Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

HydroGEN: STCH Overview

H.N. Dinh, A. Weber, A. McDaniel, R. Boardman, T. Ogitsu, H. Colon-Mercado

Presenter: Anthony McDaniel, SNL

Date: 6/13/2018

Venue: 2018 DOE Annual Merit Review

Project ID # PD148d

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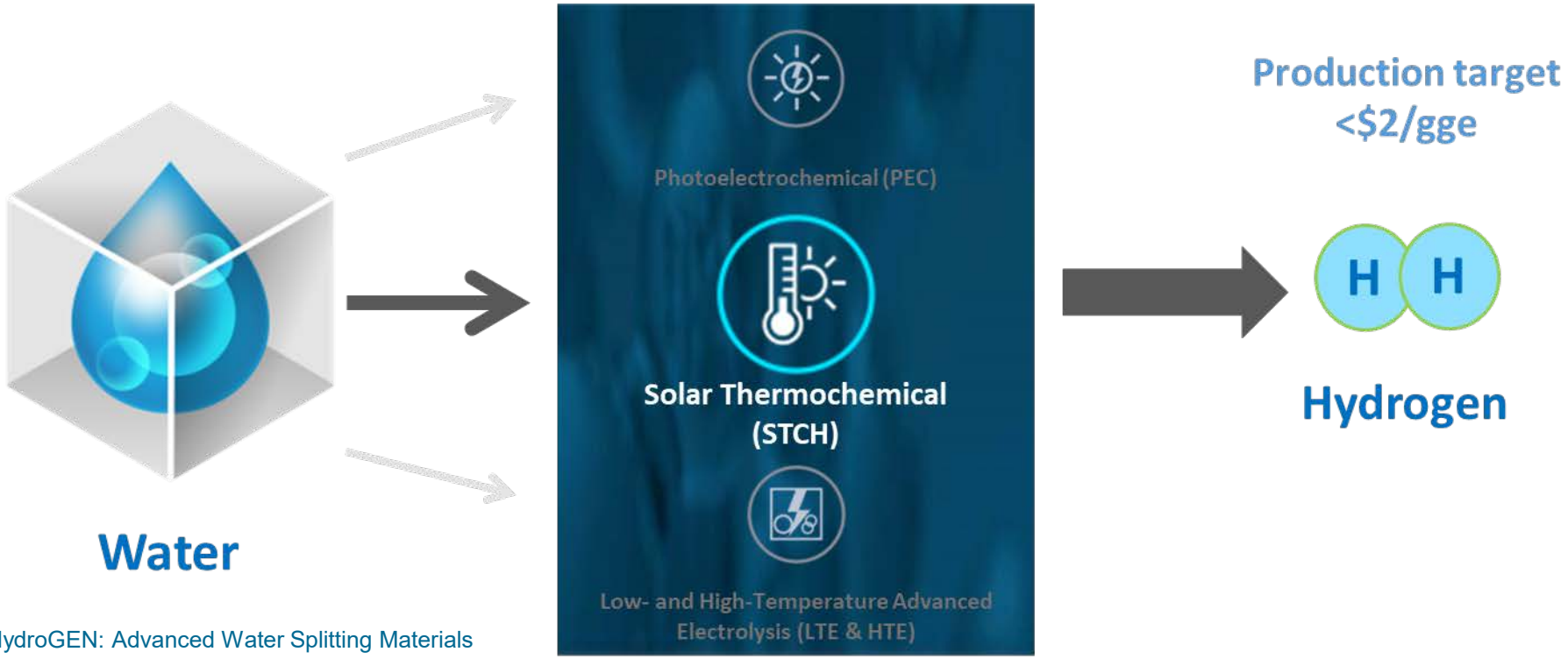
NREL NATIONAL RENEWABLE ENERGY LABORATORY | BERKELEY LAB | Sandia National Laboratories | INL Idaho National Laboratory | Lawrence Livermore National Laboratory | SRNL

Advanced Water-Splitting Materials (AWSM)

AWSM Consortium 6 Core Labs:

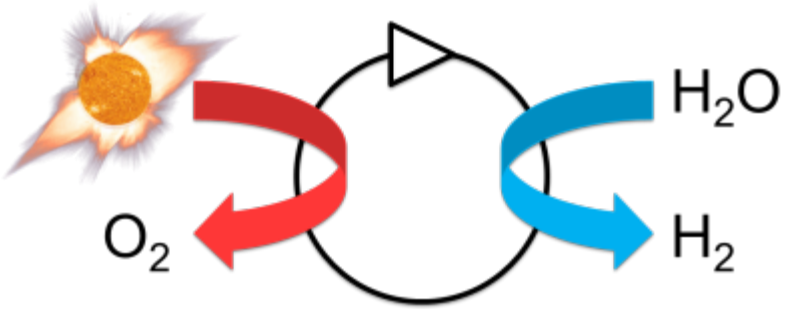
NREL National Renewable Energy Laboratory; Berkeley Lab; Sandia National Laboratories; Idaho National Laboratory; Lawrence Livermore National Laboratory; SRNL

Accelerating R&D of innovative materials critical to advanced water splitting technologies for clean, sustainable & low cost H_2 production, including:



Thermochemical and Hybrid Water Splitting Technologies

Thermochemistry



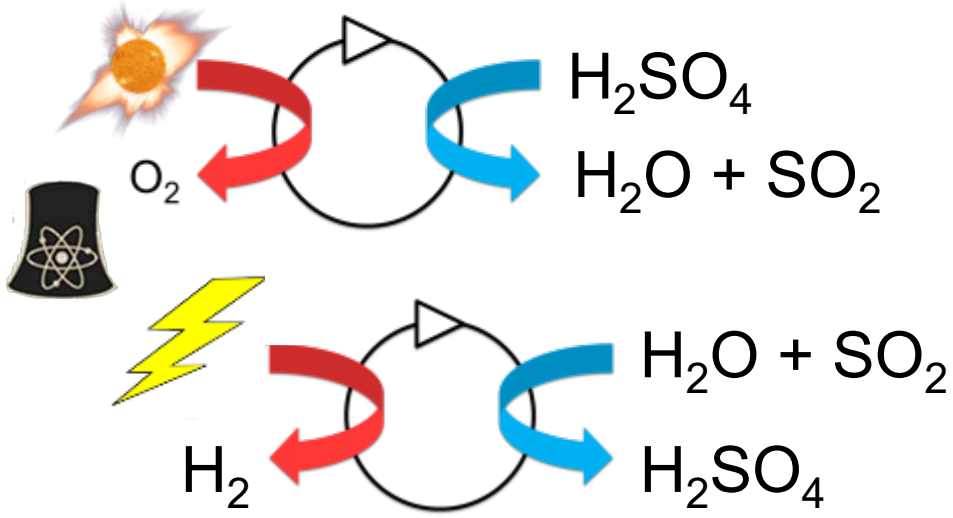
$$MO_x \rightarrow MO_{x-\delta} + \frac{\delta}{2} O_2 \quad \text{(1) Reduction}$$

