Energy Materials Network
U.S. Department of Energy

HydroGEN
Advanced Water Splitting Materials

Project ID: P148e

Cross-Cut Modeling

Contributors: Tadashi Ogitsu, Tuan Anh Pham, Brandon Wood, Joel Varley, Andrew Rowberg, Shenli Zhang, Marcos Calegari, Huyna Kwon, Alexandra Zagalskaya, Fikret Aydin (LLNL); Joel Ager, Adam Weber, Masao Suzuki (LBNL); Meng Li, Qian Zhang (INL); Stephan Lany, Mai-Anh Ha, Ross Larsen (NREL); Anthony McDaniel, Matt Witman, Sean Bishop (SNL)

Presenter: Tadashi Ogitsu, Cross-Cut Modeling Lead, LLNL

Date: May 7, 2024

DOE Hydrogen Program

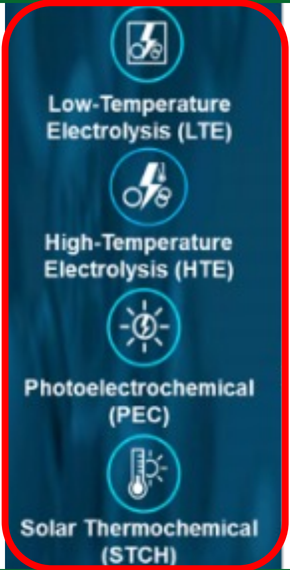
2024 Annual Merit Review and Peer Evaluation Meeting

NREL Transforming ENERGY | BERKELEY LAB | Sandia National Laboratories | INL | Lawrence Livermore National Laboratory

HydroGEN Project Goal

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

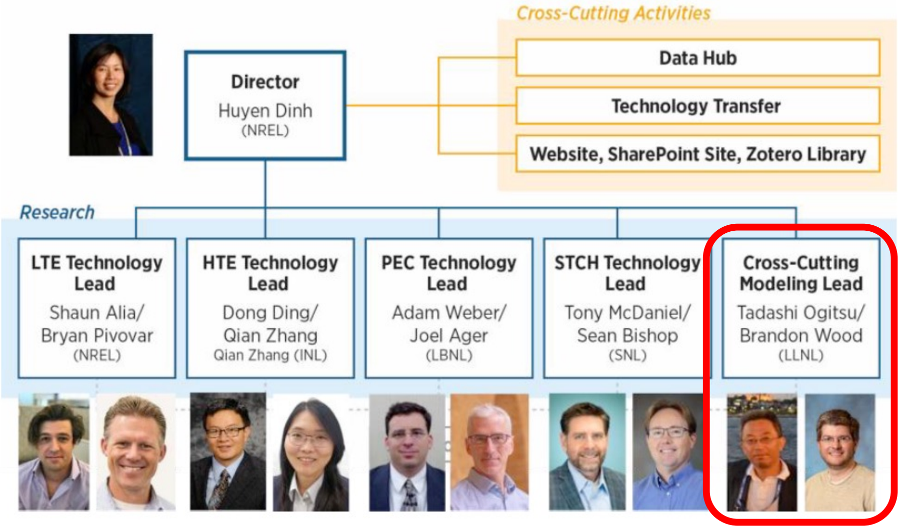
Goal: Accelerate foundational R&D of innovative materials for advanced water splitting (AWS) technologies to enable clean, sustainable, and low-cost (\$1/kg H_2) hydrogen production



H_2 Production Target: \$1/kg

HydroGEN is focused on early-stage R&D in H_2 production and fosters cross-cutting innovation using theory-guided applied materials R&D to advance all emerging water-splitting pathways for hydrogen production

