

# Photoelectrochemical Hydrogen Production

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PDP37

# Overview

## Timeline

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

## 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

## Barriers

- AP. Materials Efficiency
- AQ. Materials Durability
- AR. Bulk Materials Synthesis
- AS. Device Configuration Design
- AT. Systems Design and Evaluation

## 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**

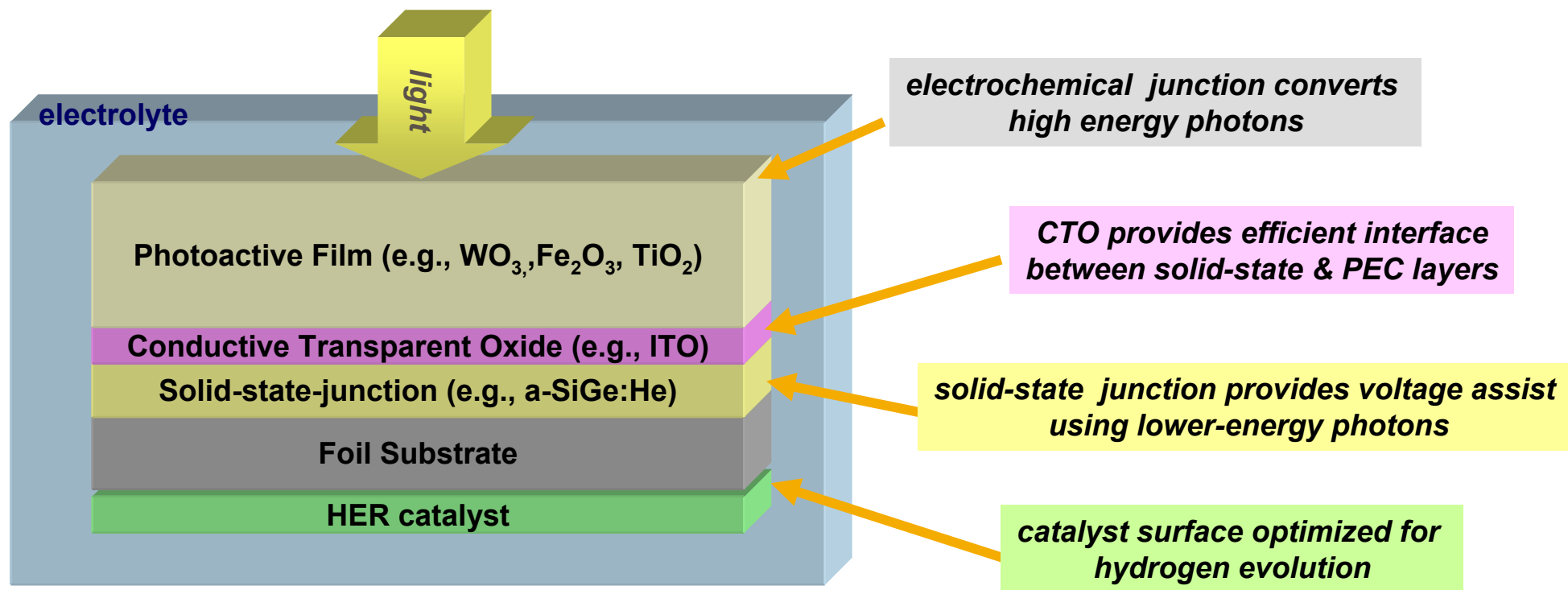
- Development of low-cost photoactive materials with 1-sun photocurrents greater than 6 mA/cm<sup>2</sup> and with sufficient durability to meet the lifetime requirement
- Development of supporting solid-state devices with sufficient current and voltage output
- Development of necessary process integration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