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

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

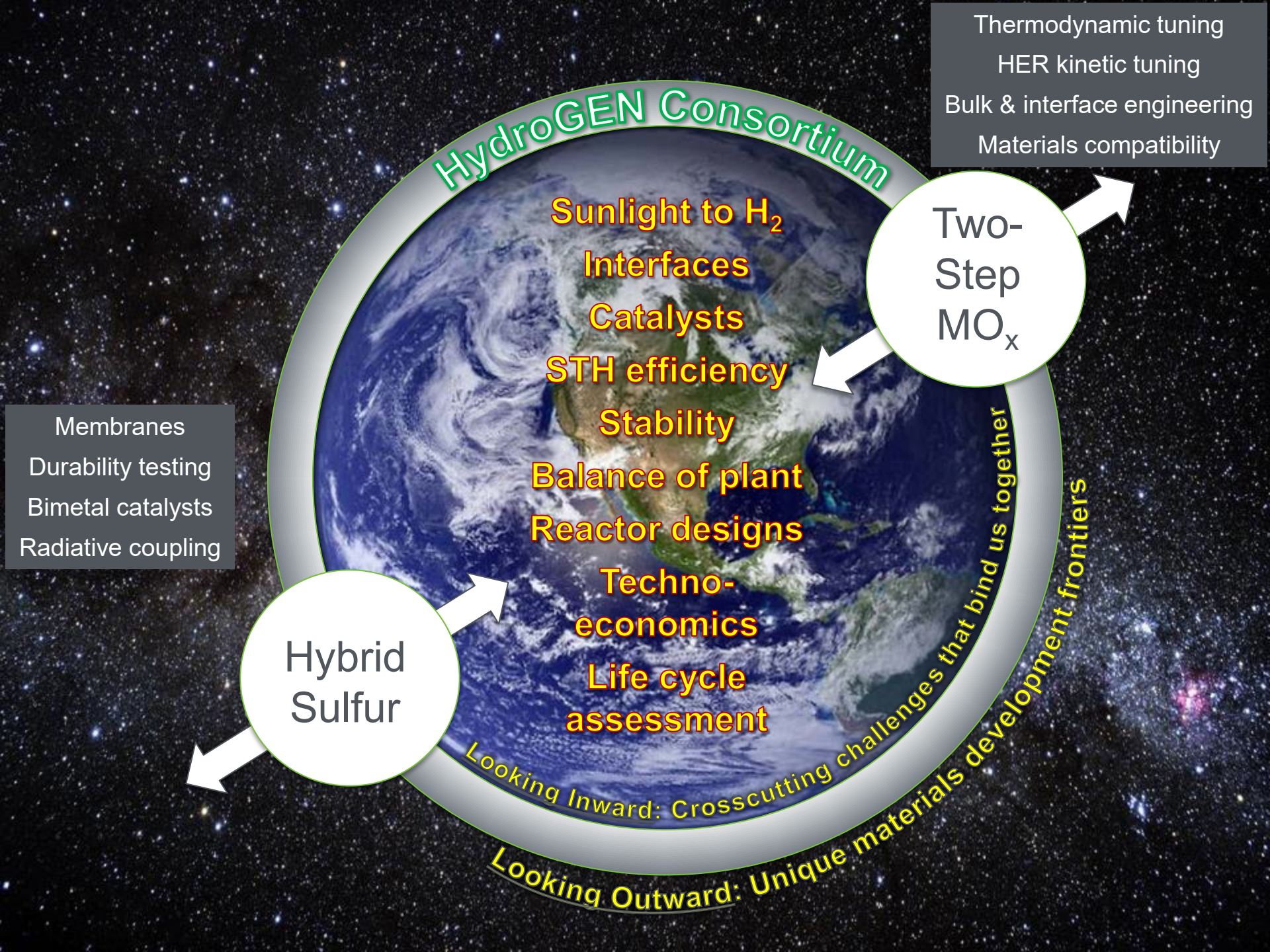
- Metal cation is redox active element in two-step cycle.

TC + Electrochemistry

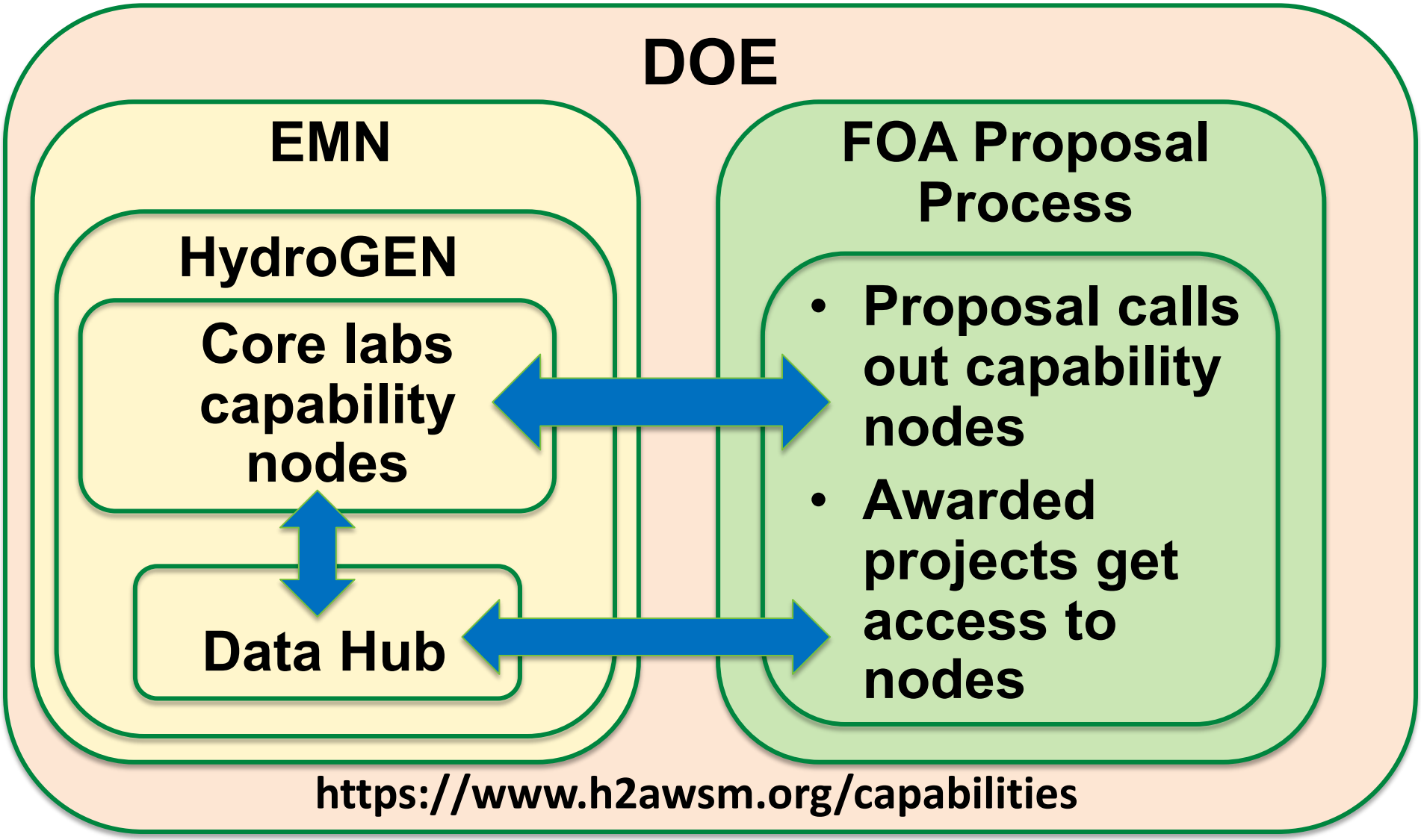


$H_2SO_4 \leftrightarrow H_2O + SO_2 + ½\ O_2$
(thermochemical; 800-900 °C)
$SO_2 + 2\ H_2O \rightarrow H_2SO_4 + H_2$
(electrochemical; 80-120 °C)
Net Reaction: $H_2O \rightarrow H_2 + ½\ O_2$

- Sulfur is redox active element in two-step cycle.


