Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Non-intermittent, Solar-thermal Processing to Split Water Continuously via a Near-isothermal, Pressure-Swing Redox Cycle

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NREL Transforming ENERGY
BERKELEY LAB Bringing Science Solutions to the World
Sandia National Laboratories
INL Idaho National Laboratory
Lawrence Livermore National Laboratory

Project Overview

Partners: University of Colorado Boulder Department of Chemical and Biological Engineering; CU Bold Center; HFTO HydroGen Consortium – NREL; OMC Hydrogen; and ETH Zurich

Project Vision: We hope to experimentally demonstrate a solar-to-fuel energy efficiency greater than 10%, representing nearly a twofold increase over the current record; and a hydrogen production rate of 1 g/h using simulated sunlight for over two weeks using a 10kW thermal HFSS to demonstrate robustness of active materials.

Project Impact: We hope to revitalize interest in STCH through both experimental demonstration and a TEA for a continuous process - developing the iron aluminate-based, STCH production approach for splitting water and establish modeling tools to simulate reactor and system performance to guide design of future reactor iterations; and to identify cost implications associated with decoupling the reactor from the solar receiver via gas heating and thermal storage using a high-temperature thermocline.

Project Goal

- Milestones & key metrics

Milestone 1.1 (Q3; 9 months): Establish congruency between power measurements determined via the flux mapping and water-cooled calorimeter-based methods.

Milestone 1.2 (Q5; 15 months): Complete existing system modifications and computationally and/or experimentally determine minimum fluidization velocity for the as-synthesized iron aluminates.

Milestone 2.1 (Q2; 6 months): Establish that (1) the elemental composition of the representative *in-house sample* agrees with the respective target values and (2) the percent relative change in equilibrated mass at 1400°C between oxygen partial pressures of 10^{-2} and 10^{-4} bar exceeds 0.8%.

Milestone 2.2 (Q4; 12 months): Replicate Milestone 2.1 for the *commercially-procured, large-scale sample*.

Milestone 3 (Q1; 3 months): Computationally identify conditions that result in peak efficiency for both isothermal and near-isothermal (ΔT < 200°C) operating modalities, ensuring that the evaluated conditions are practical.

Milestone 9.1 (Q4; 12 months): Interview prospective BOLD undergraduate students in early fall 2023 or spring 2024, one of which will be hired to work on the project.

Project Goal

- Milestones & key metrics

Go/No-Go 1 (End of Q4; 12 months)**:** Using the existing system and ~10 grams of iron aluminates, synthesized in-house, demonstrate a production capacity greater than 550 µmol g^{-1} for 5 consecutive cycles, quantify the accompanying solar-to-fuel energy efficiency, and compare measured performance with model predictions. Then, determine the mass loading required to achieve an efficiency of 10% to inform the design of the next iteration reactor (**Milestone 1.2, Task 1**), as well as dictate the geometrical configuration of the heat exchanger to be developed in **Task 4**.

Project Goal

- Milestones & key metrics

Milestone 4 (Q6; 18 months): Successfully fabricate and install a robust counter-flow gas-gas heat exchanger, which comprises RPC structures contained within the inner and annulus regions of two concentrically aligned tubes.

Milestone 5 (Q5; 15 months): Deliver ~2 kg of iron aluminates, synthesized at large scale via the optimal method determined from **Task 2**, to ETH Zürich for evaluation in their “solar mini-refinery” system.

