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Sandia National Laboratories

H_2FC Hydrogen and Fuel Cells Program

Perovskites And Particle Reactor: A Multinational Effort To Advance Solar Hydrogen

Anthony McDaniel
Sandia National Laboratories

ASME 2018 Power & Energy Conference
Lake Buena Vista, FL
June 2018

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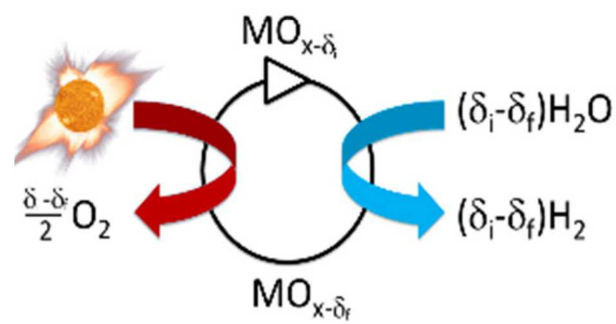
Sandia Team

Dr. Ivan Ermanoski, Dr. Kevin Albrecht, Dr. Eric Coker, Dr. Andrea Ambrosini, Dr. Josh Sugar, Mr. Jeff Roba

Material Discovery Team

- Colorado School of Mines, Golden CO.
  - Prof. Ryan O'Hayre, Prof. Michael Sanders, Ms. Debora Barcellos
  - Novel material formulations, synthesis, and screening
- Northwestern University, Evanston IL.
  - Prof. Christopher Wolverton, Dr. Antonie Emery
  - Application of quantum theory to materials screening
- Stanford University, Stanford CA.
  - Prof. William Chueh, Dr. BG Gopal, Ms. Nadia Ahlborg
  - Entropy engineering of materials

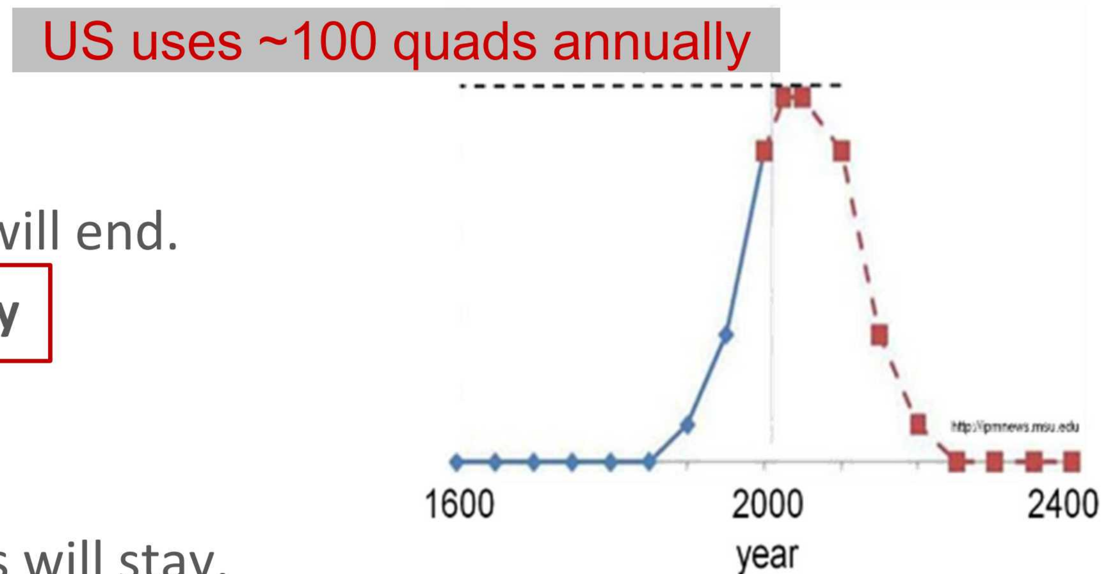


Reactor Design, Testing, and Demonstration Team

- Bucknell University, Lewisburg PA.
  - Prof. Nathan Siegel
  - Particle heat transfer, solar simulator design, CPR2 assembly and testing
- German Aerospace Center-DLR , Cologne DE
  - Dr. Christian Sattler, Dr. Justin Lapp, Dr. Abisheck Singh, Dr. Stefan Brendelberger, Mr. Johannes Grobbel
  - Solar particle receiver design, fabrication, and testing

Use Of "Mined" Carbon Is Here Today But Gone Tomorrow…Most Certainly

- Opportunities for solar-derived renewables.
  - Provide energy security
  - Mitigate climate change



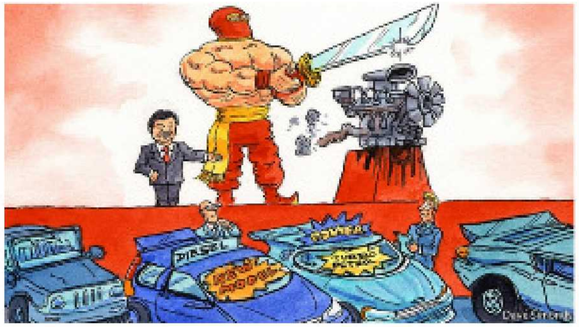
- Use of "mined" carbon will end.
  - **Burn Out** or **Fade Away**
- Chemical energy carriers will stay.
- Combustion-based energy conversion may stay.

Governments Are Driving Initiatives

Zooming ahead

China moves towards banning the internal combustion engine

Its government is developing a plan to phase out vehicles powered by fossil fuels



Browse: Home / Australasian News / Solar fuels could be Australia's biggest energy export

Solar fuels could be Australia's biggest energy export

Posted on October 16, 2015. **Australasian News.**

Author: Giles Parkinson

Source: reneweconomy.com.au

Can German auto regulators usher in the zero-emissions age?

The country's federal council, or Bundesrat, has resolved to ban all gas and diesel-powered cars by 2030.

By Joseph Dussault, Staff

The internal combustion engine, which powered the world's automobile boom, could soon be a relic of the past – at least in Germany.

The country's federal council, or Bundesrat, has resolved to ban all gas and

Netherlands looks to ban all non-electric cars by 2025

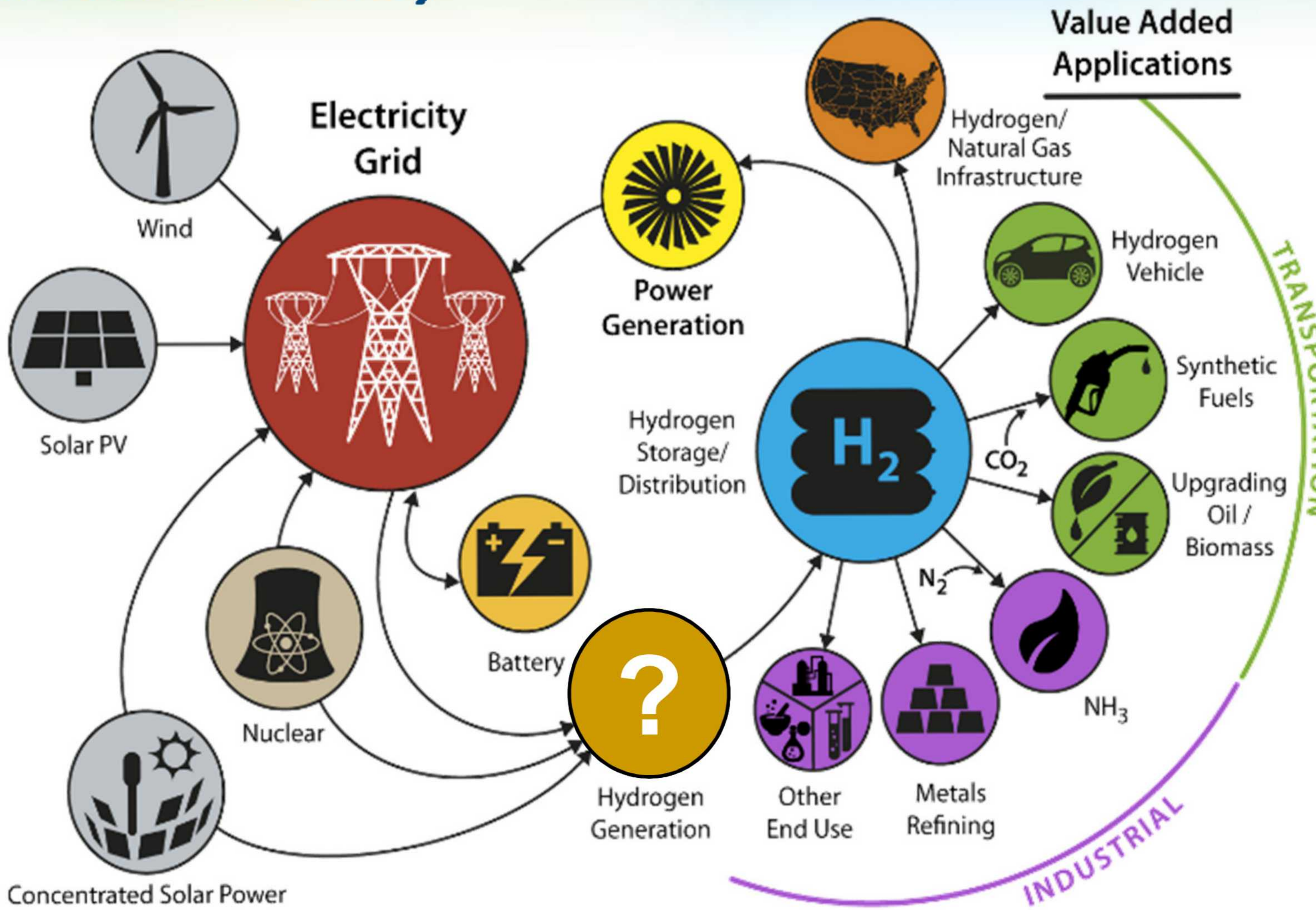
the Netherlands may only allow electric vehicles on the road.

Kick-off for world's largest electrolysis system in Mainz

In May 2014 Siemens, toget
RheinMain University of App
type of energy storage syste
button, the Chairman of the
board member Professor Sie
Mainz AG, Detlev Höhne an
Reymann, President of Rhei
production plant at the Energ
German Federal Ministry of
Storage Funding Initiative th
equipped with an electrolyze
wind farms to hydrogen from
electricity from renewable so
of up to 6 megawatts the pla

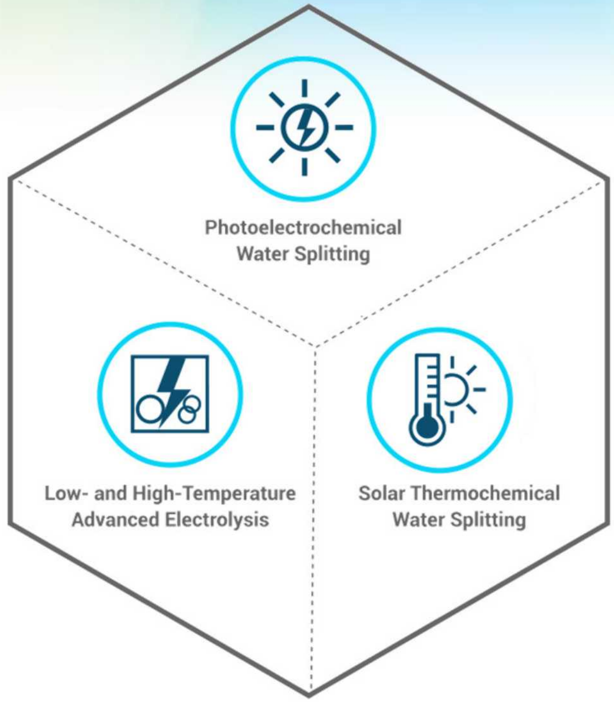
The principle of electrolysis has been tried and tested for decades. What is special about the Mainz system is that it involves highly dynamic PEM high-pressure electrolysis which is particularly suitable for high current density and can react within milliseconds to sharp increases in power generation from wind and solar sources. In this electrolyzer a proton exchange membrane (PEM) separates the two electrodes at which oxygen and hydrogen are formed. On the front and back of the membrane are precious-metal electrodes that are connected to the positive and negative poles of the voltage source. This is where the water is split. The system in Mainz will thus have a capacity relevant for bottlenecks in the grid and small wind farms.

Hydrogen Is "Gone" Today But Will Be Here Tomorrow…Mostly



Hydrogen As Far As The Eye Can See

+

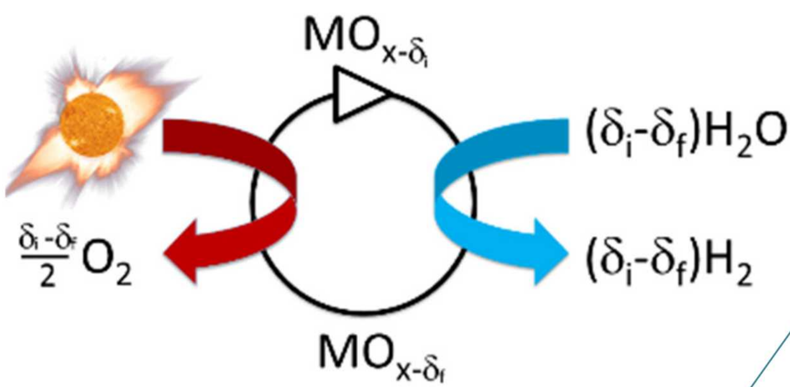


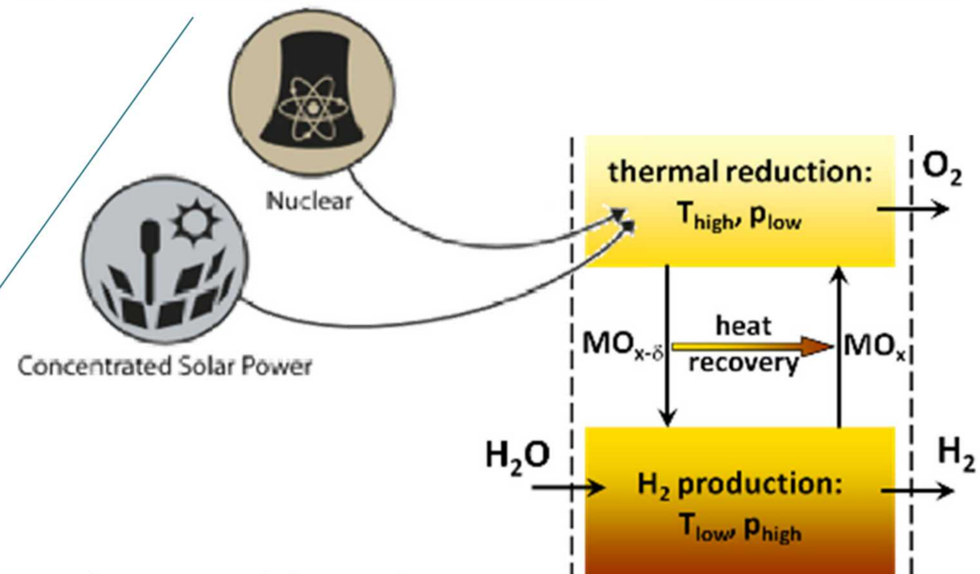
= H_2

- Global efforts underway to advance solar hydrogen production.
  - Address KEY technology challenges to advance readiness level of large scale, low cost renewable H_2
- US DOE heavily invested in developing advanced water splitting technology pathways.
  - Electrolysis, photoelectrochemical, thermochemical, microbial

Simple Concept: Heat + H_2O In, H_2 + O_2 Out

R. Perret, SAND Report (SAND2011-3622), Sandia National Laboratories, 2011.
G. J. Kolb, R. B. Diver, SAND Report (SAND2008-1900), Sandia National Laboratories, 2008.
S. Abanades, P. Charvin, G. Flamant, P. Neveu, *Energy*. **31**, 2805–2822 (2006).