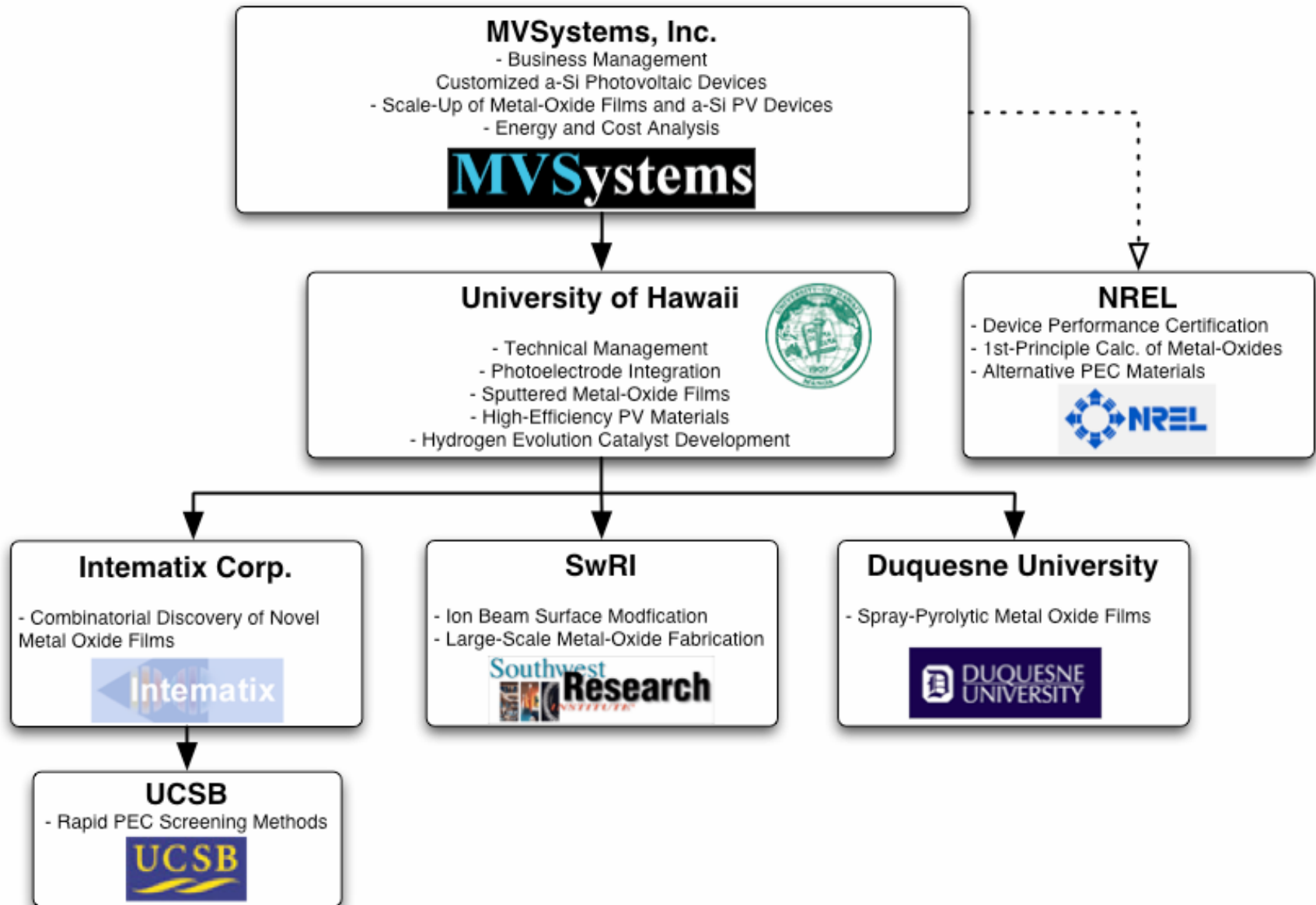
# Approach:

## 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 ( $\text{WO}_3$ ) on vacuum roll system
  - Economic/energy analysis of HPE technology based on current state and projections

