Solar hydrogen production by photoelectrochemical (PEC) water-splitting: Advancing technology through the synergistic activities of the PEC working group (PEC WG)

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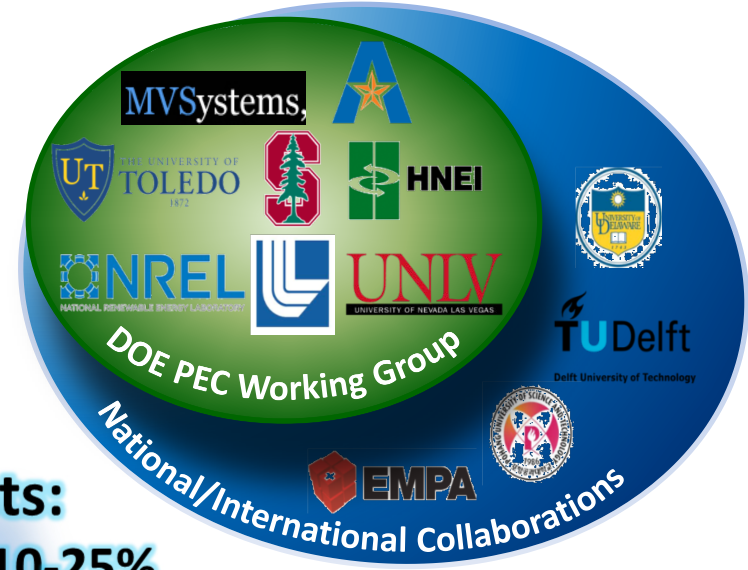
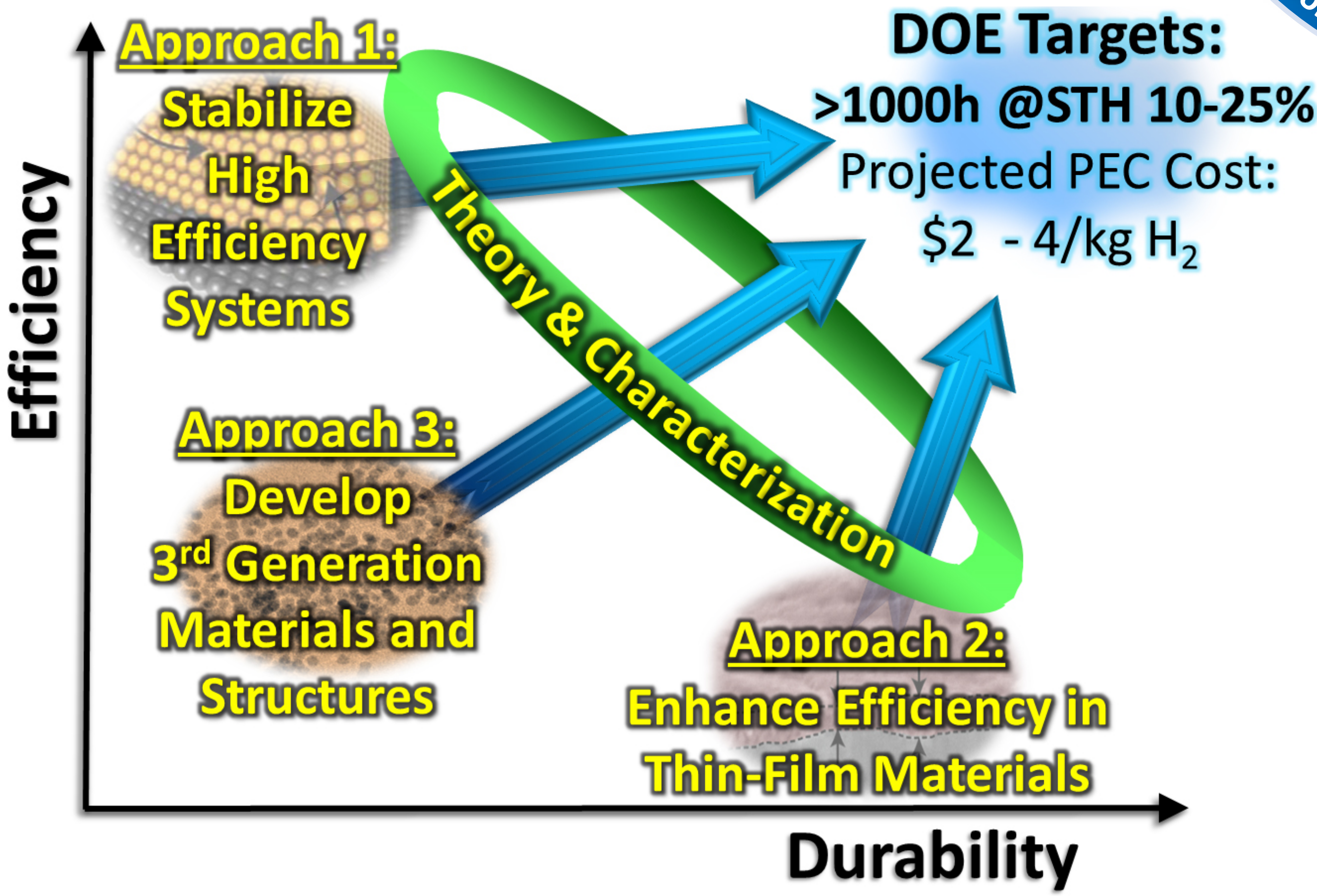
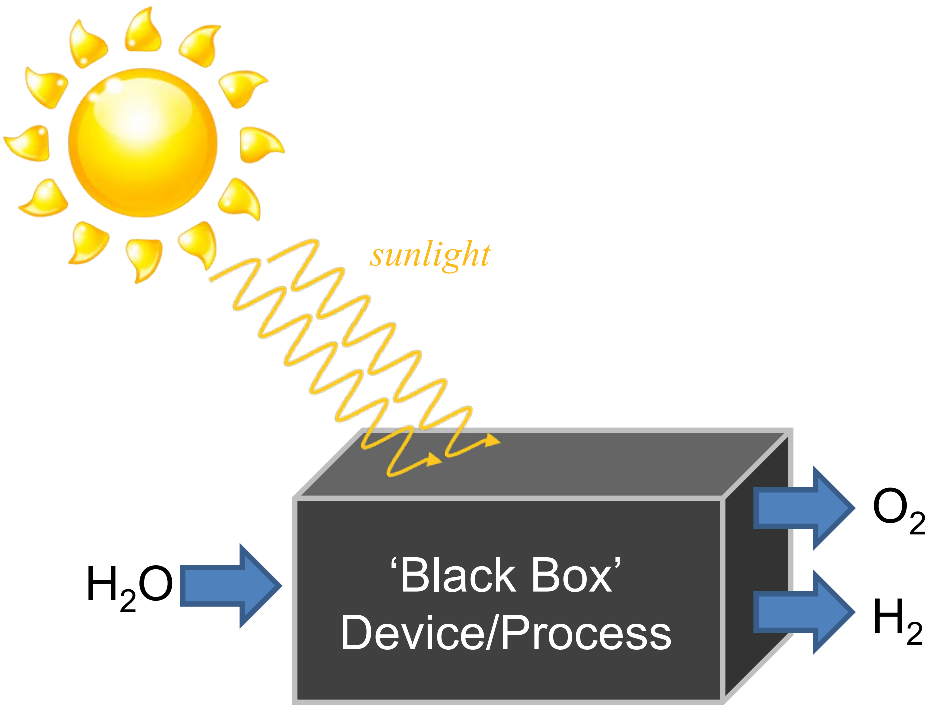
Project ID: PD033

The US DOE PEC Working Group approach towards efficient and durable solar H_2 production



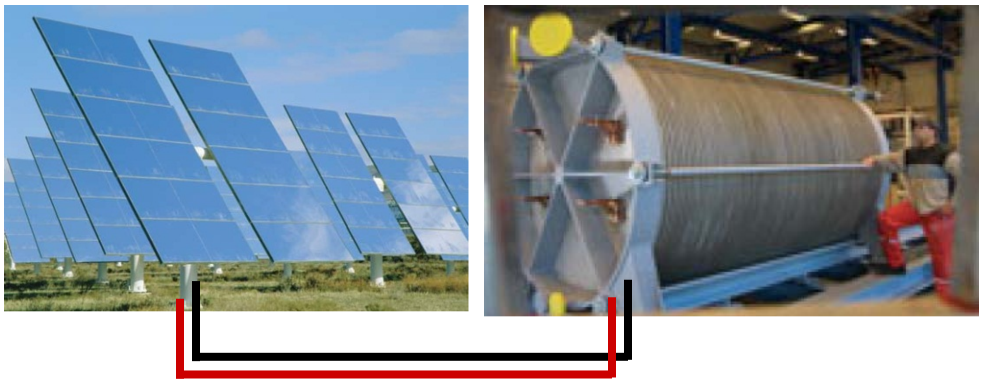


Storing solar energy in the form of chemical bonds

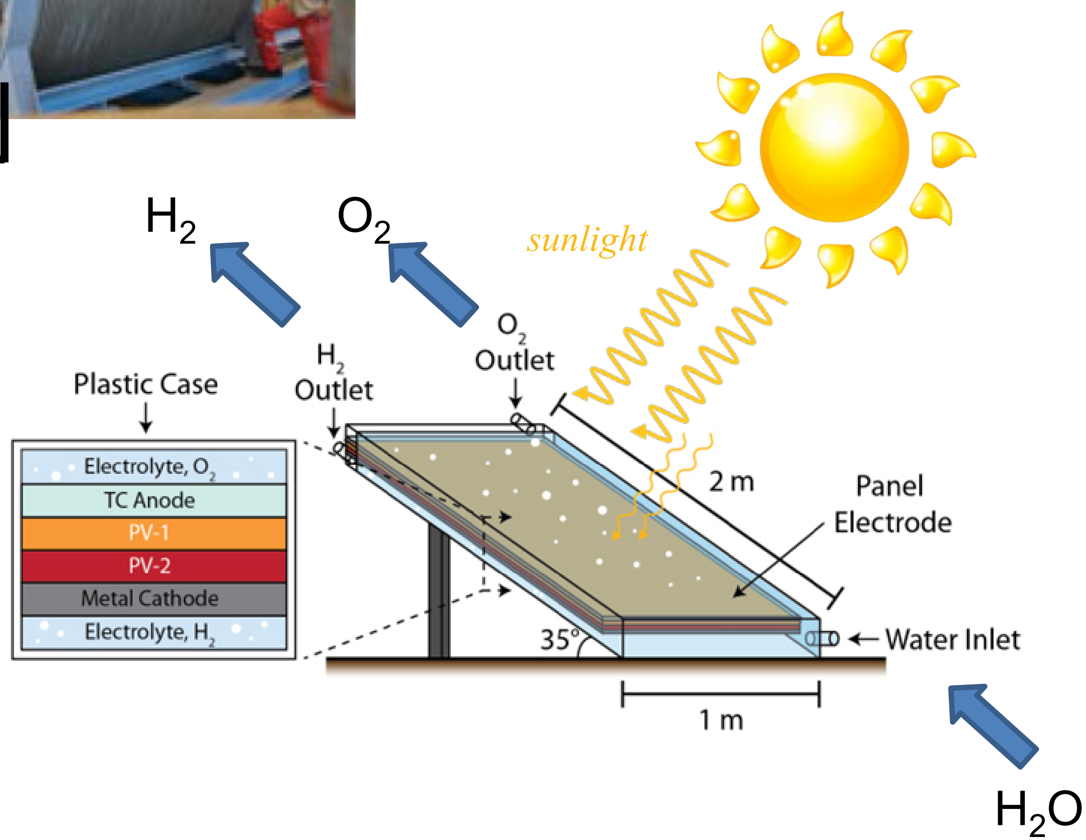


(Photo-)electrochemical schemes

Scheme 1: Separate devices for electricity generation and for H_2 production.



