Center for Alkaline Based Energy Solutions (CABES)
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Lead Institution: Cornell University
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***Mission Statement**: **CABES** seeks 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 and their impact on fuel cell and electrolyzer technologies. 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):

1. SD-1. What factors govern electrocatalysis in alkaline media?
2. SD-2. How do we understand and control transport in alkaline media?
3. SD-3. What makes energy materials durable in alkaline media?

The center integrates theory and computational methods of catalysis and interfacial structure and dynamics, the synthesis of model (electro)catalytic systems with atomic level control, ionically conducting/transporting ionomers/membranes in contact with electrodes, computational materials science to guide the synthesis of other materials, and the development of experimental tools that will provide *operando*/*in situ*, spatiotemporal characterization of systems under operation. These studies are 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. We foresee the center as providing the scientific basis for ushering in an alkaline-based energy system that utilizes abundant elements and is scalable to the needs of society.

CABES addresses fundamental issues of critical needs in energy conversion technologies, guided by the challenges articulated in the relevant DOE reports, Basic Research Needs and Round Tables. CABES SD-based approach revolves around synergistic loops. Fig. 1 presents the loop for SD-1 that integrates materials synthesis and characterization, electrochemical testing, and modeling/data science. Each component within the loop informs the others; i.e., theory may suggest new catalysts to synthesize, and characterization may suggest new structures to simulate and synthesize. With unique characterization tools to examine the structure and strain distributions in catalyst nanoparticles at atomic resolution, and at the nanoscale *in-situ* and *operando*, and electrochemical testing of both components and membrane electrode assemblies, we have information on both structure and properties to guide the synthesis, and test and inform the modeling. This enables us to explore and optimize the synthesis of catalyst nanoparticles in a systematic manner. 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. The *ab-initio* modelling of surface structure and reaction pathways will greatly benefit from our data science tools for exploring these higher-dimensional spaces.

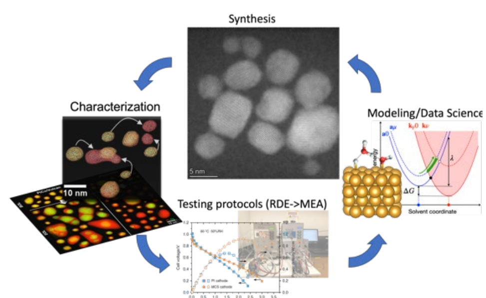

Fig. 1. SD1 synergistic research loop illustrating interactions between/among the different components of the team.

Science Driver 2 aims to achieve a fundamental understanding of how the architecture, especially of electrolyte/membrane materials, and interfaces within them, influences ion and molecule transport in electrochemical systems under alkaline conditions. The relationships between architecture and transport are investigated through the systematic preparation and study of alkaline exchange membranes (AEMs), correlated ionomers, and the respective interfaces. We have developed novel tools for their study including cryogenic transmission electron microscopy (cryo-TEM) (Fig. 2). We also assess the transport properties that result from these structures.

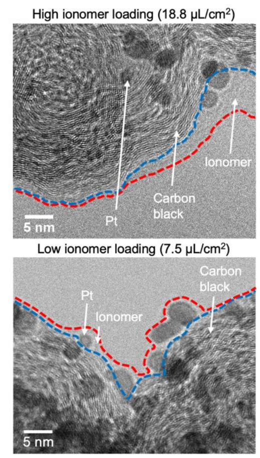

Fig. 2. Non-uniform ionomer distribution revealed by low-dose, cryo-TEM imaging of ionomer-electrocatalyst composites.

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 can we design and synthesize electrolytes with high hydroxide conductivity yet maintain their long-term durability under operating conditions. We are also focused on understanding interactions of membranes and ionomers with catalysts/supports.

We have also established a foundation of studies of non-precious metal based electrocatalysts with particular emphasis on metal-nitrogen-carbon, transition metal oxides, perovskites and spinels as well as transition metal nitrides. These studies are providing valuable design criteria for the synthesis of next generation high performance and highly stable electrocatalysts.

CABES has also developed unique experimental capabilities including cryo-TEM for the study of membranes and ionomers in contact with electrocatalysts and supports. We have developed a liquid cell incorporating electrodes on the viewing membrane in a transmission electron microscope.

For studying the role of defects in interface instability we have developed X-ray nano-diffraction and nano-fluorescence analysis to quantify structural defects in catalysts for OER. By leveraging nanoprobe diffraction, we have developed a new tool for localizing, with nanometer resolution, regions with high strain and will extend this method to nanoimaging to examine the impact of strain and defects on electrocatalysis in alkaline media; one of the main research themes of CABES.

We feel confident that CABES will help establish the basis for ushering in and enabling an alkaline-based energy technology society.

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