# Approach:

## 3. Division of Tasks



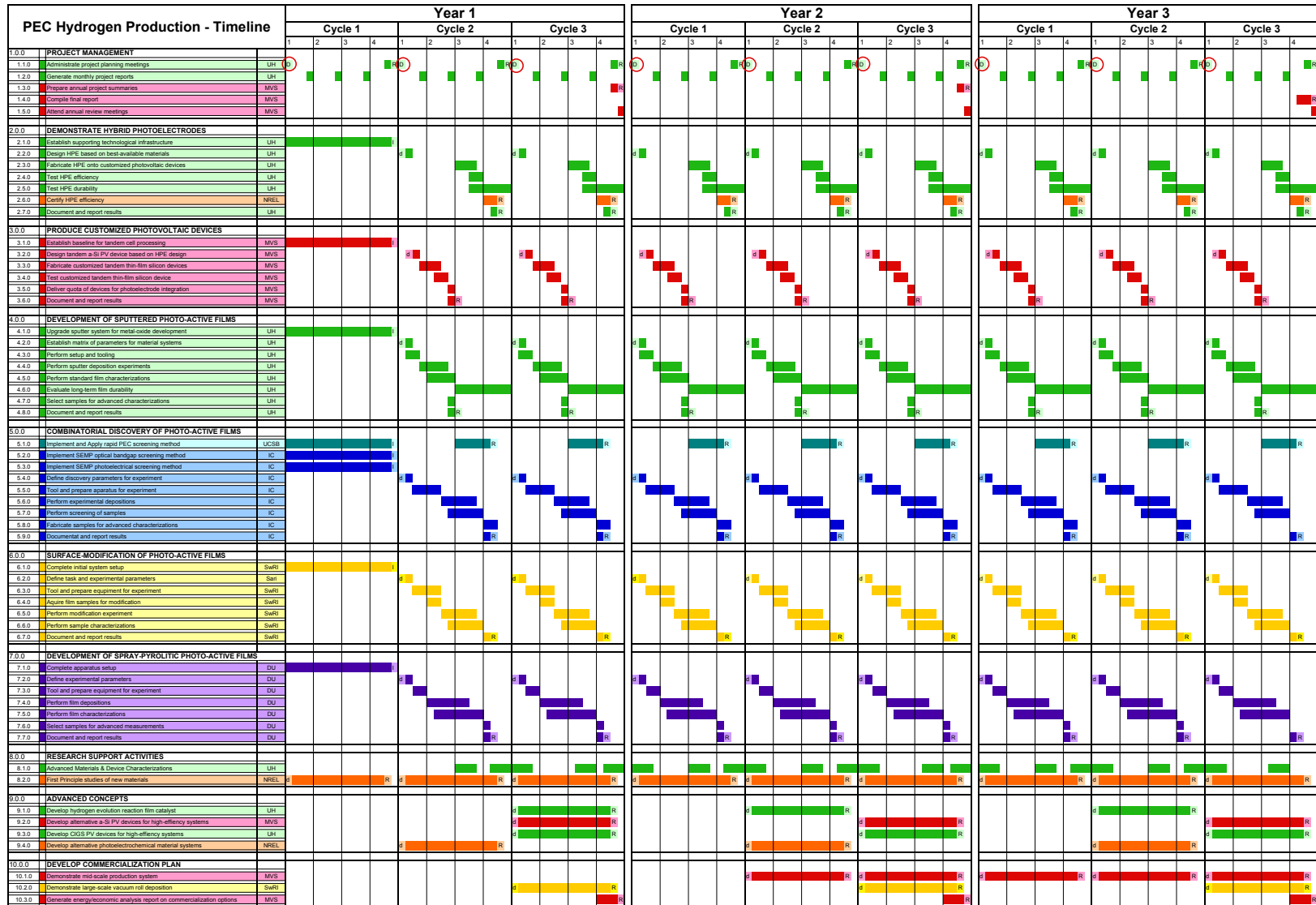
# Anticipated Progress (*no funding to date*):

## 1. Milestone Plan

	Year 1	Year 2	Year 3
<u>HPE Demonstration:</u> <i>Efficiency, lifetime targets</i>	2-4% STH 200hr	5-7% STH 500hr	7.5% STH 1000hr
<u>Materials R&amp;D:</u> <i>(PEC material) Photocurrent, Lifetime targets</i>	1.7 -3.3 mA/cm <sup>2</sup> , 200hr	4.1-5.7 mA/cm <sup>2</sup> , 500hr	6.1 mA/cm <sup>2</sup> , 1000hr
<u>Commercialization:</u>	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



Legend: I = Infrastructure established  
 D = Decision Point  
 d = definition of experiment/study  
 R = report

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 University of Hawaii UC Santa Barbara Duquesne University  
 NREL



# Anticipated Progress (*no funding to date*):

## 3. Photoactive Materials R&D Target

Performance of 6.1 mA/cm<sup>2</sup> 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

\*MVSystems 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 commercial-scale vacuum roll deposition system

# Future Work

## **Necessary work for DOE 2010 goals:**

- Material development to reach 8 mA/cm<sup>2</sup> (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<sup>2</sup> (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

**The most significant hydrogen hazard associated with this project is:**

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

*\*at 7.5% STH efficiency under 1-sun, a 4 cm<sup>2</sup> lab-scale device produces less than 1 milligram of H<sub>2</sub> 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<sub>2</sub> handling procedures & emergency protocols

*\*at 7.5% STH efficiency under 1-sun, a 4 cm<sup>2</sup> lab-scale device produces less than 1 milligram of H<sub>2</sub> per hour.*