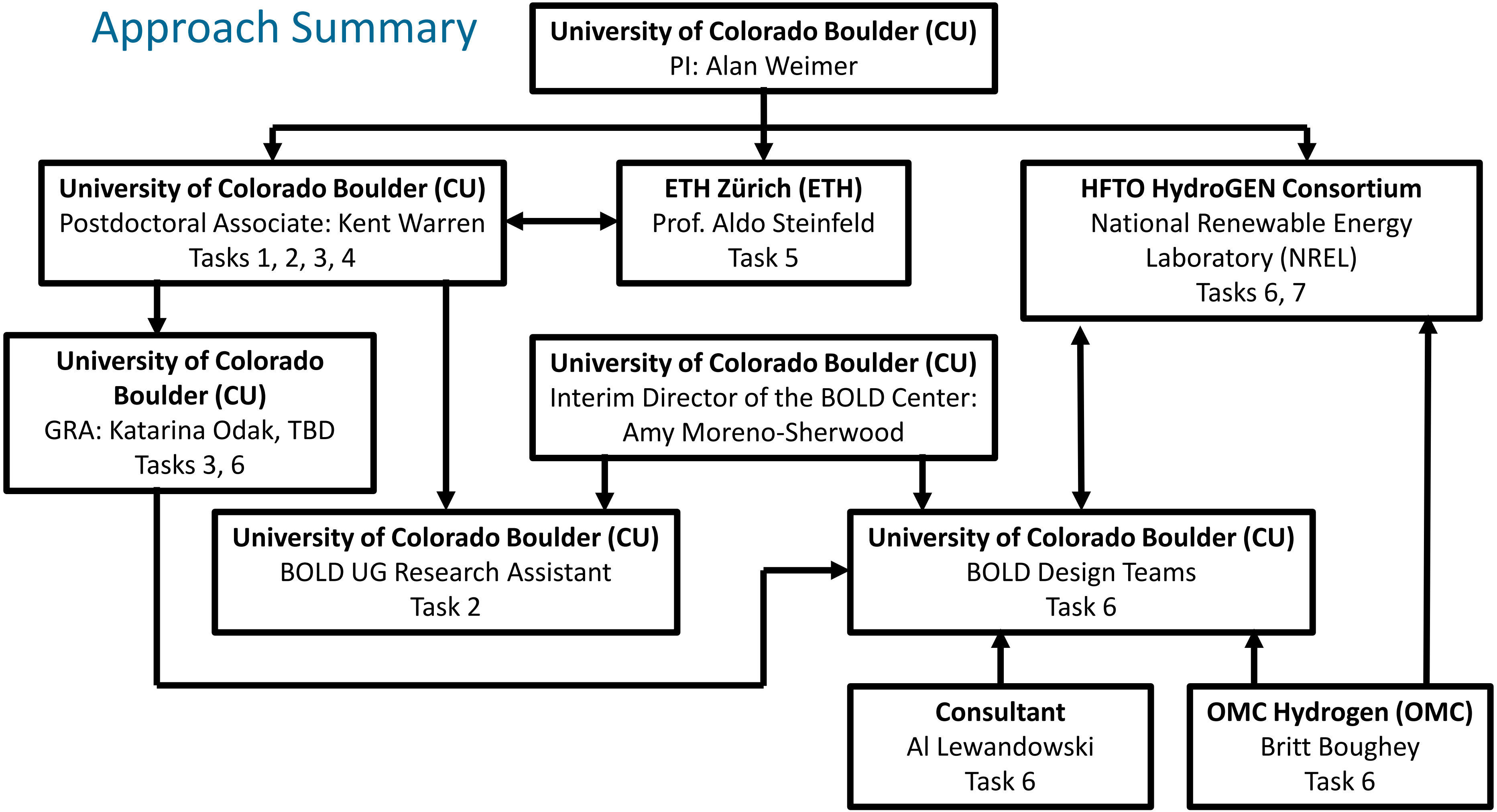
Milestone 6 (Q8; 24 months): Develop (1) a TEA that will accurately determine the process variables allowing for a 10% IRR for a H_2 selling price of \$2/kg H_2 , along with tornado plots identifying the most critical parameters and (2) a marketing report identifying commercial opportunities for each case. An analysis of the Installation Tax Credit vs the Production Tax Credit for the economics will also be carried out.

Milestone 7 (Q7; 21 months): Validate reactor model by comparing simulated O_2 evolution and H_2 production rates with experimentally measured data obtained at CU’s high-flux solar simulator facility.

Milestone 8 (Q8; 24 months): Submit list comprising instances of scientific research dissemination, including oral and poster presentations as well as scientific articles (in preparation and submitted), to EERE for review.

Milestone 9.2 (Q8; 24 months): During the spring 2025 semester in Year 2, a BOLD undergraduate capstone design team will be selected to complete the TEA, working with the project team for support.

