Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy (UNCAGE-ME)
EFRC Director: Krista S. Walton
Lead Institution: Georgia Institute of Technology
Class: 2014 – 2022

***Mission Statement**: To develop and harness a deep knowledge base in the characterization, prediction, and control of acid-gas interactions with a broad class of materials to accelerate materials discovery in acid gas separations, conversion, and utilization.*

Acid gases are ubiquitous in energy applications ranging from fuel and flue gas treatment and conversion of hydrocarbons to selective catalytic reduction of NOx and natural gas upgrading. The integrated research carried out by UNCAGE-ME (Phase I) allowed us to systematically identify materials features, common across classes of structures in some cases, that dictate how these materials behave in the presence of and/or selectively interact with acid gases. Having built this framework, the Center now seeks to harness this foundational knowledge through modeling, machine learning, and directed synthesis to accelerate materials design for acid-gas related energy technologies.

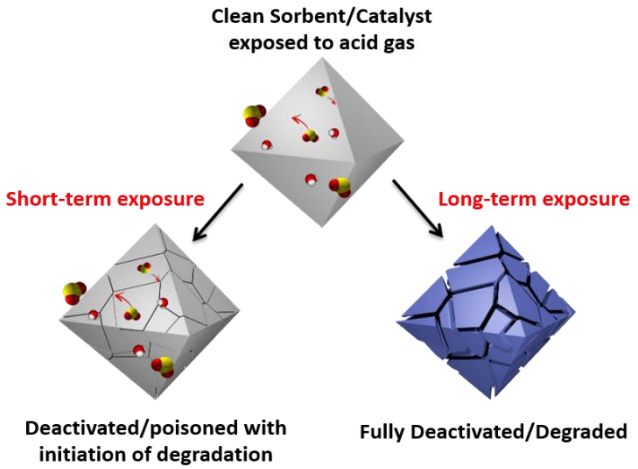

Figure 1: Changes induced in sorbents/catalysts upon short- and long-term exposure to acid gases. Materials are typically treated as passive in these environments, but can change dramatically upon exposure to SO_x, NO_x, and H_2S.

Materials-focused research for separations and catalysis often considers the materials as being passive in their process environment. In contrast, evolution of materials under working conditions due to exposure to acid gases is the norm rather than an exception. In Phase II of UNCAGE-ME, we will combine *in situ* molecular spectroscopic studies of both the surface functionalities and bulk structures of materials relevant to catalysis and separations of acid gases under conditions relevant to complex environments. Experiments will be combined with complementary data analytics and multi-scale computational and theoretical modeling of acid gas interactions with solids for targeted materials design.

Objectives

UNCAGE-ME seeks to provide a fundamental understanding of acid gas interactions with solid materials through integrated studies of the interaction of key acid gases (CO_2, NO_2, NO, SO_2, H_2S) with a broad range of materials. With our discoveries on acid gas tolerance and reactivity of materials in hand, machine learning and data analytics can now be introduced as powerful tools for elevating these unique data sets to the level of real prediction. Coupled with in situ techniques and molecular modeling, UNCAGEME is now uniquely positioned to exploit systematic data on acid gas tolerance and reactivity to achieve an unprecedented level of design, prediction, and control of catalysts, membranes, and sorbents. Insights gained by the multi-investigator, multidisciplinary teams will allow us to achieve the following long-term, 4-Year Goals set forth for the Center:

1. Develop a deep knowledge base of structure-property relationships for acid gas interactions with sorbents, membranes, and catalysts in complex mixtures applicable to broad classes of materials.

2. Leverage machine learning techniques to enable fundamental predictions of materials interacting with complex gas environments on long time scales.
3. Harness computational techniques for directing the design and synthesis of catalysts, membranes, and sorbents with targeted selectivity and reactivity.
4. Accelerate materials discovery for acid-gas separations, conversion, and utilization through the development and use of an integrated set of design tools to predict material stability and lifetime in the presence of acid gases.

Center Research Team and Scientific Organization

In Phase II of UNCAGE-ME, the Center's research framework will include cross-cutting themes to drive materials discovery for predicting targeted chemistries, porosities, and defects, and the development of self-healing materials with a focus on regeneration methods. The original mission of UNCAGE-ME will continue to motivate the Center's research. New and ambitious research goals that leverage the success of our Phase I work while bringing new, powerful research capabilities to bear will drive the Center's work.

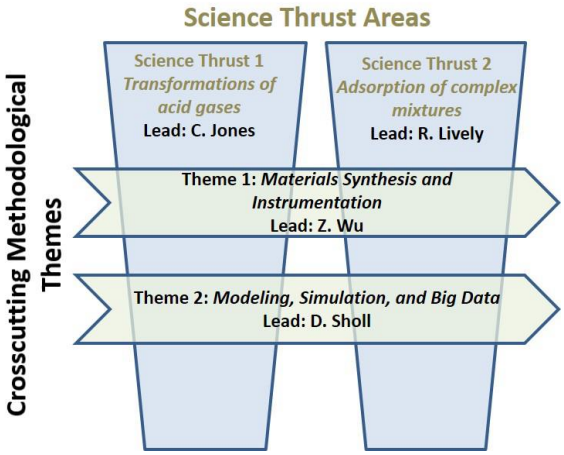

Figure 2: Overview of research thrusts/themes.

An overview of Science Thrusts and cross cutting Methodological Themes for Phase II of UNCAGE-ME is illustrated in Fig. 2. These Thrusts and Themes will work in an interconnected manner. The Science Thrusts focus on two broad strategies for developing the fundamental science for understanding and control of materials in acid gas mixtures relevant to two types of processes: (i) transformations of acid gases and (ii) adsorption of complex mixtures. The Methodological Themes are integrated across the Science Thrusts to assimilate the Center's results to predict high-performing materials, direct synthesis activities, and ultimately provide a robust, holistic design strategy that can be used more broadly by others in the field.

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