- Direct storage of solar energy in a chemical bond.
- Many hundred cycles proposed.
  - Multi-phase, multi-step, thermochemical-electrochemical hybrids
- This multinational effort focused on two-step, non-volatile MO_x.

Outline

Searching For A Perfect Material

- Navigating a highly constrained requirement space.

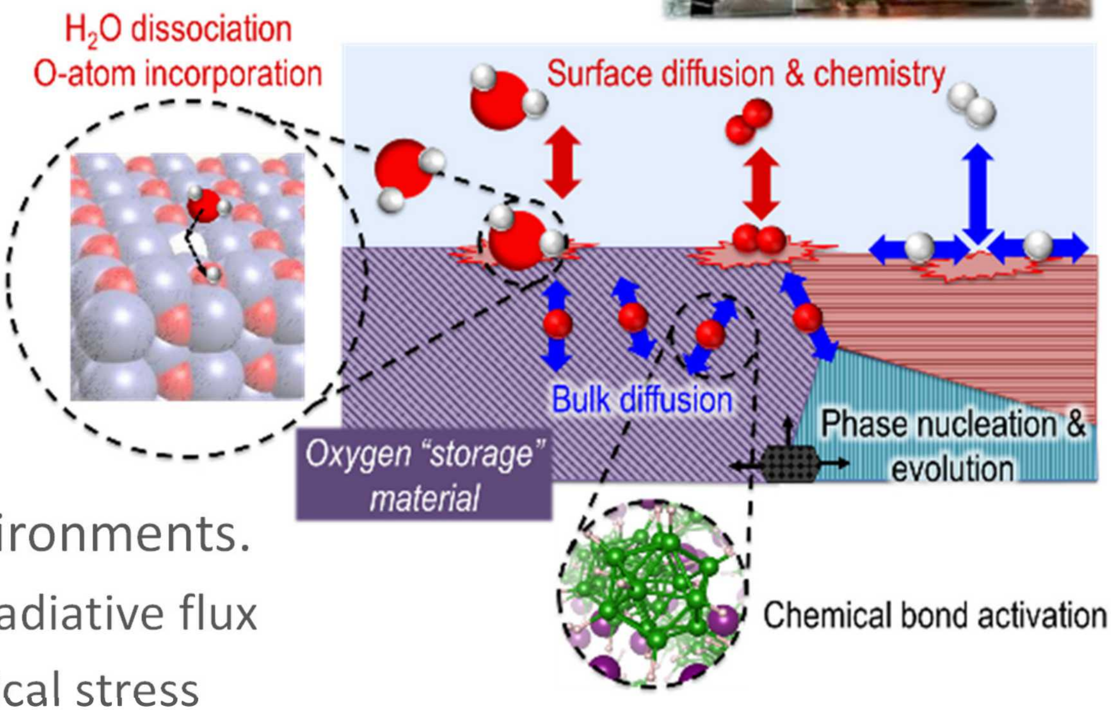

- Will perovskite (Mn) dethrone fluorite (Ce)?

Searching For A Perfect Solar Reactor

- Achieving high conversion efficiency and scalability is challenging.

STC H_2 Materials Theme: Oxygen Exchange And Transport

- Oxygen storage materials with a **twist**.
  - Thermodynamics
  - Kinetics
  - Transport
  - Gas-solid interactions
  - Solid-solid interactions



- Materials in extreme environments.
  - High temperature and radiative flux
  - High thermal and chemical stress

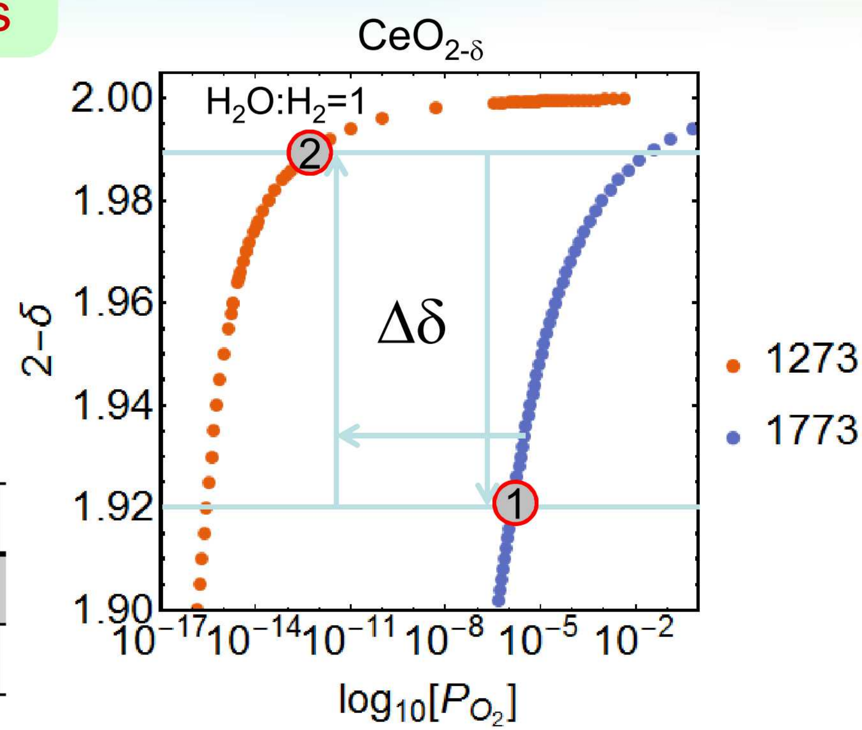
Cycle Thermodynamics: Challenge Process Economics

$\Delta\delta$ at target T_{TR} too small for CeO_2 to meet cost and efficiency targets

$$MO_x \rightarrow MO_{x-\delta} + \frac{\delta}{2} O_2 \quad \text{(1) Reduction}$$

$$MO_{x-\delta} + \delta \cdot H_2O \rightarrow MO_x + \delta \cdot H_2 \quad \text{(2) Oxidation}$$

$$\delta \cdot H_2O \rightarrow \frac{\delta}{2} O_2 + \delta \cdot H_2 \quad \text{(3) Thermolysis}$$



Process metrics (US DOE targets):

H_2 production rate	50-100mt/day
Solar-to-H_2 efficiency	>25%
H_2 production cost (US DOE)	~$3/kg

Desired cycle metrics:

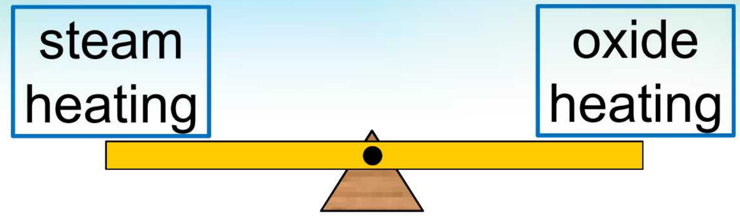
Reduction Temperature (T_{TR})	~1400ºC	
Oxidation Temperature (T_{OX})	~800ºC	
"O" activity in reduction	$\mu_{gas} < \mu_{solid}$	$\mu_{gas} \sim 10^{-6} atm$
"O" activity in oxidation	$\mu_{gas} > \mu_{solid}$	$\mu_{gas} \sim 10^{-13} atm$

Engineering challenge

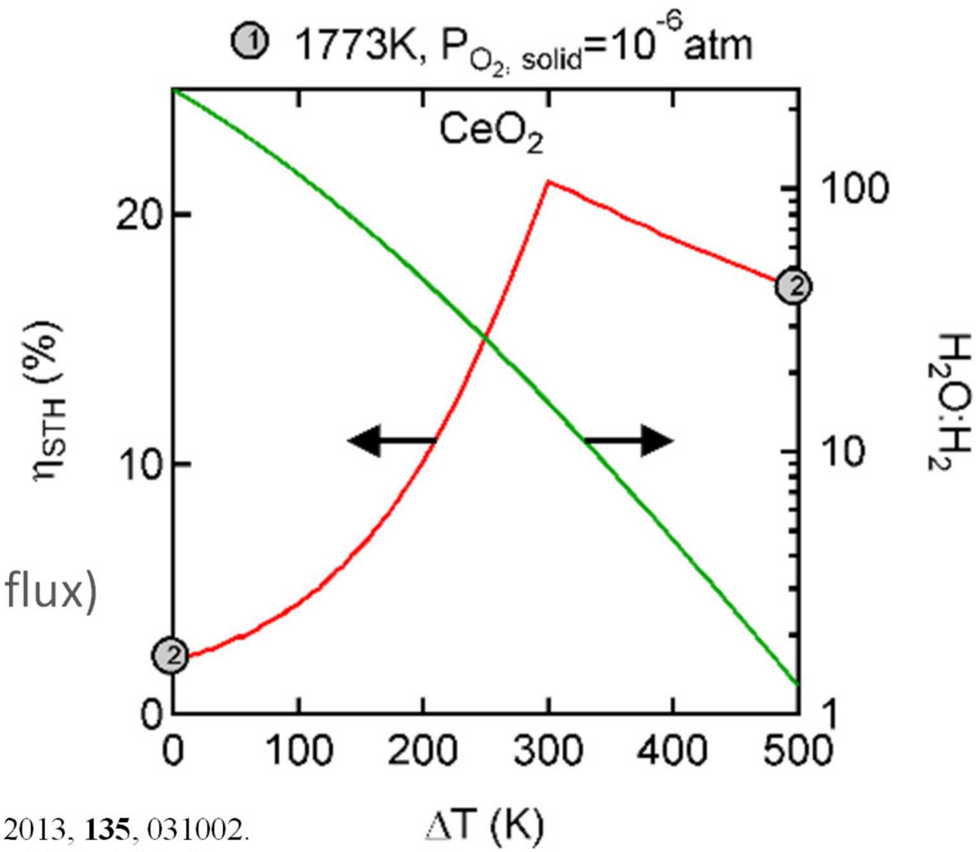
Material challenge

Navigating A Highly Constrained Space

H_2 production rate	50-100mt/day
Solar-to-H_2 efficiency	>25%
H_2 production cost (US DOE)	~$3/kg



- Low reduction temperature.
  - $T_{TR} < 1400\ ^{o}C$
- High H_2 cycle capacity.
  - $\Delta\delta > 0.1 >> CeO_2$
- High conversion.
  - $H_2O:H_2 < 10$
- AND...
  - Fast redox kinetics (match solar flux)
  - Earth abundant (cheap)
  - High durability (stable)



I. Ermanoski, N.P. Siegel, E.B. Stechel, *J. Solar Energy Engineering*, 2013, **135**, 031002.
A.H. McDaniel, *Current Opinion in Green and Sustainable Chemistry*, 2017, **4**, 37–43.

Cycle Thermodynamics: Tradeoffs Between $\Delta\delta$, T_{TR}, and $H_2O:H_2$

spinel

Fe^{2+}/Fe^{3+} systems :

- High redox capacity ($\Delta\delta$>0.1)
- Slow H_2O oxidation kinetics
- Moderate reduction <1400 °C
- Oxide matrix required

fluorite

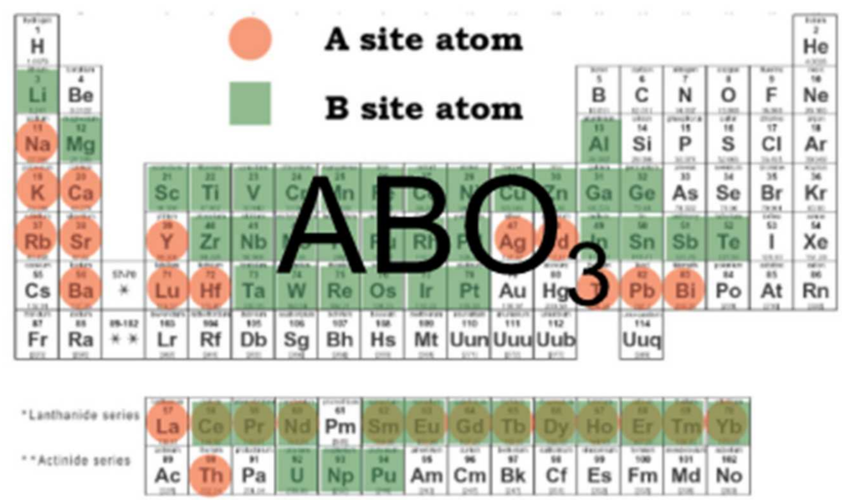
Ce^{3+}/Ce^{4+} systems:

- Low redox capacity ($\Delta\delta$<0.08)
- Fast H_2O oxidation kinetics
- Shallow reduction at 1500 °C
- Durable

perovskite

$TM^{2+}/TM^{3+}/TM^{4+}$ systems:

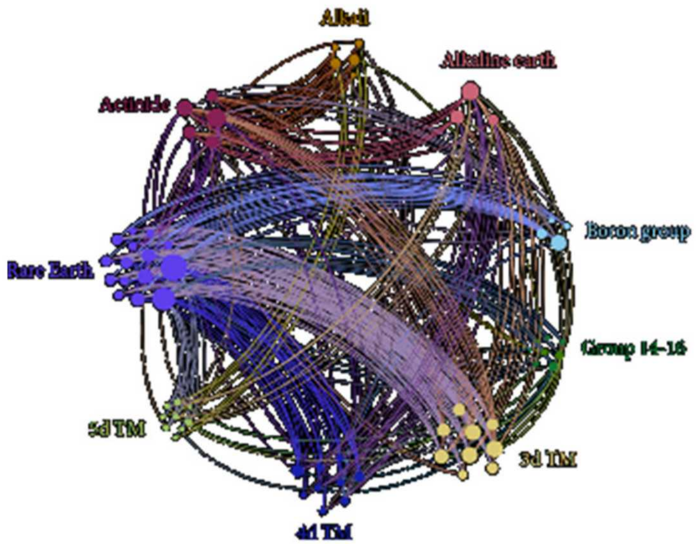
- High redox capacity ($\Delta\delta$>0.1)
- Promising H_2O oxidation kinetics
- Deep reduction <1400 °C
- Vast material space!