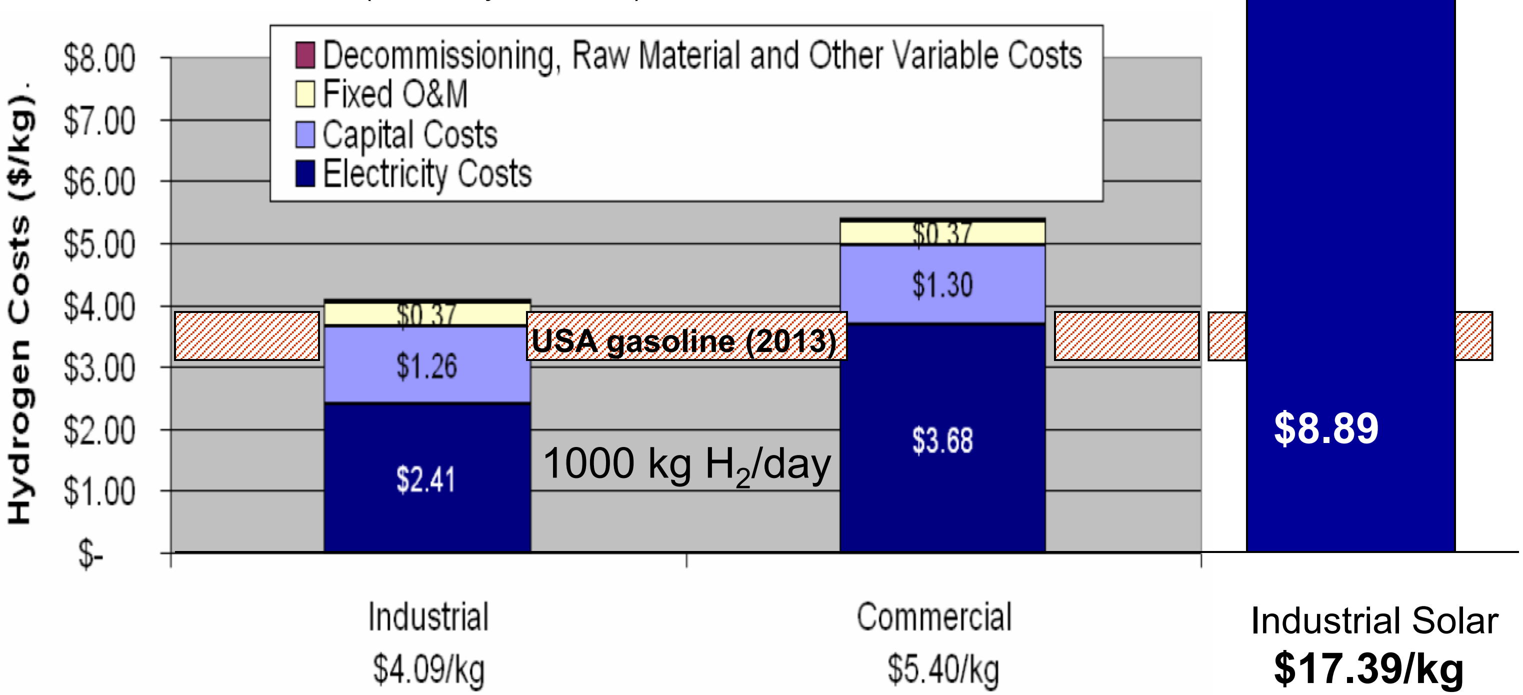
Scheme 2: One integrated device for solar harvesting and H_2 production.



Techno-Economics: PV-electrolysis

• "Electrolysis: Information and Opportunities for Electric Power Utilities"
DOE-NREL Technical Report, NREL/TP-581-40605
September 2006

• www.solarbuzz.com (February 20, 2012)



$0.045/kWh

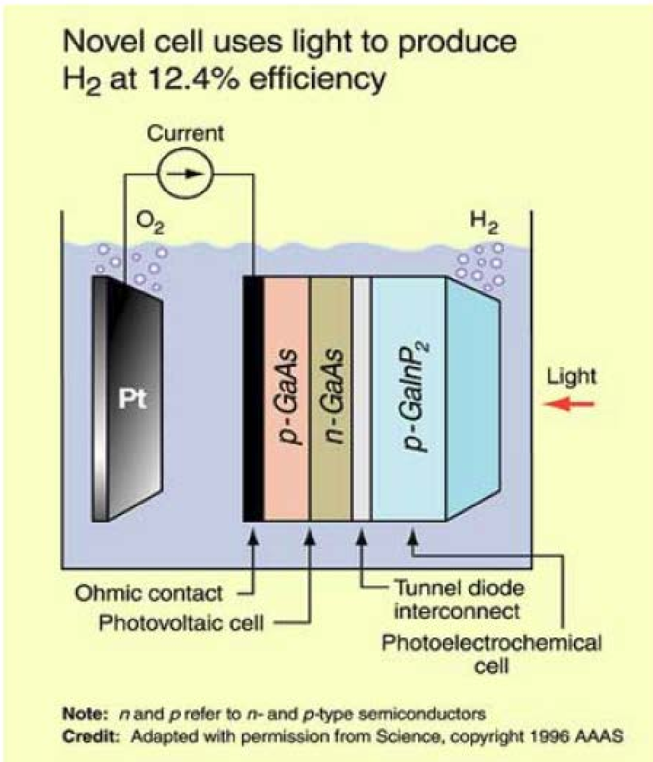
$0.069/kWh in 2005

$0.166/kWh (2012)
500 kW system
sunny climate

A world record PEC device

NREL
National Renewable Energy Laboratory

World Record Photoelectrolysis Device Science, April 17 1998.



- Direct water electrolysis.
- Unique tandem (PV/PEC) design.
- 12.4% Solar-to-hydrogen

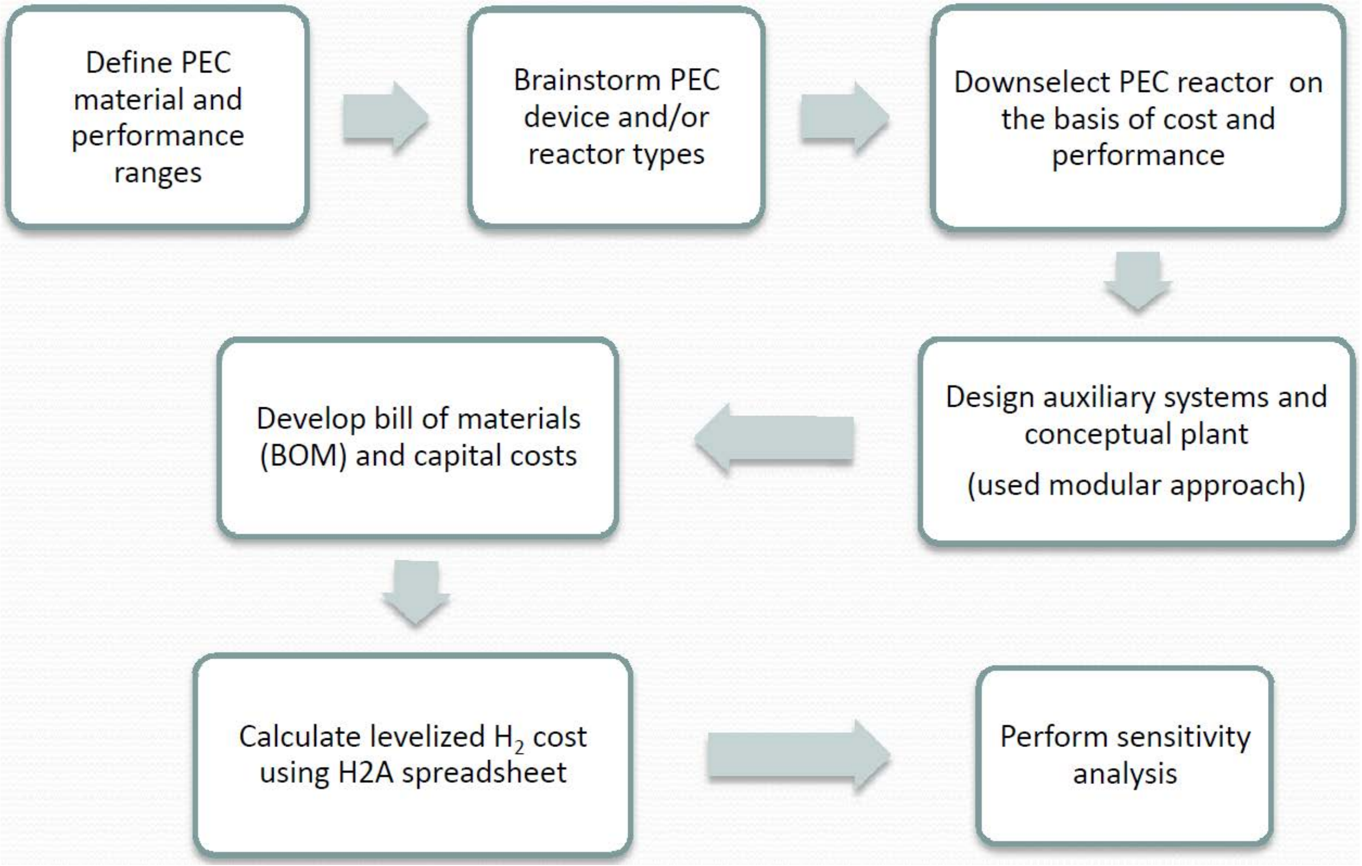
Experimental Cell

Operated for the U.S. Department of Energy by Midwest Research Institute • Battelle • Bechtel