Thermodynamic tuning
HER kinetic tuning
Bulk & interface engineering
Materials compatibility
HydroGEN Consortium
Sunlight to H_2
Interfaces
Catalysts
STH efficiency
Stability
Balance of plant
Reactor designs
Techno-economics
Life cycle assessment
Two-Step MO_x
Hybrid Sulfur
Membranes
Durability testing
Bimetal catalysts
Radiative coupling
Looking Inward: Crosscutting challenges that bind us together
Looking Outward: Unique materials development frontiers

HydroGEN-AWSM Framework



EMN HydroGEN

STCH: Solar Thermochemical & Hybrids

Barriers
- Cost
- Efficiency
- Durability

STCH Node Labs

- Sandia National Laboratories
- Idaho National Laboratory
- NREL National Renewable Energy Laboratory
- SRNL Savannah River National Laboratory
- Lawrence Livermore National Laboratory

Support through:

- Personnel
- Equipment
- Expertise
- Capability
- Materials
- Data

STCH Projects

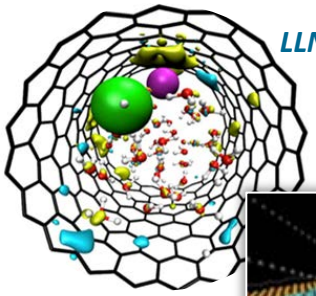
- Greenway Energy LLC — Engineering consultant in Aiken County, South Carolina
- Colorado School of Mines
- Arizona State University Sun Devils
- University of Colorado
- Princeton University 1746
- University of South Carolina
- Northwestern University

HydroGEN-AWSM Core Labs Nodes

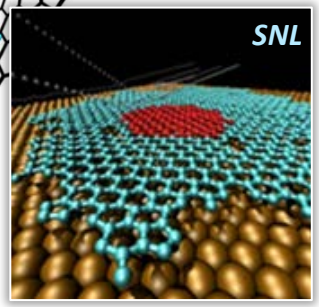
Impact

Comprising more than 80 unique, world-class capabilities/expertise in:

Materials Theory/Computation

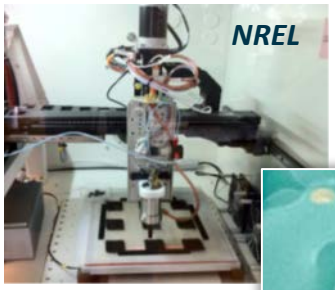


Bulk & interfacial models of aqueous electrolytes

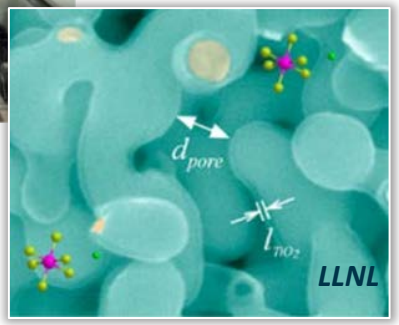


LAMMPS classic molecular dynamics modeling relevant to H_2O splitting

Advanced Materials Synthesis



High-throughput spray pyrolysis system for electrode fabrication



Conformal ultrathin TiO_2 ALD coating on bulk nanoporous gold

Characterization & Analytics

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

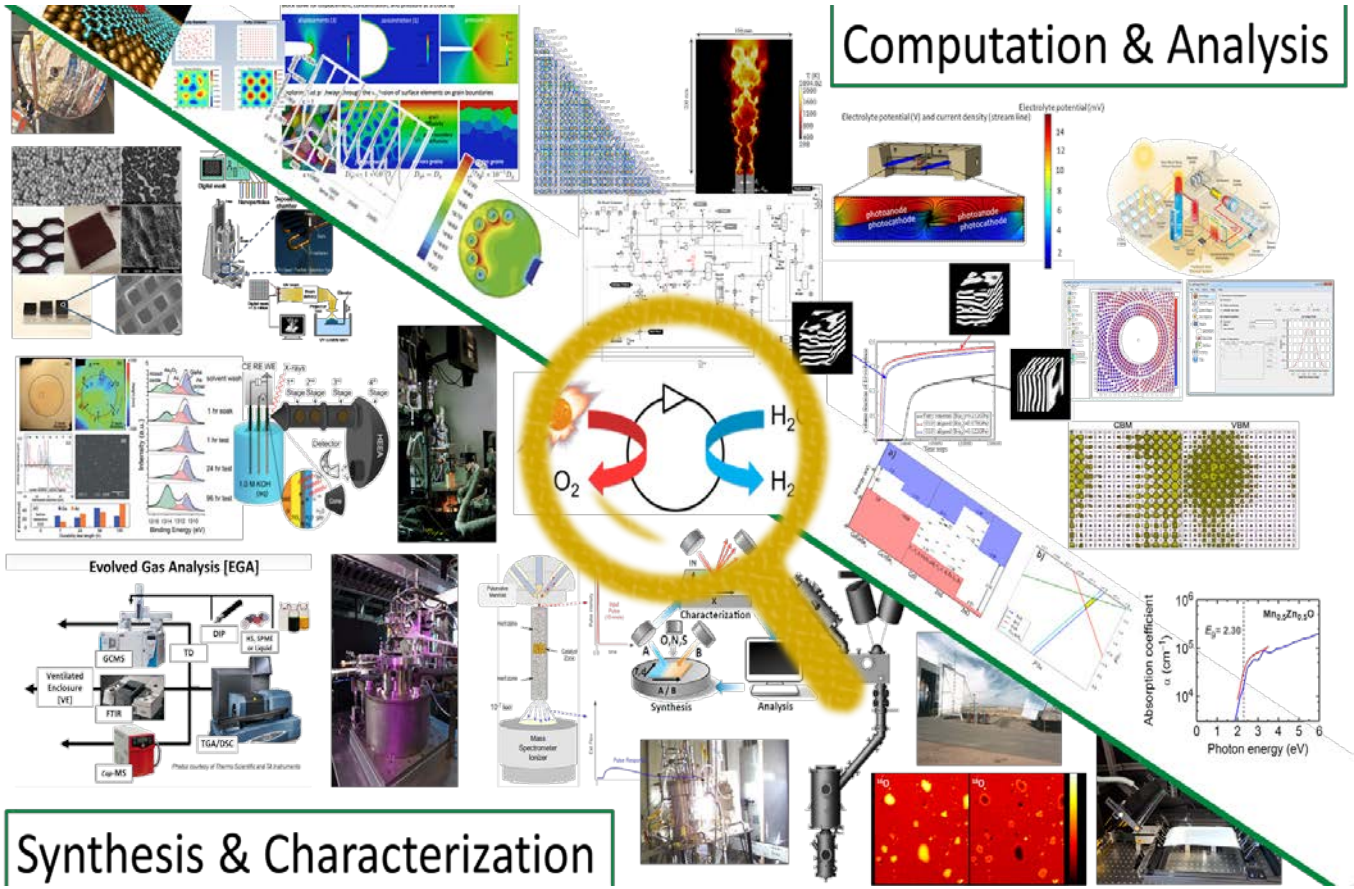
TAP reactor for extracting quantitative kinetic data

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

Website: https://www.h2awsm.org/

40 STCH Nodes Available in the Consortium

Impact



Analysis: 1 Computation: 6	Characterization: 5 Synthesis/Process: 6	Cat1
Analysis: 1 Computation: 5	Characterization: 3 Synthesis/Process: 4	Cat2
Analysis: 1 Computation: 4	Characterization: 4 Synthesis/Process: 0	Cat3

- 11 nodes from 5 National Labs supporting 5 STCH projects.

