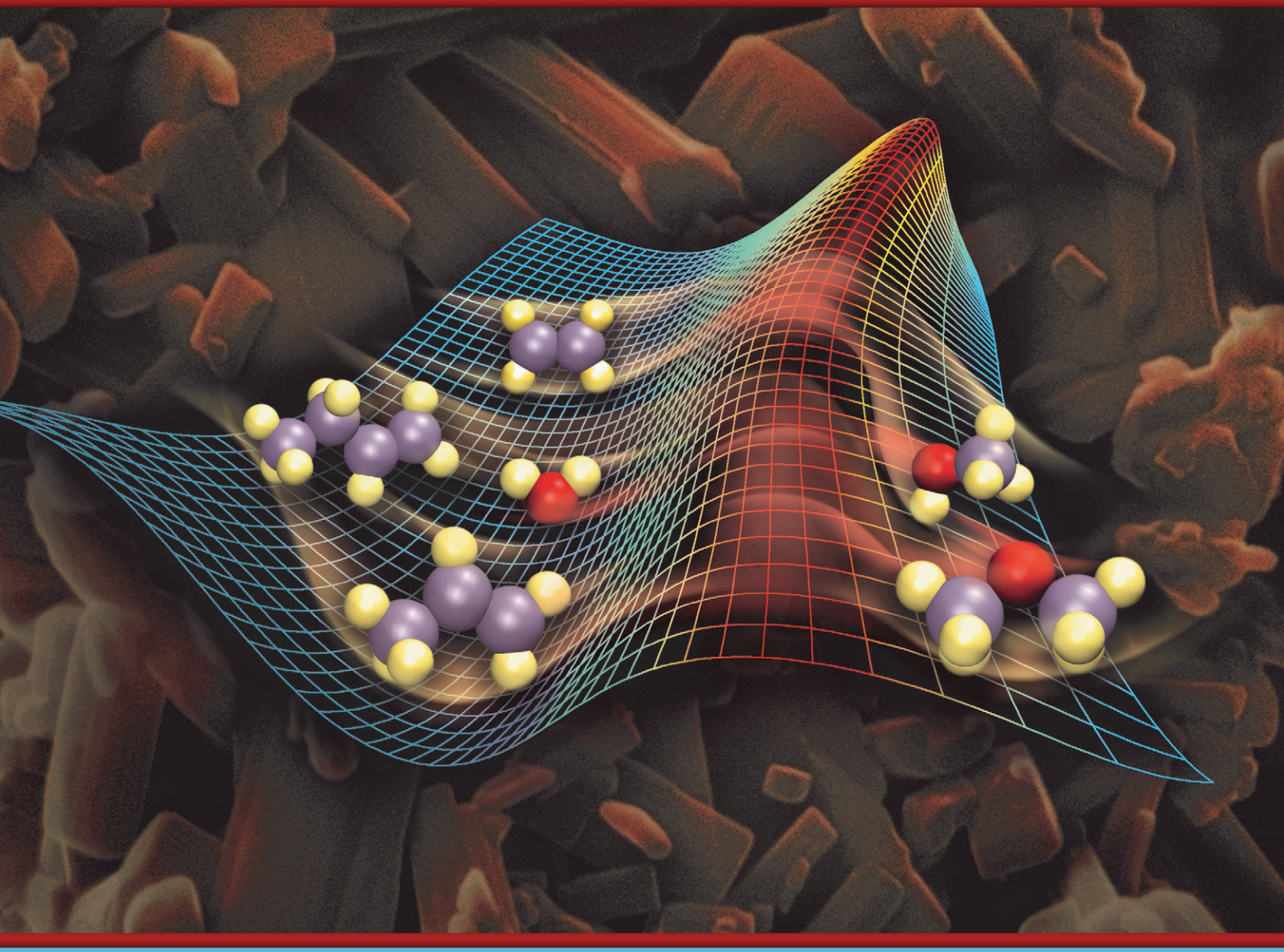
Basic Research Needs for

Catalysis Science



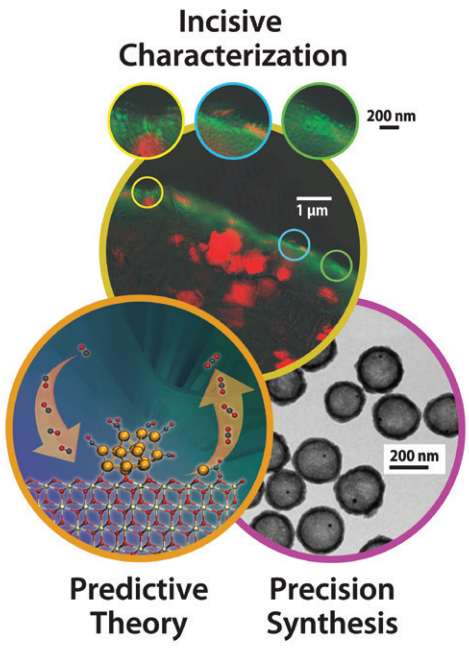
***Catalysis Science**—Harnessing complexity in catalysis to create next-generation energy technology*