Approach Summary



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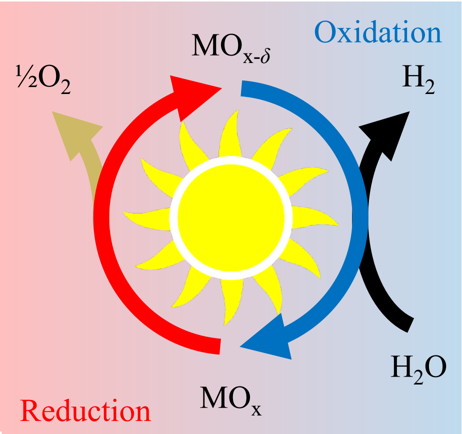
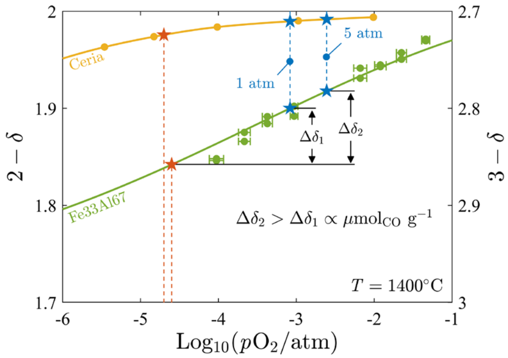
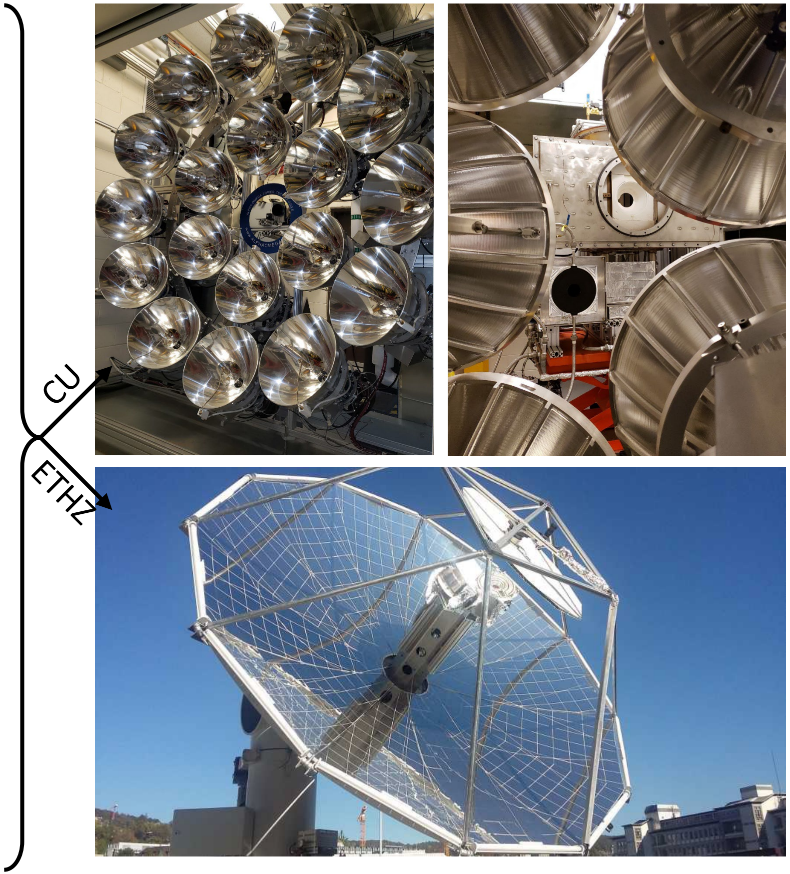






Scope of work:

1) Using both CU's HFSS and ETHZ's solar dish, demonstrate world-record efficiency for solar thermochemical fuel production. Operation will include isothermal to near-isothermal (< 150°C temperature swing), iron aluminate redox.
2) Deliver 1g H_2/hr for two weeks
3) Design, build, integrate ceramic HX for heat integration
4) Modeling
5) Develop robust TEA

Tran J. T., K.J. Warren, et al., W. (2023). *Joule*,71759-1768.

Highlight Intended Lab Node Collaborations

Lab	Node PI	Node Title	Brief Scope	Budget Period 1 Funding	Brief Scope	Budget Period 2 Funding	Total
NREL	Zhiwen Ma	Multiscale modeling node and STCH TEA node	NREL will perform components (reactor, HX, TES) and STCH system modeling and establish a TEA framework for CU STCH system and renewable integration with TES continuous.	$375, 000	Validate reactor model with CU's HFSS test. System analysis for component cost and TEA inputs and support commercial paths	$375,000	$750,000
				$375,000		$375,000	$750,000