5 Seedling Projects Awarded in FY2018

11 nodes from 5 National Labs supporting projects

Approach

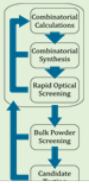
Accelerated Discovery of STCH Materials via High-Throughput Computational and Experimental Methods

PI, Ryan O'Hayre, Colorado School of Mines
Co-PI, Michael Sanders, Colorado School of Mines

Project Vision

Merging combinatorial synthesis methods with combinatorial theoretical calculations to rapidly discover new potential materials for use in two-step metal oxide cycles for STCH

POSTER ID: PD165



NODE	LAB	PI
First principles materials theory	NREL	S. Lany
(HTE) thin film combinatorial	NREL	A. Zakutayev
Laser heated SFR	SNL	A. McDaniel

Computationally Accelerated Discovery and Experimental Demonstration of High-Performance Materials for Advanced Solar Thermochemical Hydrogen Production

PI, Charles Musgrave, University of Colorado
Co-PI, Alan Weimer, University of Colorado

Project Vision

Utilize machine-learned models coupled with ab initio thermodynamic and kinetic screening calculations to accelerate the RD&D of new STCH materials

POSTER ID: PD166

NODE	LAB	PI
First principles materials theory	NREL	S. Lany
Technoeconomic analysis	NREL	G. Saur
HT-XRD & TA	SNL	E. Coker
Laser heated SFR	SNL	A. McDaniel

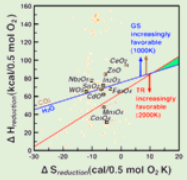
Transformative Materials for High-Efficiency Thermochemical Production of Solar Fuels

PI, Christopher Wolverton, Northwestern University
Co-PI, Sossina Haile, Northwestern University

Project Vision

Combine high-throughput computation and experiment to study the properties of novel, predicted STCH materials

POSTER ID: PD167



NODE	LAB	PI
First principles materials theory	NREL	S. Lany
Technoeconomic analysis	NREL	G. Saur
Tools for enhanced thermochem H2	NREL	D. Ginley
Mesoscale kinetic modeling	LLNL	T. W. Heo

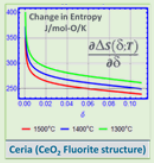
Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design for Solar Thermochemical Hydrogen

PI, Ellen Stechel, Arizona State University
Co-PI, Emily Carter, Princeton University

Project Vision

Accurate (enough) first principles calculations of the oxygen chemical potential for complex mixed ionic electronic (off-stoichiometric) doubly substituted perovskite solid solutions from which we can extract the thermodynamics

POSTER ID: PD168



NODE	LAB	PI
Tools for enhanced thermochem H2	NREL	D. Ginley
HT-XRD & TA	SNL	E. Coker
UQ Toolkit	SNL	B. Debusschere
Laser heated SFR	SNL	A. McDaniel

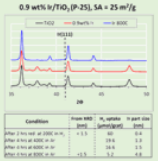
High temperature reactor catalyst material development for low cost and efficient solar driven sulfur-based processes

PI, Claudio Corgnale, Greenway Energy
Co-PI, John Monnier, University of South Carolina

Project Vision

Develop new material catalyst using our demonstrated surface free energy and electroless deposition technique, and integrate directly into a solar reactor-receiver

POSTER ID: PD169



NODE	LAB	PI
Engineering BOP of hi-temp systems	NREL	Z. Ma
Catalysts for harsh environments	INL	D. Ginosar
Flow sheet development and technoeconomic analysis	SRNL	M. Gorensek

Themes are *fundamental*:

- Computational material science, machine learning, high throughput screening, accelerated discovery

Leveraging HydroGEN Capabilities to Enable Project Success

Impact

Computation:

- First Principles Materials Theory for Advanced Water Splitting Pathways (S.Lany, NREL)
  - Role of charged defects in generating configurational entropy
  - Comp. screen material thermodynamics
- Uncertainty Quantification in Computational Models of Physical Systems (B.Debusschere, SNL)
  - Bayesian statistical uncertainty quantification to assess impact of imperfect knowledge
- Mesoscale Kinetic Modeling of Water Splitting and Corrosion Processes (T.W.Heo, LLNL)
  - Model reaction kinetics and phase dynamics

Analysis:

- Engineering of Balance of Plant for High-Temperature Systems (Z.Ma, NREL)
  - Solar reactor design and CFD model-based performance analysis
- Techno-Economic Analysis of Hydrogen Production (G.Saur, NREL)
  - H2A analysis of production pathway
- Advanced Water-Splitting Materials Requirements Based on Flowsheet Development and Techno-Economic Analysis (M.Gorensek, SRNL)
  - Conceptual design of solar plant
  - Econ-finance analysis of solar plant

Characterization:

- Development and Evaluation of Catalysts for Harsh Environments (D.Ginosar, INL)
  - Durability and performance @ hi T and low pH
- High-Temperature X-Ray Diffraction (HT-XRD) and Complementary Thermal Analysis (E.Coker, SNL)
  - *in operando* XRD, validate structure models
  - Thermal analysis, validate thermo models
- Virtually Accessible Laser Heated Stagnation Flow Reactor for Characterizing Redox Chemistry of Materials Under Extreme Conditions (A.McDaniel, SNL)
  - Measure reaction kinetics and quantify redox performance

Synthesis:

- High-Throughput Experimental Thin Film Combinatorial Capabilities (A.Zakutayev, NREL)
  - Pulsed laser deposition of compositionally-varied oxide materials libraries
  - Chemical and physical analysis of oxide films
- Computational and Experimental Tools for Enhanced Thermochemical Hydrogen Production (D.Ginley, NREL)
  - Controlled material defect engineering for DFT validation and descriptor testing

Example node: SNL

Uncertainty Quantification in Computational Models

Accomplishment

Bayesian inference of thermodynamic model parameters

$$p(\lambda|d,\mathcal{M}) = \frac{p(d|\lambda,\mathcal{M})p(\lambda,\mathcal{M})}{p(d|\mathcal{M})}$$

Bayes' rule updates prior belief in parameter values (λ) with data (d), to obtain posterior belief in the parameter values

$$z = -\ln(\delta)$$

$$u = \frac{1}{2} ln\left(\frac{P_{O_2,\mathrm{amb}}}{P_{O_2}}\right)$$

$$\beta = \left(\frac{T_{\mathrm{ref}}}{T}\right)$$

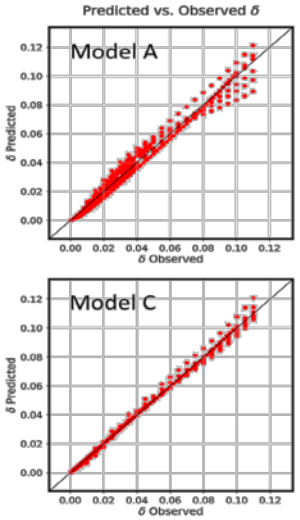
$$P_{O_2,\mathrm{amb}} = 0.20946$$

$$T_{\mathrm{ref}} = 1073.15$$

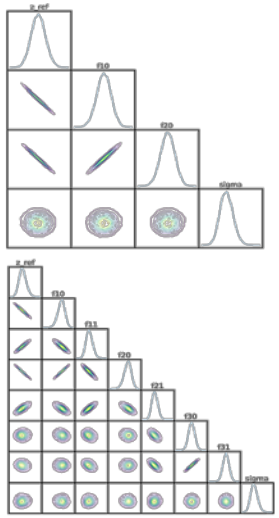
$$z = \frac{z_{\mathrm{ref}} + f_{10}(1-\beta) + f_{20}u + f_{30}u(1-\beta)}{1 + f_{11}(1-\beta) + f_{21}u + f_{31}u(1-\beta)}$$

Considered 4 models in transformed (P, T, δ) variables

Bayes Factor reveals model preference



Model C is strongly preferred because additional parameters allow better fit



Strong dependencies between some parameters

- Derive simplest possible model to fit O_2 chemical potential in solid.
  - Analytically extract material thermodynamics to solve inverse material design problem
- Uncertainty Quantification determines model parameters needed to predict thermodynamic behavior with specified uncertainty.
  - How accurate does the model have to be?
  - How does error propagation impact predictions?