DOE is very interested in a “Materials Genome” approach to material discovery and optimization

Perovskite Discovery: Identify Them, Make Them, Test Them

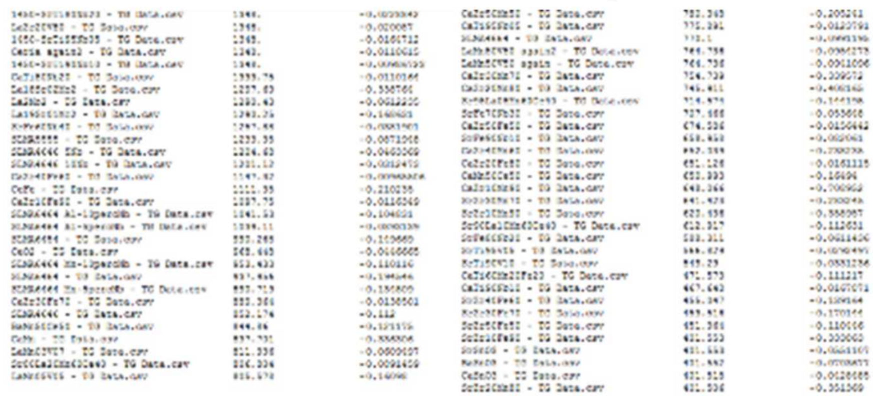
- High throughput DFT.
  - 11,000 calculations



  - 139 possible ABO_3 WS
  - Existence & $\Delta E_{f,V_O}$ (2-5eV)
  - Tested 20 compounds

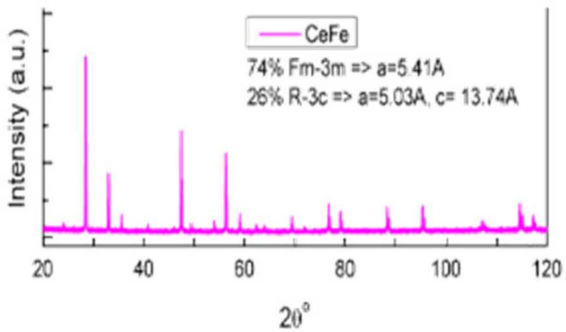
A. A. Emery, J. E. Saal, S. Kirklin, V. I. Hegde, C. Wolverton, *Chemistry of Materials*, 2016, **28**, 5621–5634.

- Chemical intuition.
  - 15 elements (Al, Ba, Ca, Ce, Fe, La, Mn, Mo, Nb, O, Sn, Sr, Ti, V, and Zr)
  - Ox. state ($Ce^{3+/4+}$, $Fe^{2+/3+}$, $Mn^{2+/3+/4+}$, $Mo^{3+/4+}$, $Sn^{2+/4+}$, $Ti^{2+/4+}$, $V^{4+/5+}$)
  - Tested ~200 compounds

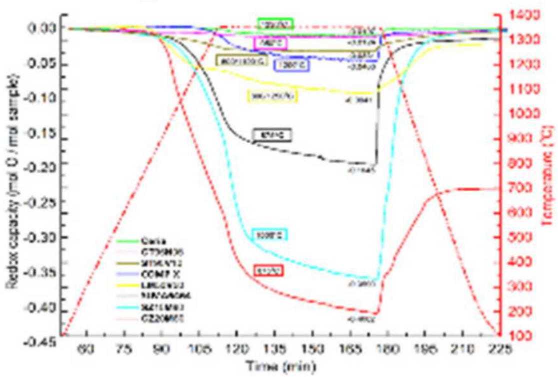


Perovskite Discovery: Identify Them, Make Them, Test Them

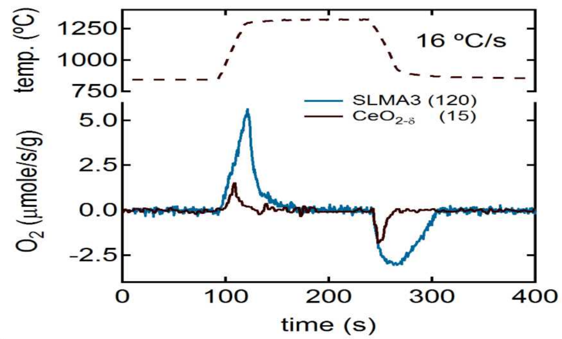
- Crystallography.
  - Phase purity



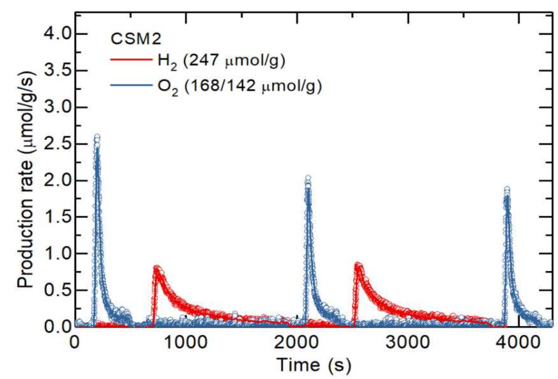
- Thermal analysis.
  - O_2 Redox activity



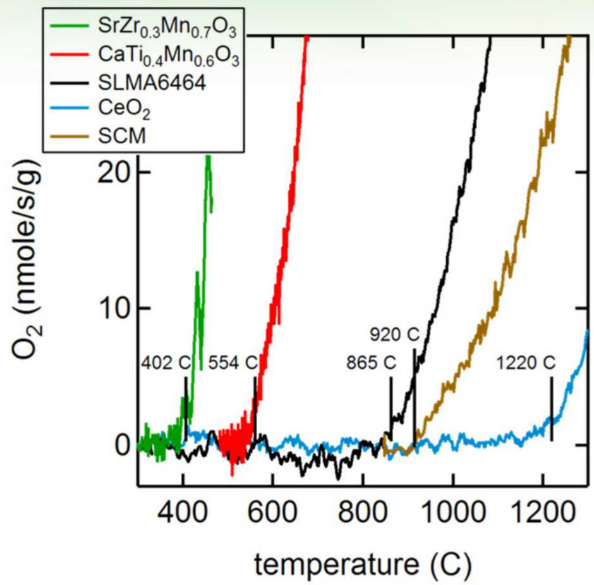
- Flow reactor.
  - O_2 Redox dynamics

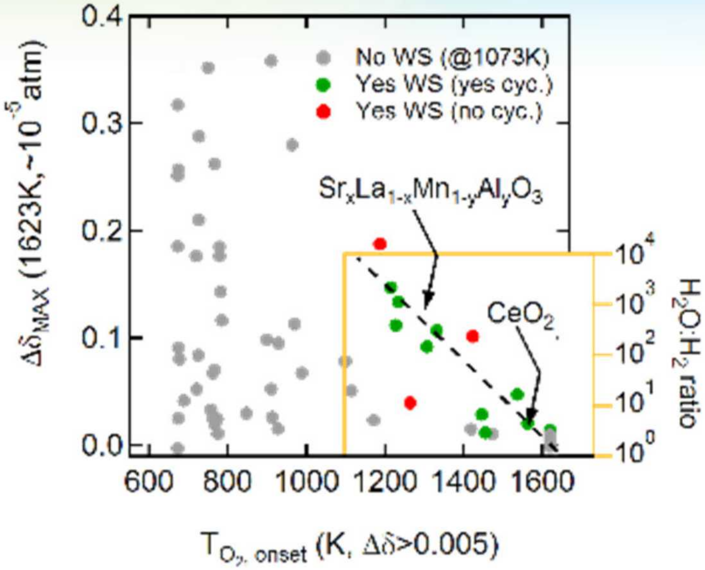


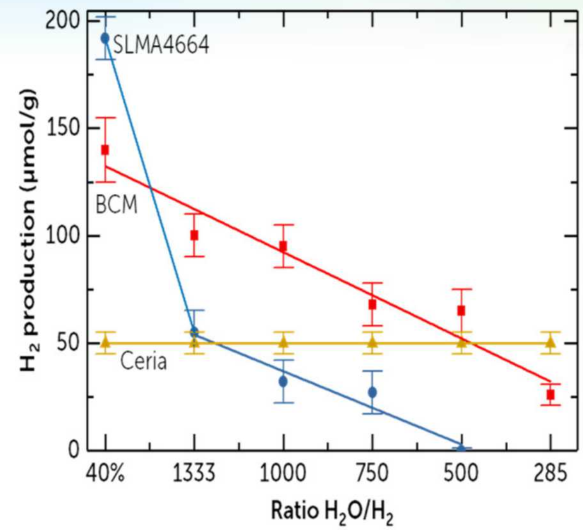
- Flow reactor.
  - Water splitting



Perovskite Discovery: Key Observations (Sum Of All ~~Fears~~ Knowledge)

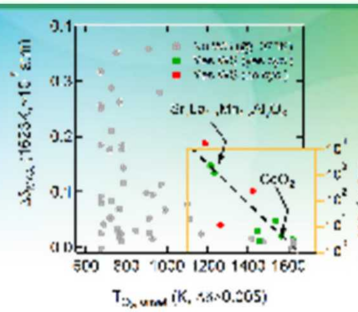






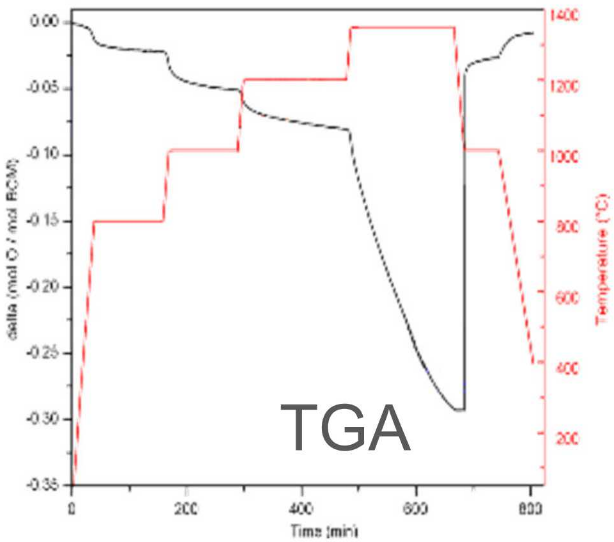
- Onset temperature for O_2 evolution correlates to ΔH_{RED} ($\Delta E_{f,Vo}$).
- Onset temperature for O_2 evolution **ALSO** correlates to WS favorability.
  - WS inactive at T_{ONSET} <1100 °C; High H_2O:H_2 ratio at T_{ONSET} <1400 °C
- Desired thermodynamic properties bounded by **KNOWN** materials.
  - SLMA and CeO_2

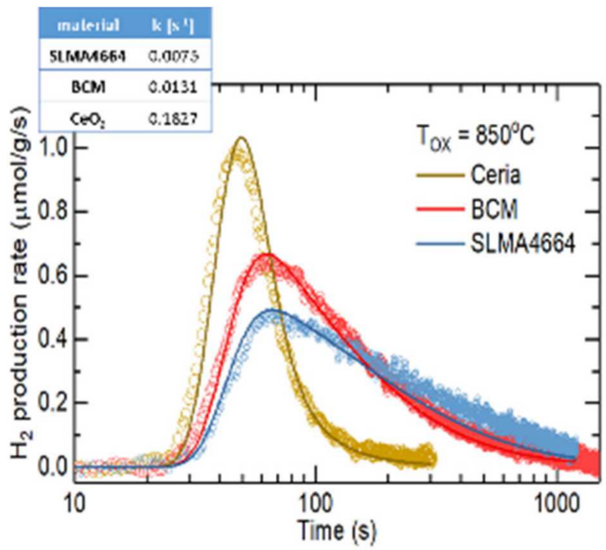
A New Perovskite: $Ba_4Ce_xMn_{1-x}O_{12}$ (BCM)

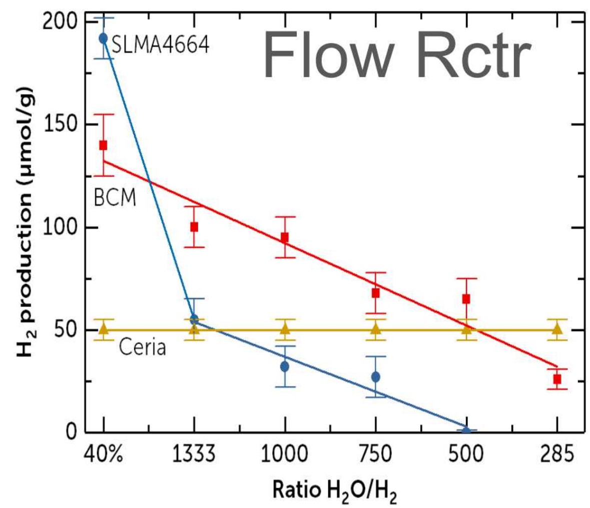


Significant O_2 loss ~1200 °C

Splits water "better" than SLMA

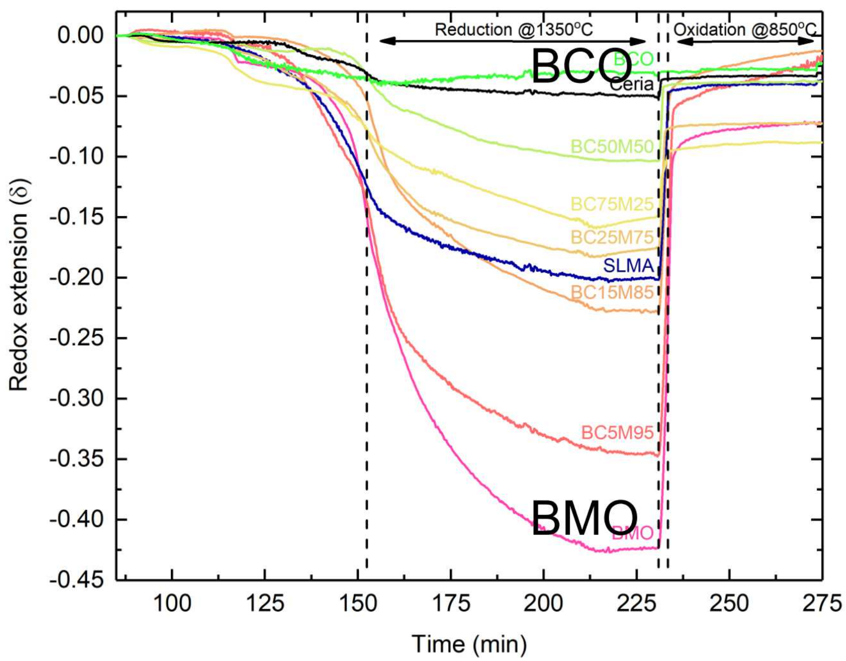


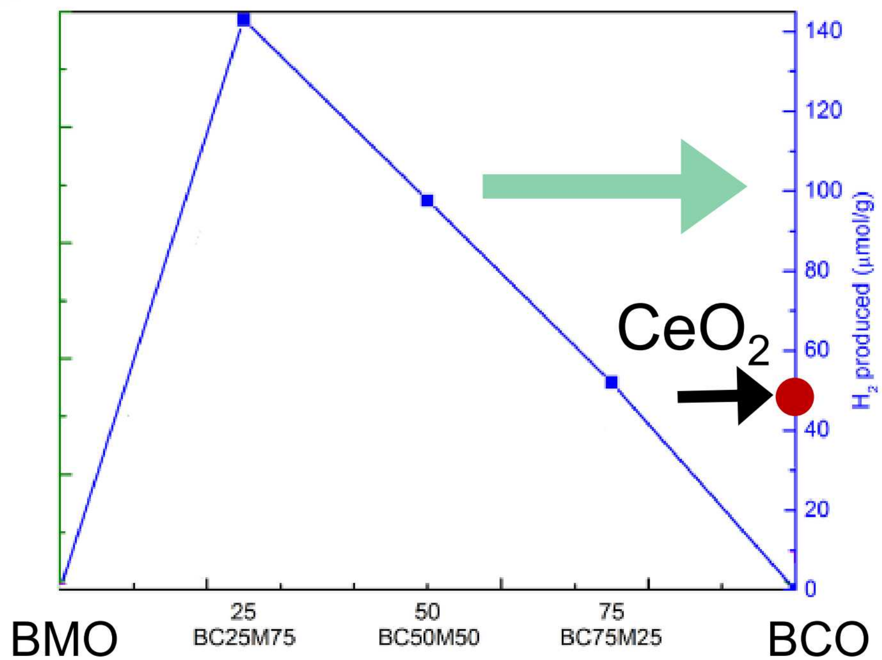




- BCM is unique when compared to known Mn-based STCH perovskites.
  - Reduces at **LOW T_{TR}** & oxidizes at **LOW $H_2O:H_2$ ratio**
  - Cerium substitutes on the **B-SITE**

