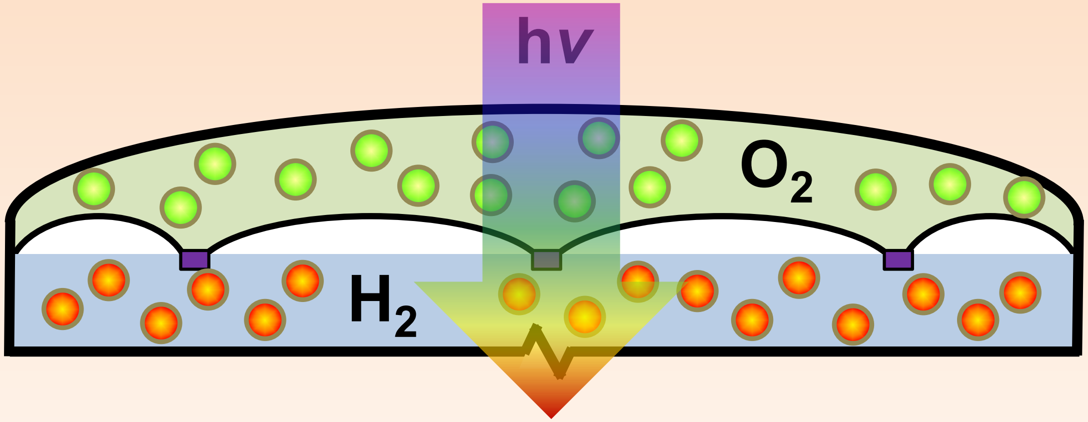
Tandem particle-slurry batch reactors for solar water splitting

Shane Ardo

University of California, Irvine



Overview

Project Timeline

- Start date: August 1, 2015
- End date: July 31, 2017

(24-month period of performance)

Budget

Project funding:	$1,248,063
– Federal funds:	$ 993,759
– UCI cost share:	$ 254,304
Funding by year	
– Year 1 spent (2/29):	$ 378,347
– Year 1 budget:	$ 685,210

Barriers Addressed

- (AG) Integrated Device Configurations
- (AH) Reactor Designs
- (AI) Auxiliary Materials
- (AJ) Synthesis and Manufacturing

Partners / Collaborators

- Device-physics modeling & simulation contributors
  - **Lawrence Berkeley National Laboratory & JCAP** (Adam Weber, *sub-recipient*)
  - **California Institute of Technology & JCAP** (Chengxiang Xiang, *sub-contracted advisor*)
- Materials Contributors
  - **Kyoto University** (Ryu Abe)
  - **Tokyo University of Science** (Akihiko Kudo)
  - **University of California, Davis** (Frank Osterloh)
  - **University of California, Riverside** (Phil Christopher)
  - **University of Houston** (Jiming Bao)
  - **University of Tokyo** (Kazunari Domen)

Relevance

Project Objective: **Experimentally validate** a laboratory-scale particle suspension reactor as a scalable technology for solar H_2 production

2015–2016 Objective: **Numerically demonstrate** the feasibility of a reactor that exhibits a 1% solar-to-hydrogen (STH) conversion efficiency

	MYRD&D Targets for a Type 2 Reactor				
Characteristics	**2011**	**2015**	**Proposed**	**2020**	**Ultimate**
H_2 Cost ($/kg)	N/A	28.60	20.00	4.60	2.10
η_{STH} (%)	N/A	1.0	1.0	5.0	10

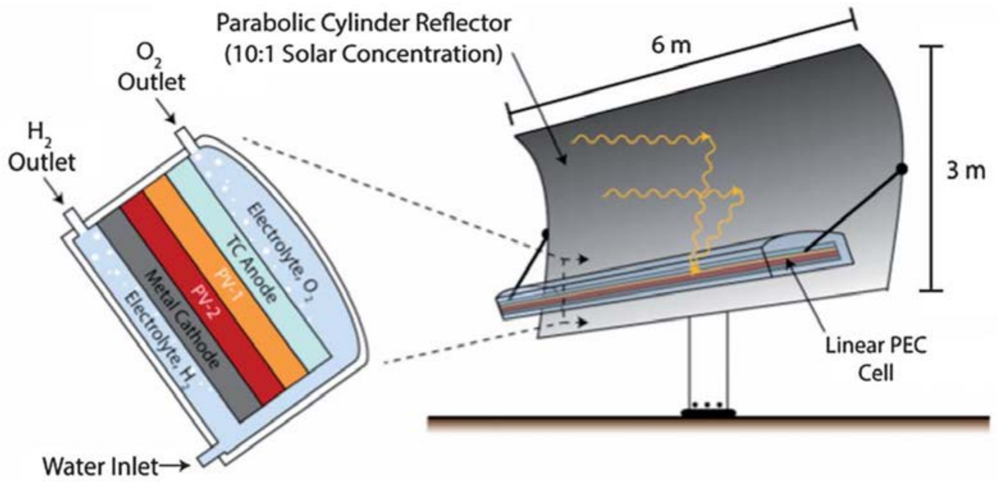
DOE Barriers	**Project Goal**
(AG) Integrated Device Configurations **(AJ) Synthesis and Manufacturing**	• Electrodeposit catalysts on light-absorber particles using bipolar electrochemistry and photoelectrodeposition
(AH) Reactor Designs	• Numerically model and simulate new designs for tandem two-compartment particle suspension reactors • Fabricate and evaluate model reactors, and assess their transport capabilities
(AI) Auxiliary Materials	• Identify the most efficient redox shuttles based on rates of mass transport and rates of electrocatalysis at carbon

Relevance

Wafers (Type 4) and Particles (Type 2)

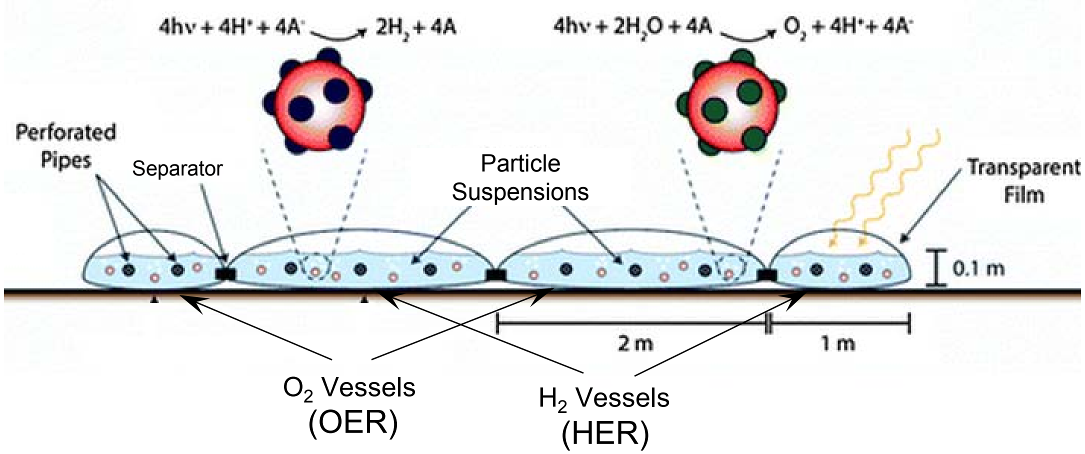
Wafer-based Design

Photoelectrodes immersed in electrolyte and illuminated with an optical concentration of 10x or more

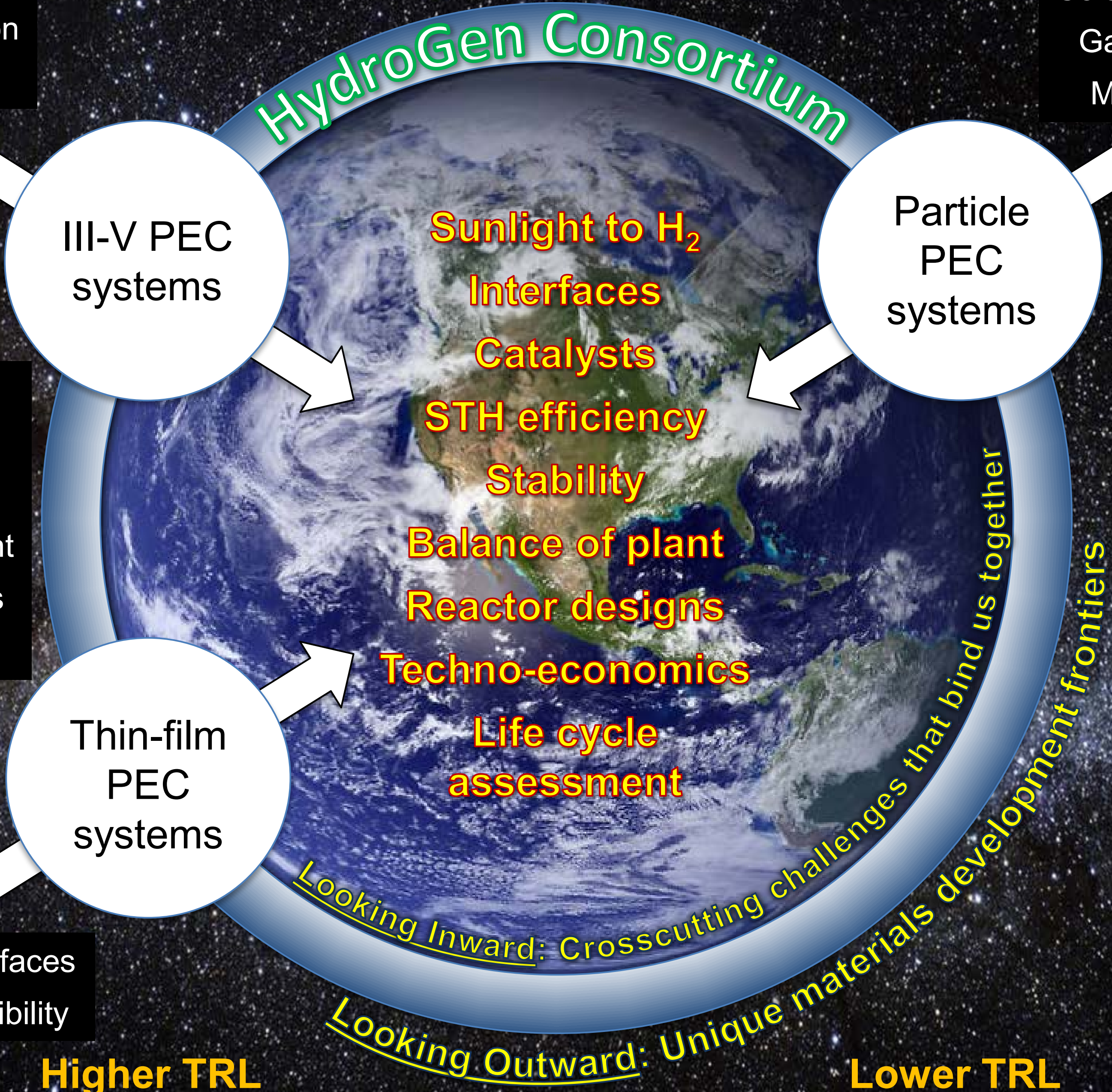


Particle-based Design

Solar water splitting reactor consisting of two particle suspensions arranged side-by-side and connected by a porous via to allow mixing of the molecular redox shuttle (A/A⁻).