Example node: NREL

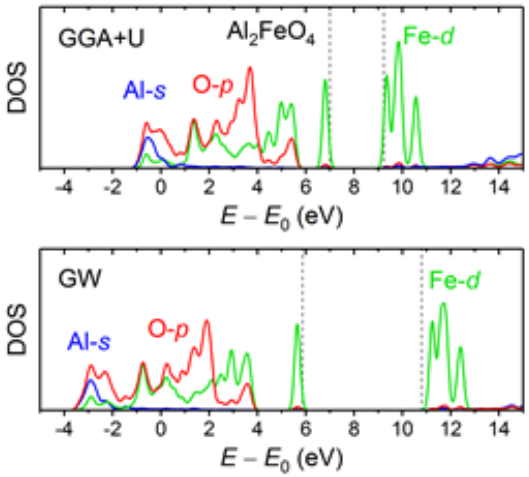
First Principles Materials Theory

Computational predictions (capabilities and expertise)

- Oxide thermochemistry
- Defect formation energies
- Defect equilibria
- Electronic structure

CU Boulder

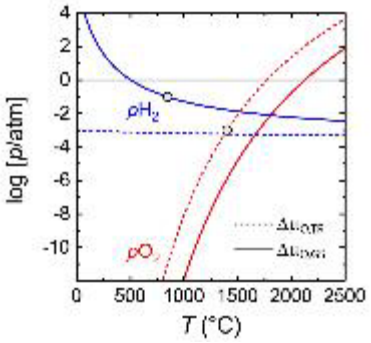
C. Musgrave, A. Holder, S. Millican

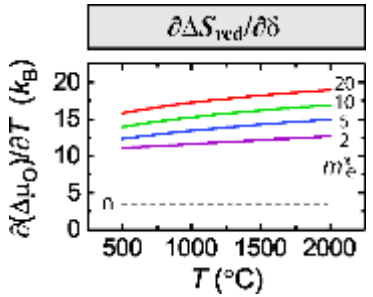


Electronic structure of hercynite in DFT and in band gap corrected GW

Basic design principles for STCH water splitting

- Optimal STCH activity by utilizing entropy due to charged defect formation

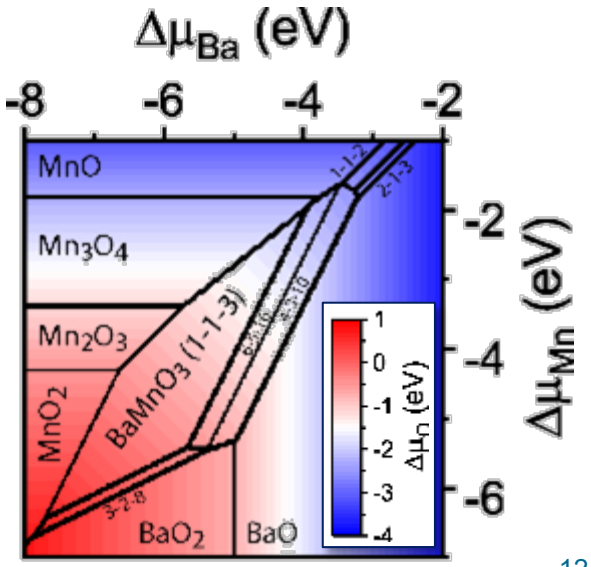




S. Lany, JCP **148**, 071101 (2018)

Colorado School of Mines

R. O'Hayre,
M. Sanders,
V. Stevanovic,
N. Kumar, J. Pan



Ba-Mn-O phase diagram in chemical potential space

Case Study: High Temperature Reactor Catalyst Material Development for Low Cost and Efficient Solar Driven Sulfur-based Processes

Collaboration

POSTER ID:

PD169

PI, Claudio Corgnale, **Greenway Energy** (GWE)
Co-PI, John Monnier, University of South Carolina

LEVEL 1 – Catalysis fundamentals
H_2SO_4 reaction catalyst understanding and development

- Catalyst performance understanding
- Catalyst development and synthesis
- Catalyst performance experimental tests

LEVEL 2 – Engineering design
H_2SO_4 reaction solar reactor design

- Novel reactor baseline configuration
- Numerical modeling of the reactor concept
- Reactor fabrication and experimental tests

LEVEL 3 – System analysis
Techno-economic analysis of the solar plant

- Novel HyS process flowsheet
- Conceptual design of the overall solar plant
- Economic-financial analysis of the solar plant

Final objective
H_2SO_4 decomposition system integrated in a solar HyS

- High energy and exergy efficiency (>20%, DOE target)
- Low hydrogen costs (<2 $/kg, DOE target)

Level 1 Action	Institution	Need for the AWSM
Catalyst development and synthesis	USC	- ***INL*** capability → run of H_2SO_4 decomposition tests at the required T, P and concentration
Catalyst tests under realistic conditions	*INL*	

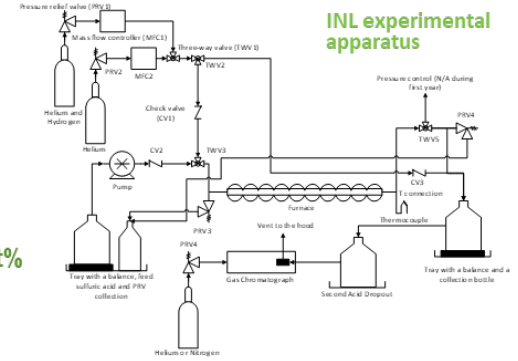
Level 2 Action	Institution	Need for the AWSM
Identification of novel solar reactor	GWE – *NREL*	- ***NREL*** has been critical to identify and optimize the novel direct solar reactor (concept being patented ROI filled)
Detailed model of the new reactor	GWE – USC	
Lab scale reactor demonstration	GWE – *NREL*	

Level 3 Action	Institution	Need for the AWSM
HyS Flowsheet	GWE – *SRNL*	- ***NREL*** capability → design of solar tower plants - ***SRNL*** capability → development of HyS process flowsheeting
Solar plant design	GWE – *NREL*	
Plant techno-economic analysis	GWE – *SRNL* - *NREL*	

INL test conditions

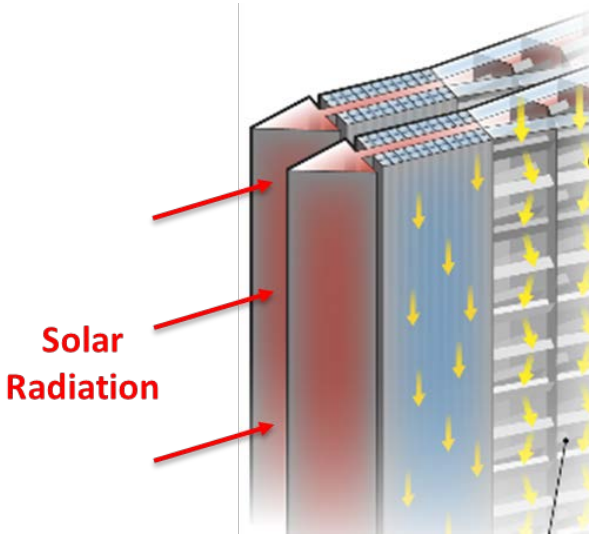
- **T up to ≈ 1000 °C**
- **P up to tens of bar**
- **H_2SO_4 conc > 90 wt%**