HydroGEN PEC Overview



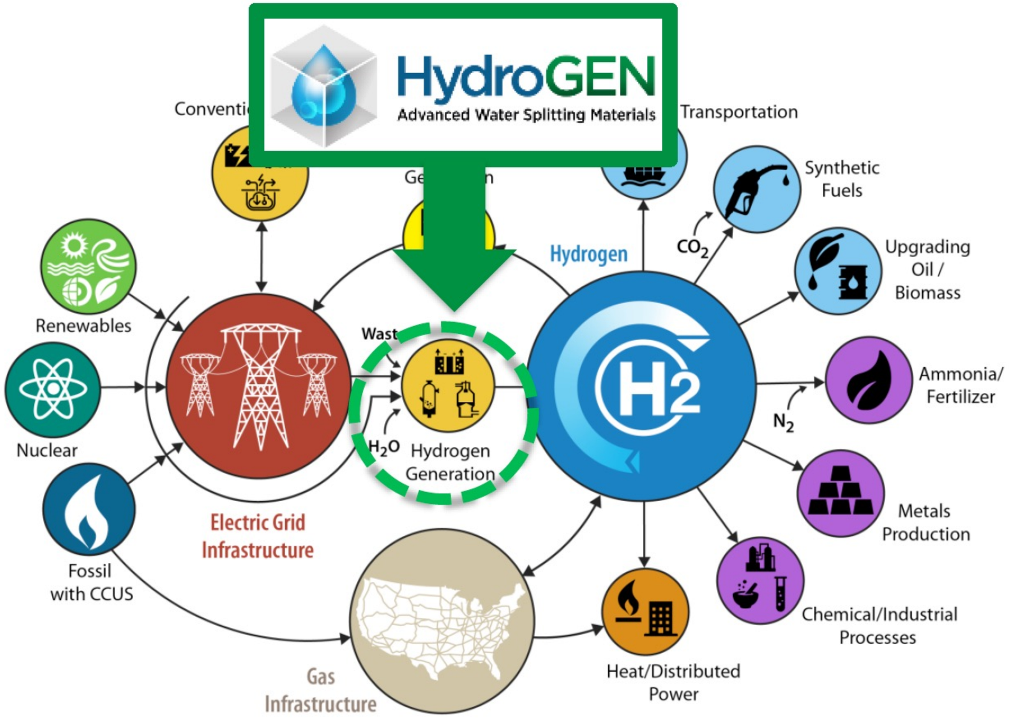
Barriers

- Efficiency
- Durability
- Cost

National Lab Cross-Cut Team

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Relevance and Potential Impact



Source: DOE Hydrogen and Fuel Cell Technologies Office, https://energy.gov/eere/fuelcells/h2-scale

Transportation and Beyond

Large-scale, low-cost hydrogen from diverse domestic resources enables an economically competitive and environmentally beneficial future energy system across sectors

Hydrogen can address specific applications that are hard to decarbonize

Today: 10 MMT H_2 in the US

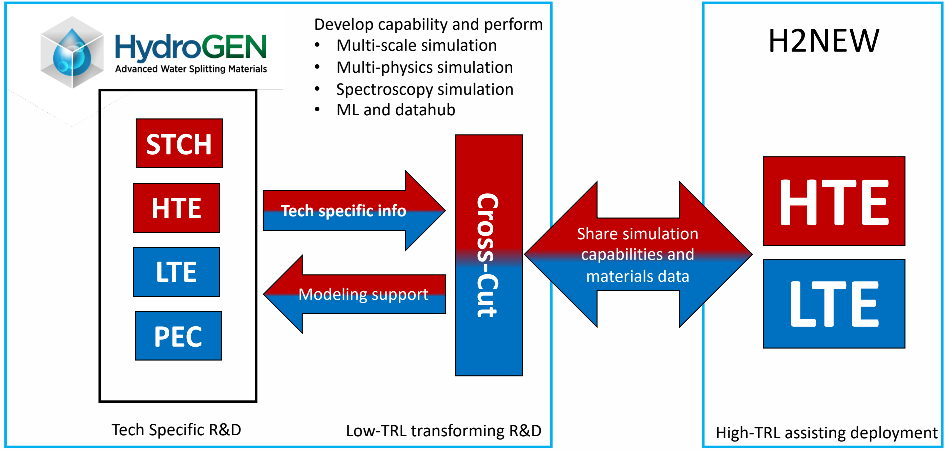
Economic potential: 2x to 4x more

Materials innovations are key to enhancing performance, durability, and reduce cost of hydrogen generation, storage, distribution, and utilization technologies key to H2@Scale

"Hydrogen at Scale (H_2@Scale): Key to a Clean, Economic, and Sustainable Energy System," Bryan Pivovar, Neha Rustagi, Sunita Satyapal, Electrochem. Soc. Interface Spring 2018 27(1): 47-52; doi:10.1149/2.F04181if.