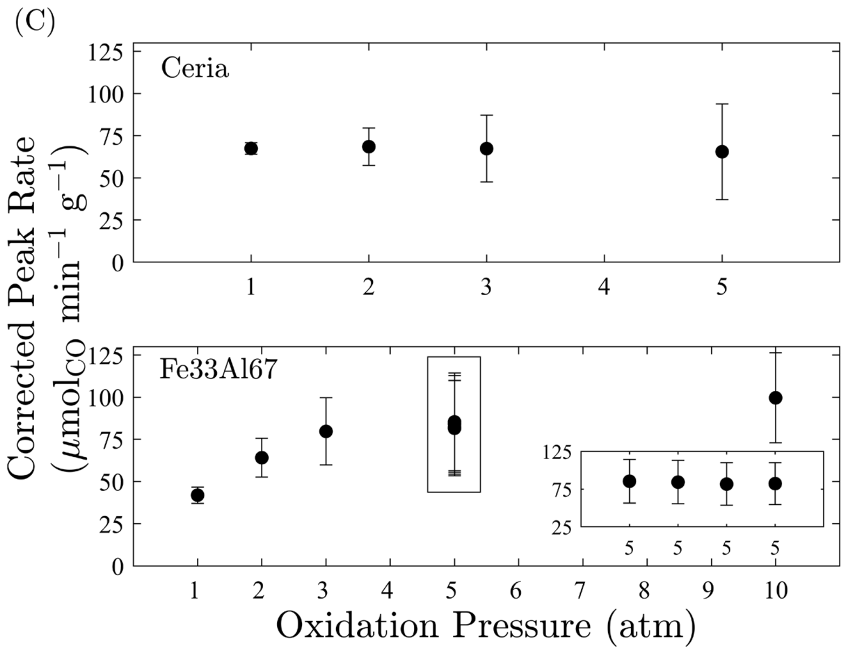
Approach Summary

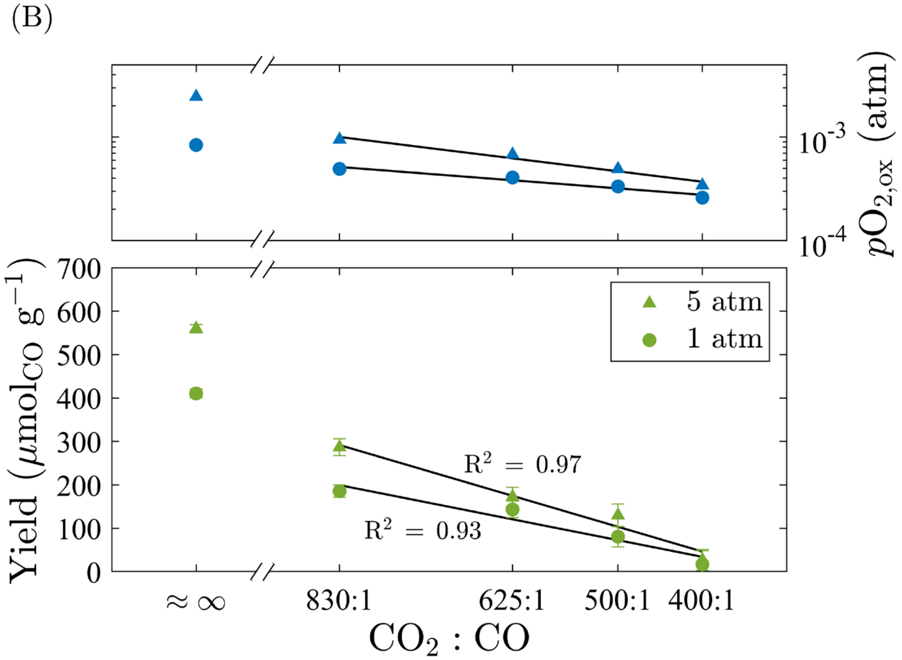
Isothermal Redox @ 1400°C

Material	Before Oxidation: $Log_{10}(pO_2/atm)$	Oxidation: Pressure (atm)	Oxidation: CO Produced (μmol g^{-1})	Reduction: O_2 Evolved (μmol g^{-1})
Ceria	-4.7 ± 0.01	1	71.1 ± 5.3	65.1 ± 0.6
		2	83.0 ± 5.2	68.0 ± 0.6
		3	83.3 ± 5.2	67.6 ± 0.6
		5	83.2 ± 5.5	83.0 ± 0.7
Fe33Al67	-4.6 ± 0.01	1	356 ± 8.1	201 ± 1.0
		2	460 ± 7.8	234 ± 1.1
		3	510 ± 7.7	256 ± 1.2
		5	588 ± 7.8	283 ± 1.2
			545 ± 7.7	282 ± 1.2
			552 ± 7.7	283 ± 1.2
			556 ± 7.7	281 ± 1.2
		10	768 ± 9.9	381 ± 1.4

Tran, J., K.J. Warren, et al, Joule, 7, 1759–1768, August 16, 2023

Approach Summary





Peak rates after accounting for the effect of gas phase dispersion and Mixing at oxidation P and 1400°C

Extent of oxidation as a function of inlet CO_2:CO ratio at P and 1400°C (top panel based on equilibrium of CO_2 thermolysis)

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2023 Team Retreat at Beaver Meadows Ranch Resort

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