Directed Search for Stable and Conductive Electrolytes for Next-Generation Proton Conducting Solid Oxide Electrolysis Cells

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DOE project award #

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Project Goals

- Identify and develop alternative proton-conducting electrolytes that improve material lifetime with respect to the state-of-the-art (SOA) and meet the P-SOEC performance targets of ≥0.8 A/cm^2 at 1.3 V/cell with ≤5 mV/khr degradation rate and a faradaic efficiency of ≥85%.

- Develop a computational database of candidate electrolytes that survey thermodynamic stability, hydrogen solubility, and hydrogen transport with respect to operating conditions

- Implement a working p-SOEC with in a packaged button cell and larger format cell to assess scale-up behavior.

Overview

Timeline and Budget

- Project Start Date: 02/02*/2024
- FY24 DOE Funding: $1,060k
- FY25 Planned DOE Funding: $1,060k
- Total DOE Funds Received to Date: $1,060k

Partners

- **Project lead:** Dr. Joel B Varley, Lawrence Livermore National Laboratory
- **Co-PI:** Dr. Wei Wu, Idaho National Laboratory, *experimental synthesis, testing and validation*
- **Potential collaborators (as part of H2LinkSc):** HEIS (Northwestern, MIT)

Barriers

Need: proton-conductivity electrolytes that exhibit higher *chemical stability* and *proton conductivity*

- **Barrier:** Existing SOA materials are complex and difficult to optimize (BCZY:X)
- **Target:** Computationally identify ”simpler” alternative chemistries and structures to experimentally synthesize and test
- **Barrier:** Synthesizing, scaling and optimizing new materials is difficult
- **Target:** Computationally identify materials most robust to varying conditions (e.g. influence of large gradients in chemical potentials and impurities) and connect with relevant experimental variables

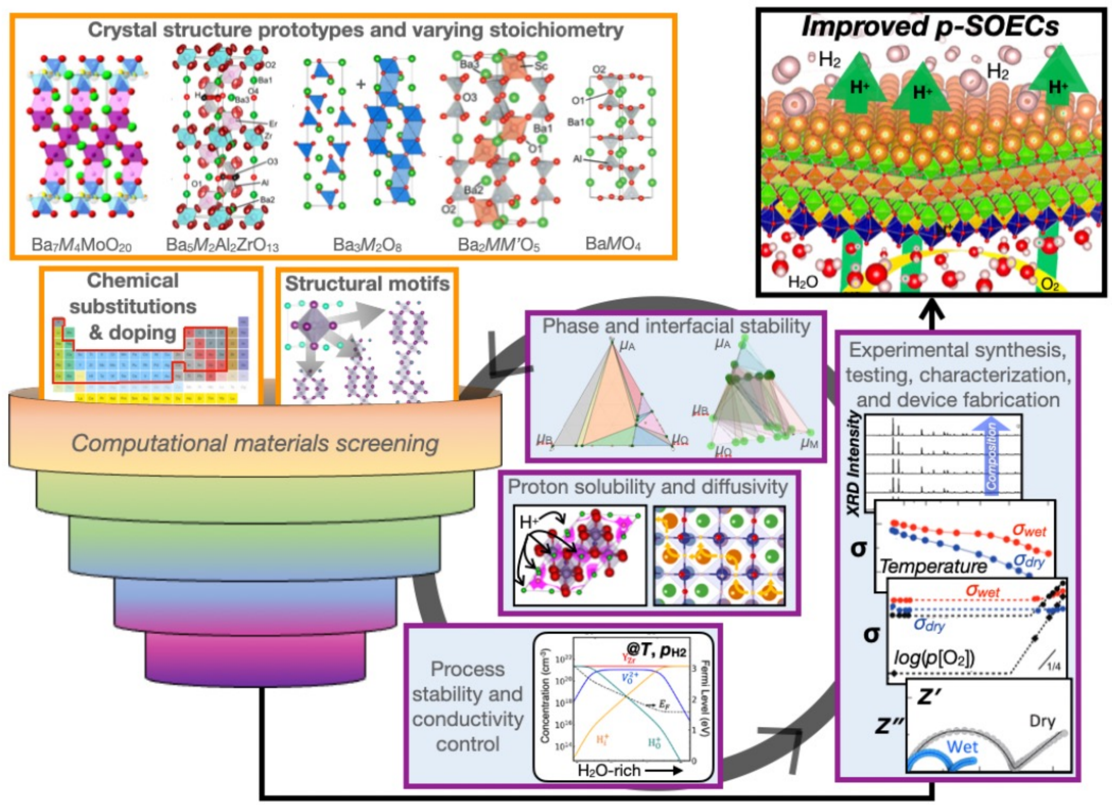
Potential Impact

- p-SOEC-based electrolyzers can operate with high efficiencies at lower temperatures but exhibit stability and degradation issues
  - Alternative electrolytes with improved stability and more facile optimization compared to existing choices (e.g. BZCY) will accelerate improvements and lower costs of P-SOECs
  - Targeted improvements in device efficiency and longevity can lead to p-SOEC devices capable of meeting the DOE's $2/kg target for electrolytic hydrogen production by 2026
- Our proposal will expand the options for viable electrolyte candidates that can lead to increased p-SOEC performance and reliability

Approach

Technical Approach

- Develop computational databases that assess alternative electrolyte structures and chemistries
  - Thermodynamic stability
  - Hydrogen solubility
  - Hydrogen transport
  - Chemical doping and alloying
- Synthesize prototype and down-selected electroytes with solid-state reaction methods
  - Electrochemical testing of performance under different temperature, hydration and environmental conditions
- Integrate and test electrolytes in p-SOEC devices
  - button cells and larger format devices