Cross-Cut Modeling Relevance and Potential Impact

Facilitate collaboration between NREL/LBNL/INL/SNL/LLNL



- Identify common aspect of computational modeling needed for four technologies
- Share node capabilities between different technologies and maximize effectiveness and efficiencies of modeling support
- Share capabilities, expertise, and knowledge between HydroGEN and H2NEW

Outcome:

- Low temperature technologies share similar needs in understanding solid-liquid interface under operation condition
- High temperature technologies share many commonalities
  - Thermodynamic analysis of alloy phase diagram including defect analysis
- Modeling effort needs to be complemented by characterization for validation

Cross-Cutting Modeling Approach

Design

- Provide **design guidance** for optimizing materials, components, and devices

Search

- Enable machine learning/data science approaches for **rapid materials discovery**

Explain

- **Deconvolute** key factors that are hard to be accessible through direct experiments

Prioritize

- **Prioritize investments** by assessing the most important factors under operating conditions

Safety in AWSM laboratories – LLNL

Lawrence Livermore National Laboratory (LLNL) is committed to protecting workers and the public, and to continual improvement in occupational health and safety (OHS) performance using the LLNL Integrated Safety Management System (ISMS). At LLNL safety and health are a priority in the planning and execution of all work activities.

In support of this policy, LLNL management and workers are committed to:

- Working safely.
- Creating a workplace that is safe, healthy, and injury/illness free.
- Utilizing LLNL hazard and risk analysis tools to identify hazards, reduce overall risk in the performance of work and to ensure a safe and healthy work environment.
- Taking responsibility and being accountable for the continuous improvement of safety and health performance at LLNL.
- Complying with applicable Environment, Safety, and Health (ES&H) laws, regulations, and other policies.
- Working together to understand the mission, the core capabilities, the risks, and opportunities associated with the work performed at the Laboratory.

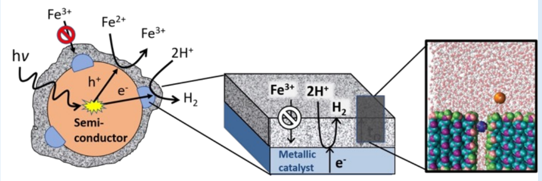
LLNL's commitment to foster and maintain a safety-conscious work environment in its facilities and in the conduct of work is based on the following principles:

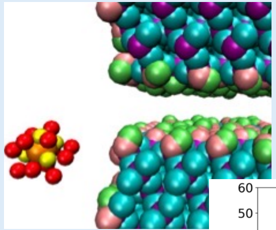
- Safety is a prerequisite for all work. Our expectation is that every worker goes home in the same or better condition than when he or she came to work.
- Worker involvement is the cornerstone of our safety culture and is essential to the successful implementation of the ISMS, International Organization for Standardization (ISO), Occupational Health and Safety Management System (OHSMS), Environmental Management System (EMS), and other ES&H program elements.
- All workers are expected to have a questioning attitude focused on hazard identification and risk reduction, promptly report all injuries and illnesses, and pause or stop work if/when they recognize that a job cannot be done safely.
- All members of the LLNL Senior Management Team, up to and including the Deputy Director and Director of LLNL, have an open door policy.
- The Deputy Director and Director of LLNL require Laboratory-wide OHS objectives and action plans to track/update progress.
- LLNL provides multiple venues for workers to express safety concerns. These include, but are not limited to their management chain, B-SAFE hotline, "Ask the Director," and the Ombuds Program.

Workers are encouraged to raise safety issues and concerns without fear of reprisal. The LLNL Senior Management Team commits to address and resolve issues and concerns in a timely manner.

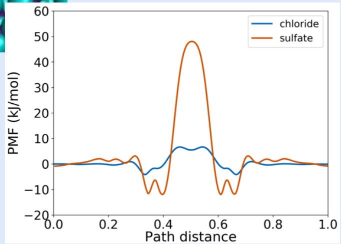
Accomplishments of low-temperature technologies (PEC/LTE)
Atomistic insights into transport, OER activities, stability

PEC: Protective layers





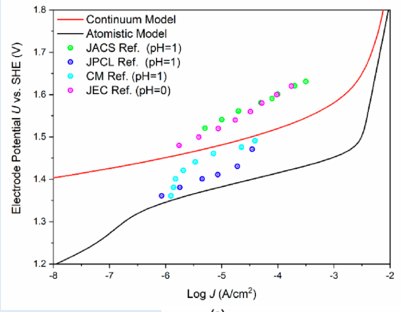
Oxide overlayer for selective transport



Aydin et al., EES Catalyst (Submitted)

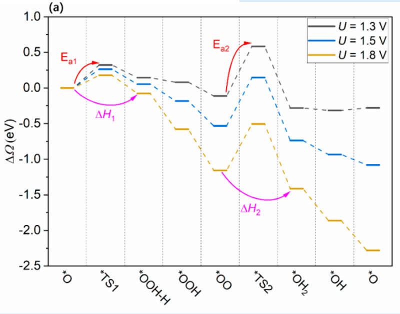
Developed **design principles** for optimizing protective layers