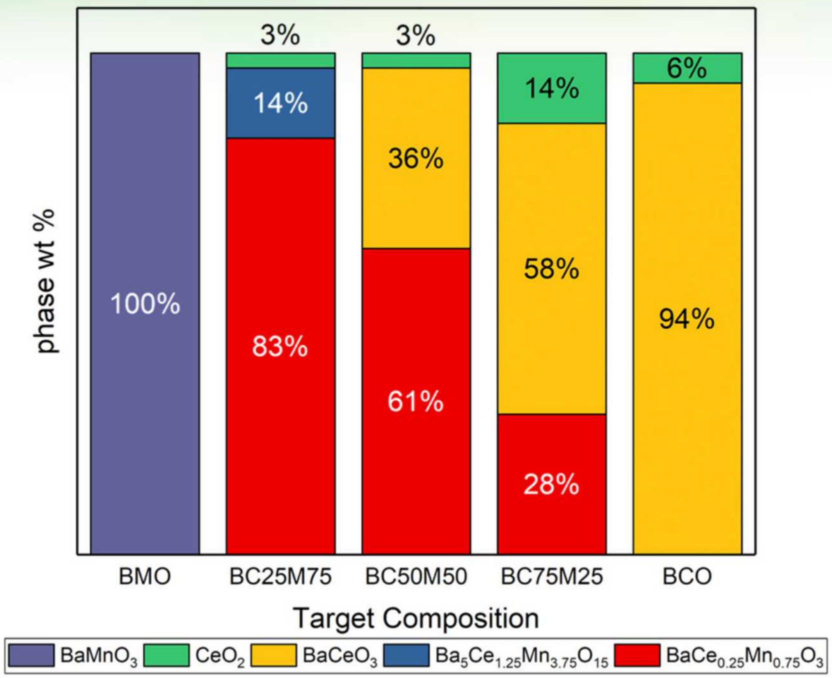
Ba-Ce-Mn-O Demonstrates Mn-dependent O_2 Redox And WS Behavior

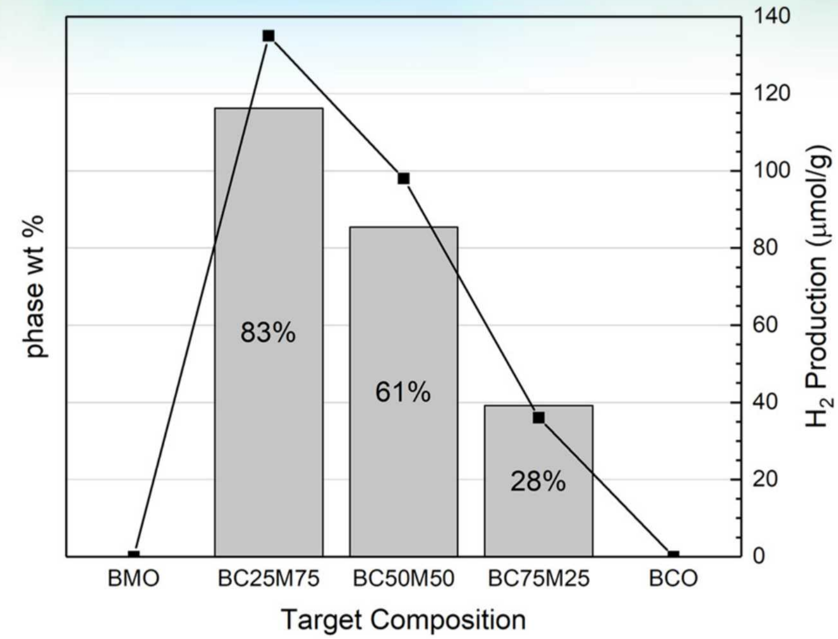




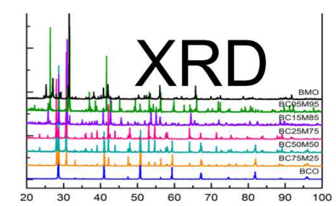
- O_2 redox extent determined by B-site Mn composition.
  - > Mn:Ce = > Δδ
- H_2 production capacity peaks at B-site Mn = 0.75.
  - T_{TR} = 1350 °C, T_{OX} = 850 °C

Ba-Ce-Mn-O Is A Mixed Phase System

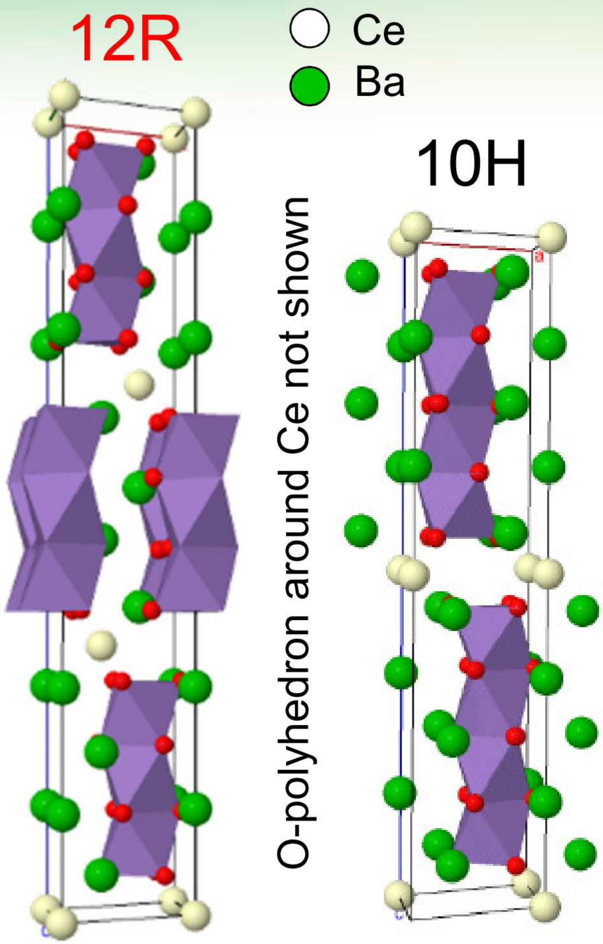


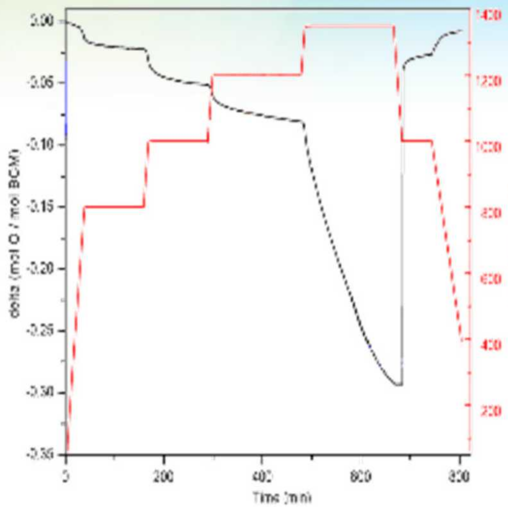


- Phases present in "as-synthesized" material are dependent on target composition.
  - CeO_2, $BaCeO_3$, Ba-Ce-Mn-O polytypes
- WS-active phase is a **LINE** compound ($BaCe_{0.25}Mn_{0.75}O_3$)

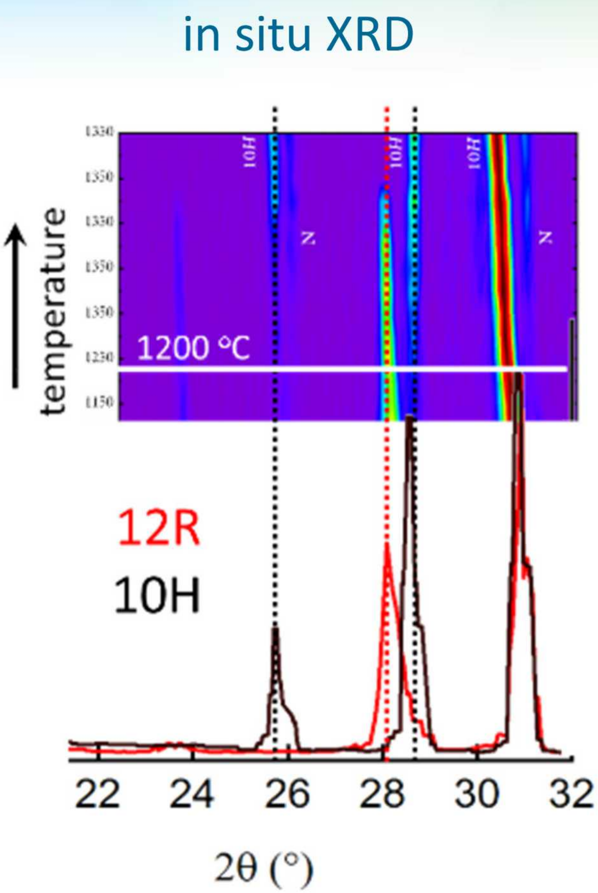


$Ba_4CeMn_3O_{12}$...Or Is It...$Ba_5Ce_{1.25}Mn_{3.75}O_{15}$?



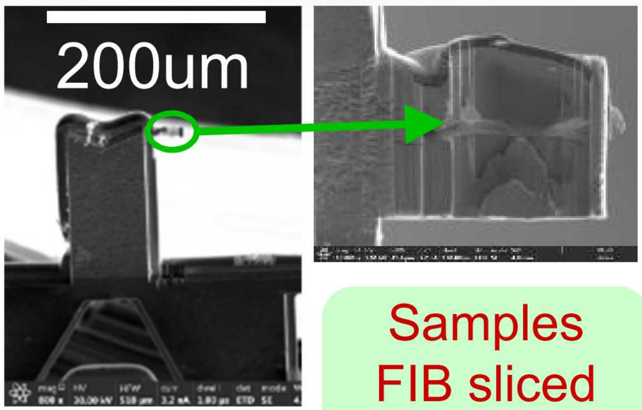


Significant O_2 loss ~1200 °C accompanied by **POLYTYPE** phase transition

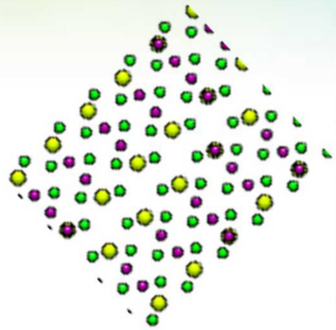


- We discovered nonstoichiometric behavior in this system.

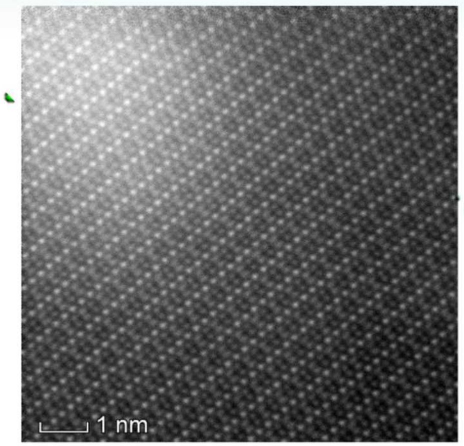
Core-hole Spectroscopy: Reveal Redox Behavior With EELS

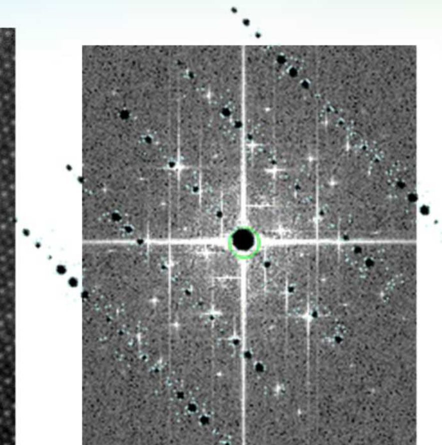


Samples FIB sliced for HRTEM



Ba
Ce
Mn

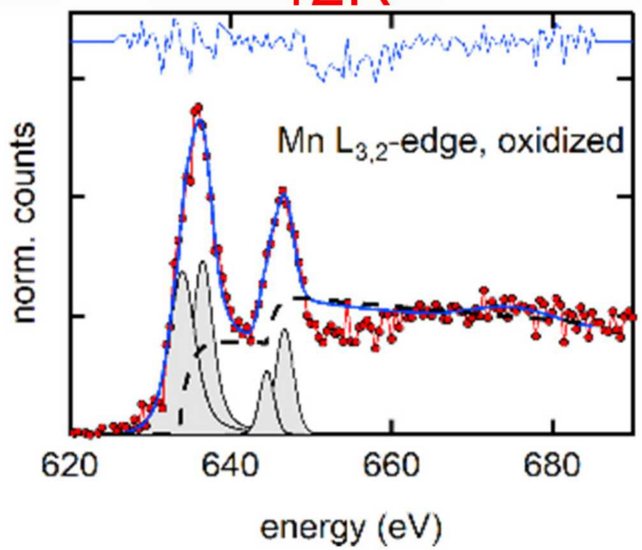




- Probe electron DOS for 12R and 10H "quenched" phases.
  - Discover where electrons go when O atoms vanish
  - Does cerium participate in redox chemistry
- Derive fundamental understanding of redox behavior.
  - Explain known materials
  - Engineer better materials

EELS Reveals: Manganese Oxidation State Changed?