Directed Technologies, Inc., DOE Report, **2009** & Pinaud, …, Ardo, …, Jaramillo, *Energy Environ. Sci.*, **2013**, *6*, 1983



HydroGen Consortium

Lower III-V costs
Optical concentration
Anti-reflection

Reactor designs
Selective catalysis
Gas separation
Mass transfer

III-V PEC systems

Particle PEC systems

Thin-film PEC systems

Bandgap tuning
Buried junctions
Durability testing
Bubble management
Non-PGM catalysts
Membranes

Sunlight to H_2
Interfaces
Catalysts
STH efficiency
Stability
Balance of plant
Reactor designs
Techno-economics
Life cycle assessment

Absorbers and interfaces processing compatibility

Looking Inward: Crosscutting challenges that bind us together

Looking Outward: Unique materials development frontiers

Higher TRL

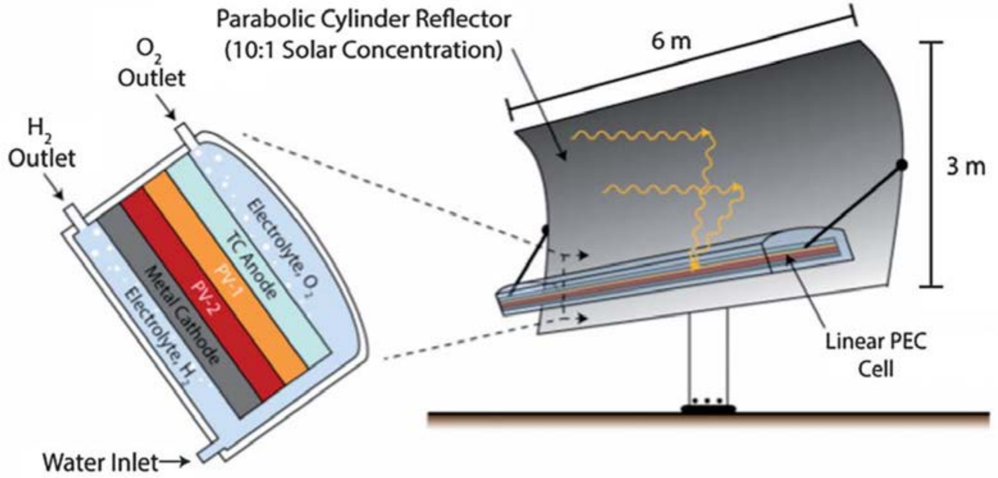
Lower TRL

Relevance

Wafers (Type 4) and Particles (Type 2)

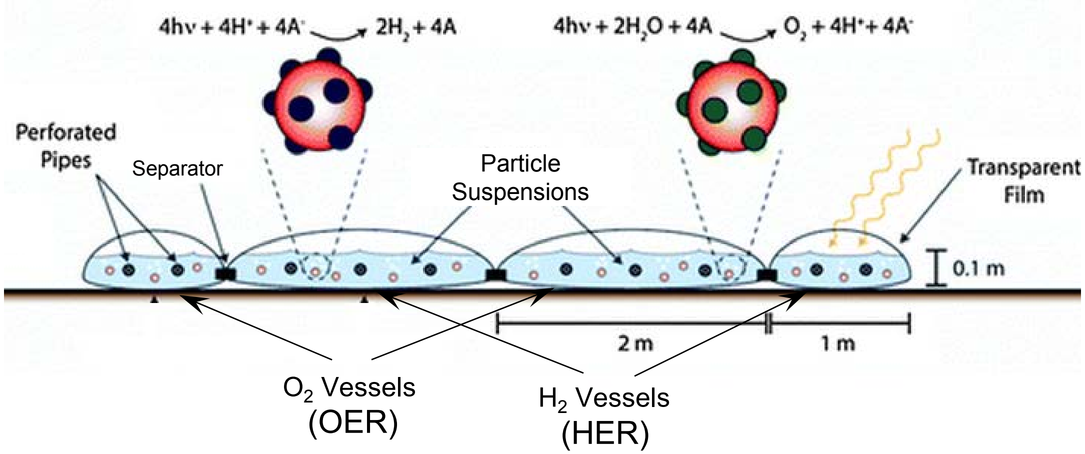
Wafer-based Design

Efficient and high-quality III-V materials with decades of prior R&D, well-understood materials properties, and often incorporated in standard device architectures with light-absorbing layers integrated with electrocatalysts



Particle-based Design

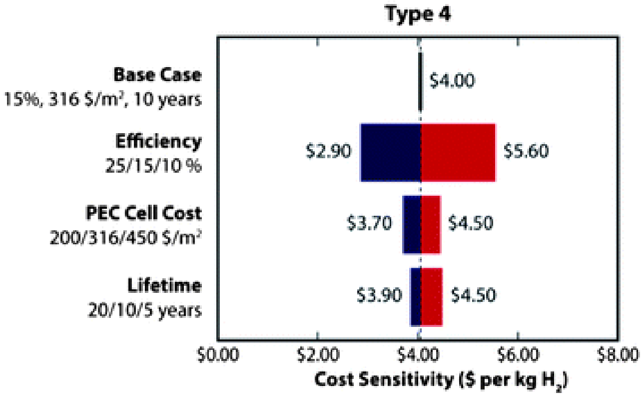
High-surface-area materials with low state-of-the-art efficiencies (as reported by only a few research groups) but with **flexibility in reactor architecture due to free-floating light absorbers**

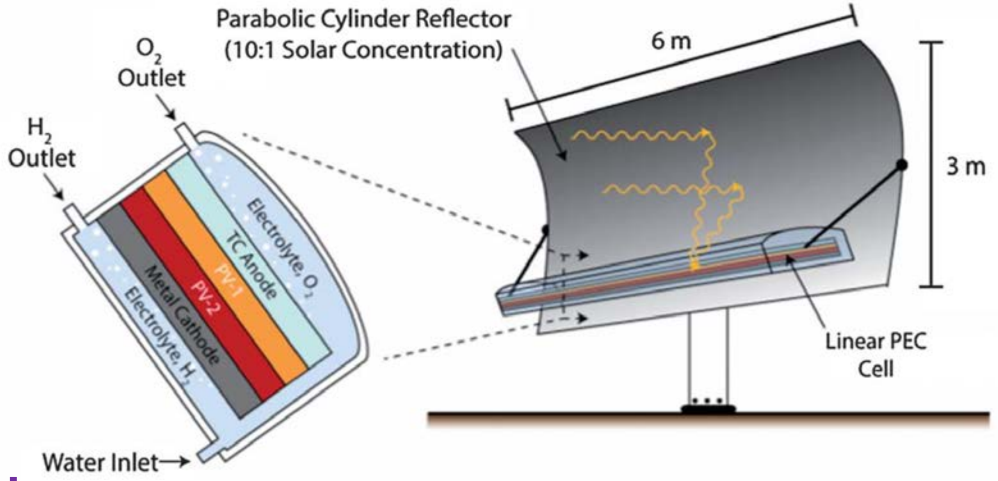


Directed Technologies, Inc., DOE Report, **2009** & Pinaud, …, Ardo, …, Jaramillo, *Energy Environ. Sci.*, **2013**, *6*, 1983

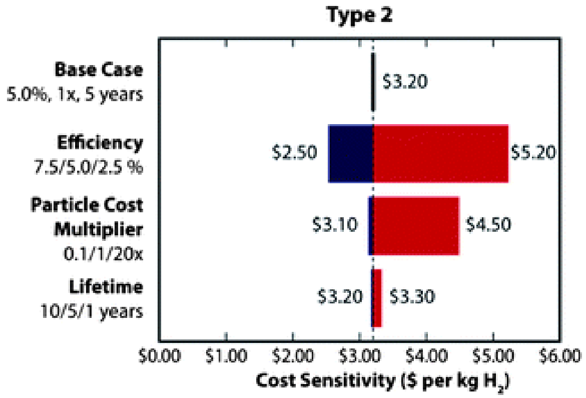
Relevance

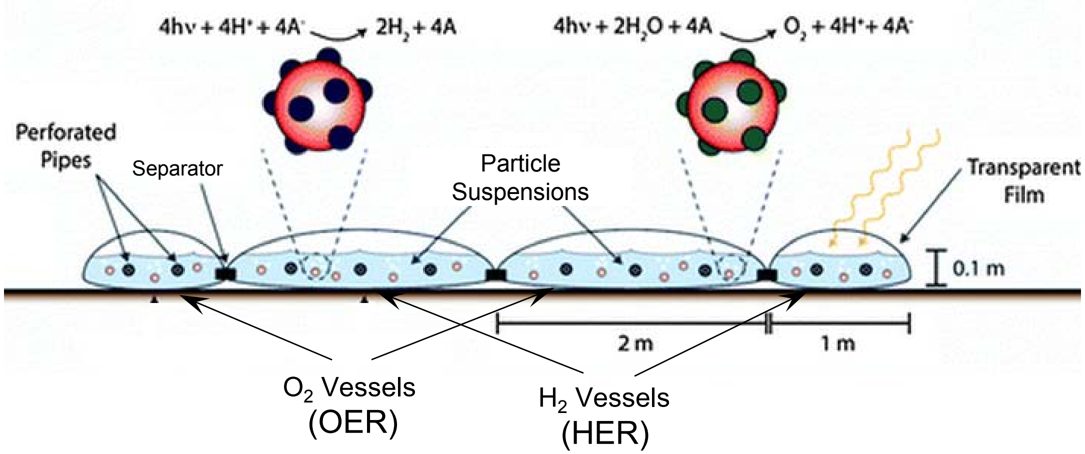
Wafers (Type 4) and Particles (Type 2)





DOE Ultimate Target: $2.10/gge H_2





Directed Technologies, Inc., DOE Report, **2009** & Pinaud, …, Ardo, …, Jaramillo, *Energy Environ. Sci.*, **2013**, *6*, 1983

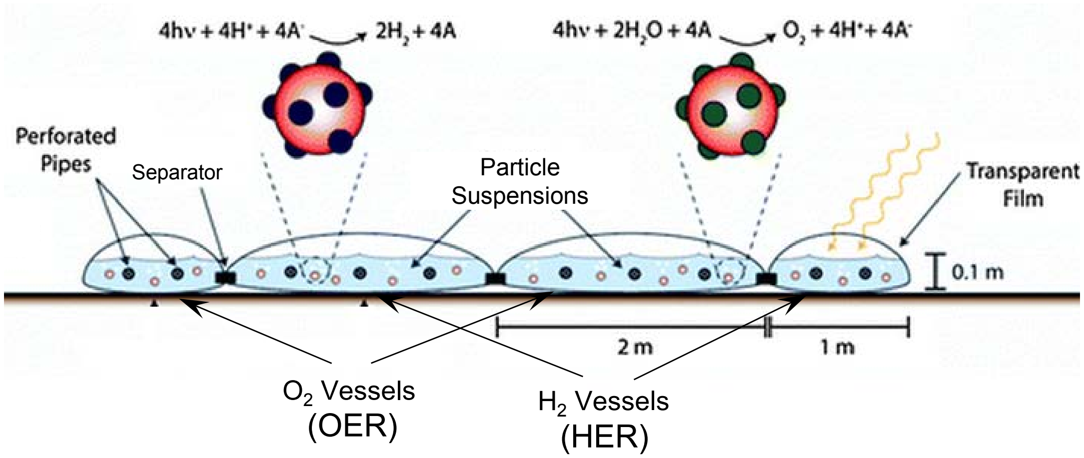
Approach: Concept

New Type 2 Reactor Design

Conventional Design

Solar water splitting reactor consisting of two particle suspensions arranged side-by-side and connected by a porous via to allow mixing of the molecular redox shuttle (A/A^-).