The big question

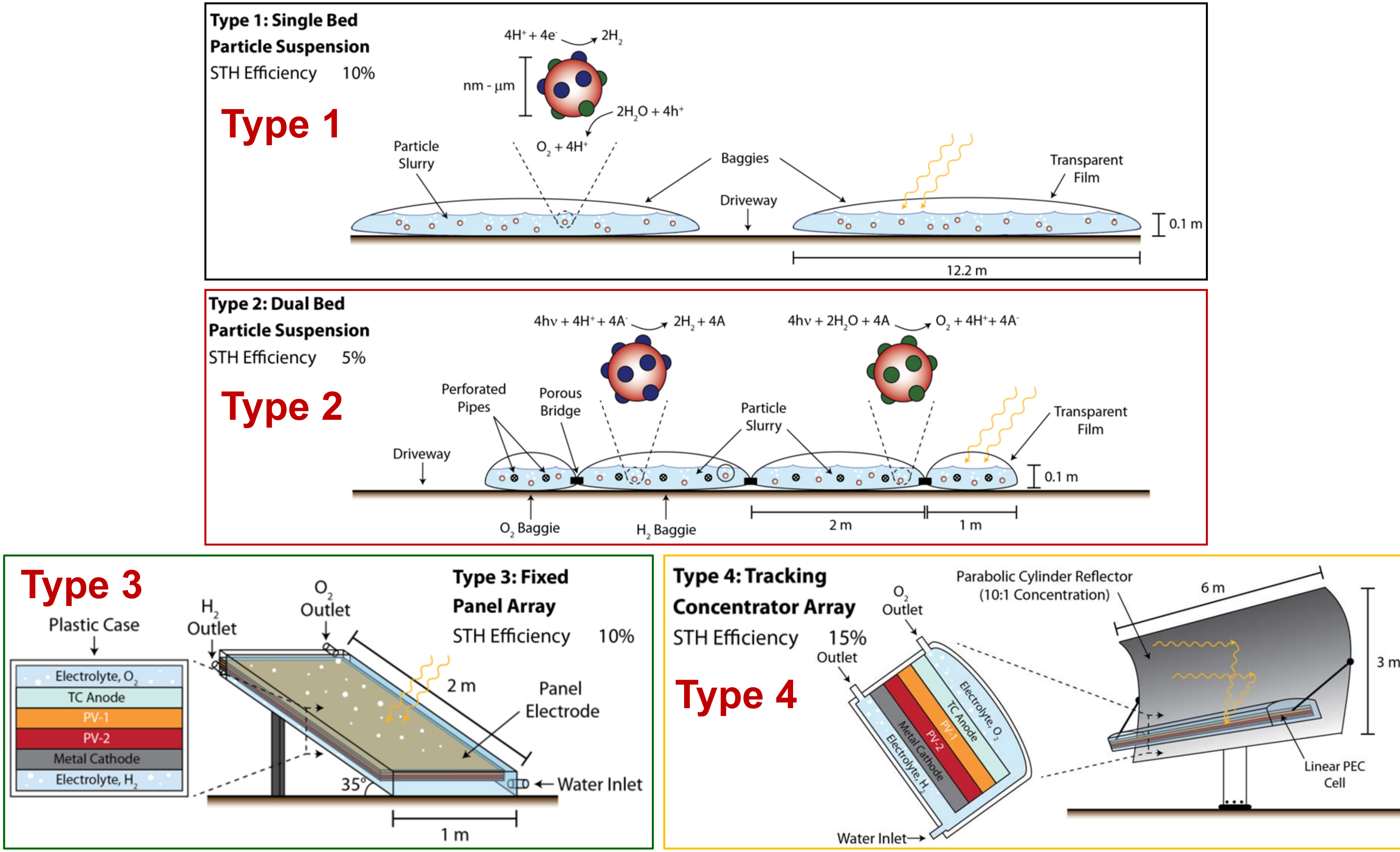
Q: Can H_2 production by solar PEC water-splitting ever be cost-effective?

To answer this question, we need a techno-economic analysis!



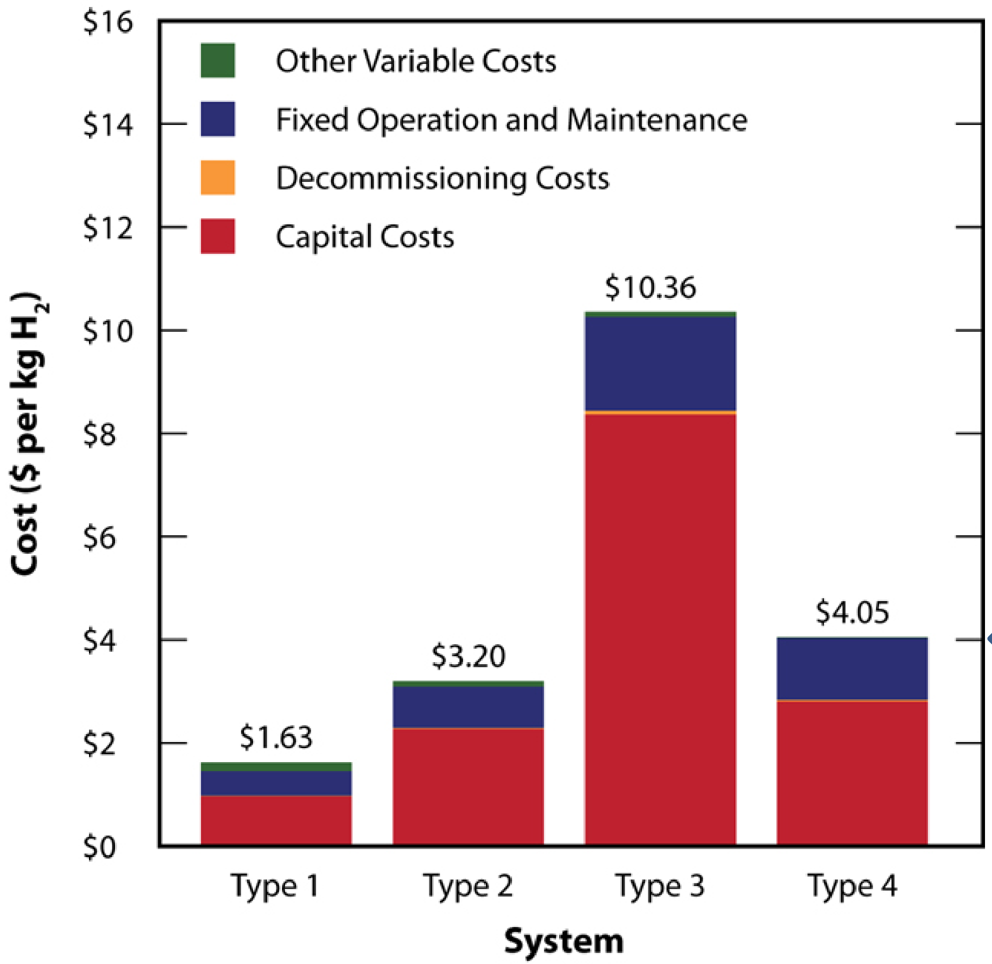
B.D. James, G.N. Baum, J. Perez, K.N. Baum, "Technoeconomic Analysis of Photoelectrochemical (PEC) Hydrogen Production", DOE Report (2009) Contract # GS-10F-009J.

Four reactor types



Which system is the most cost-effective?

Recall that 1 kg of H_2 is the energy equivalent of 1 gallon of gasoline.

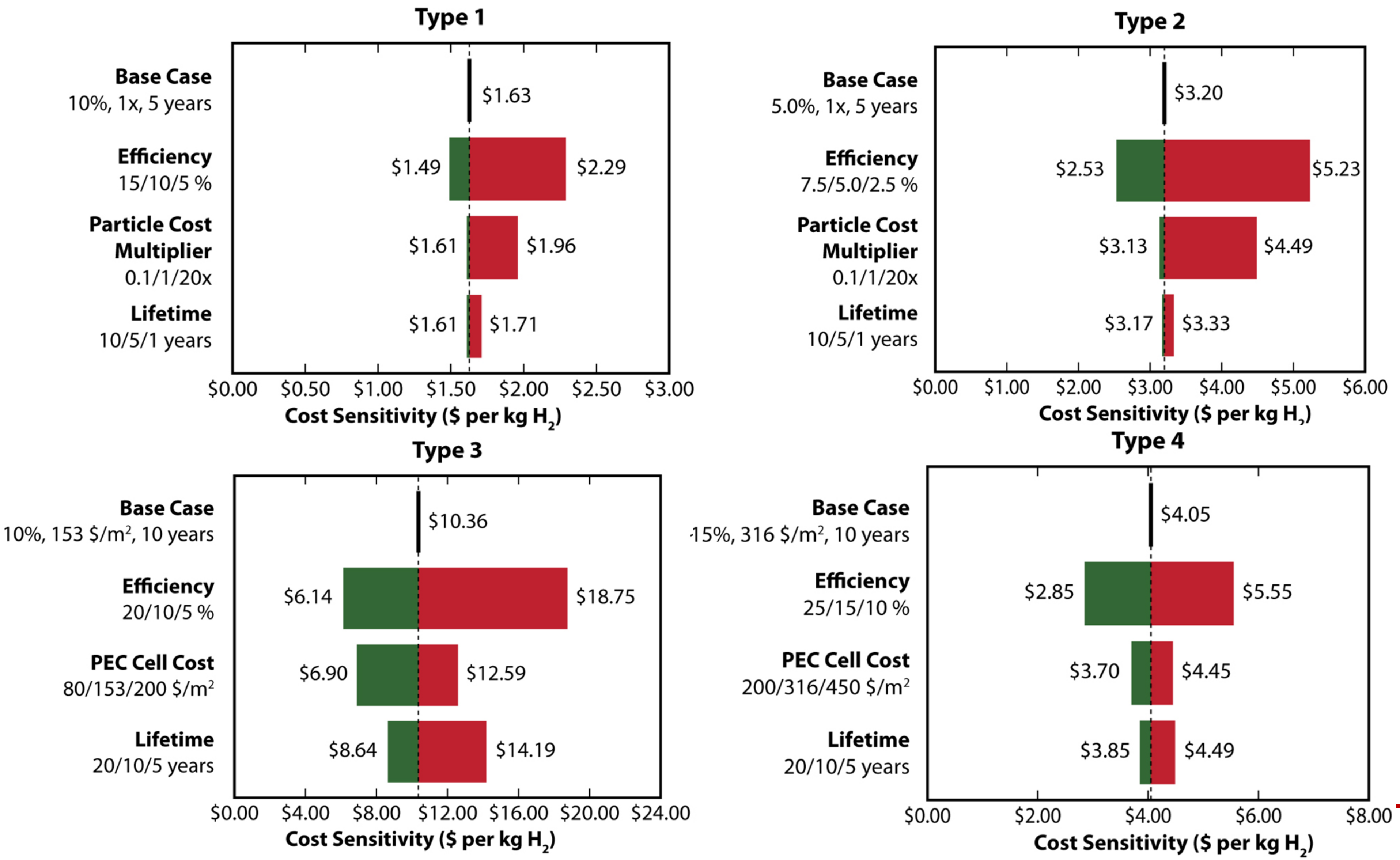


Price of 1 gallon of gasoline in the USA (2013)