INL experimental apparatus

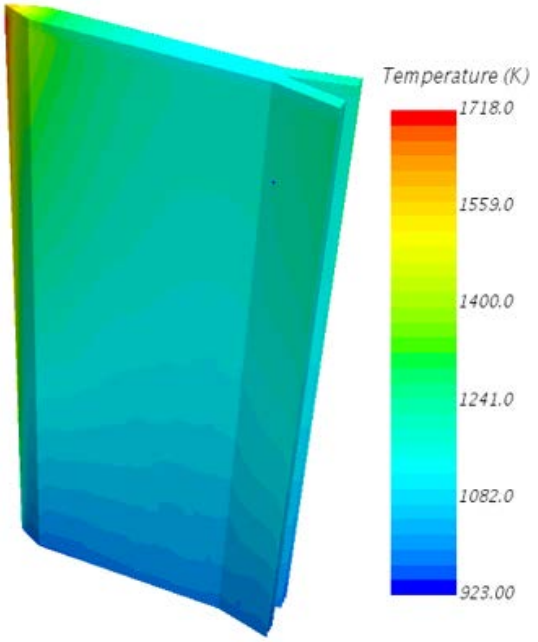


Case Study: H_2SO_4 Decomposition Reactor (GWE Seedling Project)

- Novel NREL solar cavity receiver design.
  - Direct solar irradiation of SiC receiver achieves higher operating temperature
  - Reduced volume and weight
  - No need for intermediate heat transfer fluid



- Completed preliminary large scale reactor design.
  - CFD model-based analysis
  - Verified effective heat transfer to H_2SO_4 gas
  - Predicted higher system efficiency



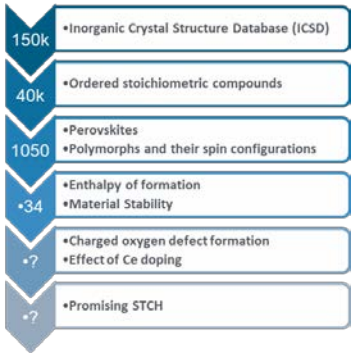
Case Study: Accelerated Discovery of STCH Materials via High-Throughput Computational and Experimental Methods

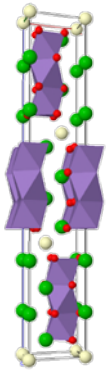
Collaboration

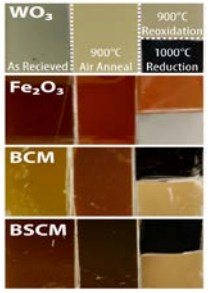
POSTER ID:

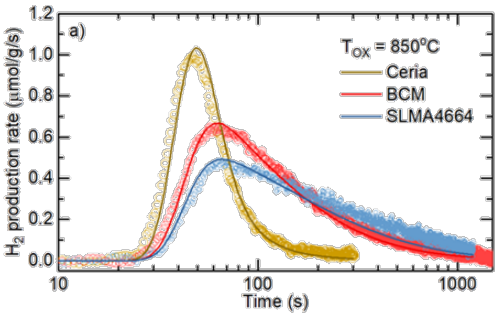
PD165

PI, Ryan O'Hayre, **Colorado School of Mines** (CSM)
Co-PI, Michael Sanders, Colorado School of Mines









Task 1: Computational

Stephan Lany
First Principles Materials Theory

- Computational resources (Peregrine)
- Expertise and guidance on research plan and execution
- Shared recent paper on charged vacancies
- Continued assistance to CSM computational team

The computational resources and expertise provided have been of the utmost importance. This was especially true in the early phase of the project.

Task 2: Combinatorial

Andriy Zakutayev
HTE Thin Film Combinatorial Capabilities

- Technical guidance on film deposition strategies
- Deposition of proof-of-concept and combinatorial library films
- Characterization of pre and post processed films
- Brought post-doc (Yun Xu) onboard to alleviate deposition bottleneck, greatly increasing the number of films available for early testing

The combinatorial film deposition capabilities are not available anywhere else and are integral to the screening plan for this project. Project success depends largely on this resource node.

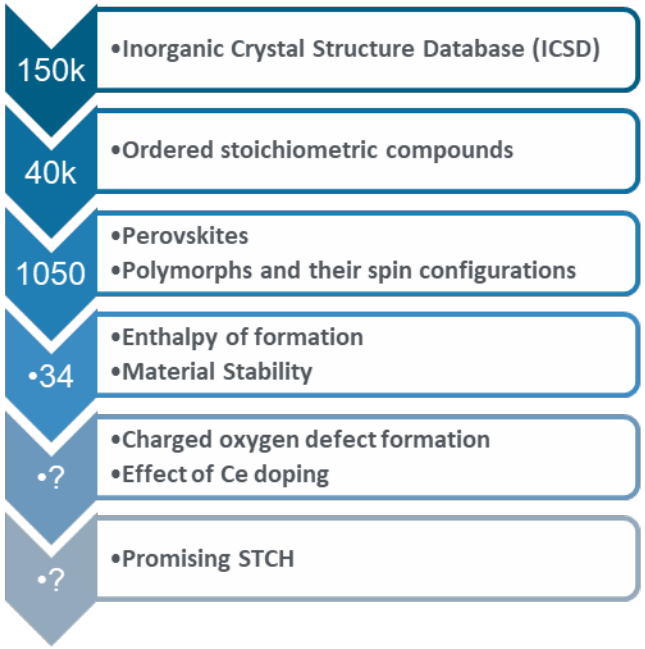
Task 3: Bulk Testing

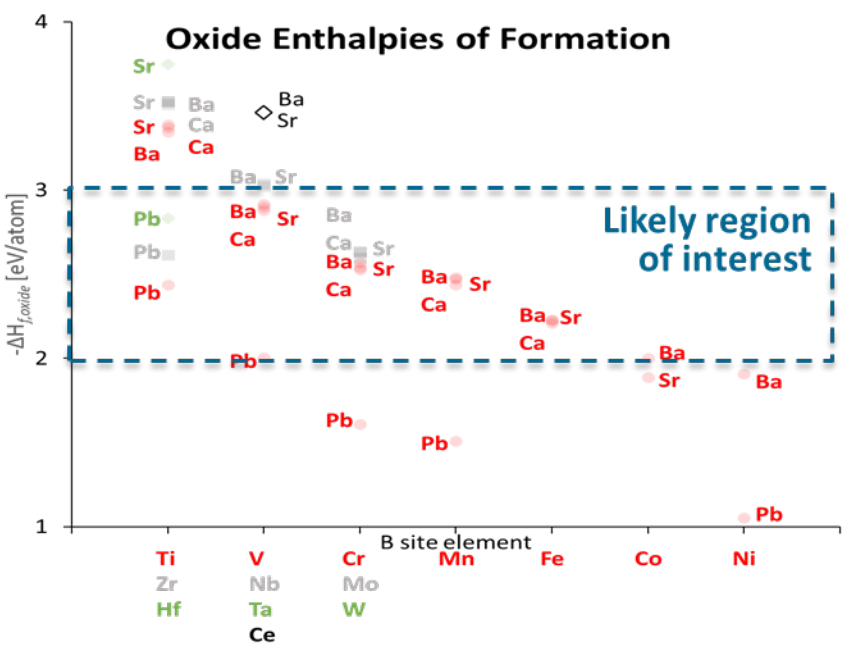
Anthony McDaniel
Laser Heated Stagnation Flow Reactor

- Discussions on durability testing of BCM and assisted with execution
- Assisted in SFR operation for testing of Compound X
- Main interface between group and pathway-specific Working Group

The SFR remains the best STCH test stand available and its continued access helps to not only verify new material performance but gives a reliable baseline for comparing to previously tested materials.