PEC: OER Activity



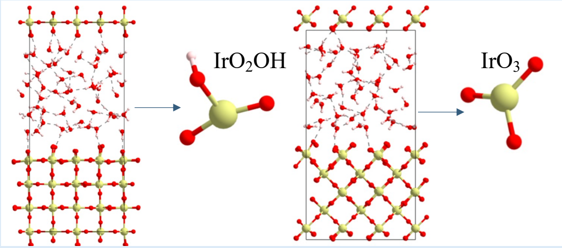
Developed models for predicting reaction kinetics

Reaction kinetics as a function of applied potentials



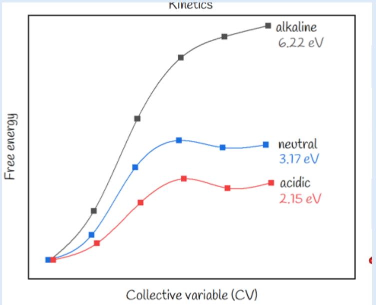
Deconvoluted impacts of operating conditions on activity

LTE: Catalyst Stability



Deconvolute impacts of **surface morphology**

Predict how **pH** influences dissolution kinetics



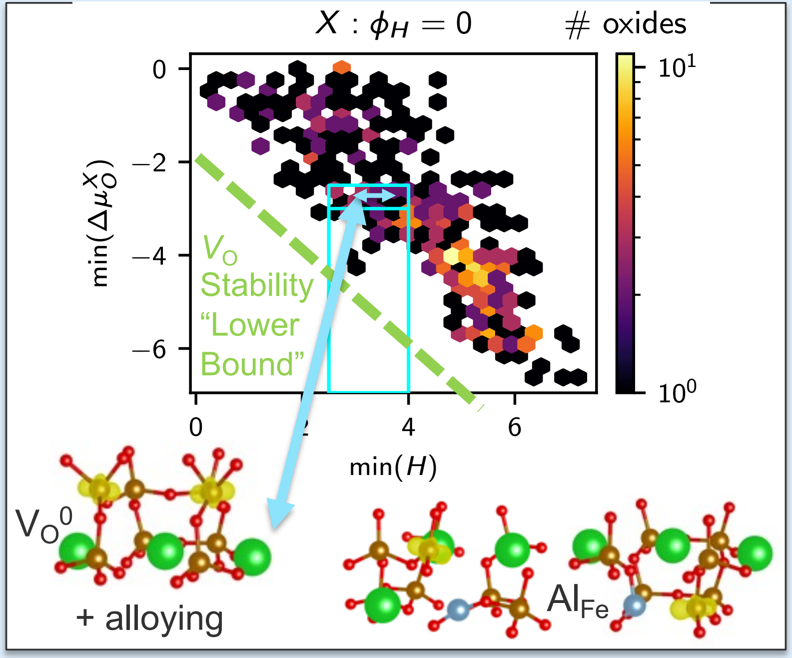
Identified **most important factors** controlling catalyst durability

Zhou et al., ACS Appl. Energy. Mater. (2023)

Zagalskaya et al., (in preparation)

Accomplishments of high-temperature technologies (STCH/HTE)
Understand stability/role of defects at operation condition

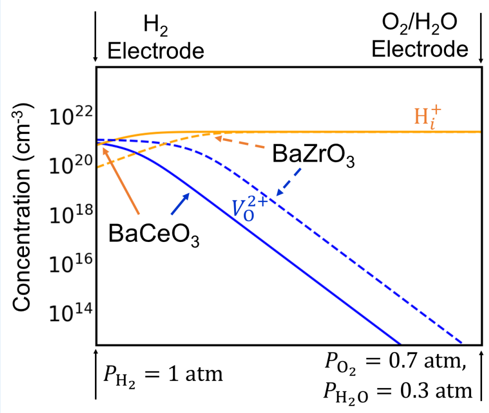
STCH: Expand dataset for oxide discovery



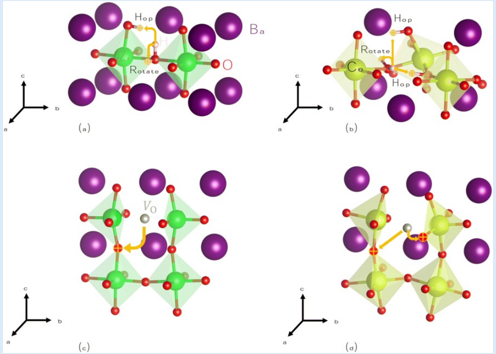
Expand and refine dataset for improving fidelity of ML models for materials discovery