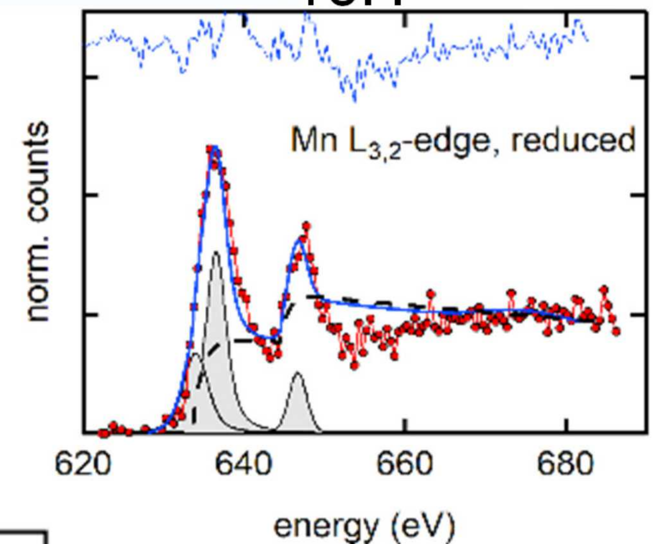
12R



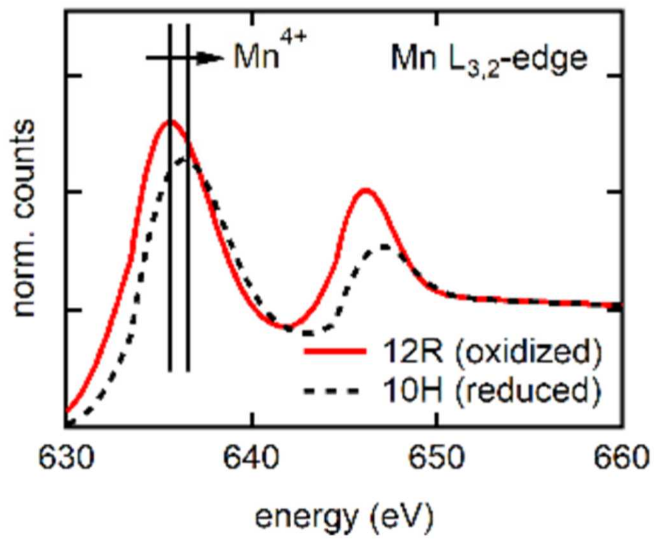
e- charge transferred to hybridized 3d system decreases hole DOS

branching ratio = Mn **REDUCED**

10H



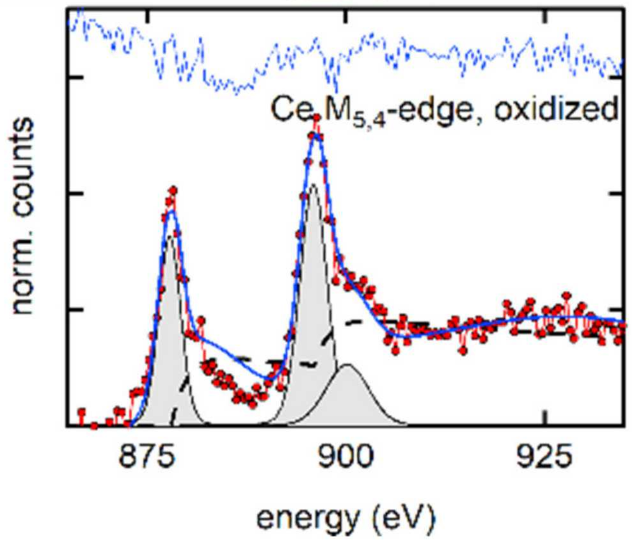
Ab inito theory required to fully interpret spectra



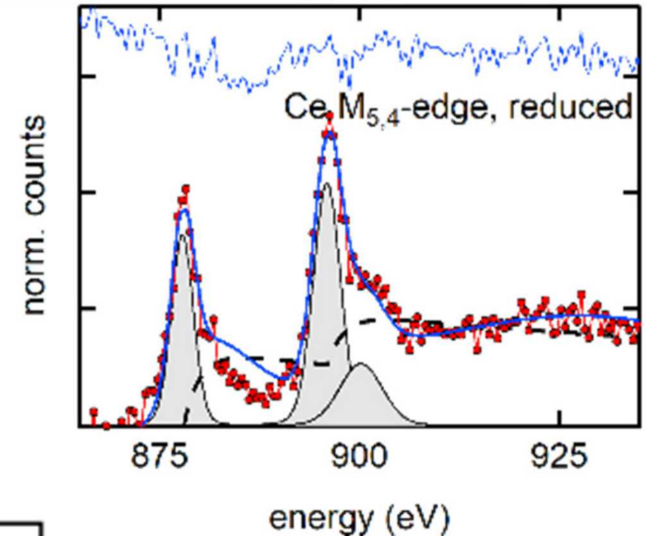
Peak shift = Mn **OXIDIZED**

EELS Reveals: Cerium Not Likely Redox Active On B-site

12R

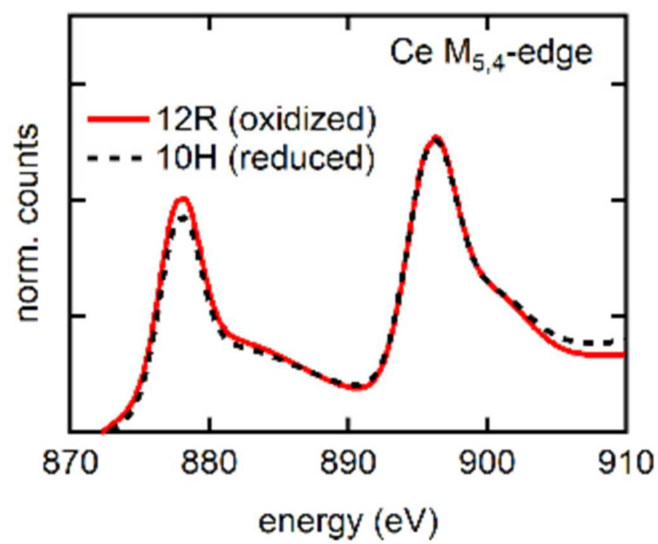


10H



4f system does not show significant changes in hole DOS

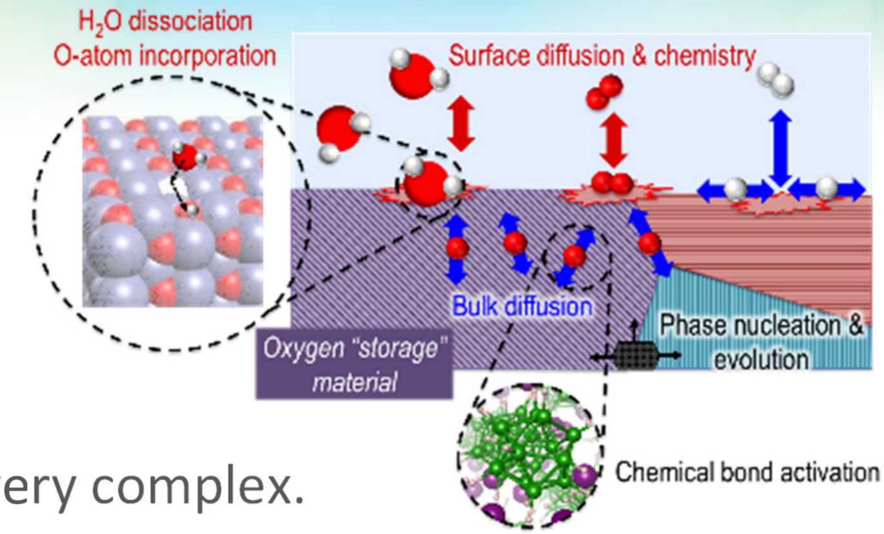
Ab inito theory required to fully interpret spectra



4f DOS is a very strong indicator of Ce oxidation state

Much Of The STCH Perovskite Story Yet To Be Told

SLOWLY marching towards developing holistic design rules for STCH materials based on first principles



- Structural transformations are very complex.
  - Exploit large entropy changes to promote water splitting favorability
  - Exploit high $[V_O^{\bullet\bullet}]$ defect concentration to promote high H_2 production
  - Exploit crystallography and solid-solid phase transitions
  - **Line compound and polytypes observed in WS with BCM**
- Ideal thermodynamics lie between CeO_2 and SLMA.

  - (AE,RE)Mn-based perovskites other than SLMA show promise
  - Balance between $\Delta\delta$ ($\uparrow$ H_2 capacity) and ΔH_R ($\downarrow$ T_{TR}) and H_2O:H_2

HydroGEN is an Energy Materials Network (EMN)

https://energy.gov/eere/energy-materials-network/energy-materials-network

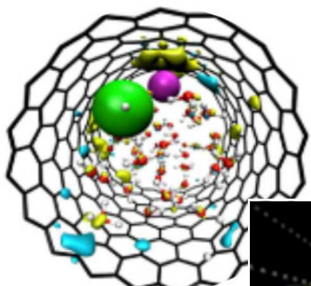
HydroGEN Advanced Water Splitting Materials

NREL, Berkeley Lab, Sandia National Laboratories, INL Idaho National Laboratory, Lawrence Livermore National Laboratory, SRNL

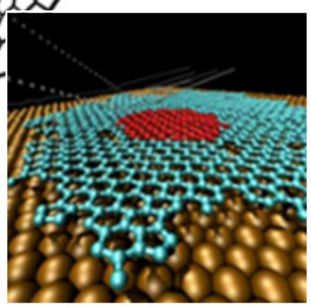
Core Labs

Comprising more than 80 unique, world-class capabilities/expertise in materials theory/computation, synthesis, and characterization & analysis:

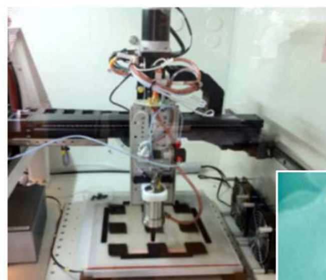
Materials Theory/Computation	Advanced Materials Synthesis	Characterization & Analysis



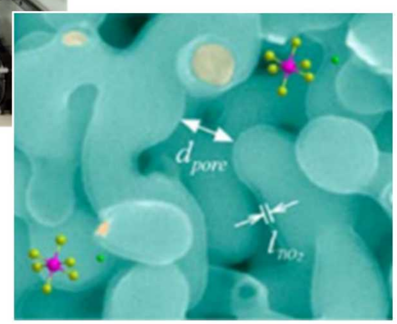
Bulk and interfacial models of aqueous electrolytes



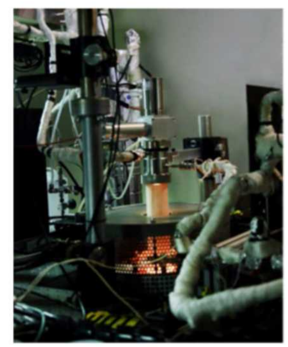
LAMMPS classic molecular dynamics modeling relevant to H_2O splitting



High-throughput spray pyrolysis system for electrode fabrication



Conformal ultrathin TiO_2 ALD coating on bulk nanoporous gold



Stagnation flow reactor to evaluate kinetics of redox material at high-T

TAP reactor for extracting quantitative kinetic data

HydroGEN fosters cross-cutting innovation using ***theory-guided applied materials R&D*** to advance all emerging water-splitting pathways for hydrogen production

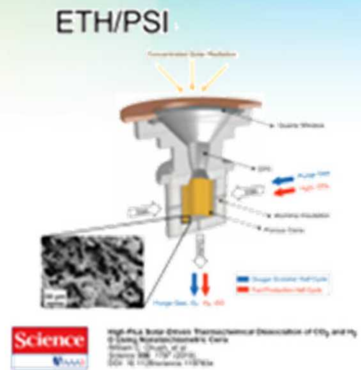
Efficiency Drives Reactor Development

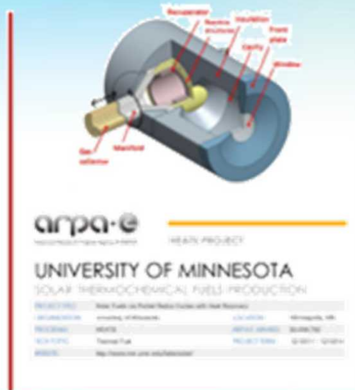
Table 3.1.7 Technical Targets: Solar-Driven High-Temperature Thermochemical Hydrogen Production [a]

Characteristics	Units	2011 Status	2015 Target	2020 Target	Ultimate Target
Solar-Driven High-Temperature Thermochemical Cycle Hydrogen Cost [b]	\$/kg	NA	14.80	3.70	2.00
Chemical Tower Capital Cost (installed cost) [c]	\$/TPD H_2	NA	4.1MM	2.3MM	1.1MM
Annual Reaction Material Cost per TPD H_2 [d]	\$/yr.-TPD H_2	NA	1.47M	89K	11K
Solar to Hydrogen (STH) Energy Conversion Ratio [e,f]	%	NA	10	20	25%
1-Sun Hydrogen Production Rate [g]	kg/s per m^2	NA	8.1E-7	1.0E-5	2.1E-6

Efficiency is a key metric for US R&D

High cost of solar collection



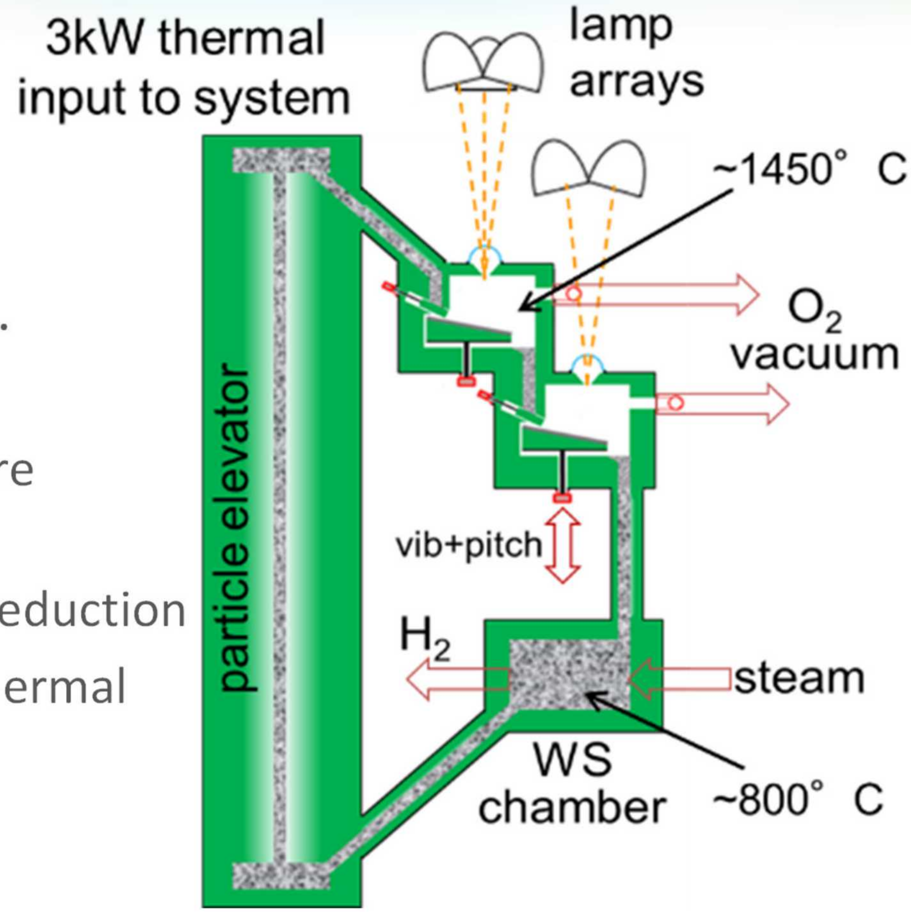


- Many different reactor designs have been proposed.
- Accurate models required to evaluate reactor performance at scale.
  - Validated by subscale systems and prototype performance