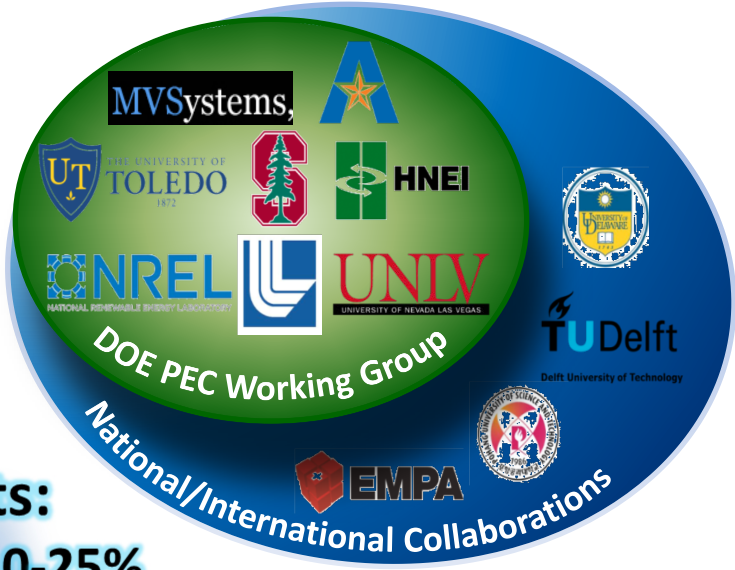
B.A. Pinaud, J.D. Benck, L.C. Seitz, A.J. Forman, Z. Chen, T.G. Deutsch, B.D. James, K.N. Baum, G.N. Baum, S. Ardo, H. Wang, E. Miller and T.F. Jaramillo (submitted, 2013).

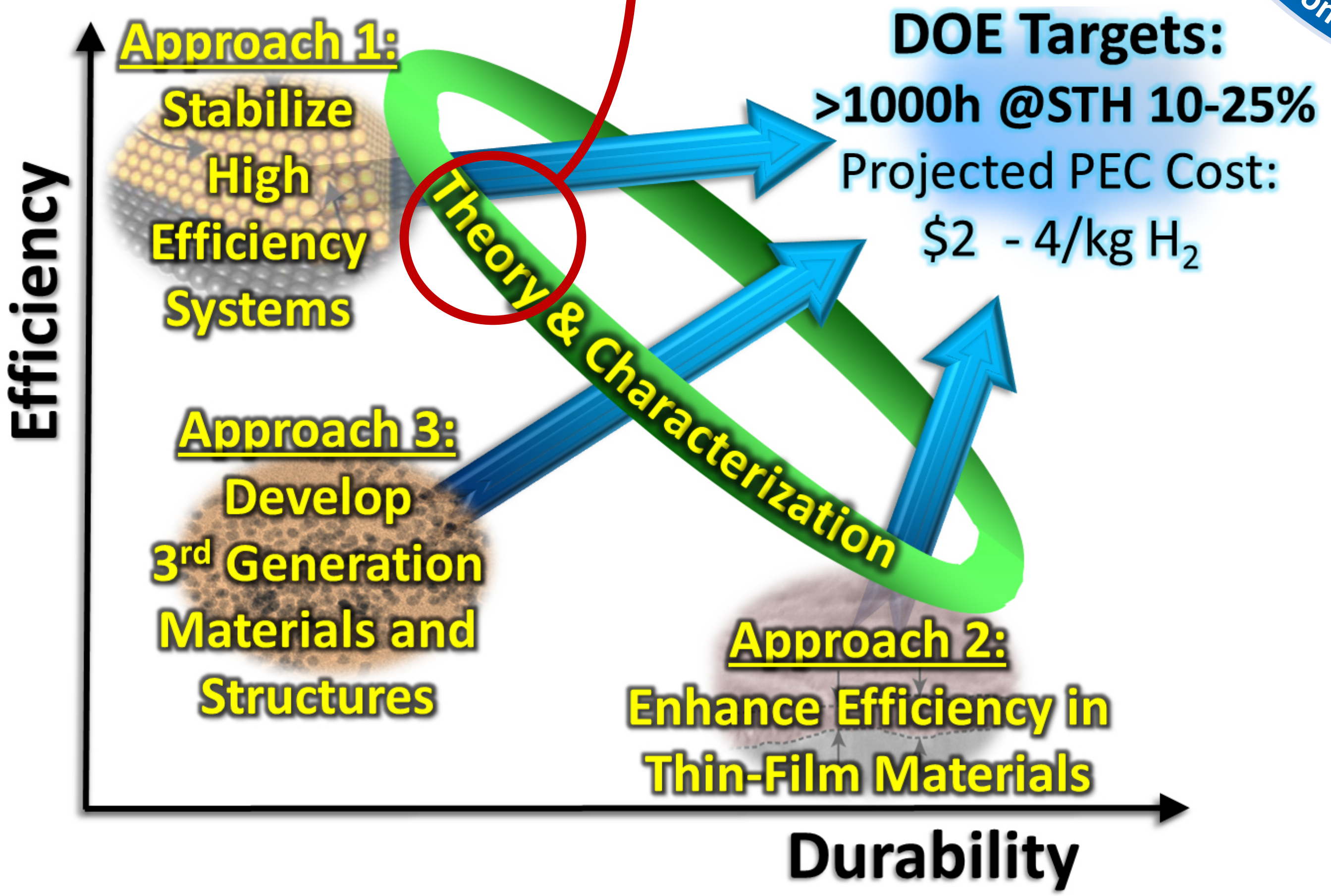
Sensitivity Analysis

How does the $/kg H_2 change if we modify our assumptions on material performance?



Just how feasible are the efficiency assumptions in the techno-economic analysis (STH 10-25 %)?





Modeling 'Realistic' PEC efficiencies

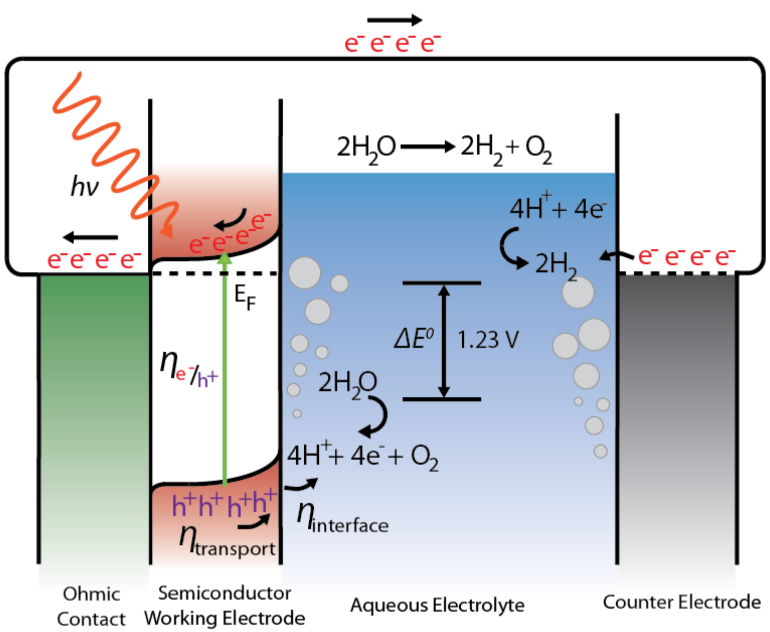
Device Options

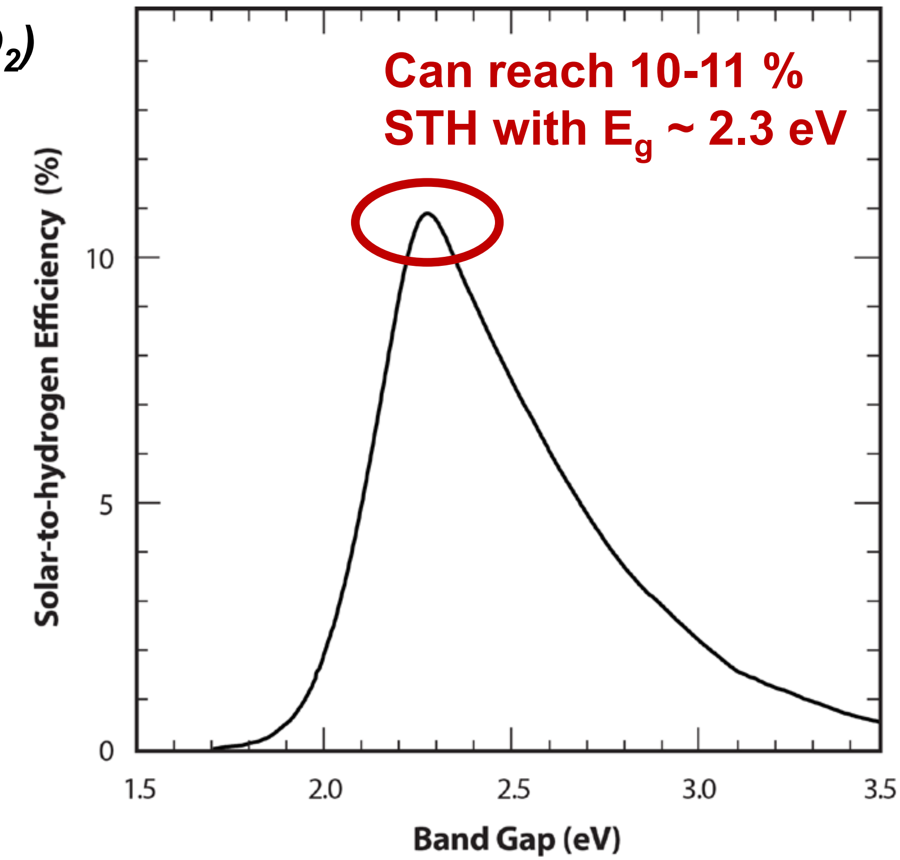
- **Solid-state V_{oc}**
  - High V_{oc} (~470mV loss)
  - Low V_{oc} (~590mV loss)
- **Catalyst Activity**
  - Precious metal (Pt/Ru)
  - Non-precious metal (MoS_2/MnO_x)
- **Shunt**
  - Zero shunt losses ($R_{sh} = \infty\ \Omega$)
  - "Significant" shunt losses $R_{sh} = 100\ \Omega$
- **Absorber Configuration**
  - Single
  - Dual stacked
  - Dual side-by-side

