Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Inverse Design of Perovskite Materials for Solar Thermochemical Hydrogen Production

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Aug. 21, 2023

Project Overview




Project Partners:

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Project Vision:

We will implement an inverse materials and reactor design approach to discover a perovskite material (ABO_3) and receiver/reactor design to achieve DOE cost targets. We will use a cascade of thermodynamic, reactor, and technoeconomic analysis (TEA) models to identify material thermodynamic fingerprints (TFP) for optimal performance

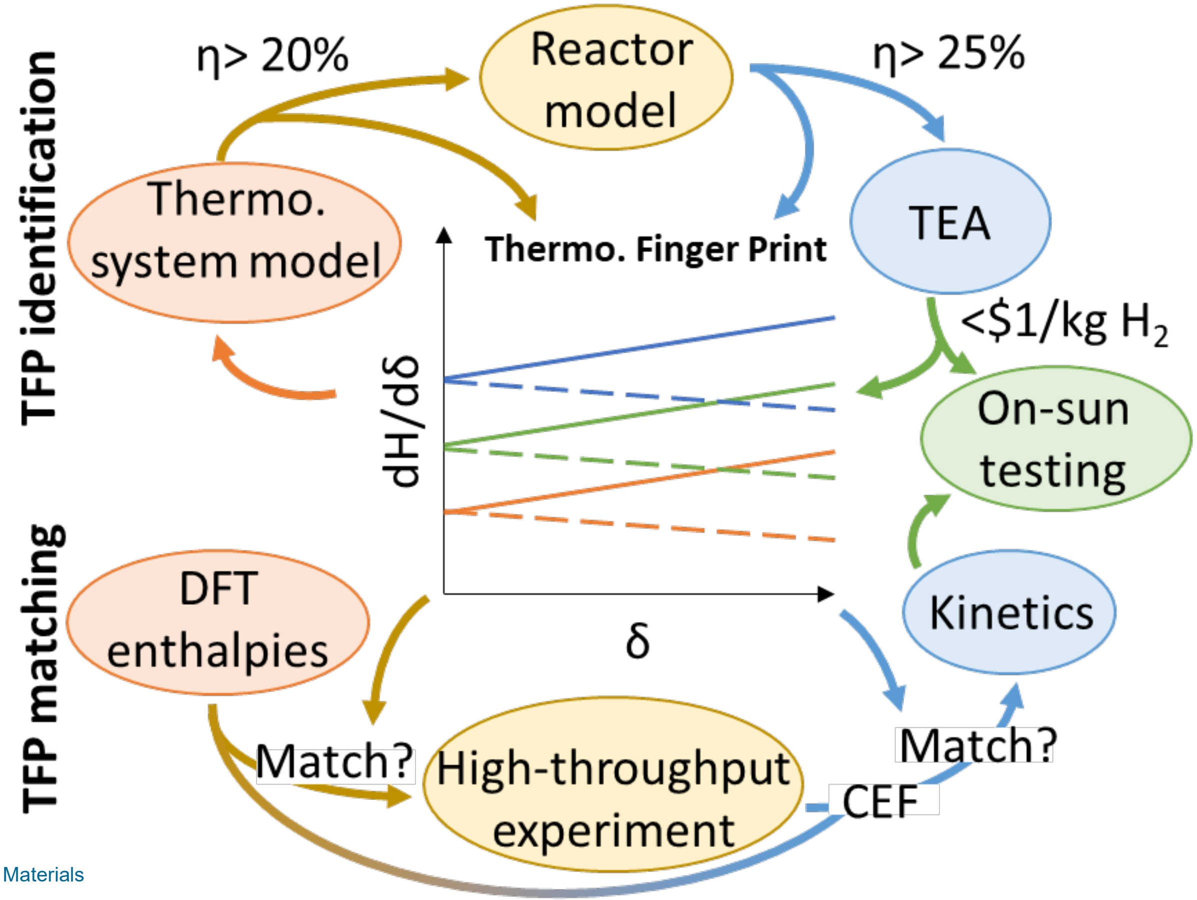
Project Impact:

Identification of at least one quinary perovskite composition ($A_{1-x}A'_xB'_yB_{1-y}O_3$) that can achieve <\$1.5/kg H_2 at scale, a 70-80% reduction from state-of-the-art CeO_2, demonstration of >1g H_2/hr production on sun, material stability for at least 100 cycles, and a reactor and plant design pathway that can achieve <\$1/kg H_2 at scale