Case Study: High Throughput Computational Materials Screening (CSM Seedling Project)





Searched prospective water splitting perovskite formulations from all possible A-B element pairs of interest.

- Selection criteria based on structural configuration, formation enthalpy, defect formation energy
- Used NREL computational resources or existing databases

Other Notable Accomplishments from Projects

Computationally Accelerated Discovery and Experimental Demonstration of High-Performance Materials for Advanced Solar Thermochemical Hydrogen Production

PI, Charles Musgrave, University of Colorado
Co-PI, Alan Weimer, University of Colorado

Project Vision

Utilize machine-learned models coupled with ab initio thermodynamic and kinetic screening calculations to accelerate the RD&D of new STCH materials

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NODE	LAB	PI
First principles materials theory	NREL	S. Lany
Technoeconomic analysis	NREL	G. Saur
HT-XRD & TA	SNL	E. Coker
Laser heated SFR	SNL	A. McDaniel

Transformative Materials for High-Efficiency Thermochemical Production of Solar Fuels

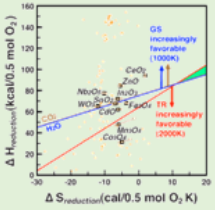
PI, Christopher Wolverton, Northwestern University
Co-PI, Sossina Haile, Northwestern University

Project Vision

Combine high-throughput computation and experiment to study the properties of novel, predicted STCH materials

POSTER ID:

PD167



NODE	LAB	PI
First principles materials theory	NREL	S. Lany
Technoeconomic analysis	NREL	G. Saur
Tools for enhanced thermochem H2	NREL	D. Ginley
Mesoscale kinetic modeling	LLNL	T. W. Heo

Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design for Solar Thermochemical Hydrogen

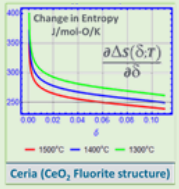
PI, Ellen Stechel, Arizona State University
Co-PI, Emily Carter, Princeton University

Project Vision

Accurate (enough) first principles calculations of the oxygen chemical potential for complex mixed ionic electronic (off-stoichiometric) doubly substituted perovskite solid solutions from which we can extract the thermodynamics

POSTER ID:

PD168



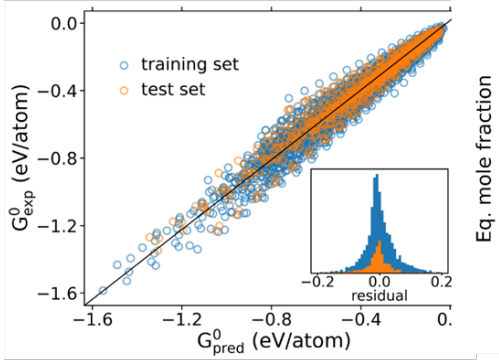
NODE	LAB	PI
Tools for enhanced thermochem H2	NREL	D. Ginley
HT-XRD & TA	SNL	E. Coker
UQ Toolkit	SNL	B. Debusschere
Laser heated SFR	SNL	A. McDaniel

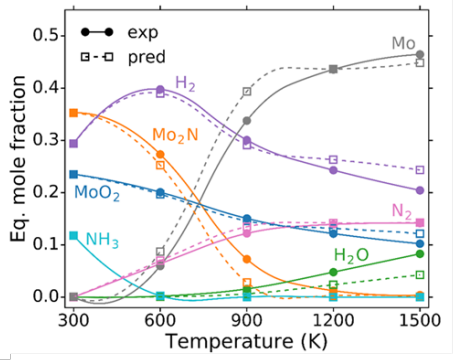
Machine Learning Accelerated Materials Discovery

Computationally Accelerated Discovery and Experimental Demonstration of High-Performance Materials for Advanced Solar Thermochemical Hydrogen Production

PI, Charles Musgrave, University of Colorado

Utilize Machine Learning (*ML*) models coupled with *ab initio* thermodynamic and kinetic screening calculations to accelerate the RD&D of new STCH materials

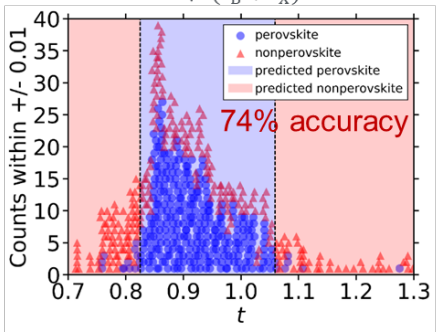




- Machine learned model for predicting the Gibbs energy, *G(T)*, with errors ~0.05 eV/atom
- Model depends on composition and 0 K calculated structure (PBE)
- Enables high-throughput rxn engineering from *ab initio* thermodynamic screening
- Collaboration with NREL

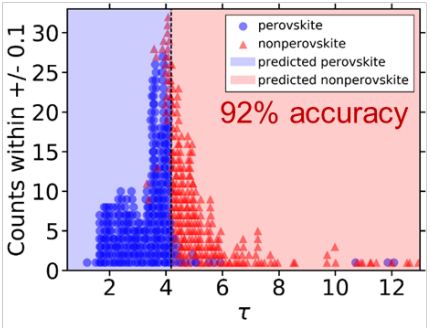
V. Goldschmidt 1926

$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$$



Bartel *et al.* 2018[2]

$$\tau = \frac{r_X}{r_B} - n_A\left(n_A - \frac{r_A/r_B}{\ln r_A/r_B}\right)$$



- Machine learned model (**τ**) for improving upon Goldschmidt's ***t*** for predicting perovskite stability
- τ – 92% vs. t – 74% accuracy for 576 experimentally characterized compounds
- Used to as 1st step in material screening to reduce required DFT calculations

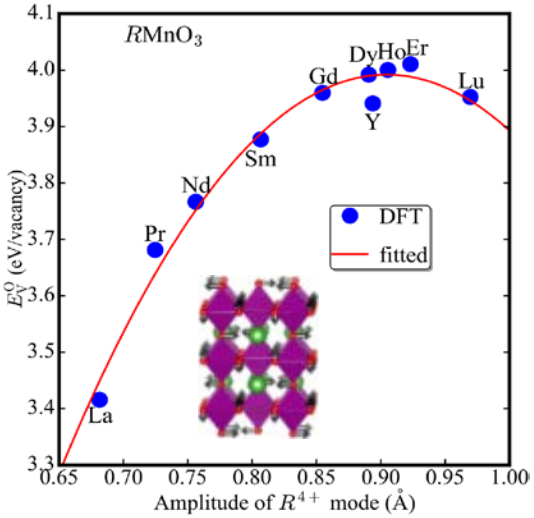
- Machine learned models trained on experimental data make application of theory faster and more reliable.

