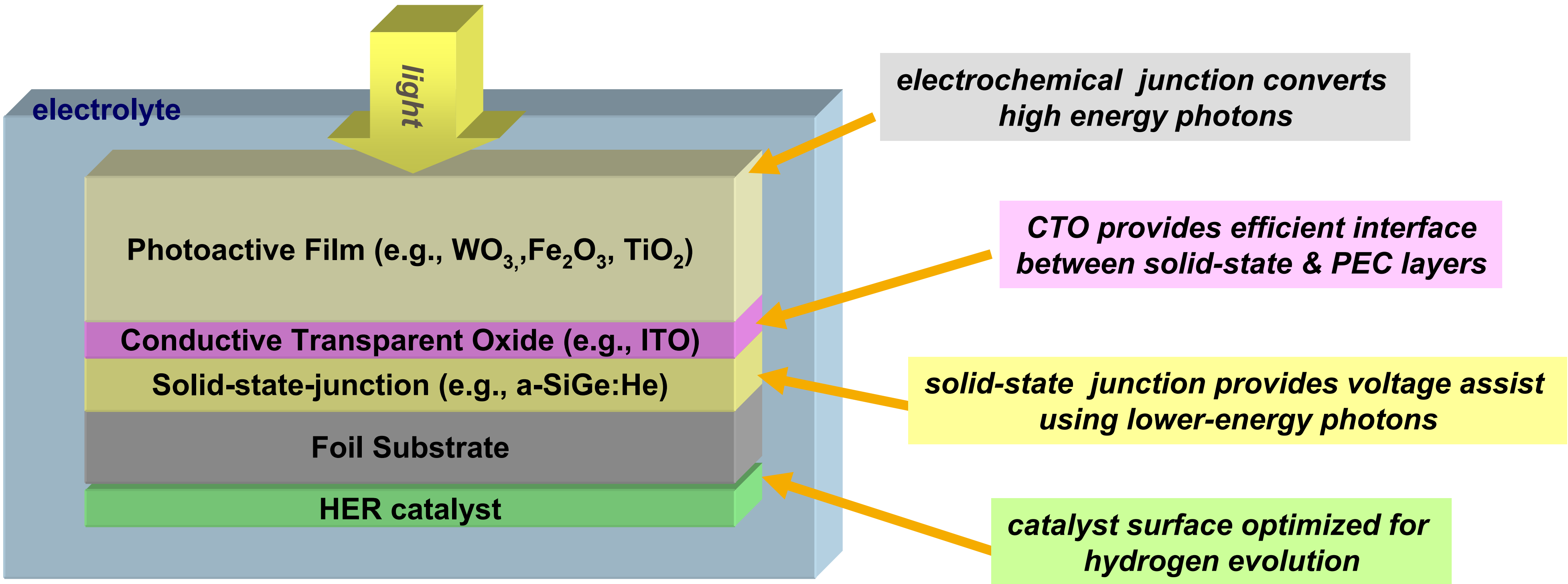
- Development of low-cost photoactive materials with 1-sun photocurrents greater than 6 mA/cm^2 and with sufficient durability to meet the lifetime requirement
- Development of supporting solid-state devices with sufficient current and voltage output
- Development of necessary process integration techniques

(2) The identification of commercialization paths toward DOE plant production cost targets

- Demonstration of materials/device fabrication process scale-up for commercialization
- Generation of an energy/economic analysis for hydrogen production cost based on the developed technology

Approach:

1. Hybrid Photoelectrode Technology*



- **Multi-junction monolithic photoelectrode for direct water splitting**
- **Focus on low-cost materials such as metal foil substrates & oxide thin films**
- **Utilize scalable fabrication processes for commercial manufacture**
- **Materials developed for HPE relevant to other multi-junction configurations**