LLNL-SNL. Nat. Comput. Sci. 3, 675 (2023)

HTE: Predict factors controlling transport



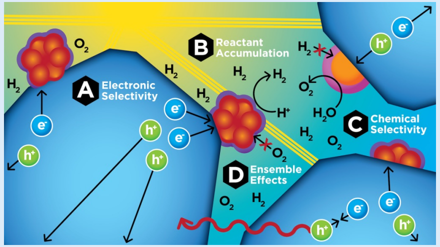
Developed guidance for optimizing **operating conditions** for enhanced ionic conductivity



Predicted impacts of **alloying** on ionic conduction

LLNL-INL. Mater. Adv. 4, 6233 (2023)

Collaboration across DOE Hydrogen Program

Centers		Activities
	**EFRC: Ensembles of Photosynthetic Nanoreactors (EPN)**	• Successfully turned a **seedling project** into a multi-million/institution EFRC project • Continue to engage with EFRCs to create **cross-pollination opportunities** between EERE and BES
ENERGY earthshots U.S. DEPARTMENT OF ENERGY	**EERC: Ionomer-based Water Electrolysis**	• Identified common interest, share data and modeling capabilities with CIWE • Developed joint project on development of multiscale simulations for **predicting ionomer degradation**
U.S. DEPARTMENT OF ENERGY DOE EPSCoR	**EPSCoR: Fe based non-PGM OER catalyst**	• Support training and **STEM education and workforce development** for hydrogen economy • LLNL team committed to **diversity and inclusion**, and career development (6 early careers with 3 female PDs)

HydroGEN Cross-Cut Seedlings: 3 new starts

P213
Shu Hu, Yale University

>200 cm^2 Type-3 PEC Water Splitting Prototype Using Bandgap-Tunable Perovskite Tandem and Molecular-Scale Designer Coatings

Node support: NREL, LBNL, LLNL

P215
Nicolas Gaillard, University of Hawaii

Semi-Monolithic Devices for Photoelectrochemical Hydrogen Production

Node support: NREL and LLNL

P217
Xin Qiang, St-Gobain

Scalable Solar Fuels Production in A Reactor Train System by Thermochemical Redox Cycling of Novel Nonstoichiometric Perovskites

Node support: NREL, SNL and LLNL

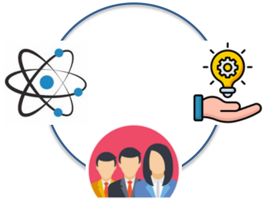
HydroGEN Cross-Cut: Future Work

Enhance modeling capabilities to achieve HFTO targets

- Develop capabilities to access impacts of materials corrosion on long-term performance
- Develop capabilities to predict how materials & usage variability influence performance and lifetime
- Address the "small data" problem to enable AI/ML approaches for materials discovery and optimization

Foster collaboration & engagement

- Foster collaboration with other offices (DOE-BES, ARPA-E)

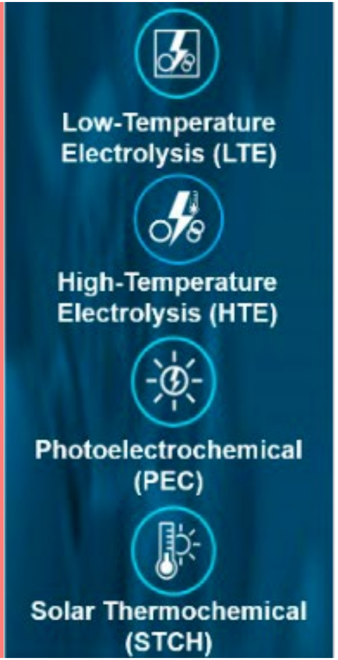


- Train next-generation workforce in multiscale simulation through partnerships with leading academic institutions
- Enable and strengthen international partnerships

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

Summary

Cross-Cutting Modeling



Supported all 4 technologies, seedling & FOA projects

5 publications & 8 invited presentations

Collaboration & engagement

- Collaboration with other offices (DOE-BES, ARPA-E, EPSCoR program)
- We continued to traine next-generation workforce in multiscale simulation through partnerships with leading academic institutions
- Enabled and strengthen international partnerships (ex. US-Japan-Korea collaboration)