Project Goal

	Key Milestones & Deliverables
Year 1	Identify compositions with > 20% STH efficiency based on the first order compound energy formalism as predicted by the thermodynamic system model
Year 2	TEA predicted cost of $2.5 /kg H_2, a 50-60% reduction compared to SOA CeO_2, using experimentally measured thermodynamics properties and bulk processing costs
Year 3	Identify perovskite compositions that can achieve <$1.5/kg H_2, demonstrate >1g H_2/hour production on sun, show stability for 100 cycles, and outline a reactor and plant design pathway that can achieve <$1/kg H_2

Approach Summary



Task 1: Project Management & Market Transfer

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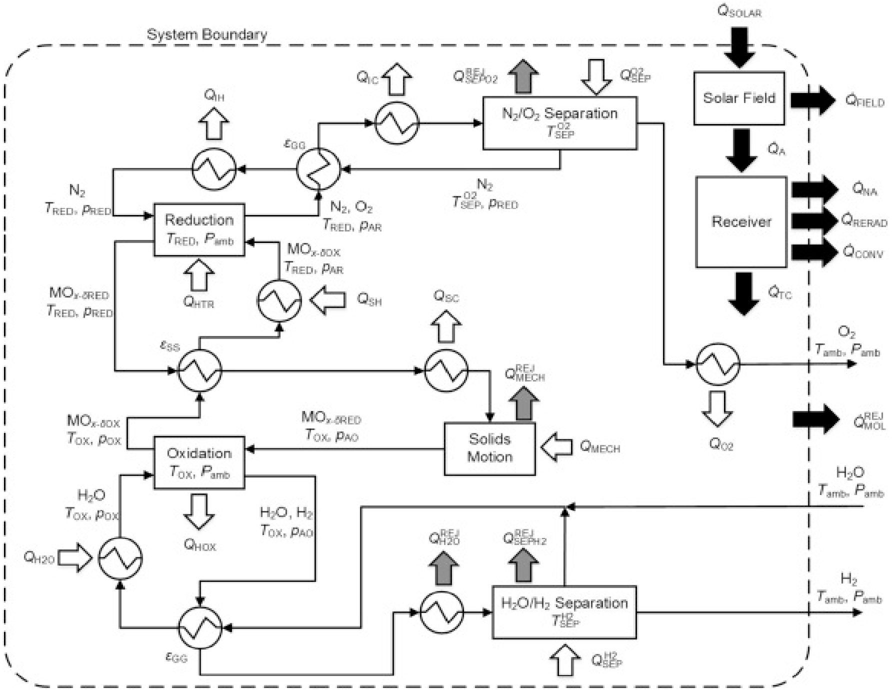
Goals:

Organize bi-weekly team meetings, cross-institution communication, prepare of reports and reviews, and develop/implement market planning

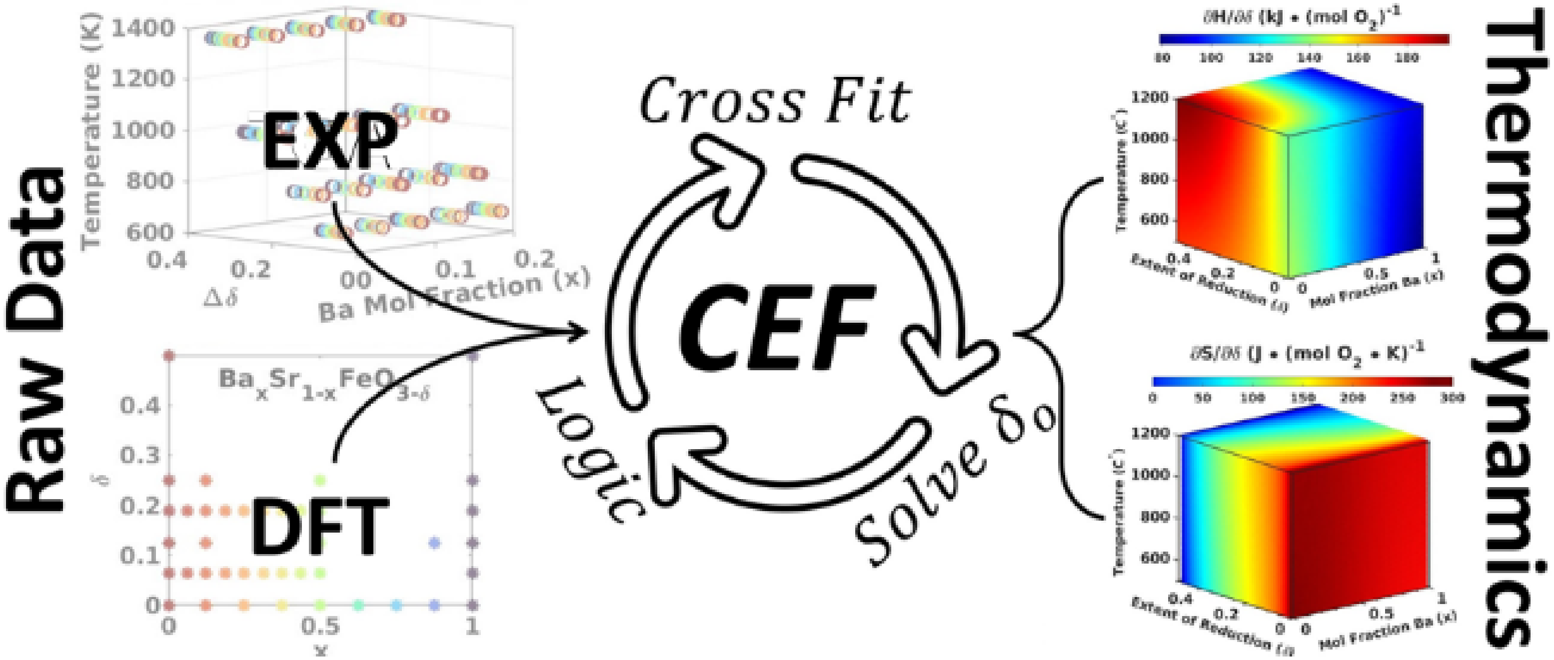
Task 2: Thermodynamic and plant level modeling & TEA



