Addressing the limitations of catalyst synthesis, characterization, and computational catalysis

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The next generation of heterogeneous catalysts that are critical to the development of advanced energy processes will probably not be discovered by systematic variations of composition and synthesis methods based on current knowledge. Even the most insightful and intuitive investigator is limited in the number of experiments and variations of independent preparation and composition variables that can be studied. Although high-throughput, parallel screening addresses this limitation, it is not a substitute for the fundamental understanding that can be gained by first principles computation, testing of the theoretical result through the experimental study of model systems, and development of next-generation synthesis methods to prepare catalysts that are computationally ideal.

To address these challenges, LSU's Energy Frontier Research Center is working to advance the state-of-the-art in both first-principles catalyst "design", and "engineering at the molecular level" so that catalysts can be prepared with specific, intentional properties designed to carry out reactions that are essential to our energy needs.