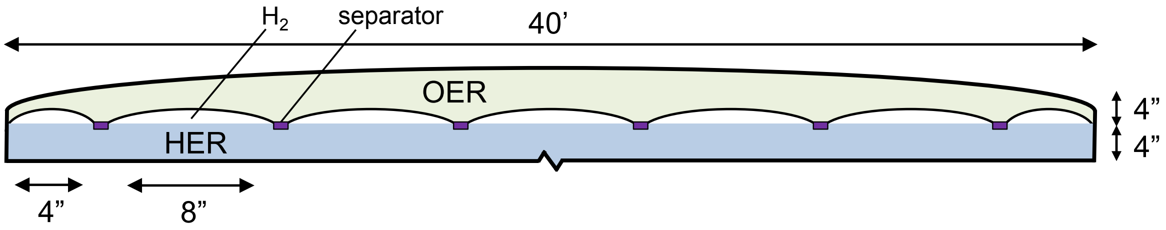
Limitation: Large mass transport distances for A/A^- and no η_{STH} benefit for the tandem design.



New Design

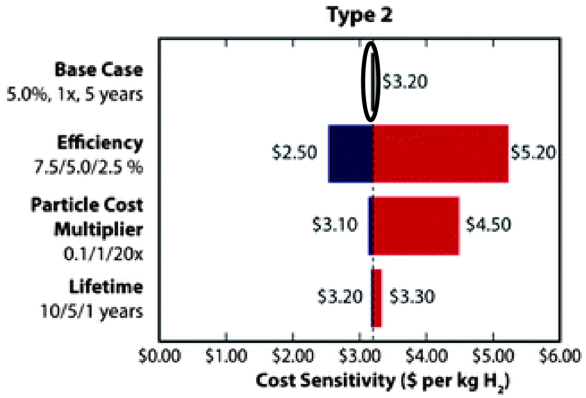
Stacked vessels afford:

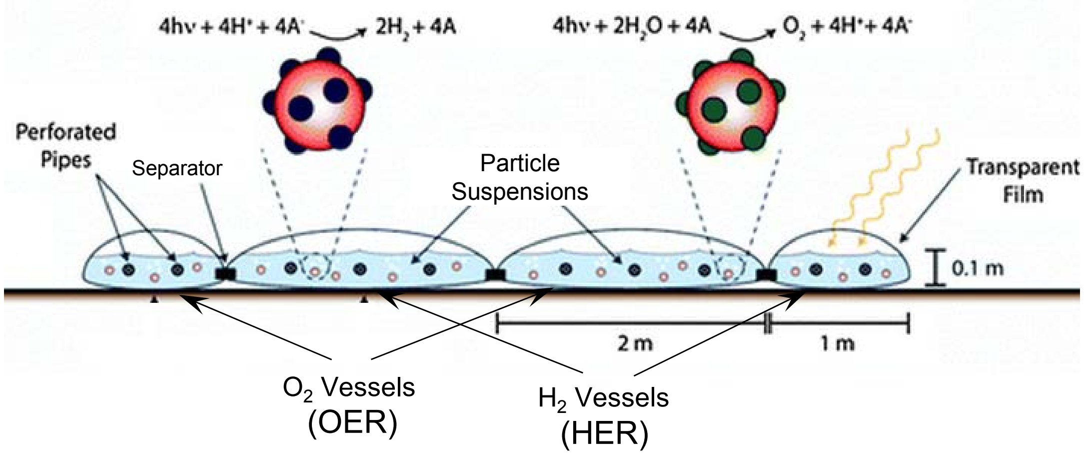
- **Small transport distances**
- **~50% increase in maximum theoretical STH conversion efficiency**
- **Reduced PVC piping & pumps**



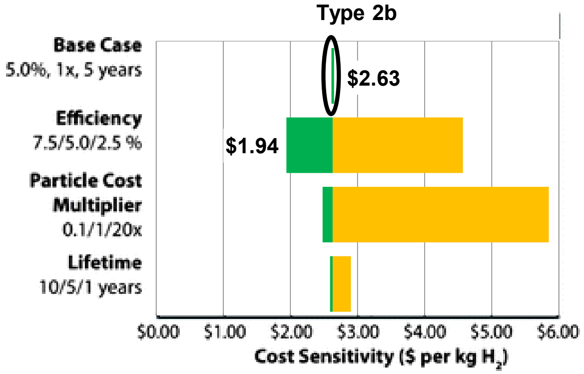
Approach: Concept

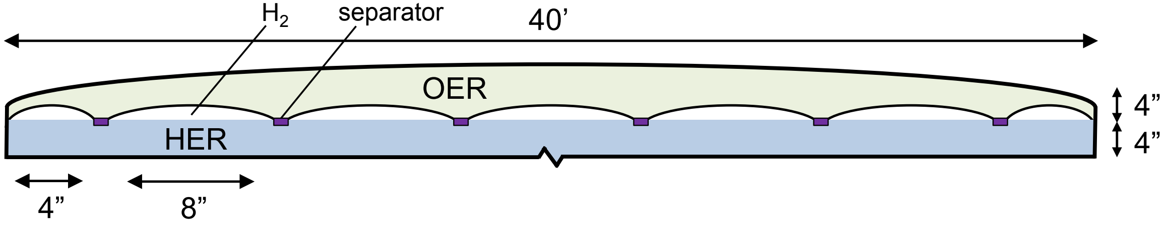
New Type 2 Reactor Design





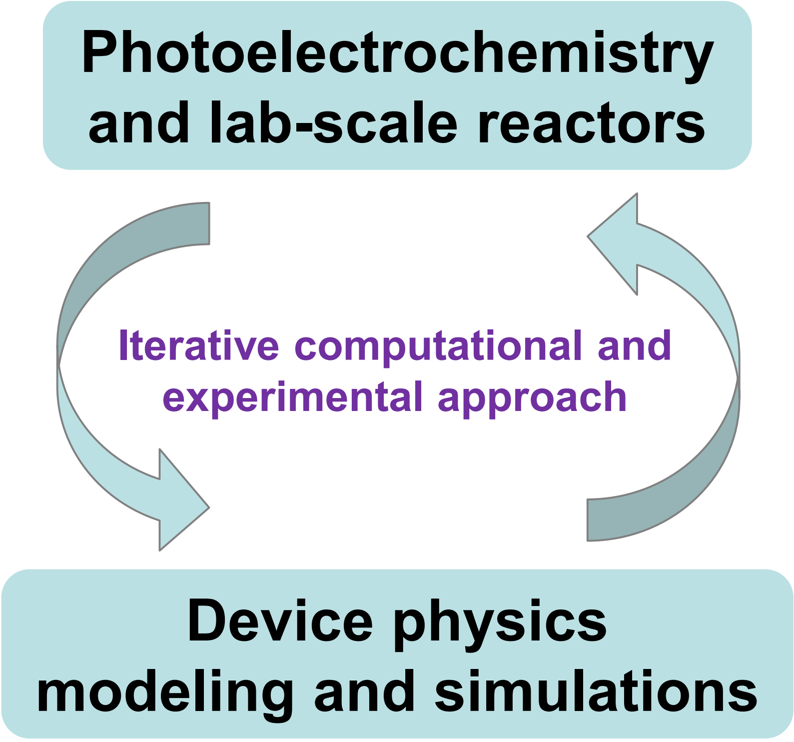
	MYRD&D Targets for a Type 2 Reactor				
Characteristics	**2011**	**2015**	**Proposed**	**2020**	**Ultimate**
H_2 Cost ($/kg)	N/A	28.60	20.00	4.60	2.10
η_{STH} (%)	N/A	1.0	1.0	5.0	10





Directed Technologies, Inc., DOE Report, **2009** & Pinaud, …, Ardo, …, Jaramillo, *Energy Environ. Sci.*, **2013**, *6*, 1983

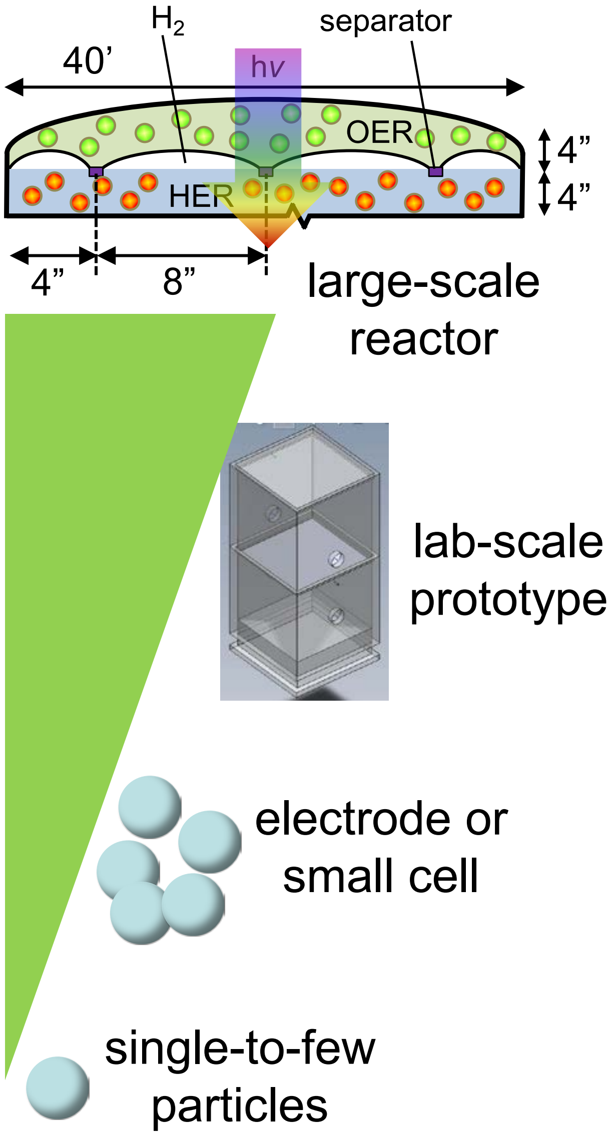
Approach: R&D



Photoelectrochemistry and lab-scale reactors

Iterative computational and experimental approach

Device physics modeling and simulations



large-scale reactor

lab-scale prototype

electrode or small cell

single-to-few particles

Approach: Milestones

Description of Milestone	Due Date (Quarter)	Percentage Complete
Task 1.0 Numerical modeling and simulation of new reactor design		
M1.1.1 Generate model that includes coupled charge transport, fluid flow, and Butler–Volmer kinetics. **(AH)**	November 1, 2015 (**Q1**)	**90%**
M1.1.2 To the model, add advanced semiconductor charge transport, i.e. generation and recombination in the bulk and at surfaces. **(AH)**	August 1, 2016 (**Q4**)	75%
D1.1.1 Go/No-Go Decision: Using 80% less pipes and 80% less pumping energy, verify 1% η_{STH}. **(AH)**	August 1, 2016 (**Q4**)	50%
M1.1.3 To the model, add electromagnetic wave propagation, thermal effects, and multi-phase flow. **(AH)**	May 1, 2017 (**Q7**)	5%
Task 2.0 Experimental evaluation of chemicals, materials, and reactors		
M2.1.1 Particle evaluation apparatus and electrocatalyst deposition apparatus using bipolar electrochemistry. **(AG, AJ)**	February 1, 2016 (**Q2**)	**75%**
M2.2.1 Maintain > 0.1% of initial redox shuttle concentration everywhere under conditions of day–night cycling. **(AI)**	May 1, 2016 (**Q3**)	60%
M2.3.1 Identify material(s) that operate at a rate consistent with > 1% η_{STH}, in any form factor and using any redox couple. **(AG)**	November 1, 2016 (**Q5**)	25%
M2.3.2 Demonstrate > 1% η_{STH} in electrode form factor. **(AG)**	February 1, 2017 (**Q6**)	0%
M2.4.1 Demonstrate > 3 standard liters of H_2 from 8 hours of solar illumination. **(AH)**	August 1, 2017 (**Q8 / end**)	0%