Goals:

Identify material performance to cost ratios and plant performance metrics required to achieve \$1/kg H_2

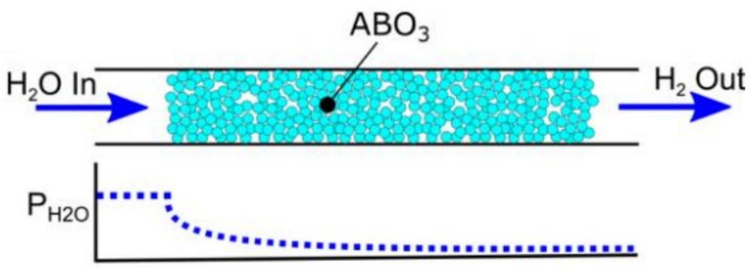
Task 3: High-Throughput Materials Development

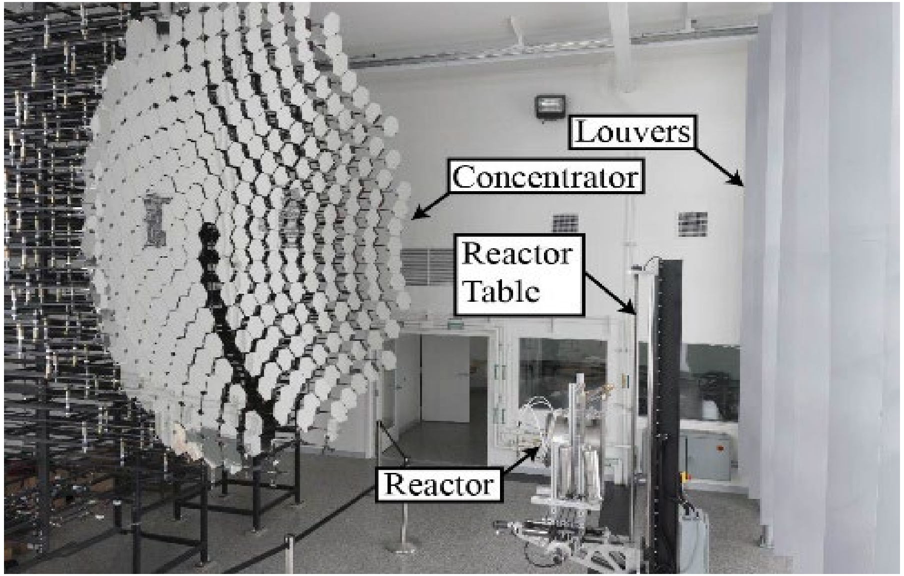


Goals:

Identify $A_{1-x}A'_xB'_yB_{1-y}O_3$ that match's ideal TFP using high throughput DFT and novel high-throughput experiments

Task 4: Reactor Design and On-Sun Demonstration





Solar furnace at Valpo

Goals:

Model, design, and experimentally test new flow reactor configurations that maximize the material utilization and therefore solar-to-fuel efficiencies.

Highlight Intended Lab Node Collaborations

Lab	Node	Scope
NREL	Techno-economic analysis	Consulting and TEA mapping
NREL	Multi-scale modeling	Consulting and reactor scale-up
Sandia	Stagnation Flow Reactor	Kinetic extraction
Sandia	High-Temp XRD	Material characterization
Sandia	Advanced Electron Microscopy	Material characterization
INL	Advanced Electrode and Solid Electrolyte Materials for Elevated Temperature Water Electrolysis	High throughput synthesis

Thank you!