J. E. Miller, A. H. McDaniel, M. D. Allendorf, *Advanced Energy Materials*. **4**, 1300469 (2014).

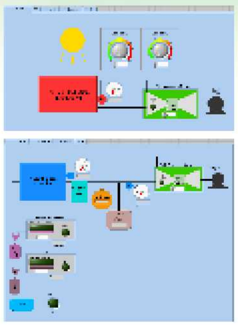
Cascading Pressure Receiver Reactor (CPR2)

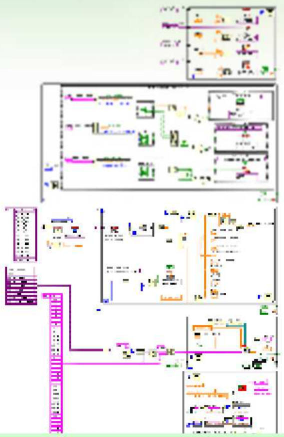
- DOE Project goals for reactor.
  - 8 hours continuous operation
  - Greater than 3 liters of H_2
- High-efficiency attributes of CPR2.
  - Continuous use of solar resource
  - Pressure cascade and temperature separation
  - Efficiency advantage of vacuum reduction
  - Efficiency advantage of non-isothermal operation
  - Only particles thermally cycled



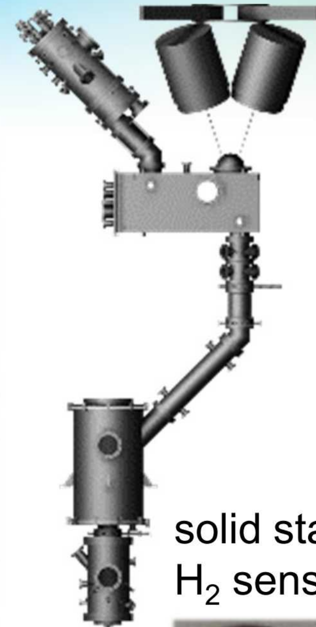
I. Ermanoski, *International Journal of Hydrogen Energy* **39**, 13114 (2014), doi:10.1016/j.ijhydene.2014.06.143.
I. Ermanoski, J. E. Miller, M. D. Allendorf, *Physical Chemistry Chemical Physics*. **16**, 8418 (2014).
N. P. Siegel, J. E. Miller, I. Ermanoski, R. B. Diver, E. B. Stechel, *Ind. Eng. Chem. Res.* **52**, 3276–3286 (2013).
I. Ermanoski, N. P. Siegel, E. B. Stechel, *J. Solar Energy Engineering*. **135**, 031002 (2013).

From Concept To Operation In 2 Years





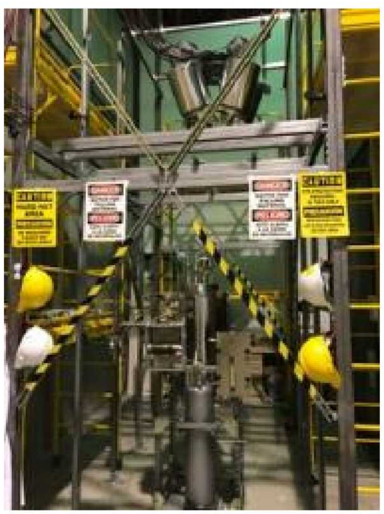
Engineering & Safety reviews complete, authorized for full operation

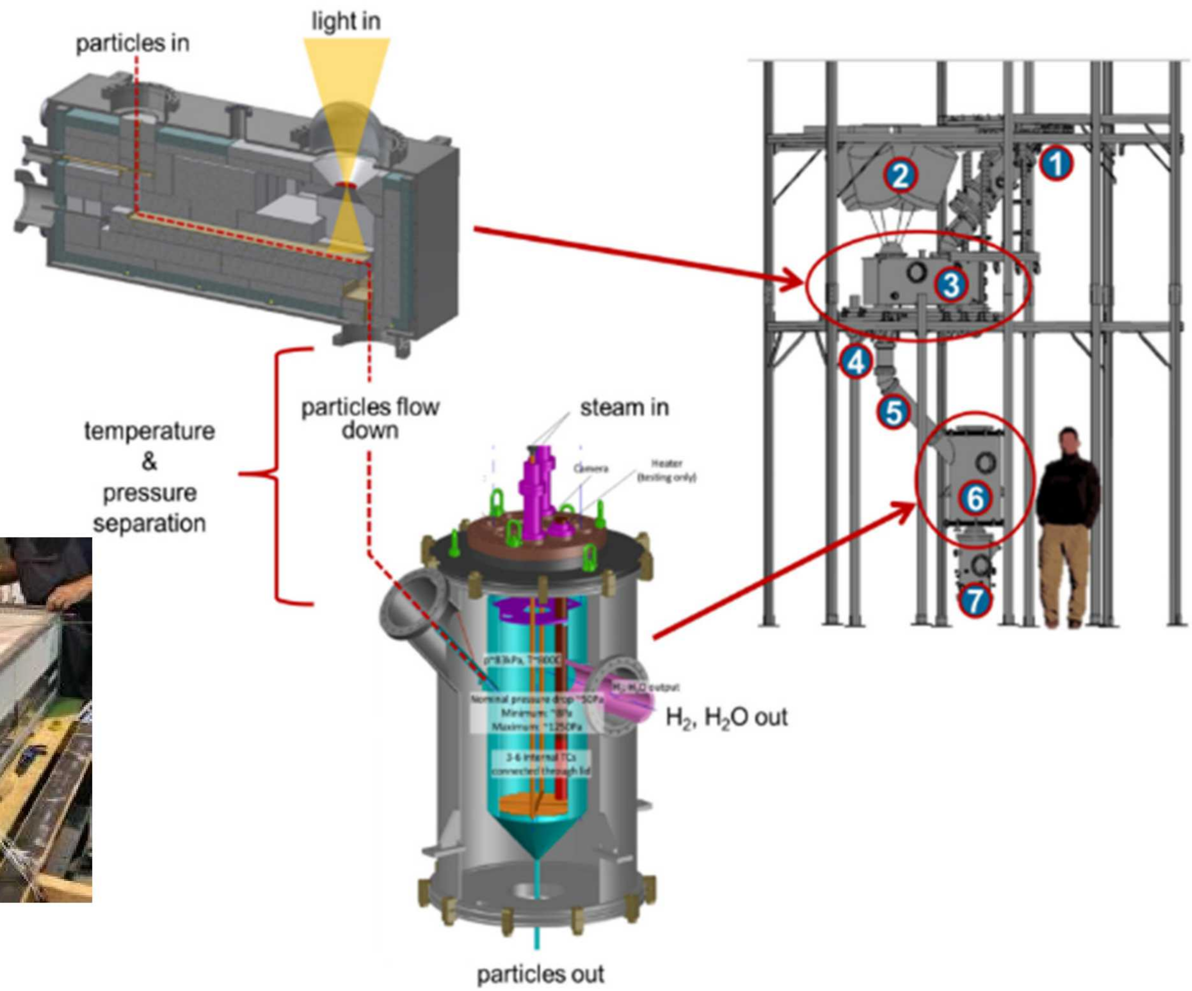


- STCH hydrogen production reactor facility specifications.
  - Vacuum system with ~10^{-4} atm base pressure at 1700 K cavity temperature
  - 10 kW_{el}, four-lamp solar simulator (~3.4 kW_{th} at cavity aperture)
  - Instrumented with ~100 TC's, optical pyrometer, motorized particle flow control, gas flow and pressure sensing/control, Sandia's MIS H2 sensor, CCTV system, etc
  - DAC is LabVIEW-based and provides measurement & control through custom GUI

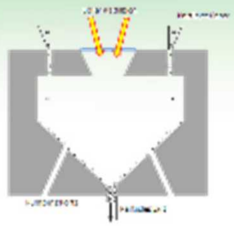
Major System Components

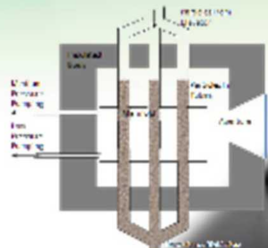
Result of a multidisciplinary collaboration between professional engineers (and one physicist) from Sandia, DLR, and Bucknell University

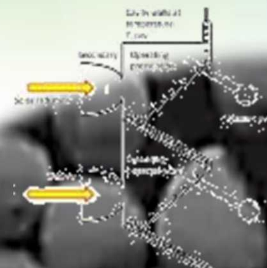


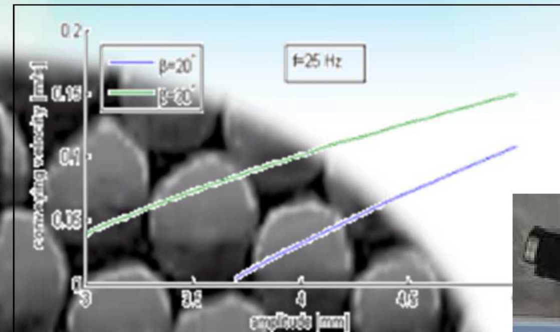


Designing the Solar Receiver



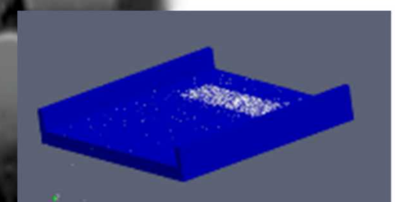


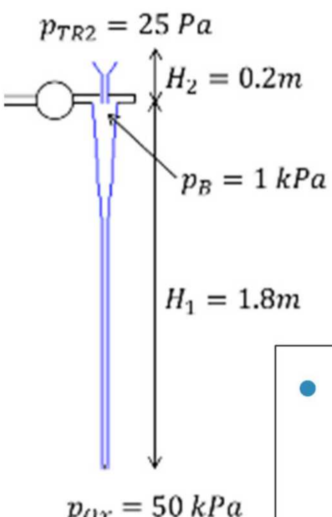


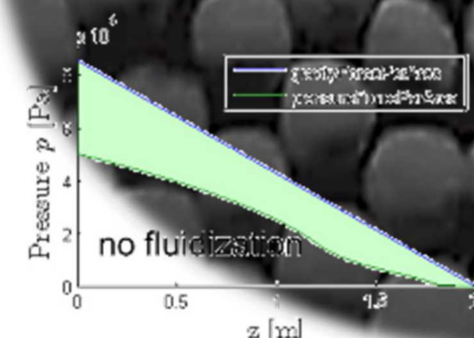


- Solar interface.
  - Direct particle irradiation

$$\frac{dp}{dz} = -\frac{\dot{m}_g}{A(z)}\frac{RT}{pMD_p}\frac{1-\phi}{\phi^3}\left[\frac{150(1-\phi)\mu}{f_c(Kn)D_p} + 1.75\frac{\dot{m}_g}{A(z)}\right]$$







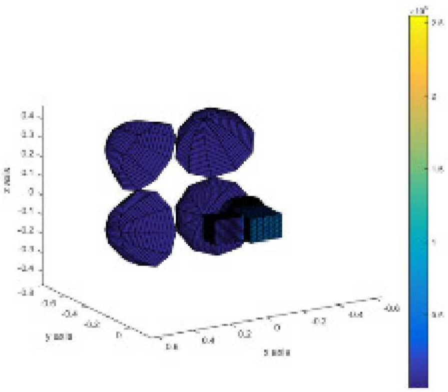
- Particle flow control.
  - Valves, vibrating plates, actuated drives

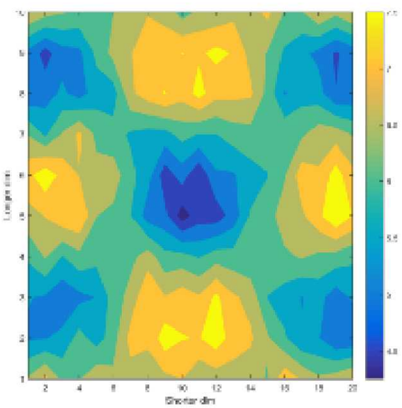
- Pressure separation.
  - Particle diameter and mass
  - Bed permeation and fluidization

Key design criteria established by detailed modeling when necessary

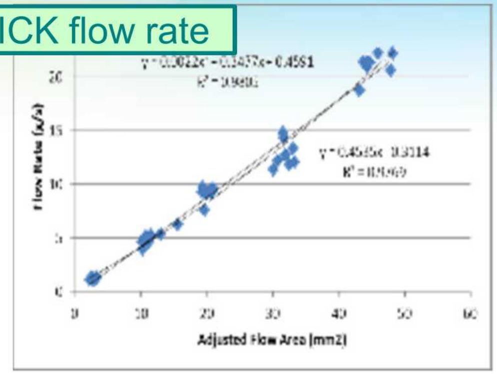
Examples Of Many Design Validation Activities