Approach: Milestones

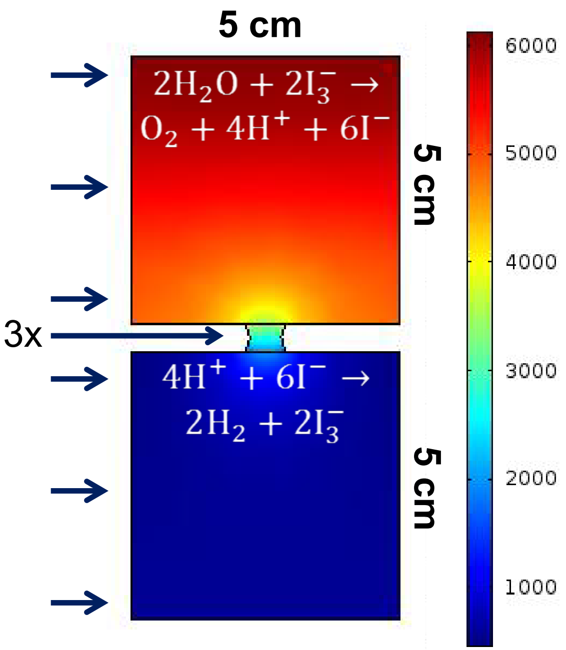
Description of Milestone	Due Date (Quarter)	Percentage Complete
Task 1.0 Numerical modeling and simulation of new reactor design		
M1.1.1 Generate model that includes coupled charge transport, fluid flow, and Butler–Volmer kinetics. **(AH)**	November 1, 2015 (**Q1**)	**90%**
M1.1.2 To the model, add advanced semiconductor charge transport, i.e. generation and recombination in the bulk and at surfaces. **(AH)**	August 1, 2016 (**Q4**)	75%
D1.1.1 Go/No-Go Decision: Using 80% less pipes and 80% less pumping energy, verify 1% η_{STH}. **(AH)**	August 1, 2016 (**Q4**)	50%
M1.1.3 To the model, add electromagnetic wave propagation, thermal effects, and multi-phase flow. **(AH)**	May 1, 2017 (**Q7**)	5%

Significant Points and Discoveries

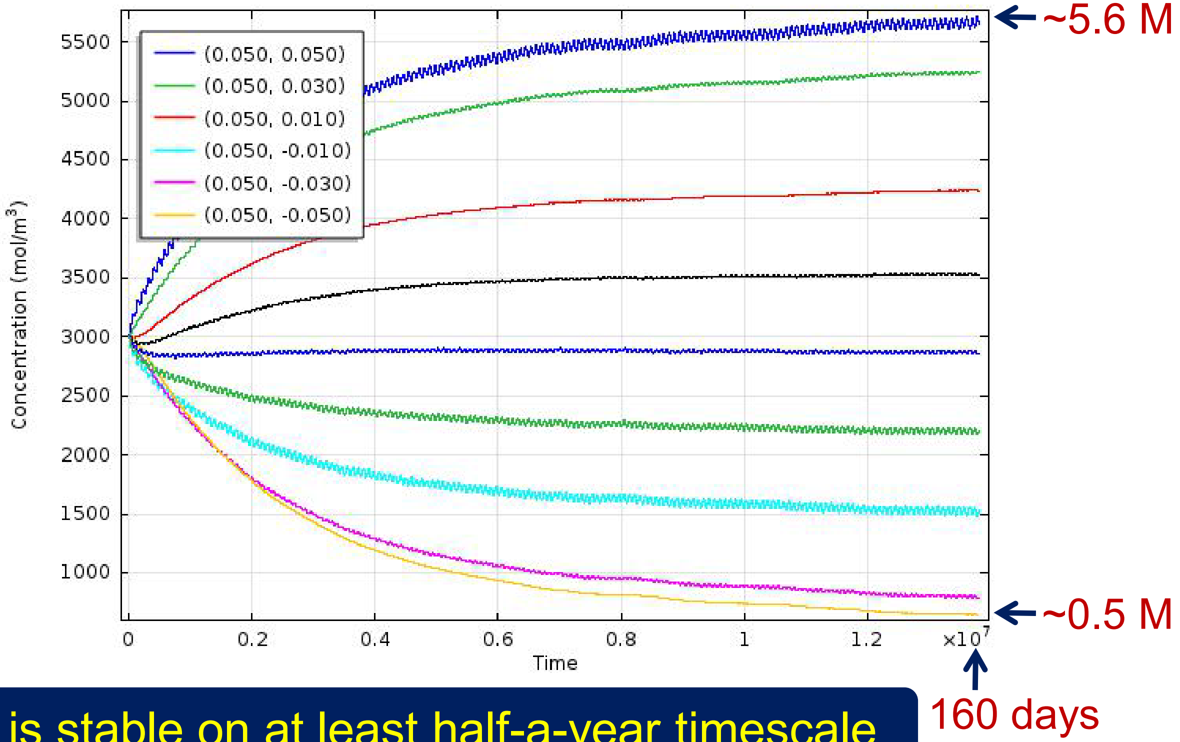
- Particles are not explicitly defined in the model.
- Migration around particles is appropriately neglected.
- Continuous Beer's Law absorption defines the maximum reaction rate along the reactor height as an input to the photodiode (or any) equation to drive the electrocatalytic reactions and determine rates of product formation (required iterative MATLAB and COMSOL communication).
- Large optical densities or thick compartments means particles close to the bottom are nearly dark and perform net shunting reverse reactions.

Accomplishments on Task 1.0

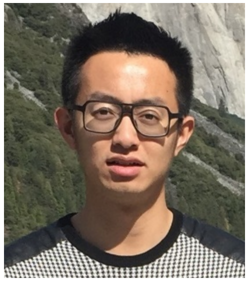
Iodide concentration @ *t* = 160 days



Time evolution of iodide concentration



Electrolyte is stable on at least half-a-year timescale



Yuanxun Shao
Chemical Engineer
(UCI Master's Student)

Toward M1.1.1

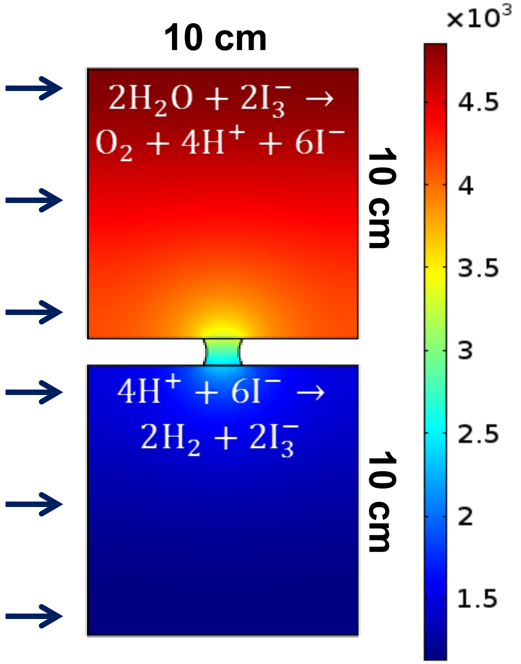
Reaction rate dictated by Beer's law absorption of solar irradiance scaled to η_{STH} = 1% and using complementary bandgap materials

Additions to future models

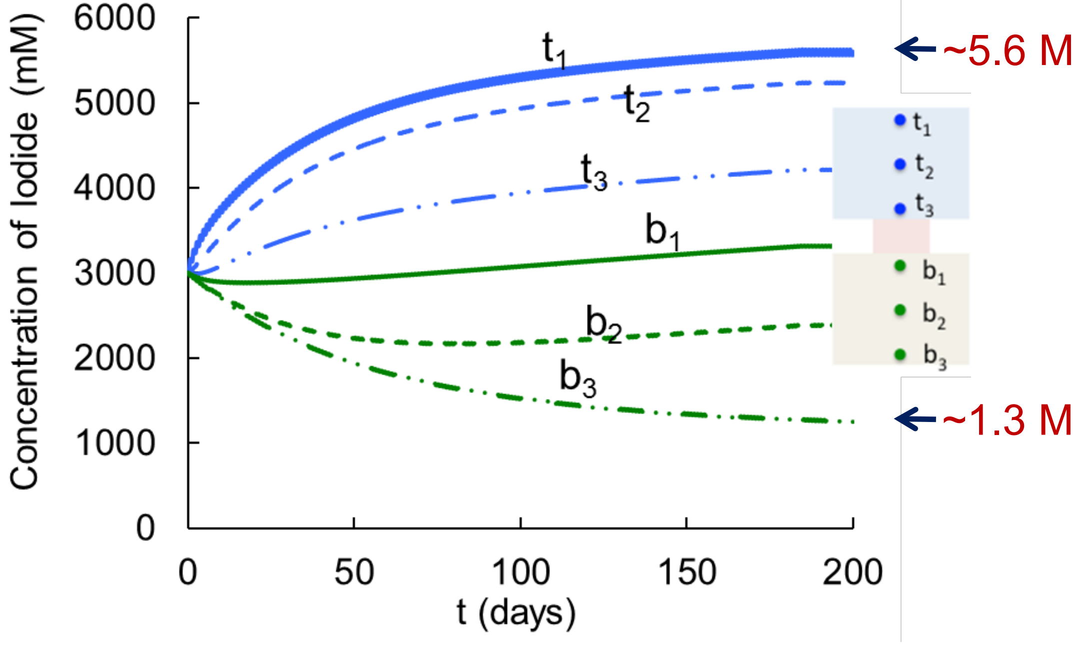
- Photovoltage
- Electrocatalysis
- Sunlight absorption by redox shuttle
- Forced convection
- Separator porosity
- Non-proton counterion for redox shuttle

Accomplishments on Task 1.0

Iodide concentration @ *t* = 200 days



Time evolution of iodide concentration



Electrolyte is stable on at least half-a-year timescale

Rohini Bala Chandran
Mechanical Engineer
(LBNL Postdoc)