DFT Enabled Materials Screening and Materials Engineering

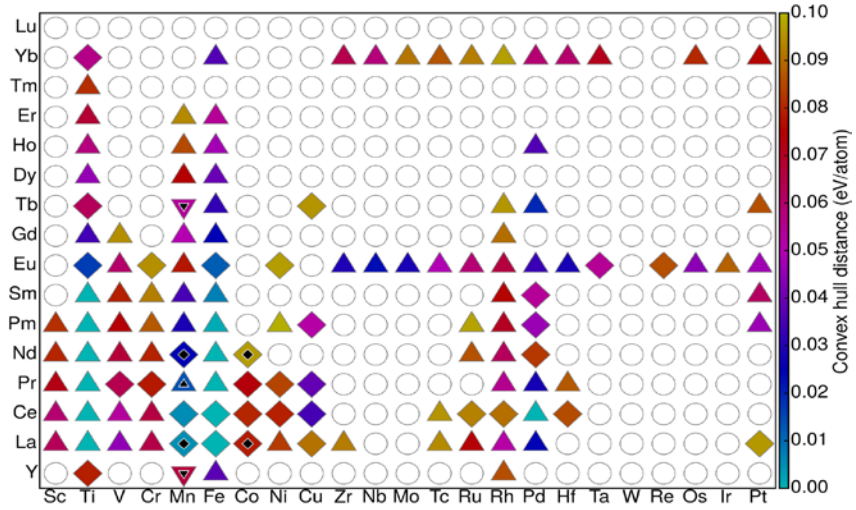
Transformative Materials for High-Efficiency Thermochemical Production of Solar Fuels

PI, Christopher Wolverton, Northwestern University

- Rare earth series ($RMnO_3$) oxygen vacancy formation energy.
  - Energy follows R^{4+} octahedral tilt amplitude quadratically
  - Can predict *and* engineer oxygen vacancy formation energy



- High throughput DFT screening of RAM_2O_6 double perovskites.
  - R=rare earth; A= alkaline earth; M=transition metal
- Large number of new stable compounds predicted.
  - Experimentally screening for redox activity

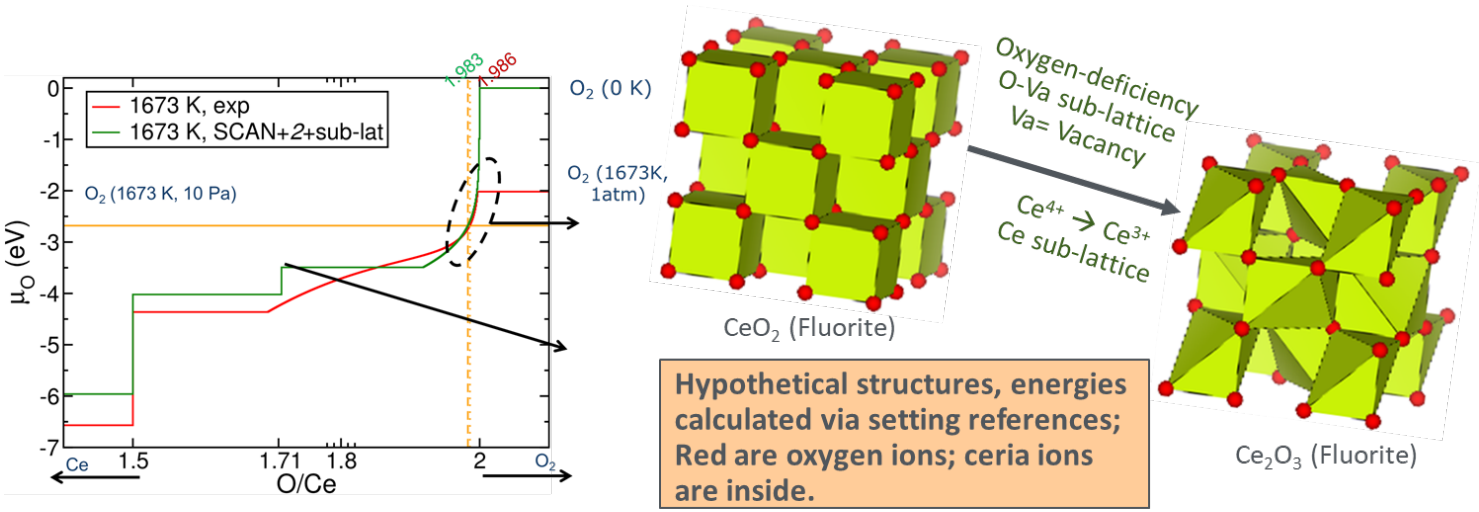


- Data in Open Quantum Mechanical Database (OQMD) used to assess new double perovskite materials.

DFT (SCAN+U) based CALPHAD Model

Mixed Ionic Electronic Conducting Quaternary Perovskites: Materials by Design for Solar Thermochemical Hydrogen

PI, Ellen Stechel, Arizona State University



Gibbs energy of $CeO_{2-\delta}$ in fluorite (F) phase; oxygen chemical potential is the derivative wrt δ; equilibrium determined by equating oxygen chemical potential to gas phase

$$G^F_{CeO_{2-\delta}} = y_{Ce^{4+}} y_O G^0_{Ce^{4+}:O} + y_{Ce^{3+}} y_O G^0_{Ce^{3+}:O} + y_{Ce^{4+}} y_{Va} G^0_{Ce^{4+}:Va} + y_{Ce^{3+}} y_{Va} G^0_{Ce^{3+}:Va} + RT\left(y_{Ce^{4+}} \ln y_{Ce^{4+}} + y_{Ce^{3+}} \ln y_{Ce^{3+}}\right) + 2RT\left(y_O \ln y_O + y_{Va} \ln y_{Va}\right) + G^F_{excess}$$

Configuration entropy: ideal solution behavior

y= Site fraction

Correction term

All Energies determined with DFT (SCAN+U)

- Oxygen chemical potential in solid calculated directly using DFT method avoids computational cost associated with modeling entropy effects.

Engagement with 2B Team and Data Hub

Accomplishment

- Collaboration with 2B Team Benchmarking Project.
- Node feedback on questionnaire & draft test framework.
  - Defining: baseline materials sets, testing protocols
- All HydroGEN STCH node capabilities were assessed for AWS technology relevance and readiness level.
- STCH data metadata definitions in development.
- Large number of STCH datasets uploaded to hub.
  - Designing custom APIs to facilitate error-free, auto-uploading

Future Work

- Leverage HydroGEN Nodes at the labs to enable successful Go/No-Go of Phase 1 projects.
  - Validate computational approach and predictive power of theory
  - Demonstrate high-throughput experimental approach to oxide discovery
  - Demonstrate enhanced material performance that validates predictions

- Enable research in Phase 2 work for some projects and enable new seedling projects.
- Work with the 2B team and STCH working group to establish testing protocols and benchmarks.
- Utilize data hub for increased communication, collaboration, generalized learnings, and making digital data public.

Any proposed future work is subject to change based on funding levels

Summary

- Developing and validating tools for accelerated materials discovery are major seedling project themes.
  - Computational material science proving effective
    - Machine learned models make application of theory faster
    - DFT-CALPHAD model accurately predicts oxygen chemical potential in CeO_2
- Supporting 5 FOA projects with 11 nodes and 11 PIs.
  - DFT modeling, materials characterization, synthesis, analysis, design
  - Personnel exchange: PIs and graduate students visit the labs
  - Collaboration: Node PIs meet regularly with projects
- Working closely with the project participants to advance knowledge and utilize capabilities and the data hub.
- Future work will include continuing to enable the projects technical progress and develop & utilize lab core capabilities.

Acknowledgements

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HydroGEN
Advanced Water Splitting Materials

Authors

Anthony McDaniel
Huyen Dinh

STCH Project Leads

Claudio Corgnale
Charles Musgrave
Ryan O'Hayre
Ellen Stechel
Chris Wolverton

Node PIs

Eric Coker
Bert Debusschere
David Ginley
Daniel Ginosar
Max Gorensek
Tae Wook Heo
Stephan Lany
Zhiwen Ma
Anthony McDaniel
Genevieve Saur
Andriy Zakutayev

Research Teams

Greenway Energy LLC
Engineering consultant in Aiken County, South Carolina

Northwestern University

NREL | BERKELEY LAB | Sandia National Laboratories | INL Idaho National Laboratory | Lawrence Livermore National Laboratory | SRNL