*Patented technology developed under DOE Grant DE-FC36-00GO10538 by U. of Hawaii

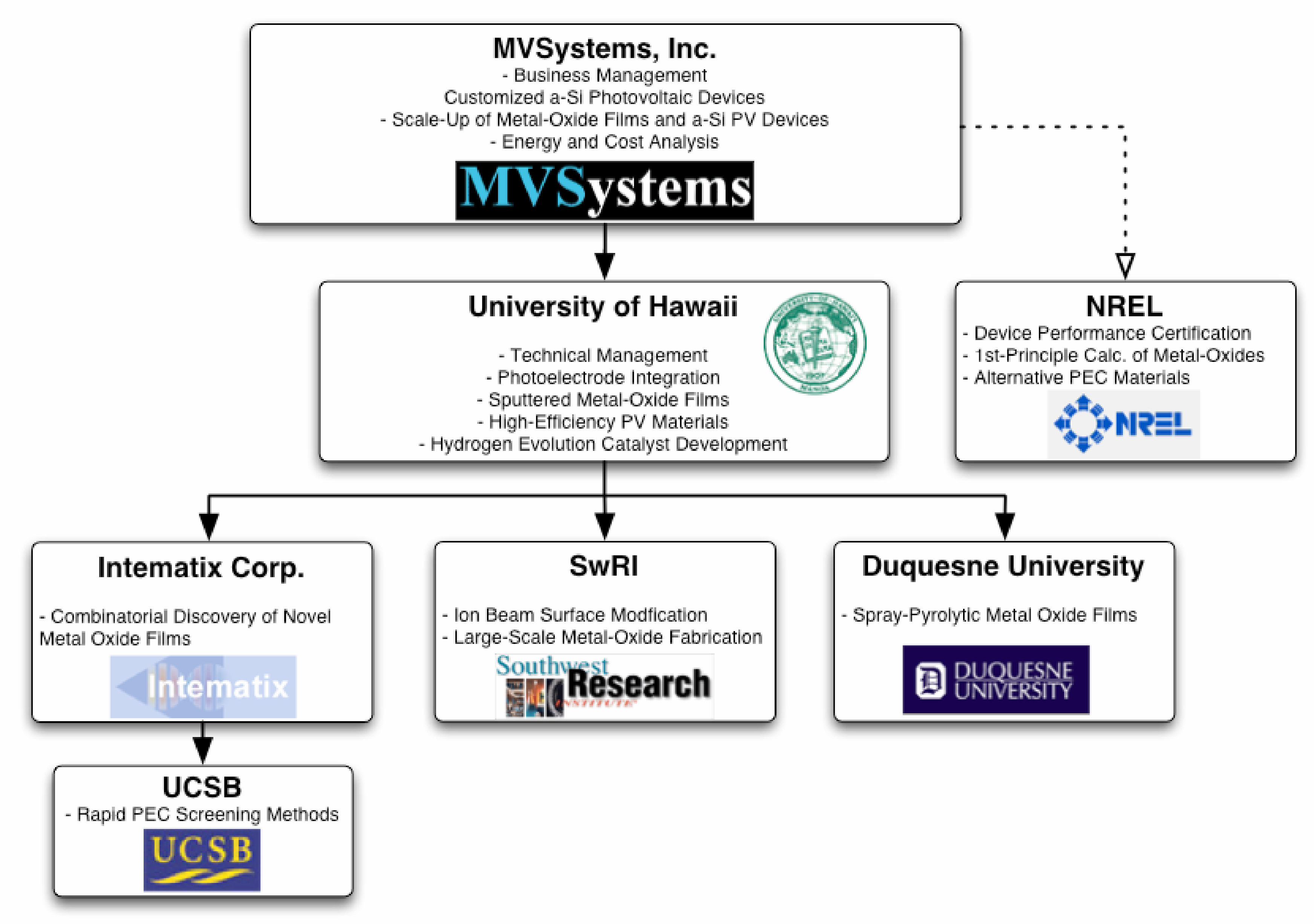
Approach:
2. Project R&D Task Breakdown

- **Accelerated R&D of Photoactive Materials**
  - High-throughput fabrication and screening of material modifications
  - doping for improved photo-response
  - film texturing for improved surface area
  - Guidance by theoretical calculations…
  - …and detailed analysis of existing high-performance materials

- **Hybrid Photoelectrode (HPE) Device Development**
  - Development of suitable solid-state junctions for device integration
  - Prototype demonstration (several cycles) based on best-available materials

- **Scale-up and Commercialization Evaluation**
  - Medium-scale fabrication of HPE component films on cluster tool
  - Large-scale fabrication of photoactive film (WO_3) on vacuum roll system
  - Economic/energy analysis of HPE technology based on current state and projections