Toward M1.1.1 & M1.1.2

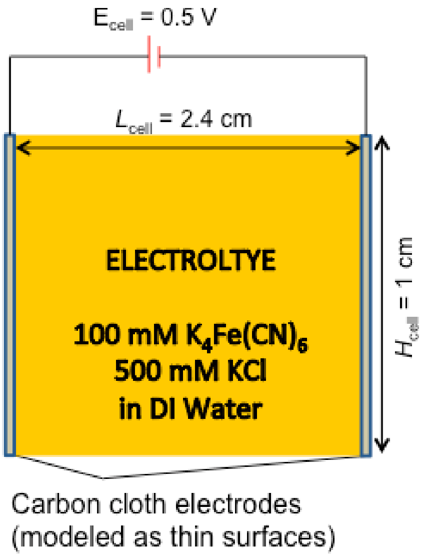
Reaction rate dictated by **experimental** Beer's law absorption of solar fluence (TiO_2 and $Rh:SrTiO_3$) to drive **ideal photodiode behavior** with coupled **Butler–Volmer electrocatalytic parameters**

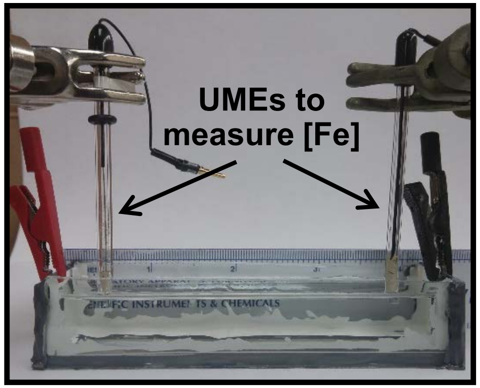
Additions to future models

- Photovoltage ✓
- Electrocatalysis ✓
- Sunlight absorption by redox shuttle
- Forced convection
- Separator porosity
- Non-proton counterion for redox shuttle

Accomplishments on Task 1.0

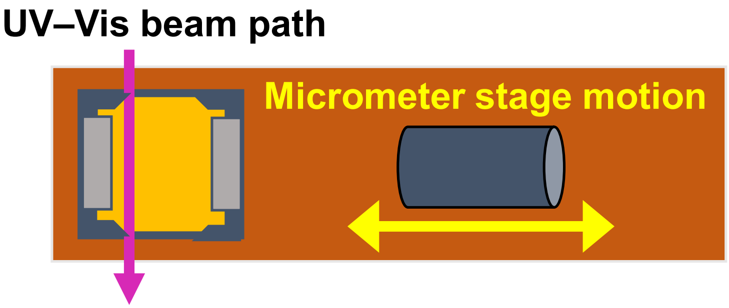
Side View



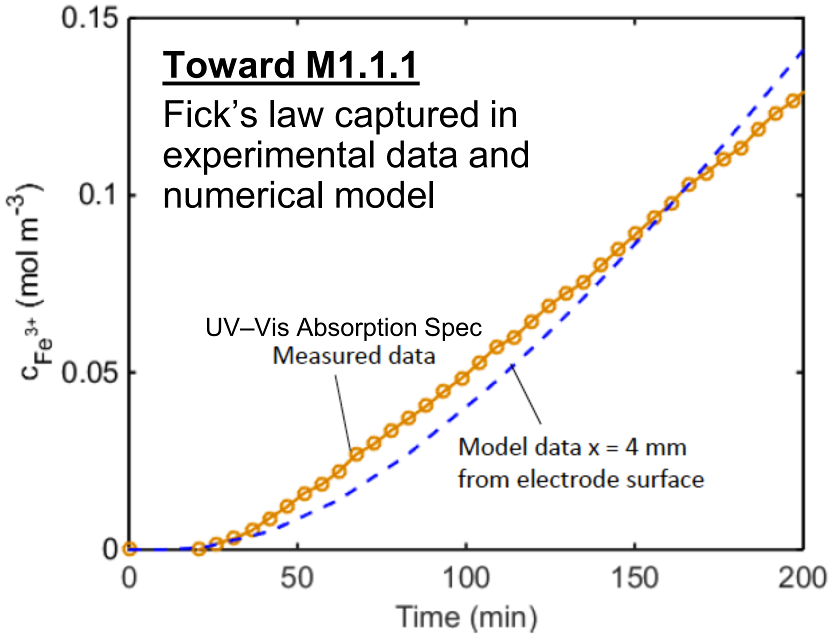


(new cell)

Top View



Theoretical diffusion observed experimentally



Toward M1.1.1

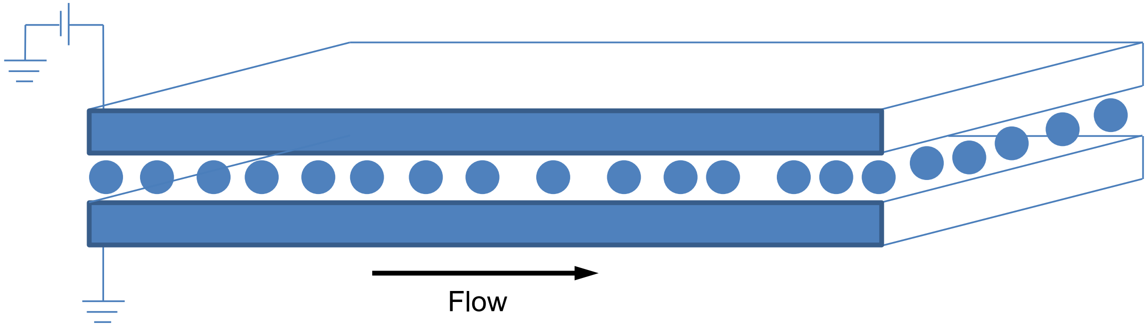
Fick's law captured in experimental data and numerical model

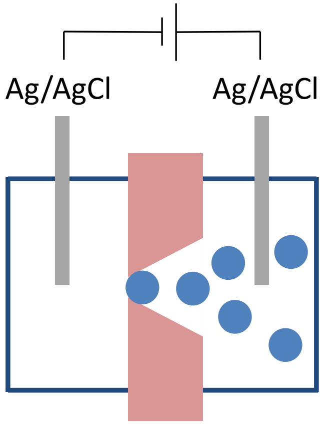
Rohini Bala Chandran
Mechanical Engineer
(LBNL Postdoc)

Kevin Tkacz
Materials Scientist
(UCI Ph.D. Student)

William Gaieck
Materials Scientist
(UCI Ph.D. Student)

Approach: Milestones

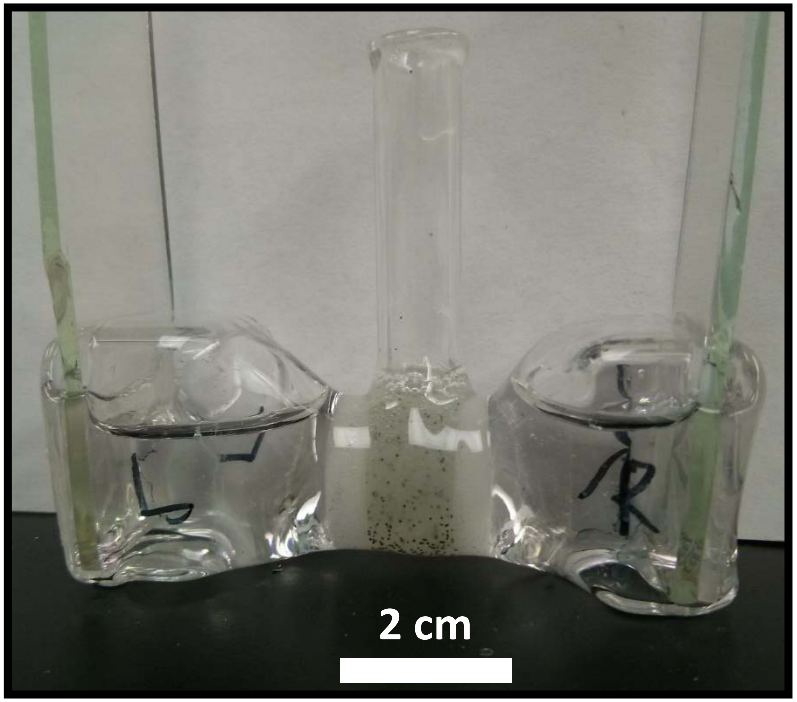




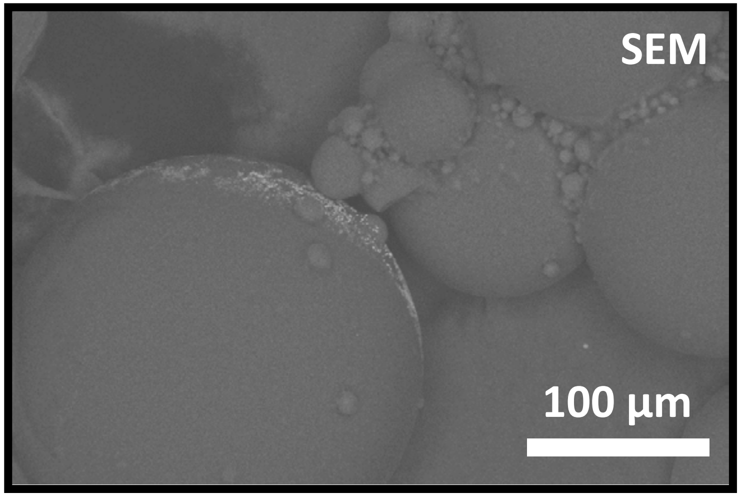
Task 2.0 Experimental evaluation of chemicals, materials, and reactors

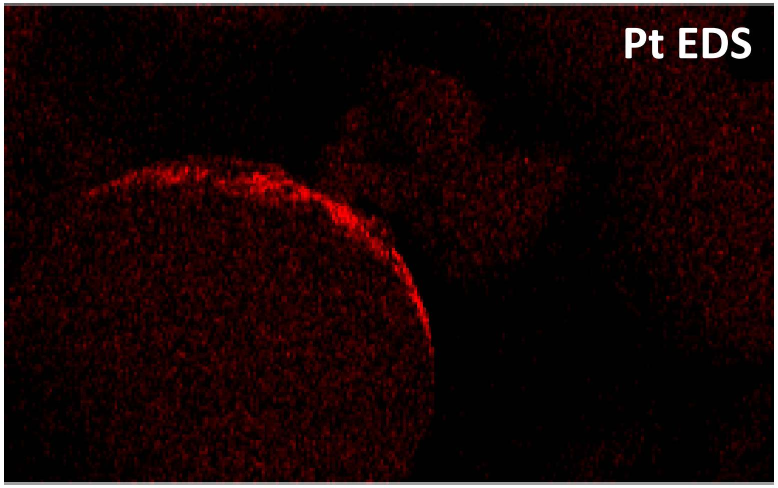
Description of Milestone	Due Date (Quarter)	Percentage Complete
M2.1.1 Particle evaluation apparatus and electrocatalyst deposition apparatus using bipolar electrochemistry. **(AG, AJ)**	February 1, 2016 (**Q2**)	**75%**
M2.2.1 Maintain > 0.1% of initial redox shuttle concentration everywhere under conditions of day–night cycling. **(AI)**	May 1, 2016 (**Q3**)	60%
M2.3.1 Identify material(s) that operate at a rate consistent with > 1% η_{STH}, in any form factor and using any redox couple. **(AG)**	November 1, 2016 (**Q5**)	25%
M2.3.2 Demonstrate > 1% η_{STH} in electrode form factor. **(AG)**	February 1, 2017 (**Q6**)	0%
M2.4.1 Demonstrate > 3 standard liters of H_2 from 8 hours of solar illumination. **(AH)**	August 1, 2017 (**Q8 / end**)	0%