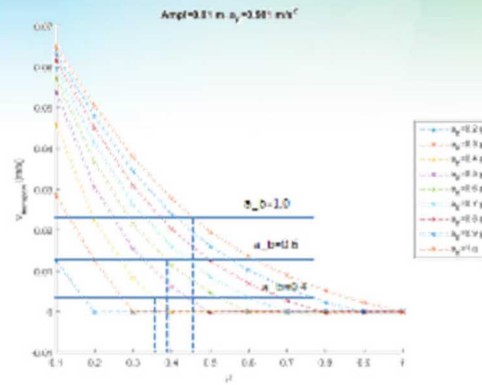
calculate flux on particles



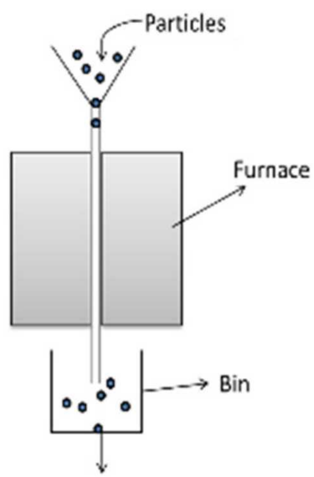


calibrate SLIP-STICK flow rate

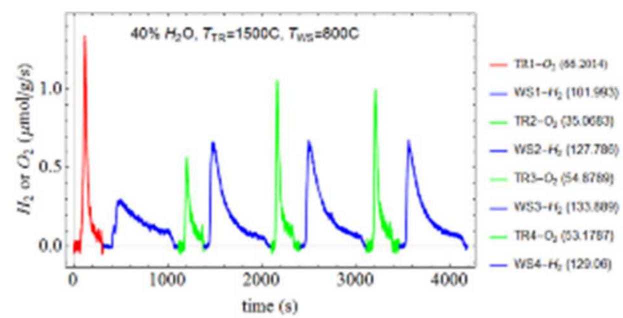


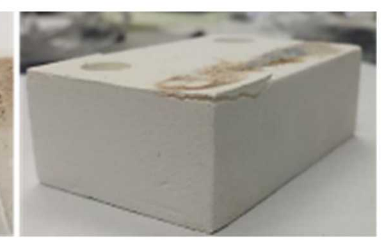


evaluate particle flow at high T



test chemical & thermal stress on materials



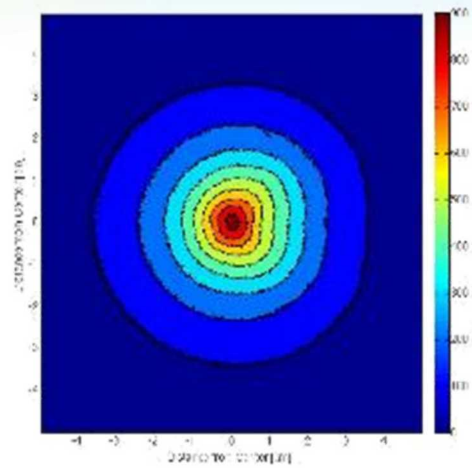


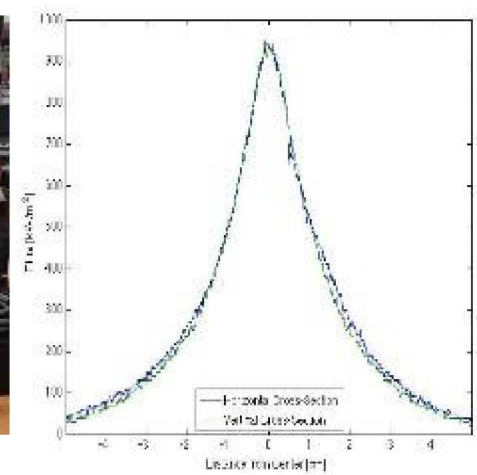
Qualify design choices to mitigate risk of CPR2 failure

Solar Simulator Powers CPR2

J. P. Roba and N. P. Siegel, *Solar Energy*, 2017, **157**, 818–826.0

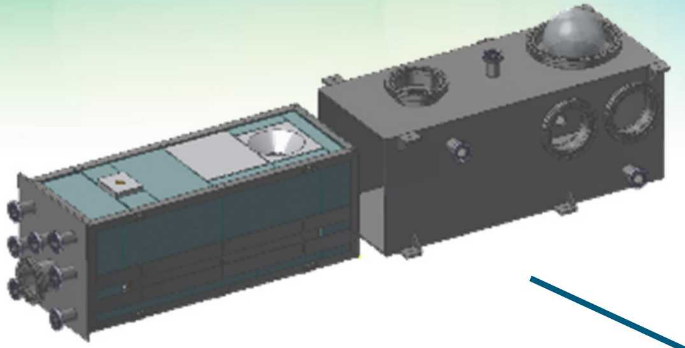
- Designed in collaboration with Bucknell University.
  - Each module houses a 2.5 kW short-arc Xe bulb
  - Each module independently focused into the CPR2 receiver aperture
- Design validated by flux mapping combined with ray tracing calculations.

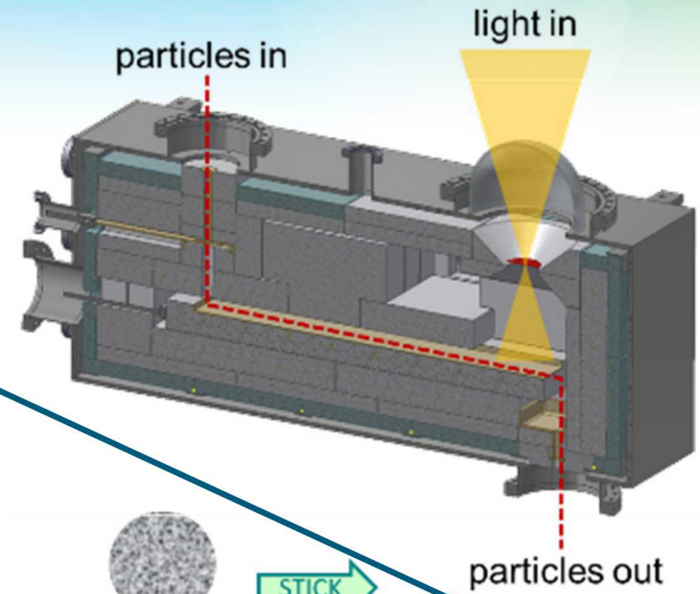




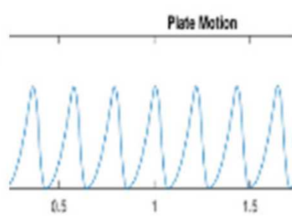
Provide 3.4 kW_{th} of simulated concentrated solar power into aperture

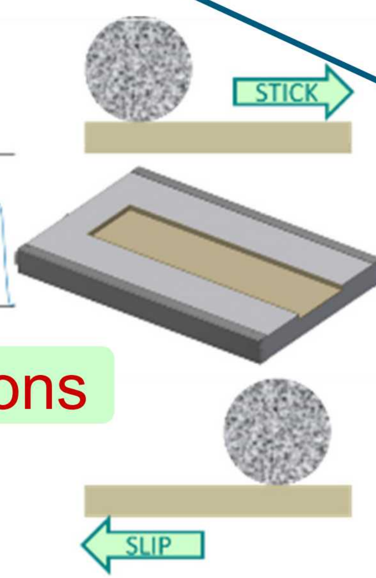
Ultra-high Temperature Solar Receiver





- Designed in collaboration with DLR and Bucknell University.
  - High vacuum, P_{TR} <.0001 atm
  - Radiant cavity, T_{wall} = 1500 °C
  - Direct illumination of particles
  - Control particle flow rate and particle irradiation time





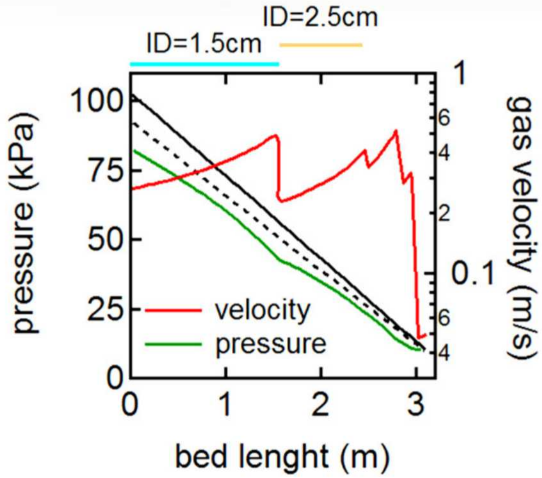
Precise control of oxide reduction conditions

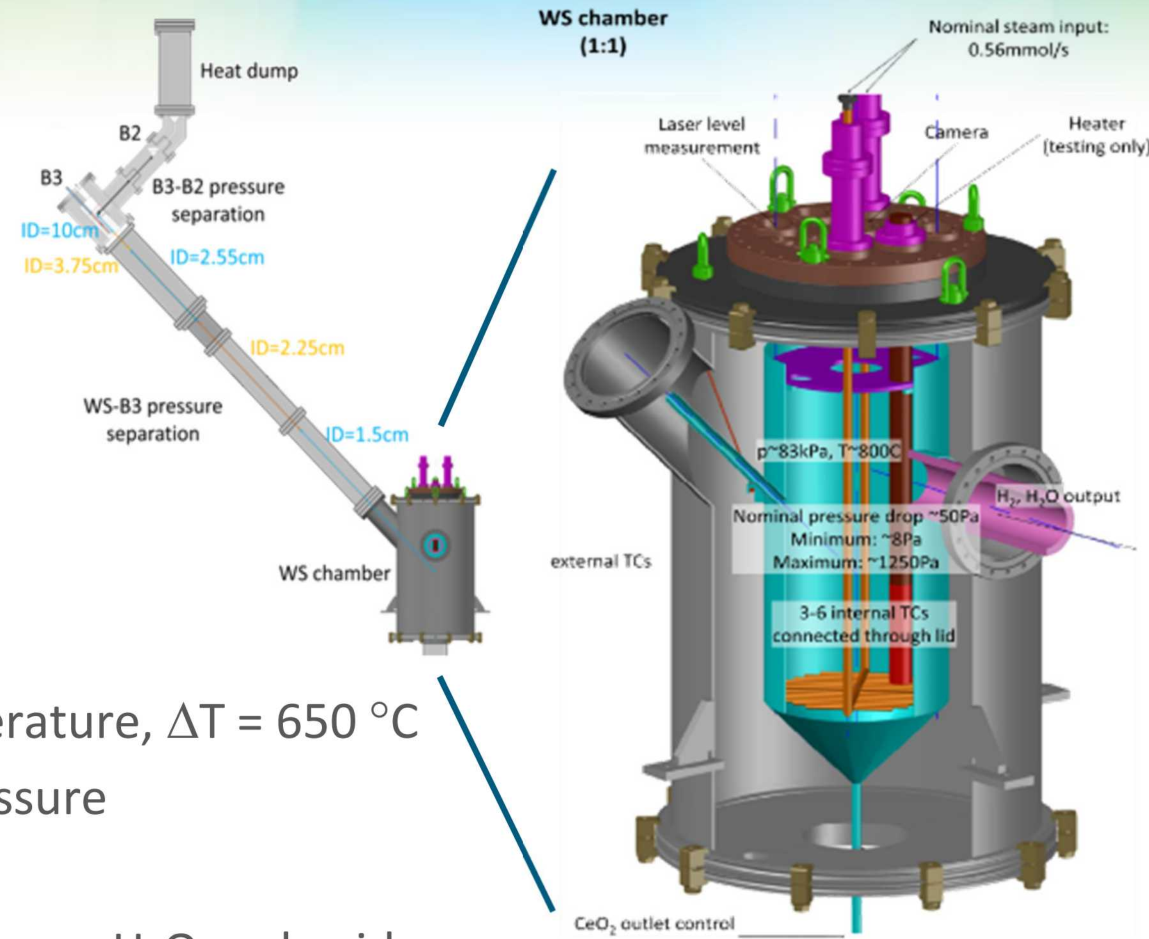
- Design validated by numerical models, ray tracing, particle flow tests, etc...

A. Singh, J. Lapp, J. Grobbel, S. Brendelberger, J. P. Reinhold, L. Olivera, I. Ermanoski, N. P. Siegel, A. McDaniel, M. Roeb and C. Sattler, *Solar Energy*, 2017, **157**, 365–376.

Pressure Separation And Water Splitting Chamber

1700 × pressure reduction without fluidization of moving particle bed

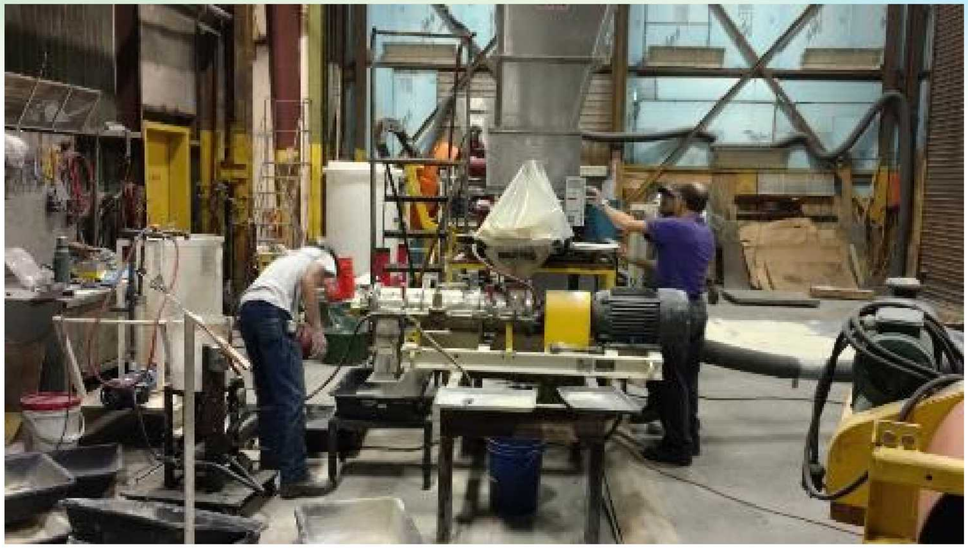




- Designed by Sandia.
  - Quench particle temperature, $\Delta T = 650$ °C
  - Stand off 0.84 atm pressure
  - Separate O_2 from H_2
  - Long contact time between H_2O and oxide

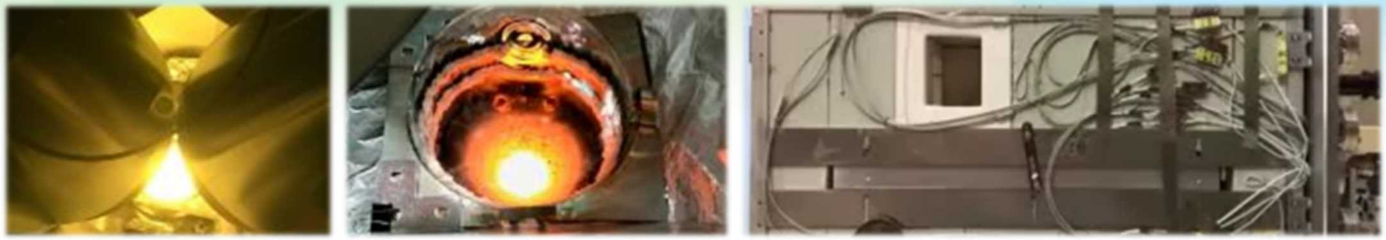
Increased H_2 production efficiency with pressure separation and countercurrent flow between H_2O and oxide

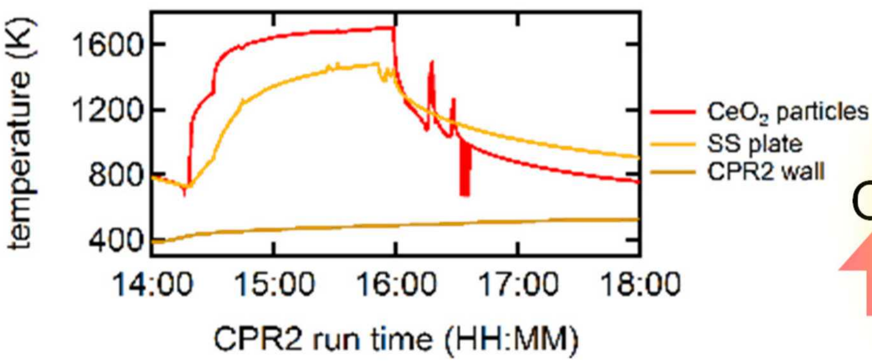
Acquired 150 kg CeO_2 For CPR2 Demonstration