Approach

Milestones and Deliverables

- **Q1:** Initialization of electrolyte stability database
- **Q2:** Synthesis protocol for prototype electrolytes $Ba_7Nb_4MoO_{20}$ and Ba_2ScAlO_5
- **Q3:** Delivery of first electrolyte stability database with down-selected candidates
- **Year 1 Go/No-Go:** Demonstrated synthesis protocol and initial property characterization of at least 1 computationally-identified electrolyte
- **CBP:** Have a summer student intern generate and present their results

Approach: Safety Planning and Culture

- **A Hydrogen Safety Plan was not required for our project submission.**

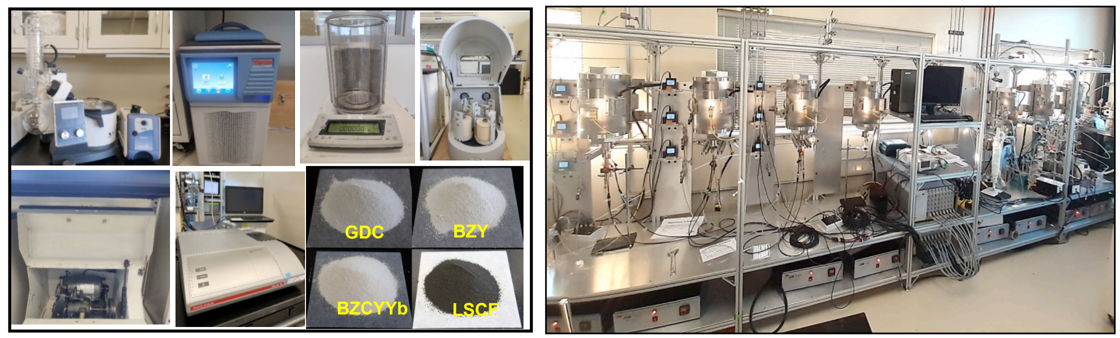
Accomplishments and Progress

This is a new project and has not been reviewed previously

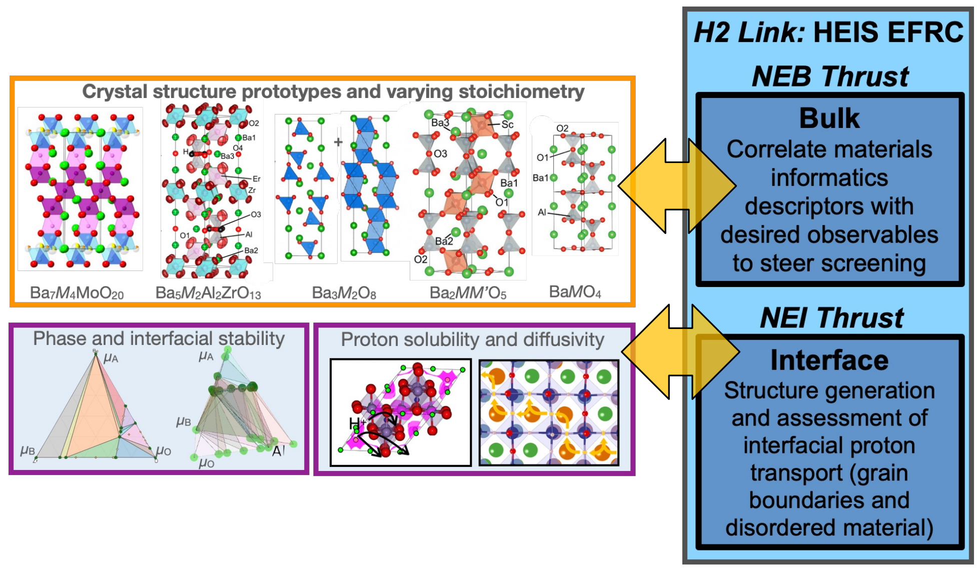
- Funding received at LLNL, with budgeting issues related to partners being resolved

Collaboration and Coordination

- **Project collaborators:**
  - Dr. Wei Wu (Idaho National Lab)
  - **Project roles:** Manage experimental synthesis, characterization and device fabrication and testing efforts



- **Planned Project collaborators:**
  - HEIS (Hydrogen in Energy and Information Sciences) EFRC (H2LinkSc)
    - Prof. J. Rondinelli (Northwestern)
    - Prof. B. Yildiz (MIT)
    - Prof. C. Wolverton (Northwestern)
  - HydroGEN consortia: assisting with testing and scale-up of cells, and process optimization



DEIA/Community Benefits Plans and Activities

Outreach activities and increased participation

- Coordinating with LLNL Discovery Center to create hydrogen technology-focused outreach efforts to young students and under-represented groups within the community and Bay Area.
- Bringing on summer students each year from minority serving institutions and/or under-privileged backgrounds

- **Fostering Energy Equity**
  - Alignment with Justice40, and exploring opportunities for developing chemical technician curricula for local and regional high school graduates and community colleges across Idaho (e.g. College of Southern Idaho).

Remaining Challenges and Barriers

To be determined!

- Population of electrolyte databases and actualizing predicted materials will take time and effort.
- Many calculations to do and experiments to perform!

Proposed Future Work

FY24: Initial population of computational databases related to thermodynamic stability and hydrogen solubility; initial development of prototype electrolyte (Ba2 and Ba7) synthesis and testing protocols.

FY25: Population of computational databases related to chemical doping/alloying stability and hydrogen transport; Development of down-selected electrolyte and implementation into p-SOEC device.

FY26: Performance optimization of down-selected electrolytes with respect to hydration, stoichiometry and processing.

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

Mandatory Summary Slide

Project has just started

- Population of a computational database on candidate proton-conducting electrolytes is just beginning.
- Initial synthesis and characterization efforts will soon be underway!