Single-absorber devices

Calculated theoretical limits for a 'realistic' STH efficiency as a function of bandgap, taking into account:

- ***Reaction overpotentials (H_2 and O_2)***
- ***Entropic losses ($V_{ph} < E_g$)***
- ***Shunts***





Seitz L, Chen Z, Pinaud B, Benck J, Chakthranont P, Forman A, Jaramillo T.F. (*in preparation* 2012)

Single-absorber devices

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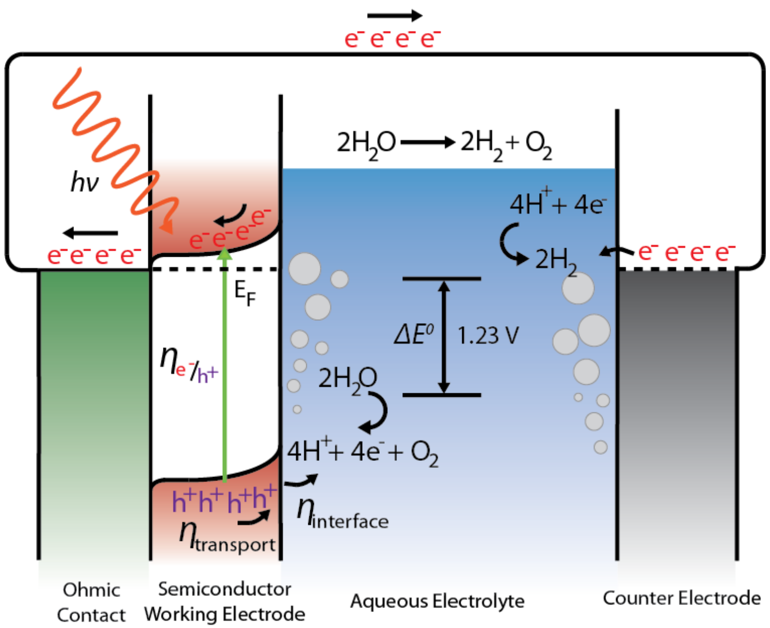
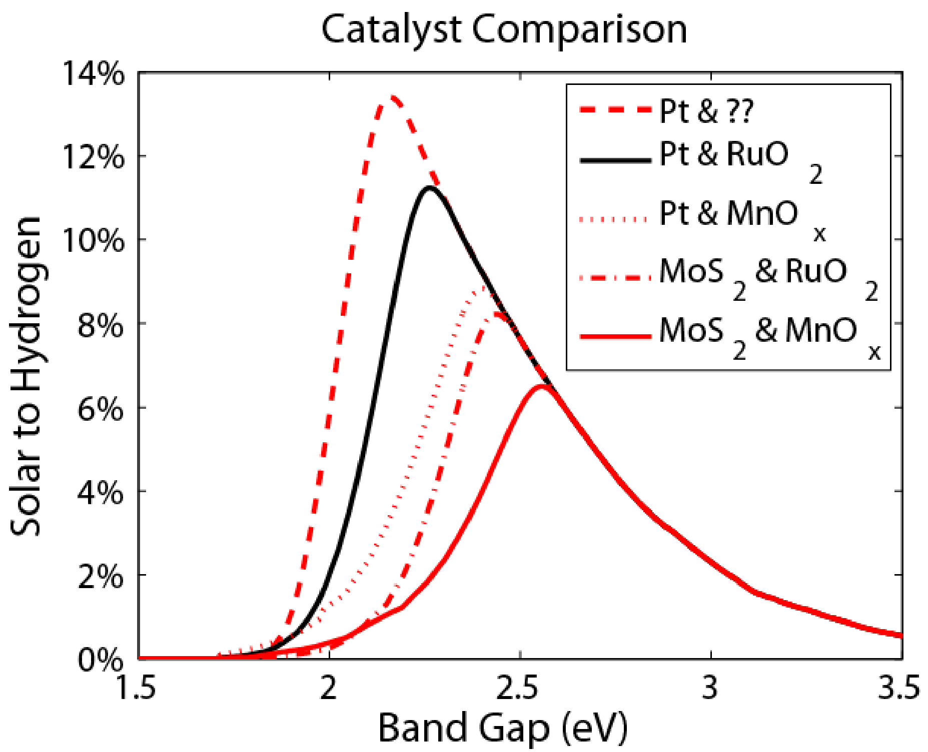
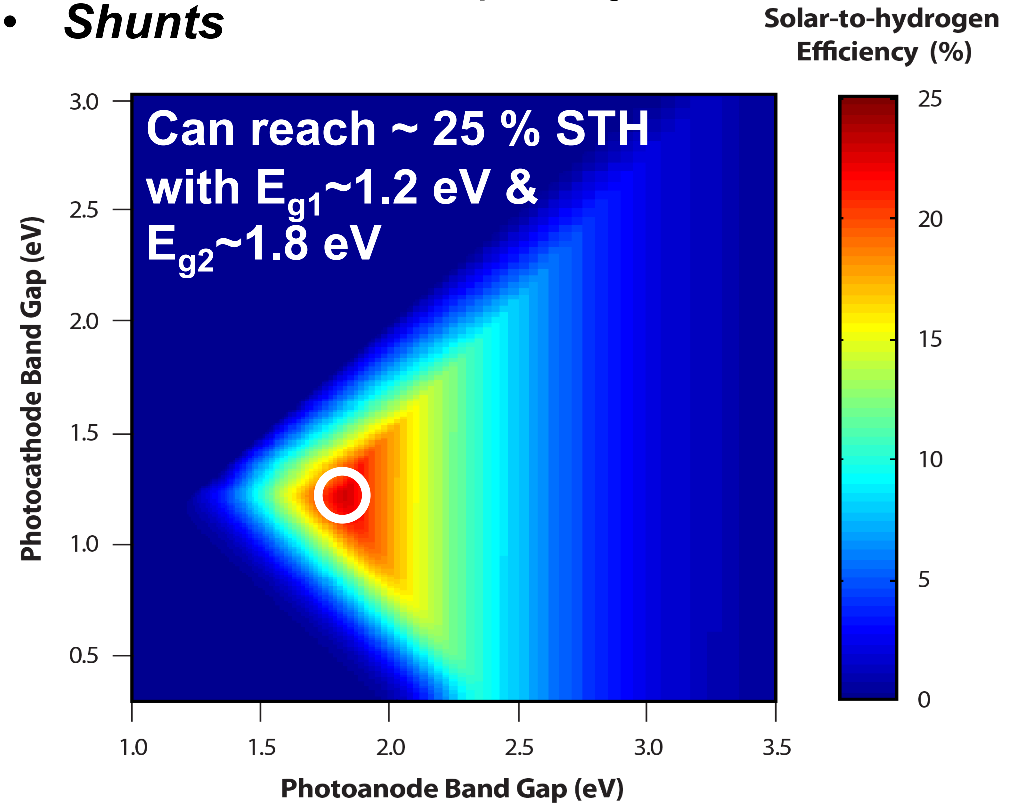


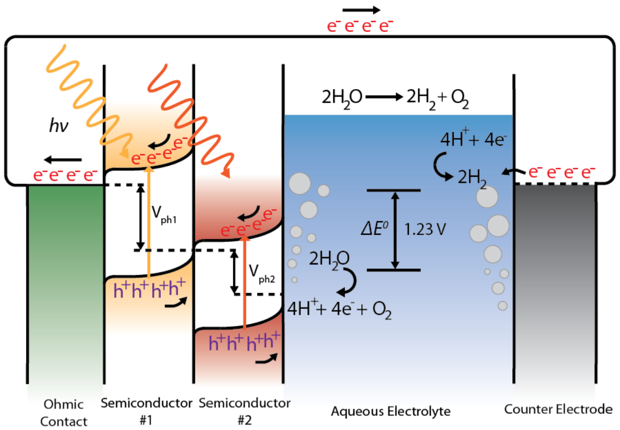


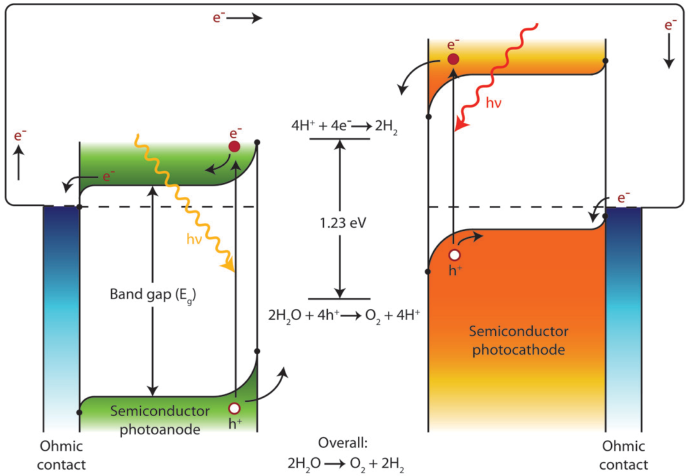
Multi-junction or Tandem Devices

Calculated theoretical limits for a 'realistic' STH efficiency as a function of bandgap, taking into account:

- ***Reaction overpotentials (H_2 and O_2)***
- ***Entropic losses ($V_{ph} < E_g$)***
- ***Shunts***





