Center for Alkaline Based Energy Solutions (CABES)
EFRC Director: Héctor D. Abruña
Lead Institution: Cornell University
Class: 2018 – 2026

Mission Statement*: To advance the scientific understanding of the fundamental factors governing electrocatalysis and electrochemical energy conversion in alkaline media.*

CABES, the *Center for Alkaline Based Energy Solutions* aims to achieve a detailed understanding of the nature, structure, and dynamics of electrocatalysis in alkaline media. We seek a detailed understanding of the nature, structure, and dynamics of fuel cell systems operating in alkaline media. CABES integrates theory and computational methods, synthesis of electrocatalysts and novel membrane materials and the development of experimental tools that will provide *in situ*, spatiotemporal characterization of systems under operation. Our programmatic focus and vision are based on 3 fundamental science drivers (SDs): **SD-1**. What factors govern electrocatalysis in alkaline media? **SD-2.** How do we understand and control transport in alkaline media? **SD-3.** What makes energy materials durable in alkaline media?

The center's integrated approach is aimed at greatly accelerating the development of electrocatalysis in alkaline media by generating the fundamental knowledge for the rational development of new materials and architectures as well as experimental and computational tools necessary for, and critical to, a fundamental understanding of these processes. We foresee the center as providing the basis for ushering an alkaline-based energy technology society with emphasis on fuel cells and electrolyzers.

CABES addresses fundamental issues of critical need and importance in energy conversion technologies, guided by the challenges articulated in the relevant DOE reports, Basic Research Needs and in support of two Energy Earthshots (Hydrogen and Long Duration Storage). CABES' advances are highlighted in authoritative and comprehensive review articles (Y. Yang, C. R. Peltier…H. D. Abruña; "*Electrocatalysis in Alkaline Media and Alkaline Membrane-Based Energy Technologies*" Chem. Rev. 2022, 122, 6, 6117–6321). Qihao Li, Andrés Molina Villarino… David A. Muller, Geoffrey W. Coates, Piotr Zelenay, and Héctor D. Abruña "*Anion Exchange Membrane Water Electrolysis: The Future of Green Hydrogen*" Journal of Physical Chemistry C (2023), 127(17), 7901-7912

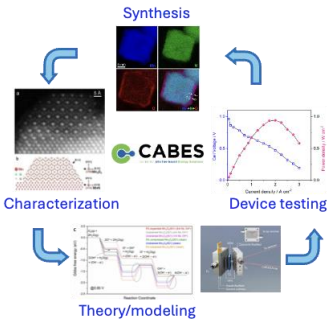

Fig. 1. SD1 synergistic research loop illustrating interactions between/among the different components of the team.

CABES' SD-based approach revolves around synergistic loops enabled by the center's three cross-cutting disciplines: materials synthesis and characterization, modeling/data science and *operando* analysis (including device testing). Fig. 1 presents the loop for SD-1. Work of each discipline within the loop informs the others; i.e. theory may suggest new catalysts to synthesize, or characterization helps refine modeling. We have expanded our previously successful strategy of strain-engineering the surfaces of nanoparticles by tuning the core composition to enhance reactivity. We also introduce high-entropy materials to increase the catalyst design space and stability options, as the "cocktail effect" from incorporating many different elements leads to unique chemical and electronic environments, as well as strain. The *ab-initio* modelling of surface structure and reaction pathways will greatly benefit from our data science tools for exploring these higher-dimensional spaces. (Fig.2)

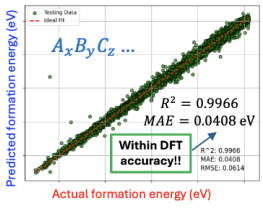

Fig.2 Predicted and actual formation energies of multicomponent catalyst candidates.

Science Driver 2 is focused on how the architecture, especially of electrolyte/membrane materials, and interfaces within them, influences ion, molecular, and electronic transport in electrochemical systems under alkaline conditions. The

relationships between architecture and transport are investigated through the same integrated approach employed in SD-1. Systematic synthesis alkaline exchange membranes (AEMs), correlated ionomers, (including new synthetic strategies that afford structural control) and the respective interfaces between/among ionomers, catalysts, and supports are analyzed with analytical and theoretical/computational local probes of critical parameters. We also assess the transport properties that result from these structures, through measurements of water uptake, water permeability, hydroxide ion conductivity, in AEM fuel cells and AEM water electrolyzers.

The aim of Science Driver 3 is to understand what makes energy materials durable in alkaline media. Efforts are organized around fundamental questions that include degradation pathways in alkaline media of membranes and ionomers during transport of OH^- and how high performing and durable electrolytes be designed and synthesized. We are also focused on understanding interactions of membranes and ionomers with catalysts/supports.

Theory and Computation, as a cross-cut effort, informs the most promising directions to pursue by employing Cahn-Hilliard dynamical studies, Joint Density Functional Theory modeling and machine learning potentials. Fig. 2. Additionally, machine learning and artificial intelligence approaches are accelerating the search for new electrocatalysts and improving understanding of transport phenomena.

Fig.3 Electron microscope dedicated to operando studies.

CABES *operando* methods cross-cut effort, has developed unique experimental capabilities including cryo-TEM for the study of membranes and ionomers in the electrode environment. We developed a liquid cell incorporating electrodes on the viewing membrane in a transmission electron microscope to observe electrochemical processes in their native environment at the nanometer scale. We have acquired an electron microscope exclusively dedicated to operando measurements (Perseus), which we believe is the only one of its kind. (Fig.3) CABES has developed X-ray nano-diffraction and nano-fluorescence analysis to quantify structural defects in catalysts for OER. We have developed a new tool for localizing, with nanometer resolution, regions with high strain, by leveraging nanoprobe diffraction, and will extend this method to nanoimaging to enable us to examine the impact of strain and defects on electrocatalysis in alkaline media. With unique characterization tools to examine the structure and strain distributions in catalyst nanoparticles at atomic resolution, and at the nanoscale, *in-situ*, *operando* and device testing of both components and membrane electrode assemblies, we have information to guide the synthesis, and test and inform the modeling.

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