Accomplishments on Task 2.0



2-electrode measurement



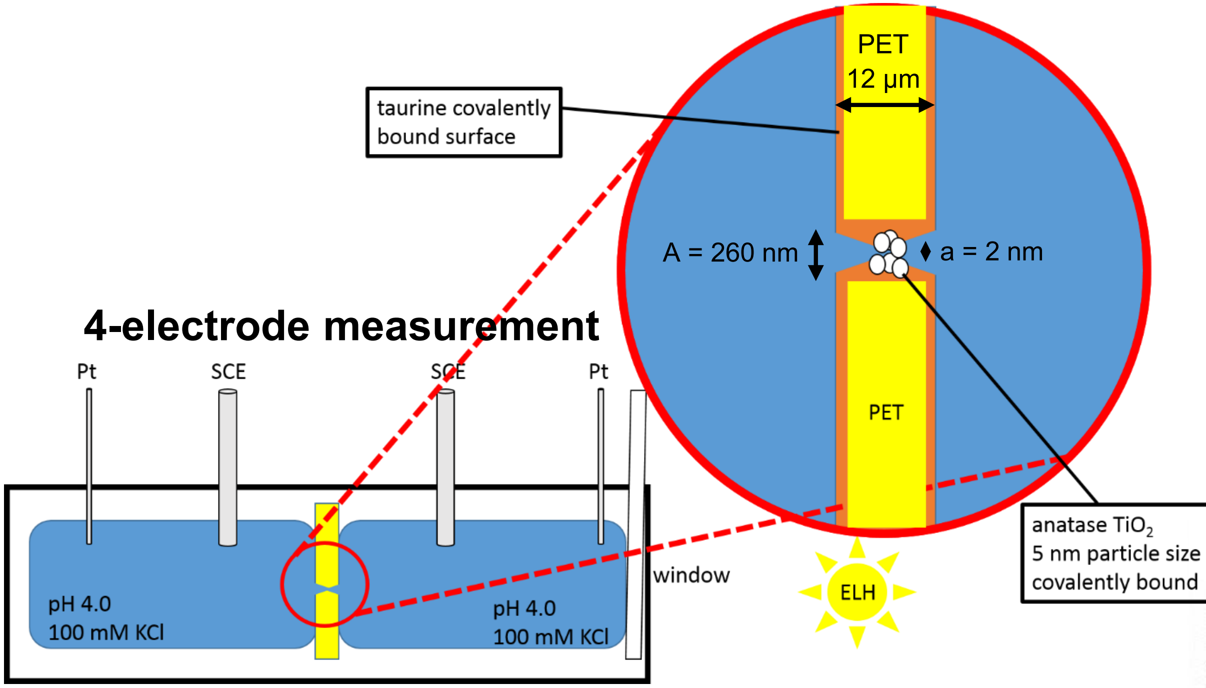


Vitreous carbon particles with bipolar Pt electrodeposition (E_{app} = 200 V for 1.5 min)

William Gaieck
Materials Scientist
(UCI Ph.D. Student)

Deposition of electrocatalysts on < 400 µm diameter carbon

Accomplishments on Task 2.0

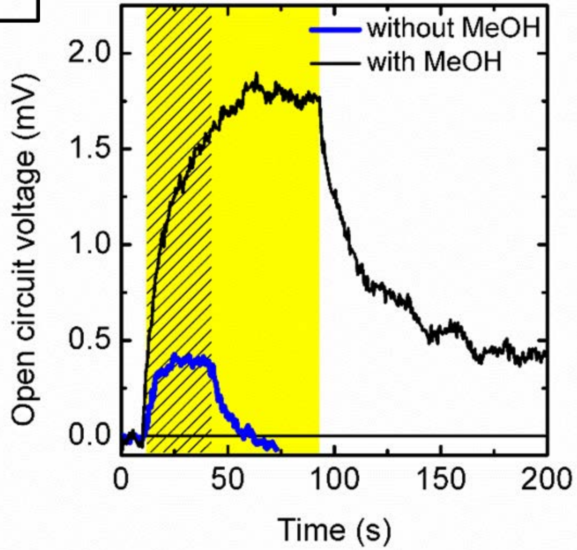


* Similar behavior observed from V_{oc} data on the microsecond timescale and binned into histograms

Christopher Sanborn
Organic Chemist
(UCI Ph.D. Student)

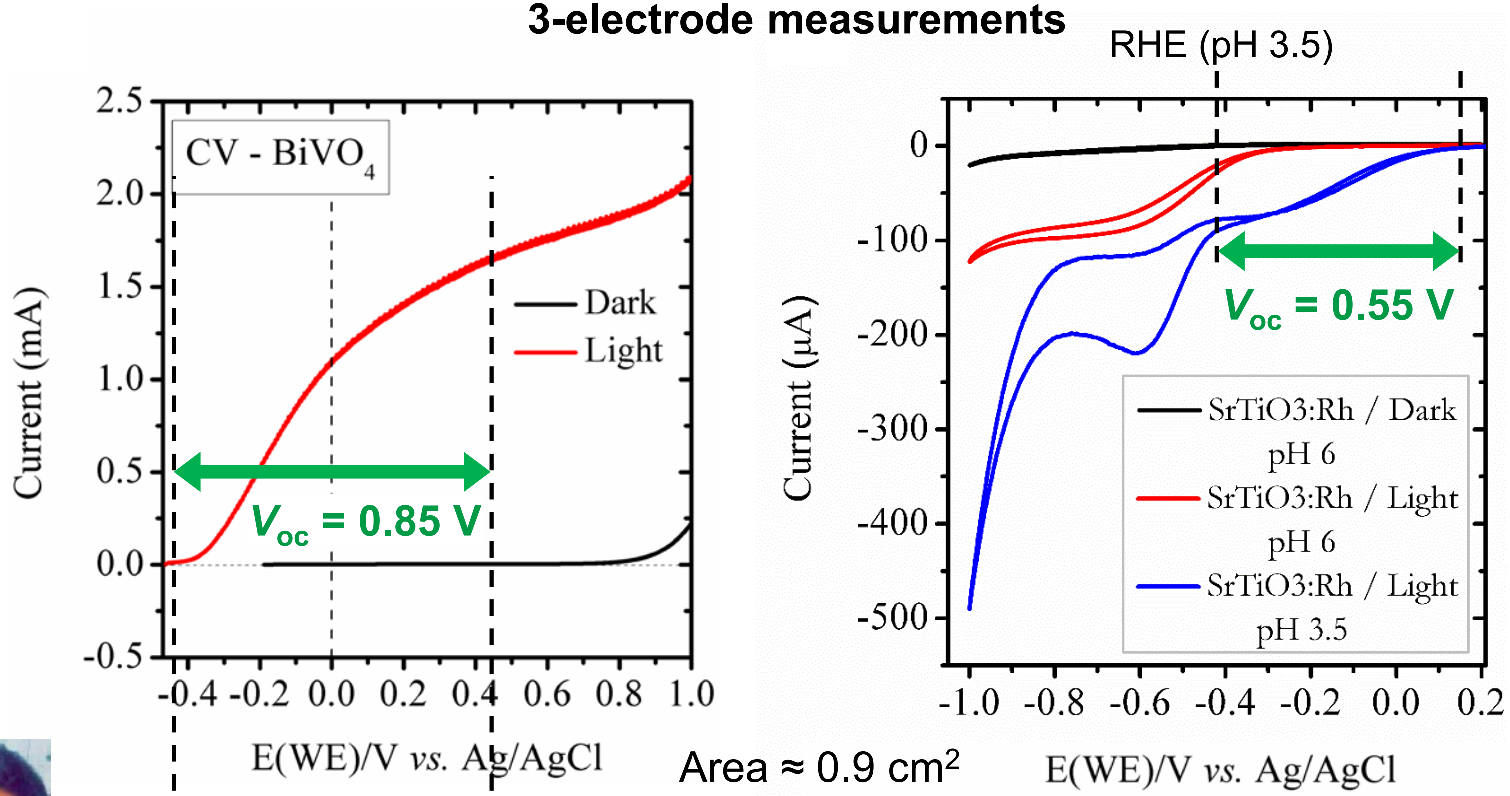
Kevin Tkacz
Materials Scientist
(UCI Ph.D. Student)

Observed photovoltage from "single" particle(s) indicates charging due to conduction-band electrons



Accomplishments on Task 2.0

3-electrode measurements



RHE (pH 10) + 1.23 V

Houman Yaghoubi
Electrical Engineer
(UCI Postdoc)

Rh-modified SrTiO$_3$ and BiVO$_4$ will generate > 1.23 V, but limited by Rh:SrTiO$_3$ $J \approx 0.1$ mA cm^{-2}

Response to previous year reviewers’ comments

This project was not reviewed last year.

Collaborations

Primary team members *(funded)*

- Lawrence Berkeley National Laboratory (Federal Lab) & Joint Center for Artificial Photosynthesis (DOE Hub)
  - **Adam Weber (sub-recipient)**: Core numerical device-physics modeling and simulation effort, specifically chemical engineering and multi-physics

- California Institute of Technology (University) & Joint Center for Artificial Photosynthesis (DOE Hub)
  - **Chengxiang Xiang (sub-contracted advisor)**: Expertise in numerical device-physics modeling and simulation effort, specifically semiconductor physics and ray tracing

Additional team members with expertise in particle materials synthesis *(unfunded)*

- Kyoto University, **Ryu Abe ($Rh:SrTiO_3$, $BiVO_4$)**
- Tokyo University of Science, **Akihiko Kudo ($Rh:SrTiO_3$, $BiVO_4$)**
- University of California, Davis, **Frank Osterloh ($Rh:SrTiO_3$, $BiVO_4$)**
- University of California, Riverside, **Phil Christopher (GaN:ZnO)**
- University of Houston, **Jiming Bao (CoO)**
- University of Tokyo, **Kazunari Domen (GaN:ZnO)**

Remaining Challenges and Barriers

Task 1.0 Numerical modeling and simulation of new reactor design

- Introduce fluid flow into the model to enable simulation of forced convection, e.g. by electrolyte pumping.
- Introduce advanced semiconductor charge transport into the model, i.e. generation and recombination in the bulk and at surfaces, to more accurately model the particle photophysics.
- **Go/No-Go Decision Point: Using 80% less pipes and 80% less pumping energy, verify 1% η_{STH} over time.**
- Introduce electromagnetic wave propagation, thermal effects, and multi-phase flow into the model to make it more realistic.

Task 2.0 Experimental evaluation of chemicals, materials, and reactors

- Use bipolar electrochemistry to measure single particle photovoltages, as inputs into the numerical models.
- Use bipolar electrochemistry to deposit electrocatalysts on sub-micron-sized particles.
- Maintain > 0.1% of initial redox shuttle concentration everywhere in the reactor under conditions of day–night cycling as an indicator of long-term availability of the redox shuttle.
- Identify material(s) that operate at a rate consistent with > 1% η_{STH}, in any form factor and using any redox couple, and then in electrode form factor, as prerequisites to the final deliverable.