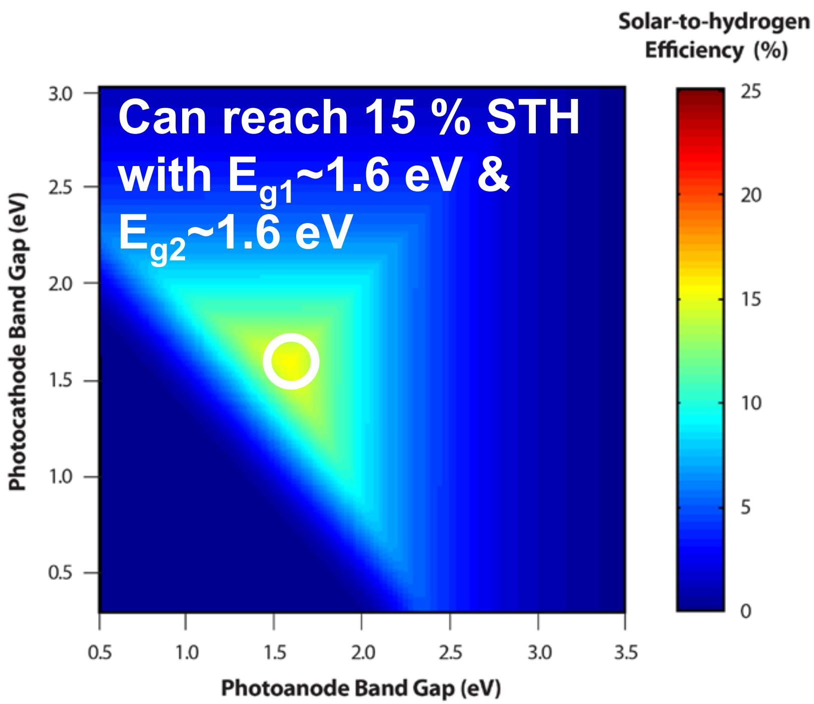


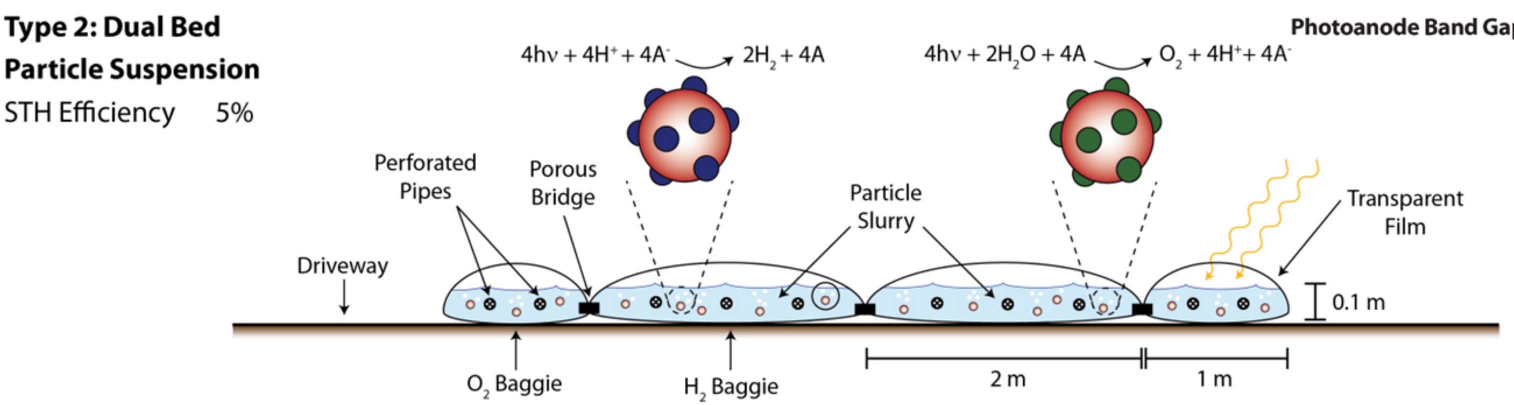
Seitz L, Chen Z, Pinaud B, Benck J, Chakthranont P, Forman A, Jaramillo T.F. (*in preparation* 2012)

Side-by-side Devices

Calculated theoretical limits for a 'realistic' STH efficiency as a function of bandgap, taking into account:

- ***Reaction overpotentials (H_2 and O_2)***
- ***Entropic losses (V_{ph} < E_g)***
- ***Shunts***



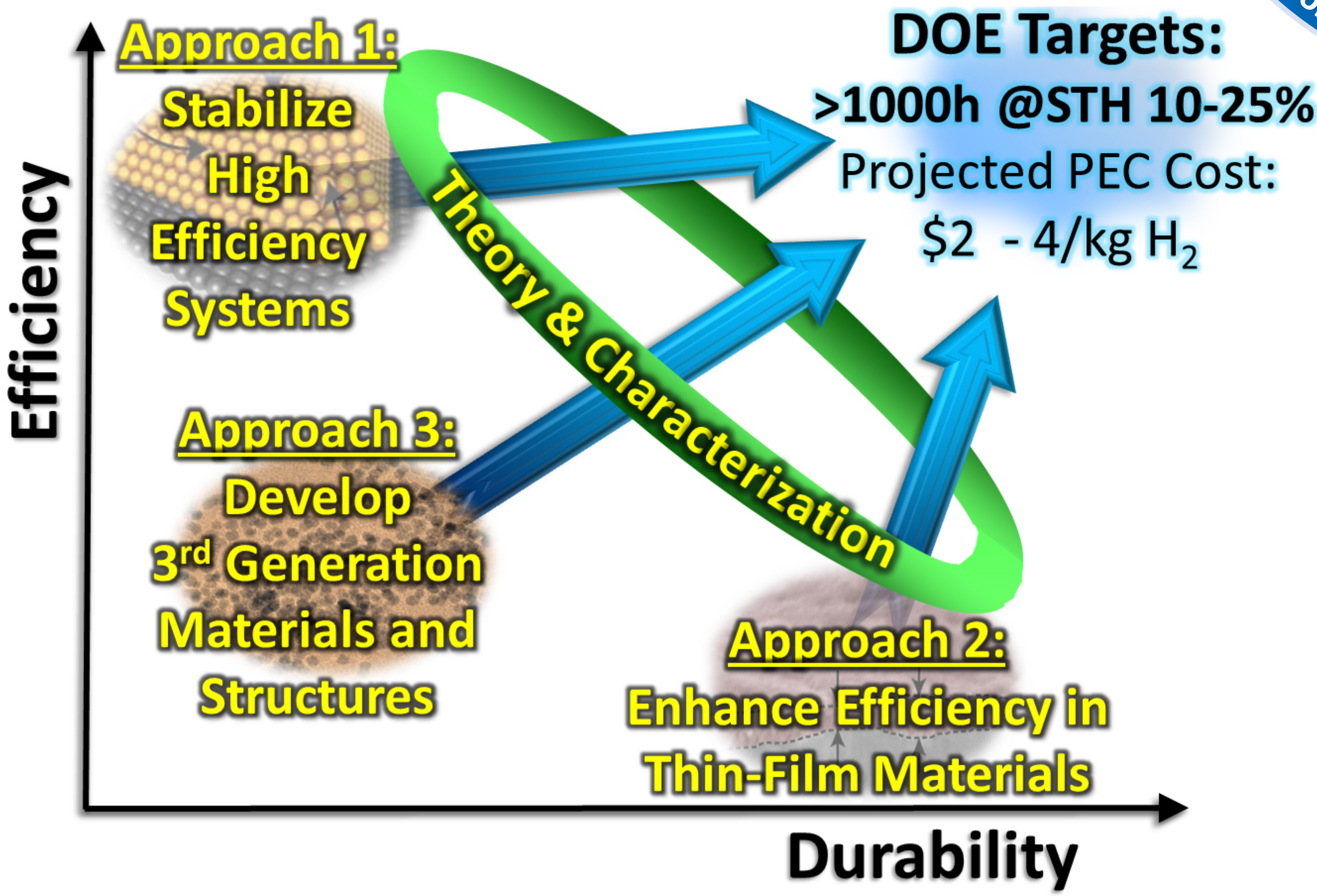


Seitz L, Chen Z, Pinaud B, Benck J, Chakthranont P, Forman A, Jaramillo T.F. (*in preparation* 2012)

The US DOE PEC Working Group approach towards efficient and durable solar H_2 production