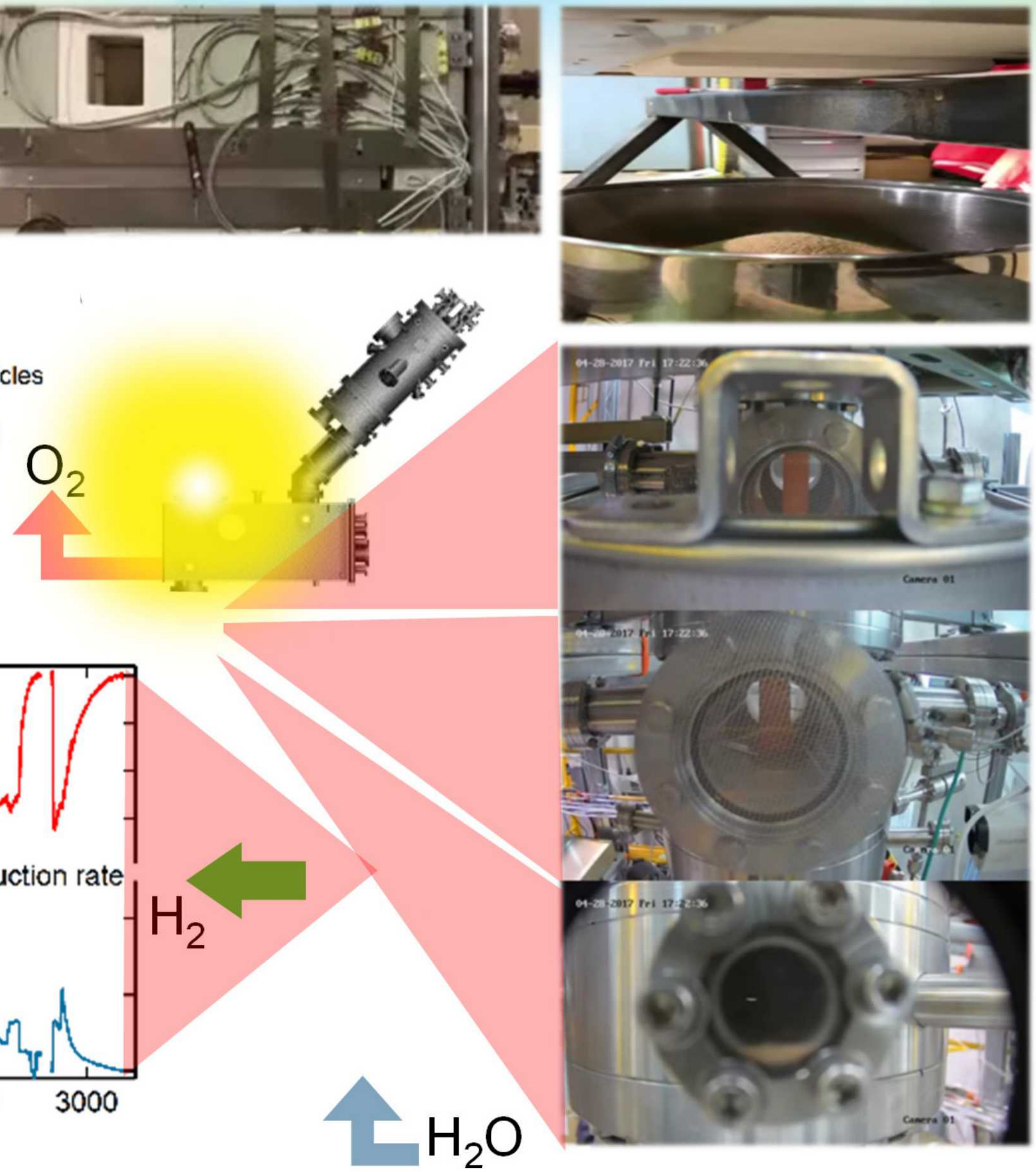


- Manufacturing **ODYSSEY**.
  - Raw powder acquired from CA supplier
  - Pelletized in PA
  - Calcined in OH
  - Quality control tested in CO
  - Shipped to NSTTF SNL/NM
- Particle size distribution critical (300±200 µm).

Marching Towards Solar H_2 Production At Scale

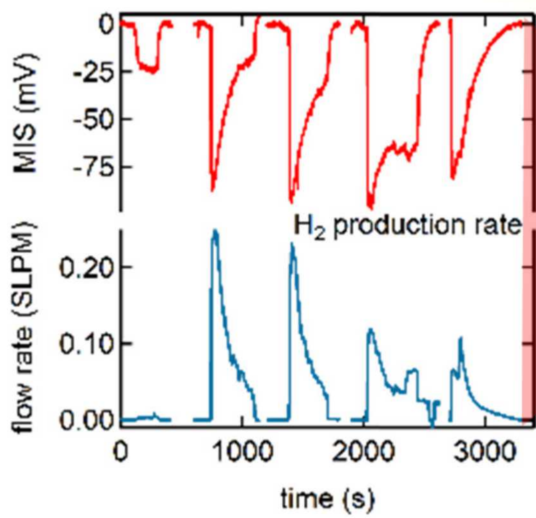




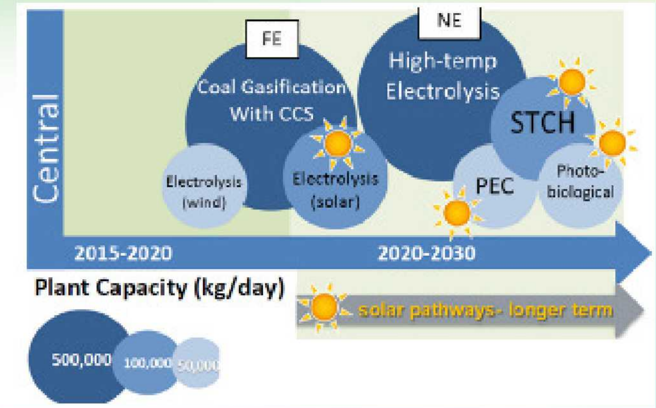


T_{TR}~1700 K

0.25 SLPM peak H_2 rate

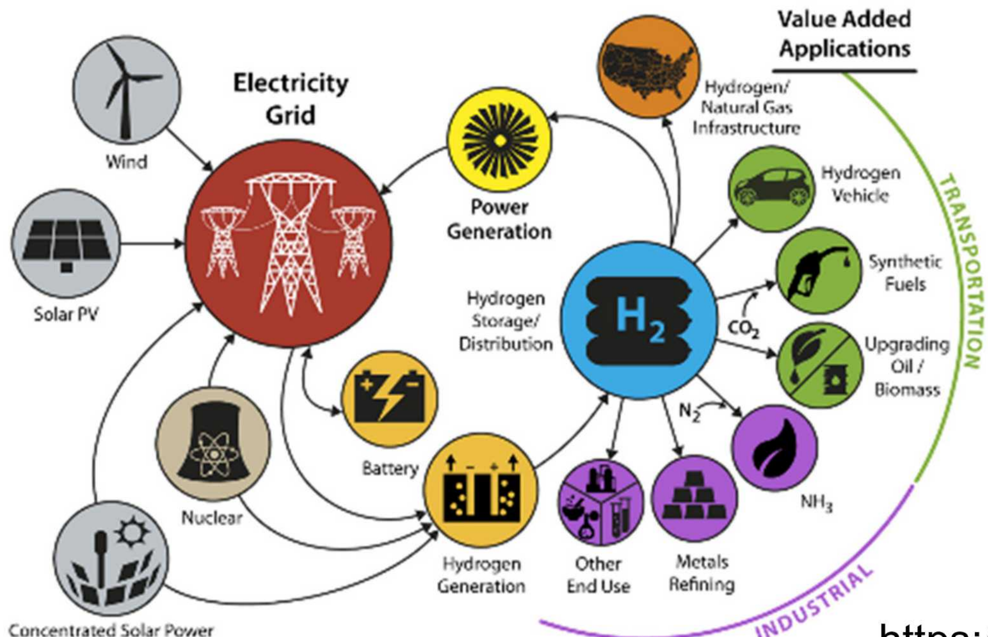


US DOE Vision For H_2 Production And Utilization



HydroGEN
Advanced Water Splitting Materials

http://h2awsm.org



H2@Scale℠
U.S. Department of Energy

https://www.energy.gov/eere/fuelcells/h2-scale

Acknowledgments (Funded By US DOE/FCTO)

Sandia Team

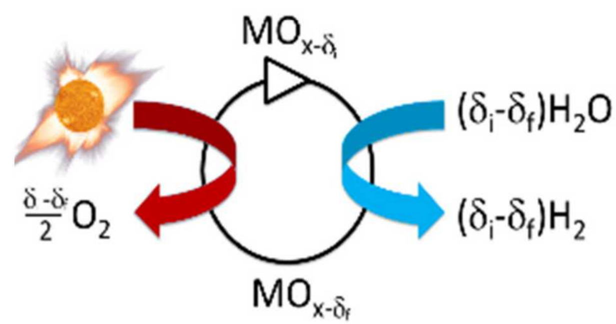
Dr. Ivan Ermanoski, Dr. Kevin Albrecht, Dr. Eric Coker, Dr. Andrea Ambrosini,
Dr. Josh Sugar, Mr. Jeff Roba

Material Discovery Team

- Colorado School of Mines, Golden CO.
  - Prof. Ryan O'Hayre, Prof. Michael Sanders, Ms. Debora Barcellos
  - Novel material formulations, synthesis, and screening
- Northwestern University, Evanston IL.
  - Prof. Christopher Wolverton, Dr. Antonie Emery
  - Application of quantum theory to materials screening
- Stanford University, Stanford CA.
  - Prof. William Chueh, Dr. BG Gopal, Ms. Nadia Ahlborg
  - Entropy engineering of materials

Reactor Design, Testing, and Demonstration Team

- Bucknell University, Lewisburg PA.
  - Prof. Nathan Siegel
  - Particle heat transfer, solar simulator design, CPR2 assembly and testing
- German Aerospace Center-DLR , Cologne DE
  - Dr. Christian Sattler, Dr. Justin Lapp, Dr. Abisheck Singh, Dr. Stefan Brendelberger, Mr. Johannes Grobbel
  - Solar particle receiver design, fabrication, and testing



Nature's Thermochemical Water Splitting Process

Source: iStock

Our challenge is to develop efficient and scalable *solar*-powered reactors producing 100,000 kg H_2/day without melting houses

Desired Material Behavior Defined by Process Economics

- Redox capacity (MO_x/H_2).
  - Oxide heating and material inventory
- Redox kinetics.
  - Cycle time and material inventory
- Earth abundance.
  - Raw materials
- Reduction temperature (T_{TR}).
  - Heliostats (solar concentration)
  - Reactor construction materials
- Steam requirement ($H_2O:H_2$).
  - Steam heating and water use
- Durability.
  - Material replacement

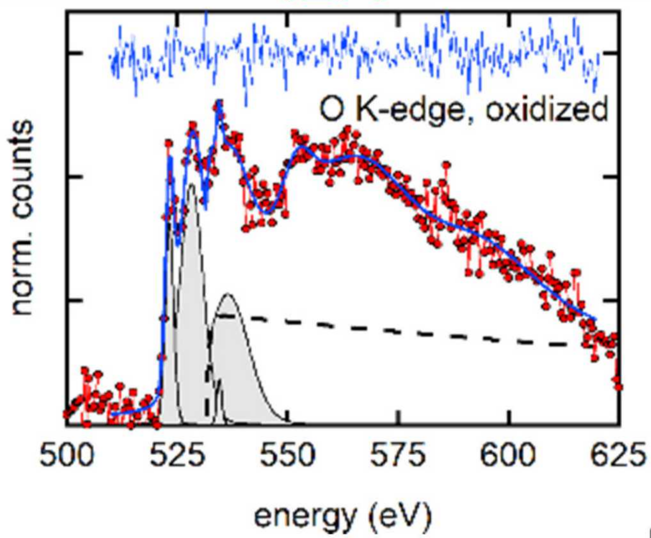
PROPERTY	IDEAL	
Redox Capacity	HIGH	<10:1 (MO_x/H_2)
Redox Kinetics	FAST	~sec (match flux)
Earth Abundance	HIGH	$>10^3/10^6$ Si
T_{TR} @ Reduction	LOW	~1400°C
H_2O/H_2 @ Oxidation	LOW	<5:1 ($H_2O:H_2$)
Durability	HIGH	>10 years

Commercial viability key driver when competing against steam methane reforming or electrolysis.

J. E. Miller, A. H. McDaniel, M. D. Allendorf, *Advanced Energy Materials*. **4**, 1300469 (2014).
I. Ermanoski, J. E. Miller, M. D. Allendorf, *Physical Chemistry Chemical Physics*. **16**, 8418 (2014).

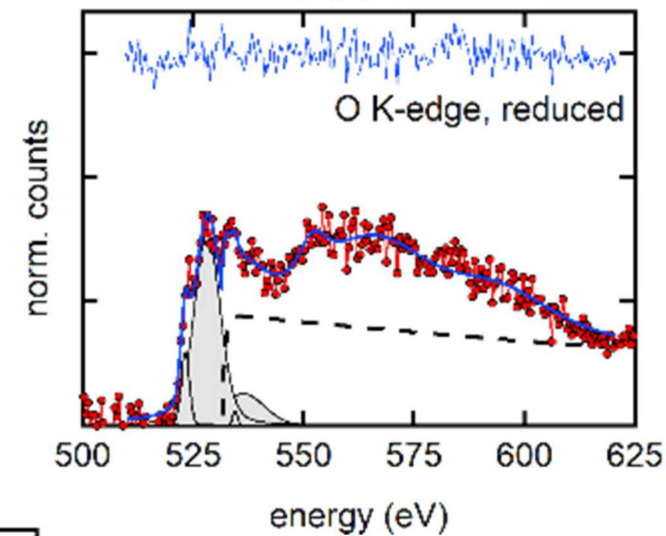
EELS Reveals: Effect Of Reduction On O-M Bonding

12R

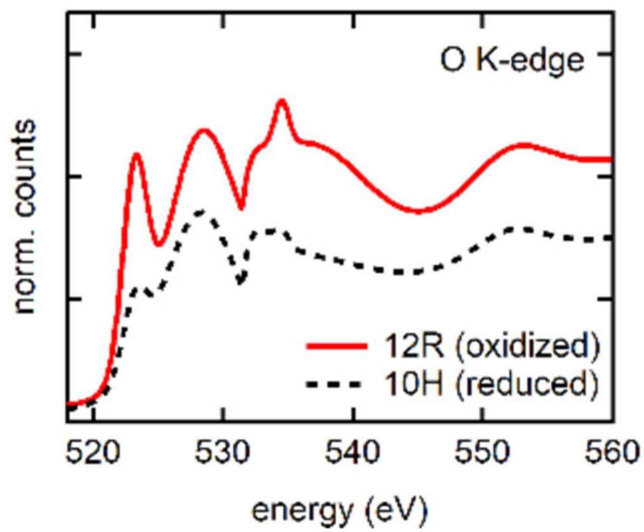


e^- charge transferred to hybridized 2p system decreases hole DOS

10H



Ab inito theory required to fully interpret spectra



Subtle variation in extended edge oscillations