Final Deliverable: Demonstrate > 3 standard liters of H_2 from 8 hours of solar illumination.

Proposed Future Work

2015–2016 Objective **(FY16)**: **Numerically demonstrate** the feasibility of a reactor that exhibits $\eta_{STH} = 1\%$

Description of Milestone – Solution	Due Date (Quarter)	Percentage Complete

Task 1.0 Numerical modeling and simulation of new reactor design

D1.1.1 Go/No-Go Decision: Using 80% less pipes and 80% less pumping energy, verify 1% η_{STH} **– Introduce forced convection**	August 1, 2016 (**Q4**)	50%

Task 2.0 Experimental evaluation of chemicals, materials, and reactors

M2.3.1 Identify material(s) that operate at a rate consistent with > 1% η_{STH}, in any form factor and using any redox couple **– Explore alternative syntheses for high-quality materials**	November 1, 2016 (**Q5**)	25%

Proposed Future Work

2015–2016 Objective **(FY16)**: **Numerically demonstrate** the feasibility of a reactor that exhibits η_{STH} = 1%

Project Objective **(FY17)**: **Experimentally validate** a laboratory-scale particle suspension reactor as a scalable technology for solar H_2 production

Description of Milestone – Solution	Due Date (Quarter)	Percentage Complete
Task 1.0 Numerical modeling and simulation of new reactor design		
D1.1.1 Go/No-Go Decision: Using 80% less pipes and 80% less pumping energy, verify 1% η_{STH} **– Introduce forced convection**	August 1, 2016 (**Q4**)	50%
M1.1.3 To the model, add electromagnetic wave propagation, thermal effects, and multi-phase flow – **Introduce multiple physics**	May 1, 2017 (**Q7**)	5%
Task 2.0 Experimental evaluation of chemicals, materials, and reactors		
M2.3.1 Identify material(s) that operate at a rate consistent with > 1% η_{STH}, in any form factor and using any redox couple **– Explore alternative syntheses for high-quality materials**	November 1, 2016 (**Q5**)	25%
M2.3.2 Demonstrate > 1% η_{STH} in electrode form factor **– Introduce electrocatalysts by photoelectrochemical deposition**	February 1, 2017 (**Q6**)	0%
M2.4.1 Demonstrate > 3 standard liters of H_2 from 8 hours of solar illumination **– Combine particles and reactor designs**	August 1, 2017 (**Q8 / end**)	0%

Project Summary

Project Objective: **Experimentally validate** a laboratory-scale particle suspension reactor as a scalable technology for solar H_2 production

Relevance	Techno-economic analyses of side-by-side particle suspension compartments suggest that H_2 cost may be inexpensive.
Approach	Stack the compartments to realize the tandem efficiency advantage and shorten the mass transport distance so that fewer pumps and pipes are needed.
Technical Accomplishments	Using a validated device physics model, demonstrated stable operation of a 1% STH stacked tandem reactor for over 200 days. Also used bipolar electrochemistry to deposit electrocatalysts and measure the photoresponse of single-to-few particles jammed in a plastic sheet. Also, synthesized and characterized efficient photoelectrodes consisting of Rh-modified $SrTiO_3$ or $BiVO_4$.
Collaborations	Several, including modeling experts and particle synthesis experts.
Proposed Future Work	Add additional device physics to the numerical models and synthesize high quality metal-oxide particles.

Technical Backup Slides

Motivation

Table 5 Summary of all direct capital expenditures and installation costs for the four different 1 TPD net H_2 production plant modules

	Type 1, single bed particle suspension		Type 2, dual bed particle suspension		Type 3, fixed panel array		Type 4, tracking concentrator array	
Reactor subassembly	Baggies	$133 077	Baggies	$791 250			Tracking/ concentrating	$2 035 420
	Particles	$22 679	Particles	$40 798	PEC cells	$8 238 271	PEC cells	$1 072 904
	Other	$56 501	Other	$60 886	Other	$105 074	Other	$26 886
Reactor subassembly total	$212 257		$892 934		$8 343 345		$3 135 209	
Gas processing subassembly	Compressor	$526 302						
	Condenser	$13 765	Compressor	$315 884	Compressor	$759 481		
	Intercoolers	$30 655	Condenser	$10 626	Condenser	$16 607	Condenser	$7098
	PSA	$107 147	Intercoolers	$23 334	Intercoolers	$36 389	Piping	$26 673
	Piping	$6416	Piping	$6811	Piping	$104 861		
Gas processing subassembly total	$684 283		$356 654		$917 338		$33 771	
Control system total	$173 944		$440 826		$319 862		$279 774	
Direct capital cost total	$1 070 485		$1 690 414		$9 580 545		$3 448 755	
Reactor cost per capture area (uninstalled)	$2.21 per m^2		$6.55 per m^2		$154.95 per m^2		$92.41 per m^2	
System Cost per capture area (uninstalled)	$19.76 per m^2		$18.46 per m^2		$204.81 per m^2		$126.51 per m^2	
Installation	Excavation	$46 259	Excavation	$124 672	Panels/reactor	$1 076 962	Reactors	$746 385
	Baggies/piping	$21 534	Baggies/piping	$291 441	Piping	$30 843	Piping	$10 521
	Gas processing	$203 361	Gas processing	$104 953	Gas processing	$243 743	Gas processing	$2129
	Control system	$52 183	Control system	$132 248	Control system	$95 959	Control system	$83 932
Installation cost total	$323 337		$653 314		$1 447 507		$842 967	
Total capital cost with installation	$1 393 822		$2 343 728		$11 028 052		$4 291 722	

Directed Technologies, Inc., DOE Report, **2009** & Pinaud, …, Ardo, …, Jaramillo, *Energy Environ. Sci.*, **2013**, *6*, 1983

DOE–EERE, H2A Analysis, http://www.hydrogen.energy.gov/h2a_production.html

Materials options: "<u>Type 2</u>"

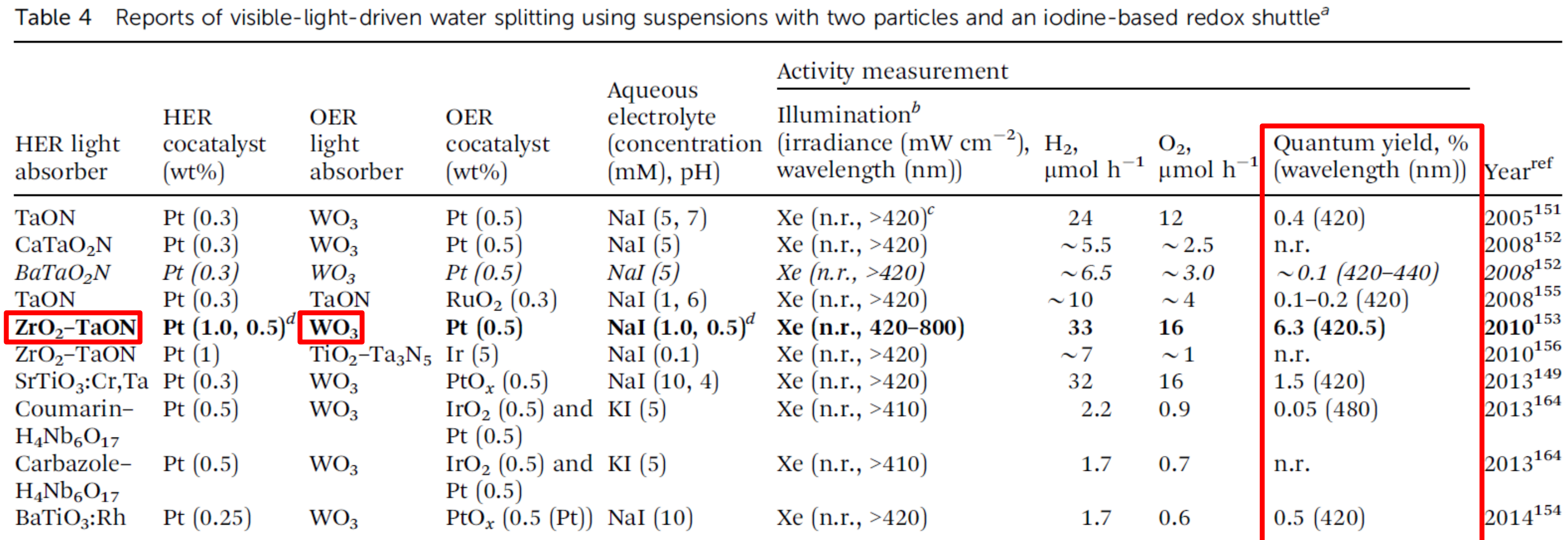


Table 4 Reports of visible-light-driven water splitting using suspensions with two particles and an iodine-based redox shuttle[a]

					Activity measurement				
HER light absorber	HER cocatalyst (wt%)	OER light absorber	OER cocatalyst (wt%)	Aqueous electrolyte (concentration (mM), pH)	Illumination[b] (irradiance (mW cm^{-2}), wavelength (nm))	H_2, μmol h^{-1}	O_2, μmol h^{-1}	Quantum yield, % (wavelength (nm))	Year[ref]
TaON	Pt (0.3)	WO_3	Pt (0.5)	NaI (5, 7)	Xe (n.r., >420)[c]	24	12	0.4 (420)	2005[151]
$CaTaO_2N$	Pt (0.3)	WO_3	Pt (0.5)	NaI (5)	Xe (n.r., >420)	~5.5	~2.5	n.r.	2008[152]
$BaTaO_2N$	*Pt (0.3)*	*WO_3*	*Pt (0.5)*	*NaI (5)*	*Xe (n.r., >420)*	*~6.5*	*~3.0*	*~0.1 (420–440)*	*2008[152]*
TaON	Pt (0.3)	TaON	RuO_2 (0.3)	NaI (1, 6)	Xe (n.r., >420)	~10	~4	0.1–0.2 (420)	2008[155]
ZrO_2–TaON	**Pt (1.0, 0.5)[d]**	**WO_3**	**Pt (0.5)**	**NaI (1.0, 0.5)[d]**	**Xe (n.r., 420–800)**	**33**	**16**	**6.3 (420.5)**	**2010[153]**
ZrO_2–TaON	Pt (1)	TiO_2–Ta_3N_5	Ir (5)	NaI (0.1)	Xe (n.r., >420)	~7	~1	n.r.	2010[156]
$SrTiO_3$:Cr,Ta	Pt (0.3)	WO_3	PtO_x (0.5)	NaI (10, 4)	Xe (n.r., >420)	32	16	1.5 (420)	2013[149]
Coumarin–$H_4Nb_6O_{17}$	Pt (0.5)	WO_3	IrO_2 (0.5) and Pt (0.5)	KI (5)	Xe (n.r., >410)	2.2	0.9	0.05 (480)	2013[164]
Carbazole–$H_4Nb_6O_{17}$	Pt (0.5)	WO_3	IrO_2 (0.5) and Pt (0.5)	KI (5)	Xe (n.r., >410)	1.7	0.7	n.r.	2013[164]
$BaTiO_3$:Rh	Pt (0.25)	WO_3	PtO_x (0.5 (Pt))	NaI (10)	Xe (n.r., >420)	1.7	0.6	0.5 (420)	2014[154]