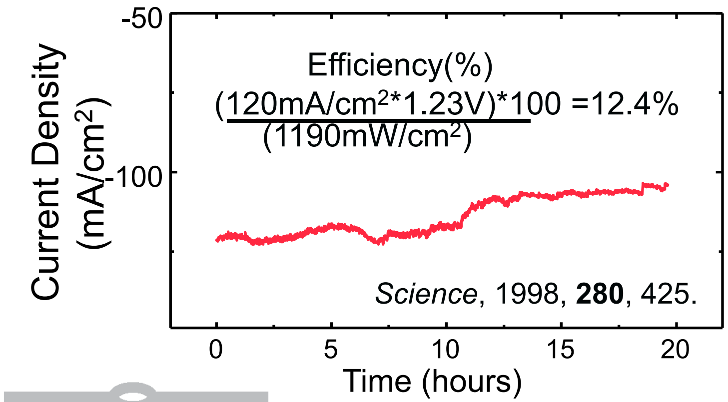
DOE PEC Working Group

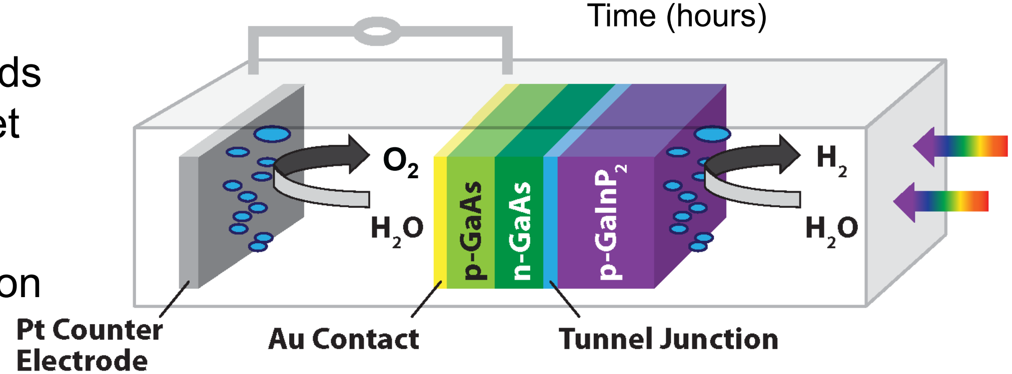
National/International Collaborations

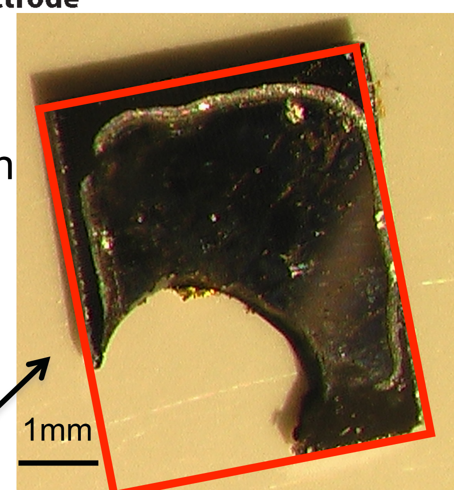


Approach #1 (NREL): Stabilizing High Efficiency Materials & Devices

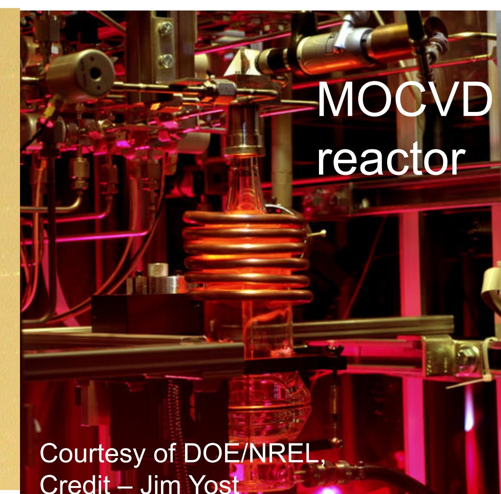
- High Efficiency
  - Work with single-crystal (high purity) semiconductors composed of Group IIIA an VA *p*-block elements (III-V)
  - Unrivaled photovoltaic efficiencies
- $GaInP_2$/GaAs Tandem
  - Only demonstrated system that exceeds unbiased 10% solar-to-hydrogen target
    - 12.4% with Pt-black counter electrode, >16% with RuO_2 CE
  - Metal organic chemical vapor deposition (MOCVD) synthesis
    - Synthesis by NREL's III-V team
- Focus: Improve Durability
  - High efficiency III-V's prone to degradation during PEC operation
  - Need enhanced corrosion resistance to meet both efficiency and durability targets







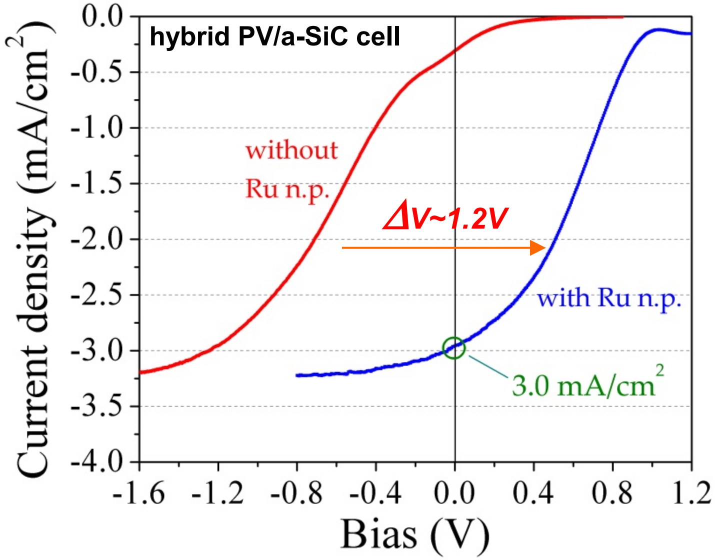
p-$GaInP_2$/GaAs tandem after 24 hours of operation in 3M H_2SO_4



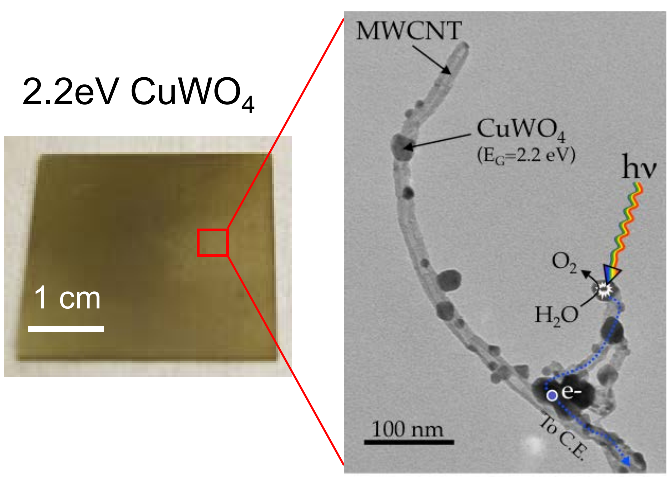
Approach #2 (MVSystems / HNEI): Improving thin-film efficiency

The MVS/HNEI research team is accelerating the development of three important thin-film material classes with high potential for reaching low-cost H_2 PEC production.

a-SiC: surface energetics management

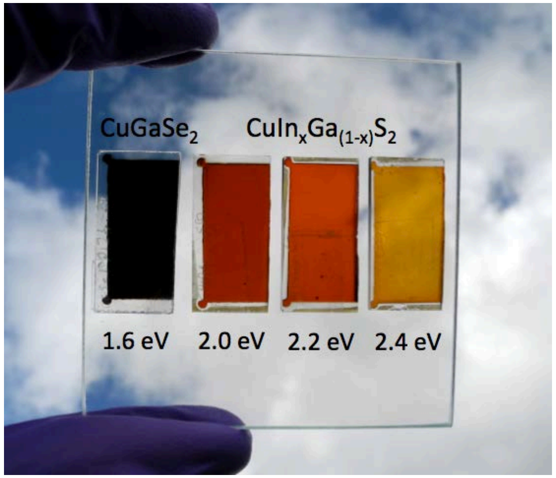


Development of new metal oxides

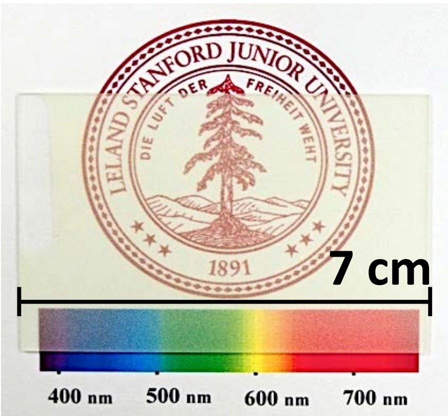


$CuWO_4$-CNT nanocomposite

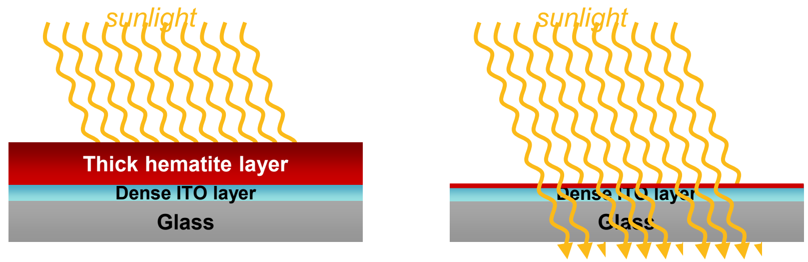
Chalcogenides bandgap engineering



Approach #3 (Stanford Univ.): 3rd Generation Device Structures, High Surface Area Scaffolds for PEC Materials



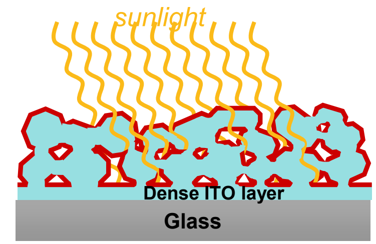
Conventional Planar Devices



Low IQE (long charge trans.)
High loading (high OD)
Low device performance

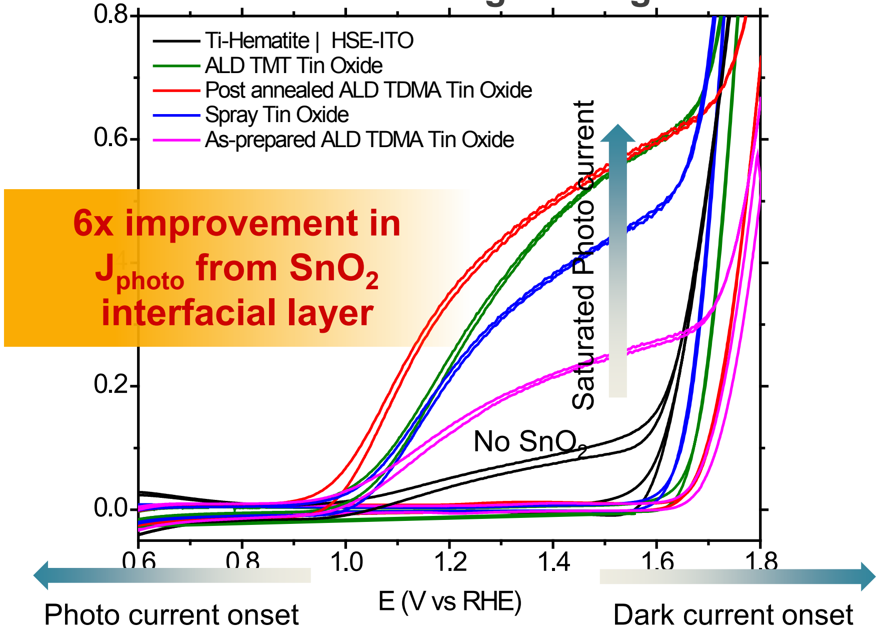
High IQE (short charge trans.)
Low loading (low OD)
Low device performance