Approach:
3. Division of Tasks



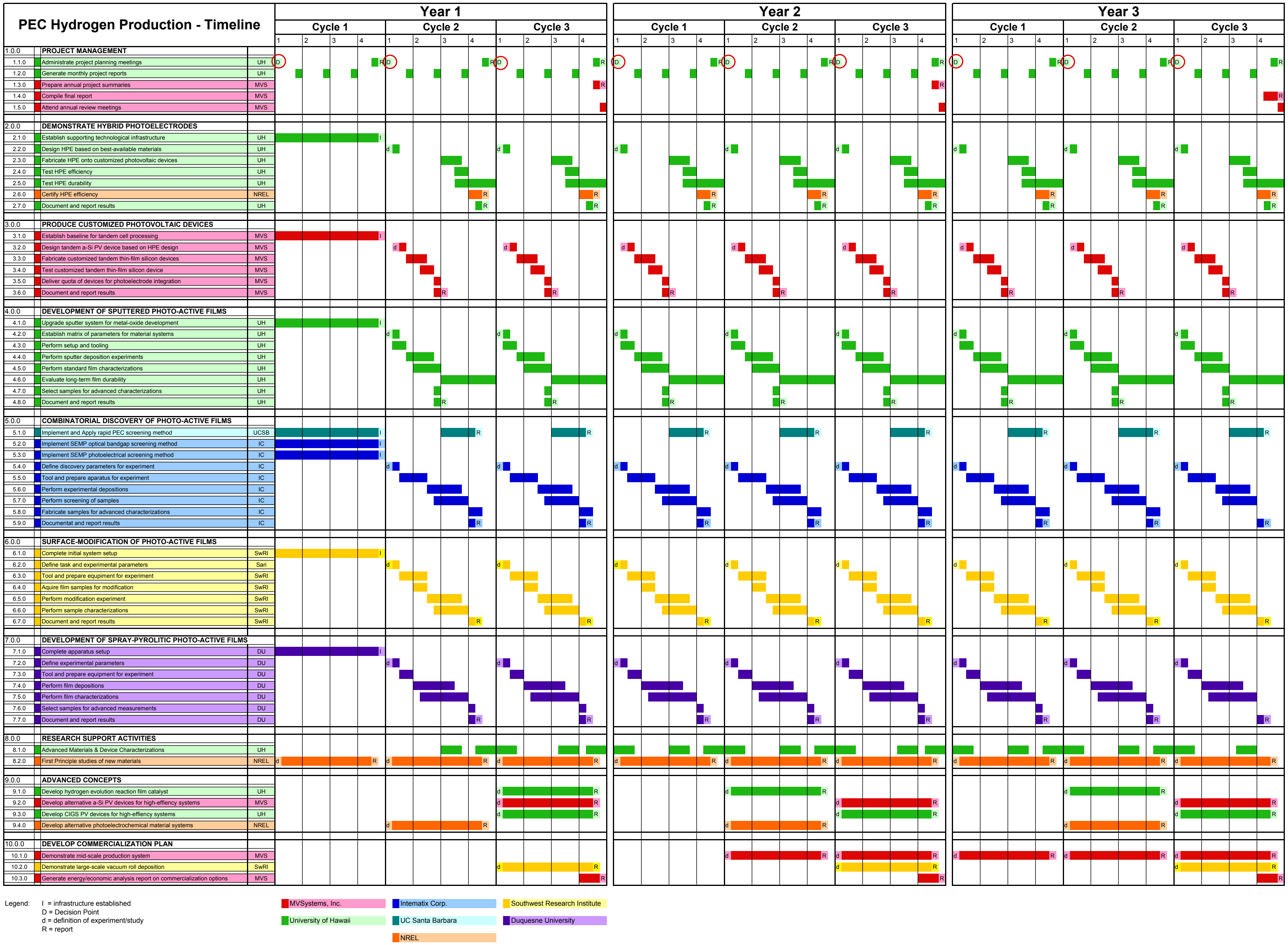
Anticipated Progress *(no funding to date):*

1. Milestone Plan

	Year 1	Year 2	Year 3
HPE Demonstration: ***Efficiency, lifetime targets***	2-4% STH 200hr	5-7% STH 500hr	7.5% STH 1000hr
Materials R&D: ***(PEC material) Photocurrent, Lifetime targets***	1.7 -3.3 mA/cm^2, 200hr	4.1-5.7 mA/cm^2, 500hr	6.1 mA/cm^2, 1000hr
Commercialization:	Energy/Economics analysis report	Reel-to-reel cass. deposition of PEC materials/devices	Vacuum roll deposition of PEC materials

Anticipated Progress *(no funding to date):*

2. Proposed Task Integration Chart



Anticipated Progress *(no funding to date):*

3. Photoactive Materials R&D Target

Performance of 6.1 mA/cm^2 with 1000hr durability- achieved through:

1. **Combinatorial Discovery of PEC Materials (barrier AP):**
   - Adaptation of combinatorial ion beam sputtering to metal oxide films
   - Development of high-throughput bandgap screening technique
   - Development of high-throughput PEC screening technique
   - Fabrication & screening of 1000s of metal oxide compounds

2. **Advanced Analysis and High-Performance Materials (barrier AP,AQ):**
   - Analysis of high-performance (high-temp. process) samples
   - PEC analysis (IPCE, Mott Schottky..)
   - Surface analysis (XRD, SEM, AFM)
   - Identification of suitable hosts and dopants by first-principles calculations

3. **Film Modifications for efficiency and durability (barrier AP,AQ):**
   - Ion beam texturing: effect on surface area, overpotentials/film stress
   - Ion implantation: controlled doping of PEC material

4. **HPE-Compatible Process Development (barrier AP,AQ, AS):**
   - Low-temperature sputter deposition of most promising compounds

Anticipated Progress *(no funding to date):*
4. HPE Performance Target

Performance of 7.5% STH with 1000hr durability- achieved through:

1. Development of improved Hybrid Photoelectrodes (barrier AS):
- Optimized HPE Design for best available PEC materials
- HPE fabrication/device completion
- Identification of failure modes/ durability issues

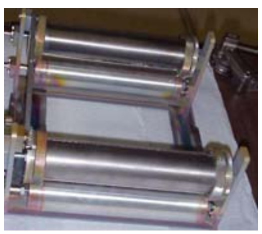
2. Production of customized photovoltaic devices for HPE (barrier AS):
- Design of current-matched a-Si-based tandem devices
- Fabrication of tandem devices with appropriate bottom- and top- layers

Anticipated Progress *(no funding to date):*

5. Commercialization Targets

MVSystems

1. **Completion of Energy/Economic Analysis (barrier AT):**
   - Assessment of feasibility of large-scale implementation of HPE technology



2. **Demonstration of Intermediate Scale Fabrication of HPE Devices (barrier AR):**
   - Device fabrication using reel-to-reel cassettes* in a cluster tool environment

*MV**Systems** patented approach for reel to reel cassette (US patent #6,258,408B1)

Southwest Research Institute

3. **Demonstration of Large Scale Fabrication of HPE Devices (barrier AR):**
   - Material fabrication using commerical-scale vacuum roll deposition system

Future Work

Necessary work for DOE 2010 goals:

- Material development to reach 8 mA/cm^2 (requires E_G<2.3 eV for top-junction)
- Device optimization (bottom junctions) to reach 10% STH
- Plant design and construction, goal 8% STH, 1000 hrs min. lifetime

Necessary work for DOE 2015 goals:

- Material development to reach 10 mA/cm^2 (requires E_G<2.0 eV for top-junction)
- Device optimization (bottom junctions) to reach 12% STH
- Plant design and construction, goal 10% STH, 5000 hrs min. lifetime

Publications and Presentations

None - no funding yet.

Reviewers Comments

This project is new, and was not reviewed in 04.

The May 04 review included comments regarding PEC research in general:

"Sufficient funding in this area for long term development is lacking, however some progress was made since last year. A concern of reviewers is that this area represents a "splintered" collection of smaller projects, and that a dedicated, multi-disciplinary program that is well organized and integrated should be put in place"

Response: ***These comments are well founded and fairly accurate. The collaborative work initiated in this project represents a significant first step toward a well-organized and dedicated multi-disciplinary program to advance the development of commercial PEC hydrogen production systems.***

Hydrogen Safety

<u>The most significant hydrogen hazard associated with this project is:</u>

Accumulation of small amounts of hydrogen during long-term testing of prototype devices.*

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at 7.5% STH efficiency under 1-sun, a 4 cm^2 lab-scale device produces less than 1 milligram of H_2 per hour.

Hydrogen Safety

Our approach to deal with this hazard is as follows:

- **Utilize extensive hydrogen safety plans developed by HNEI for the "Hawaii Fuel Cell Test Facility". Elements include:**
  - Complete database of relevant codes and standards
  - Failure modes and effects analysis (FMEA)
  - Review by industrial partner of FMEA and safety compliance
  - Generation of in-house safety manuals

- **For this project, MVSystems will implement the appropriate safety plans to accommodate the small quantities of hydrogen produced in the lab-scale PEC experiments*, including:**
  - Specification of adequate ventilation of the laboratory space
  - Training of personnel in H_2 handling procedures & emergency protocols

at 7.5% STH efficiency under 1-sun, a 4 cm^2 lab-scale device produces less than 1 milligram of H_2 per hour.