Domen

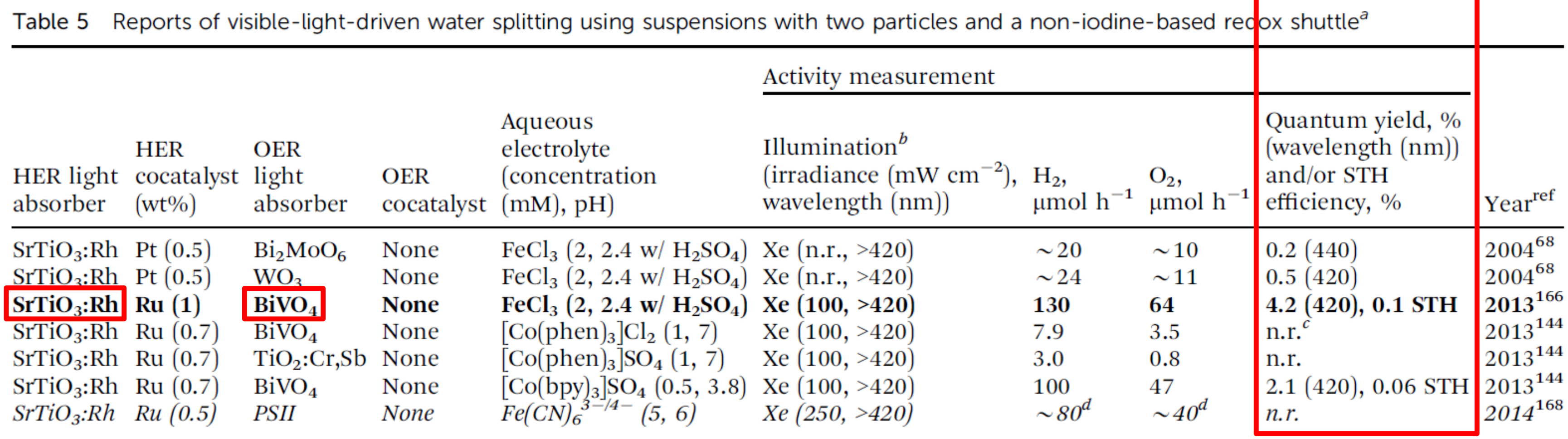


Table 5 Reports of visible-light-driven water splitting using suspensions with two particles and a non-iodine-based redox shuttle[a]

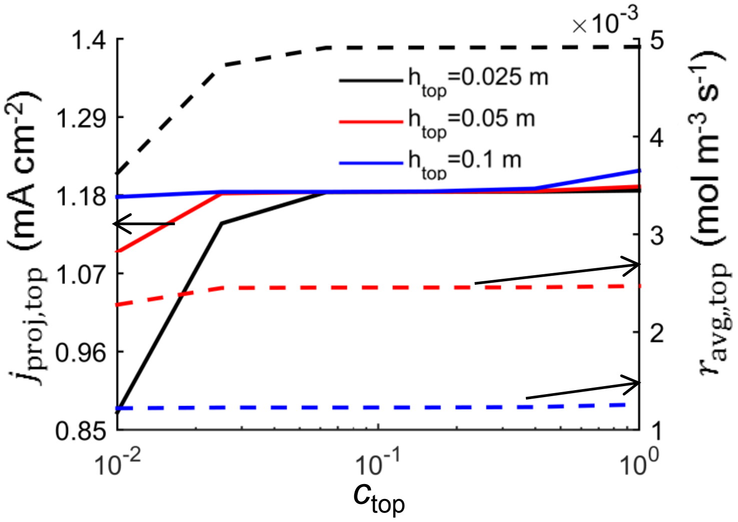
					Activity measurement				
HER light absorber	HER cocatalyst (wt%)	OER light absorber	OER cocatalyst	Aqueous electrolyte (concentration (mM), pH)	Illumination[b] (irradiance (mW cm^{-2}), wavelength (nm))	H_2, μmol h^{-1}	O_2, μmol h^{-1}	Quantum yield, % (wavelength (nm)) and/or STH efficiency, %	Year[ref]
$SrTiO_3$:Rh	Pt (0.5)	Bi_2MoO_6	None	$FeCl_3$ (2, 2.4 w/ H_2SO_4)	Xe (n.r., >420)	~20	~10	0.2 (440)	2004[68]
$SrTiO_3$:Rh	Pt (0.5)	WO_3	None	$FeCl_3$ (2, 2.4 w/ H_2SO_4)	Xe (n.r., >420)	~24	~11	0.5 (420)	2004[68]
$SrTiO_3$:Rh	**Ru (1)**	**$BiVO_4$**	**None**	**$FeCl_3$ (2, 2.4 w/ H_2SO_4)**	**Xe (100, >420)**	**130**	**64**	**4.2 (420), 0.1 STH**	**2013[166]**
$SrTiO_3$:Rh	Ru (0.7)	$BiVO_4$	None	$[Co(phen)_3]Cl_2$ (1, 7)	Xe (100, >420)	7.9	3.5	n.r.[c]	2013[144]
$SrTiO_3$:Rh	Ru (0.7)	TiO_2:Cr,Sb	None	$[Co(phen)_3]SO_4$ (1, 7)	Xe (100, >420)	3.0	0.8	n.r.	2013[144]
$SrTiO_3$:Rh	Ru (0.7)	$BiVO_4$	None	$[Co(bpy)_3]SO_4$ (0.5, 3.8)	Xe (100, >420)	100	47	2.1 (420), 0.06 STH	2013[144]
$SrTiO_3$:Rh	*Ru (0.5)*	*PSII*	*None*	*$Fe(CN)_6^{3-/4-}$ (5, 6)*	*Xe (250, >420)*	*~80[d]*	*~40[d]*	*n.r.*	*2014[168]*

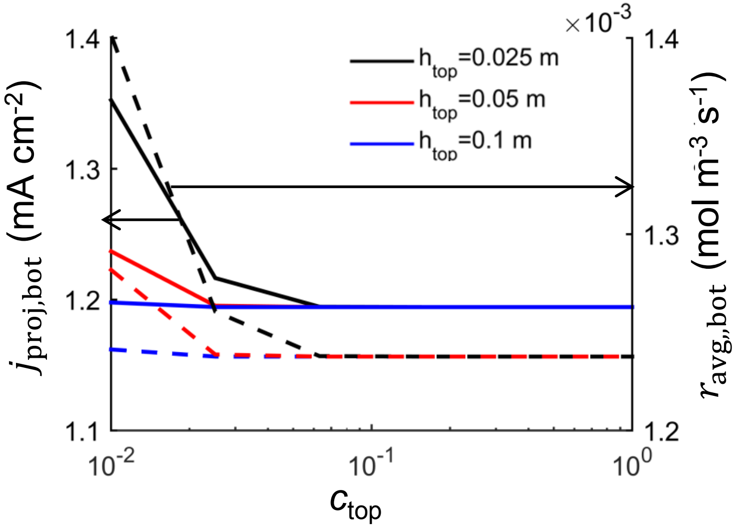
Kudo & Abe (+ UCD)

Fabian, …, Ardo, *Energy Environ. Sci.*, **2015**, *8*, 2825

Effects of Top Compartment Photocatalyst Concentration and Reactor Height

Model Parameter	Top Values	(Bot)tom Values
Compartment height, ***h***	**0.025, 0.05, 0.1 m**	0.1 m
Photocatalyst concentration, ***c***	**0.01 – 1 g L^{-1}**	0.002 g L^{-1}
Photocatalyst bandgap, $\boldsymbol{E_g}$	**3.1, 2.5 eV**	2.5 eV
OER/HER reverse saturation current density, $\boldsymbol{j_r}$	**10^{-10} – 10^{-18} A m^{-2}**	**10^{-10} – 10^{-18} A m^{-2}**
OER/HER exchange current density, $\boldsymbol{j_o}$	10^{-4} A m^{-2}	1.5 A m^{-2}



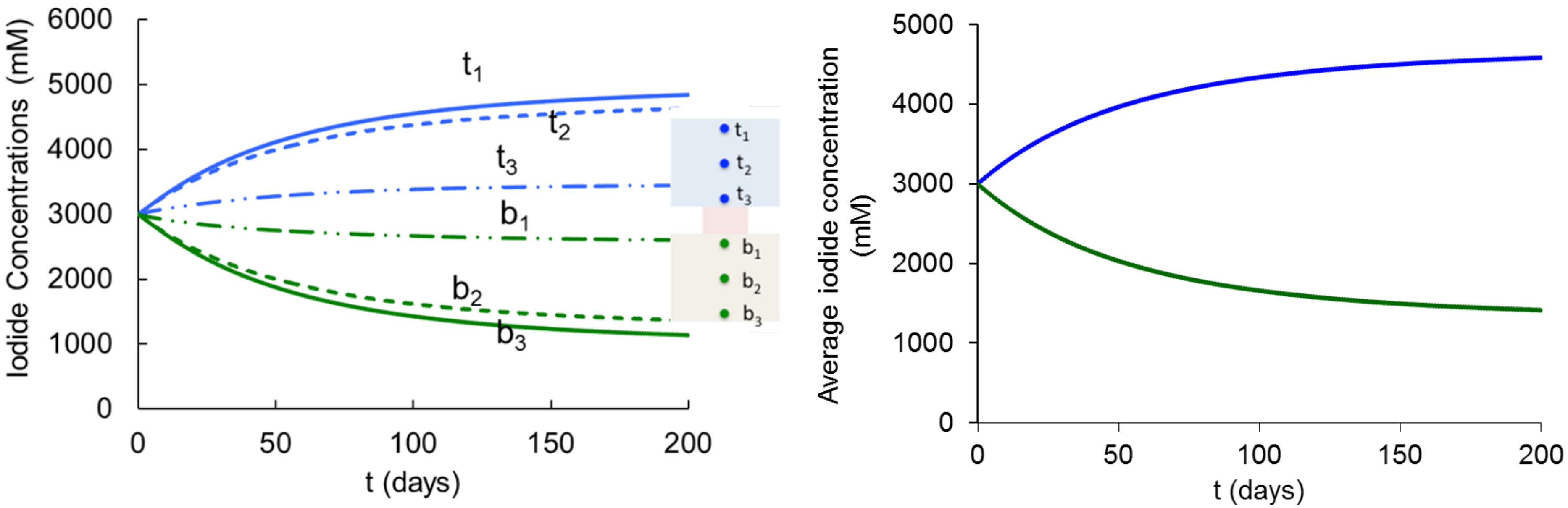


* Mass transport effects not included in these simulations

Model Parameters for Transient Simulations

	TOP (OER)	BOTTOM (HER)
Photocatalyst Concentration	TiO_2 0.01 g/L	$SrTiO_3$:Rh 0.002 g/L
Height	10 cm	10 cm
j_r	10^{-18} A m^{-2}	10^{-10} A m^{-2}
j_o	10^{-4} A m^{-2}	1.5 A m^{-2}
A_0	14.2 m^2 m^{-3}	8.6 m^2 m^{-3}
Particle Diameter	1 µm	1 µm

Model with Complete Scattering



* Assumed homogeneous reaction rates