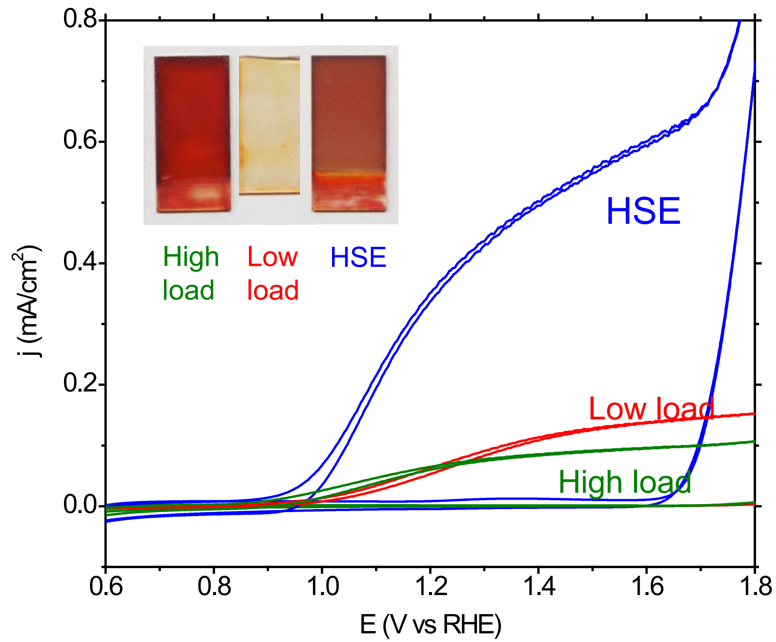
HSE Support



High IQE
High loading (high OD)
High device performance

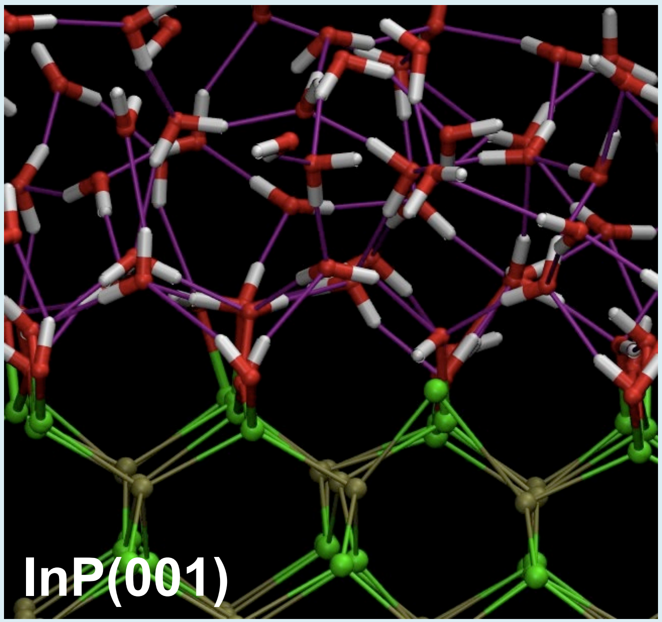
Interfacial Engineering



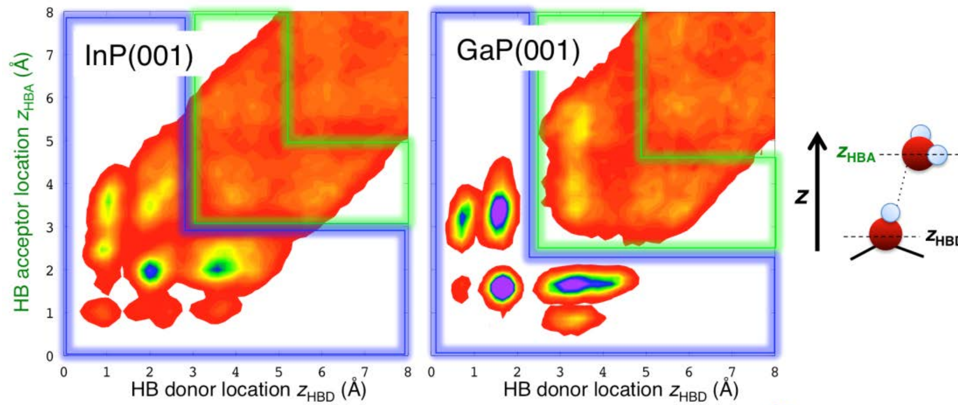


Theory at the molecular-scale (LLNL): Ab-initio molecular dynamics (MD) to investigate the electrode-electrolyte interface

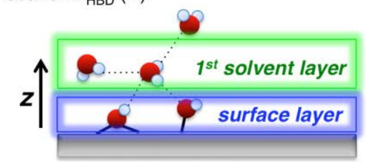
Ab-initio molecular dynamics simulations of water-InP and water-GaP interfaces



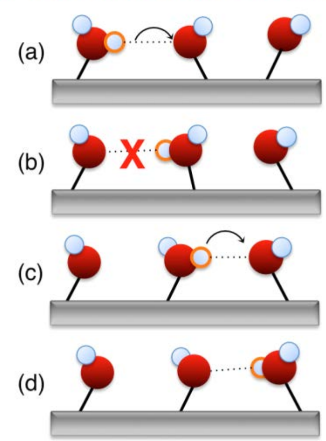
Experimental observation: Pt loading on GaP(001) improves the conversion efficiency *only a little* [ChemPhysChem 13, 3053 (2012)]



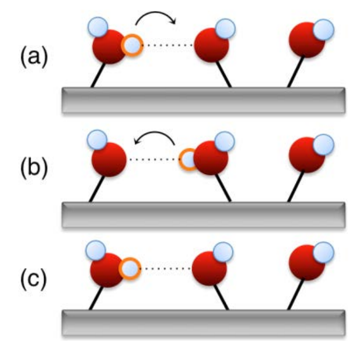
- InP HB network explores a broader phase space
- GaP HB network prohibits interchange between most topologies



InP-water interface: good h+ transport



GaP-water interface: bad h+ transport



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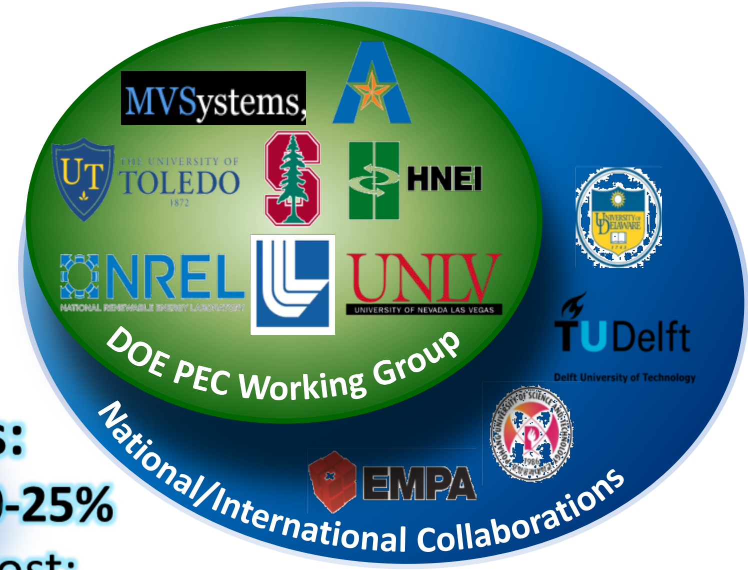

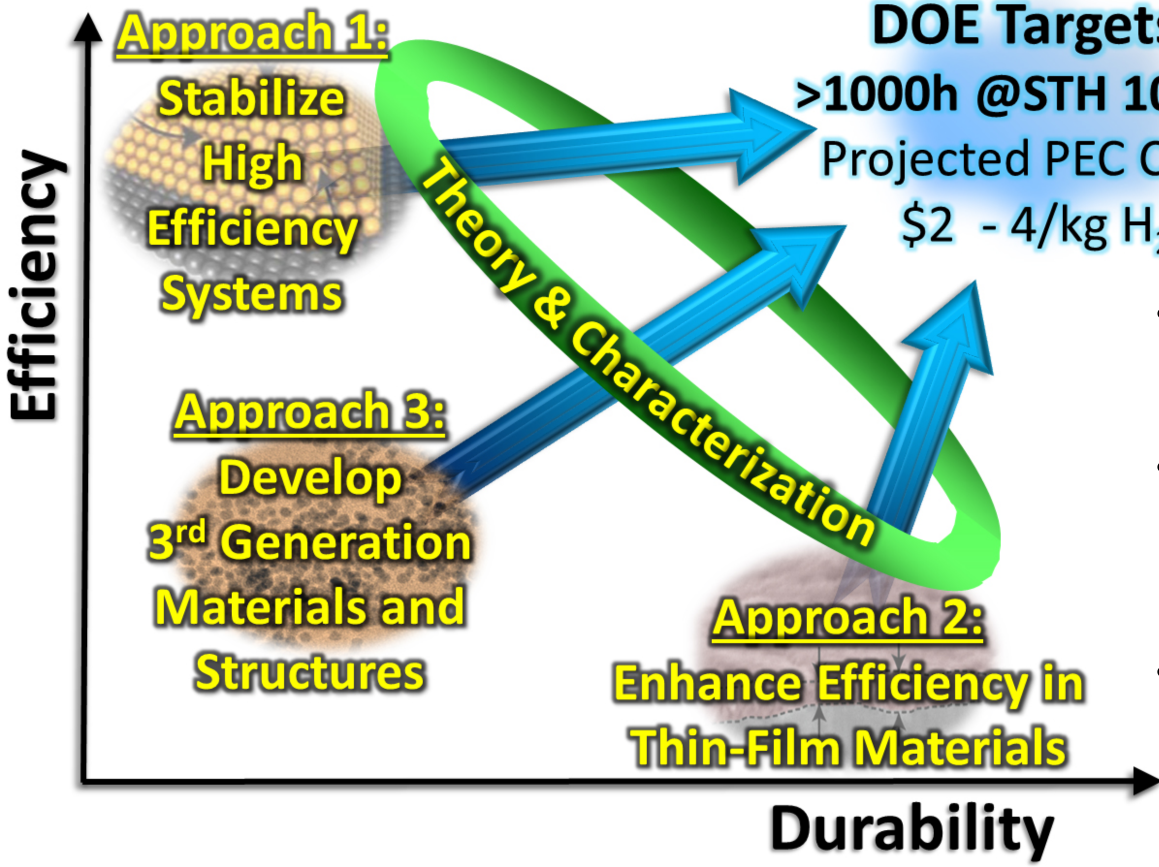

Summary

- Technologically, PEC water-splitting has already been accomplished.
- A techno-economic analysis shows that it is possible to reach cost targets if materials with appropriate properties can be developed.
- A feasibility study shows that these properties are within reach based on the current state of materials development.
- The PEC WG is collaborating synergistically to accelerate R&D efforts.