Catalysis Science—Realizing efficient catalytic processes to increase the diversity of resources for production of chemicals and energy

Catalysis is the core of modern chemical conversions—the production processes for the vast majority of our fuels and chemicals use catalysts. Solid and molecular catalysts increase chemical transformation rates (reactivity) by lowering energy barriers for chemical reactions and can increase the yield of desired products (selectivity) by controlling the relative rates of competing reactions. High catalytic reactivity and selectivity reduce the required energy input, the number of process steps, and unwanted byproducts in the overall catalytic conversion. New catalysts will enable more efficient chemical transformations of raw materials and interconversion of the energy stored in chemical bonds with thermal and electrical energy. Advancing our understanding of and ability to control catalyzed reactions is essential to ensure the long-term economic viability of the energy and chemical industries.

Over the past decade, advances in the characterization of working catalysts, theory and computation, and high-precision chemical and materials synthesis have enabled impressive progress in catalysis science. This progress has provided detailed insight into how reactions occur and has led to increased appreciation of the intrinsic complexity of catalytic processes. Understanding this complexity has further enabled advances in areas as diverse as high-temperature transformation of hydrocarbons, low-temperature conversion of highly functionalized bio-derived compounds, highly selective synthesis of complex molecules, and improved electrochemical processes. By integrating the knowledge gained from studies of homogeneous, heterogeneous, and biological catalysts, we are beginning to understand and take advantage of the remarkably diverse capabilities of catalysts based on multifunctional molecular complexes, functionalized porous materials, and stabilized nanostructures and single atoms.

A Basic Research Needs workshop held in May 2017 identified five Priority Research Directions that address complexity in catalysis science. This emerging and transformative approach will lead to catalysts with unprecedented reactivity and selectivity for use in critical energy and chemical technologies. The full report will be available at https://science.energy.gov/bes/community-resources/reports/.



Deeper understanding of catalyst complexity requires new methods to probe catalytic phenomena at the atomic/molecular level, during catalyst operation, and on time and length scales commensurate with the formation of key reaction intermediates. Recent advances in precision synthesis and powerful new characterization methods have transformed our ability to probe catalyst structure–reactivity relationships experimentally; and developments in theory and simulation allow more accurate, realistic modeling of larger catalytic systems. Future advances in catalysis science depend on transformative capabilities in synthesis, characterization, and theory to allow control of interfacial interactions, multimodal in situ/operando characterization, models spanning multiple time/length scales, identification of rare/metastable active states of catalysts, and resolution of reaction mechanisms with atomic precision.

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Priority Research Directions

- **Design catalysts beyond the binding site**

  Key question: *How do we elucidate the cooperative interactions among the binding site, reacting molecules, and the surrounding environment to enable the design of catalyst structures that precisely control chemical reactions?*

  Enzymes, nature's catalysts, combine binding sites (localized regions that promote bond breaking/making in the reacting molecule) with precise positioning of nonreacting components that influence reaction barriers and control access to the binding site. Atomic-level, three-dimensional design of robust nonbiological catalysts that precisely positions both reacting and nonreacting components will enable fast and selective chemical transformations for energy applications under conditions currently not possible.

- **Understand and control the dynamic evolution of catalysts**

  Key questions: *How do we monitor and direct changes in catalysts during their life cycles and relate them to varying reactivity and selectivity? How do we design catalysts that adapt to varying feed composition and reaction conditions and ultimately can be reactivated?*

  Catalysts are inherently dynamic materials whose local and extended structures change continuously, beginning with assembly of the components into a catalytically active architecture and continuing as the catalyst interacts with reacting molecules. These changes impact the chemical and physical properties of the catalyst and hence have profound consequences for its performance and lifetime.

- **Manipulate reaction networks in complex environments to steer catalytic transformations selectively**

  Key questions: *How do we control the kinetics of multiple reactions at all relevant length scales to direct reaction pathways in catalytic reaction cascades, especially for multicomponent mixtures? How do we understand and integrate interdependent steps that may occur over different time and energy domains?*

  Many emerging chemical feedstocks have diverse, variable compositions whose transformations involve interconnected reaction pathways depending upon process conditions. Mastering these challenging chemical conversions requires integrating catalyst design to control reaction kinetics with strategies to direct nanoscale transport and separations.

- **Design catalysts for efficient electron-driven chemical transformations**

  Key questions: *How do we design selective, efficient electron-driven chemical processes at electrically conducting interfaces and use mechanistic understanding of those processes to discover new electrocatalytic systems with high energy efficiencies?*

  Electrocatalytic systems interconvert chemical and electrical energy by harnessing the flow of electrons to form and break chemical bonds. Designing electrocatalytic systems with tailored electronic states and controlled interfacial environments will allow electrocatalysis with high selectivity and energy efficiency.

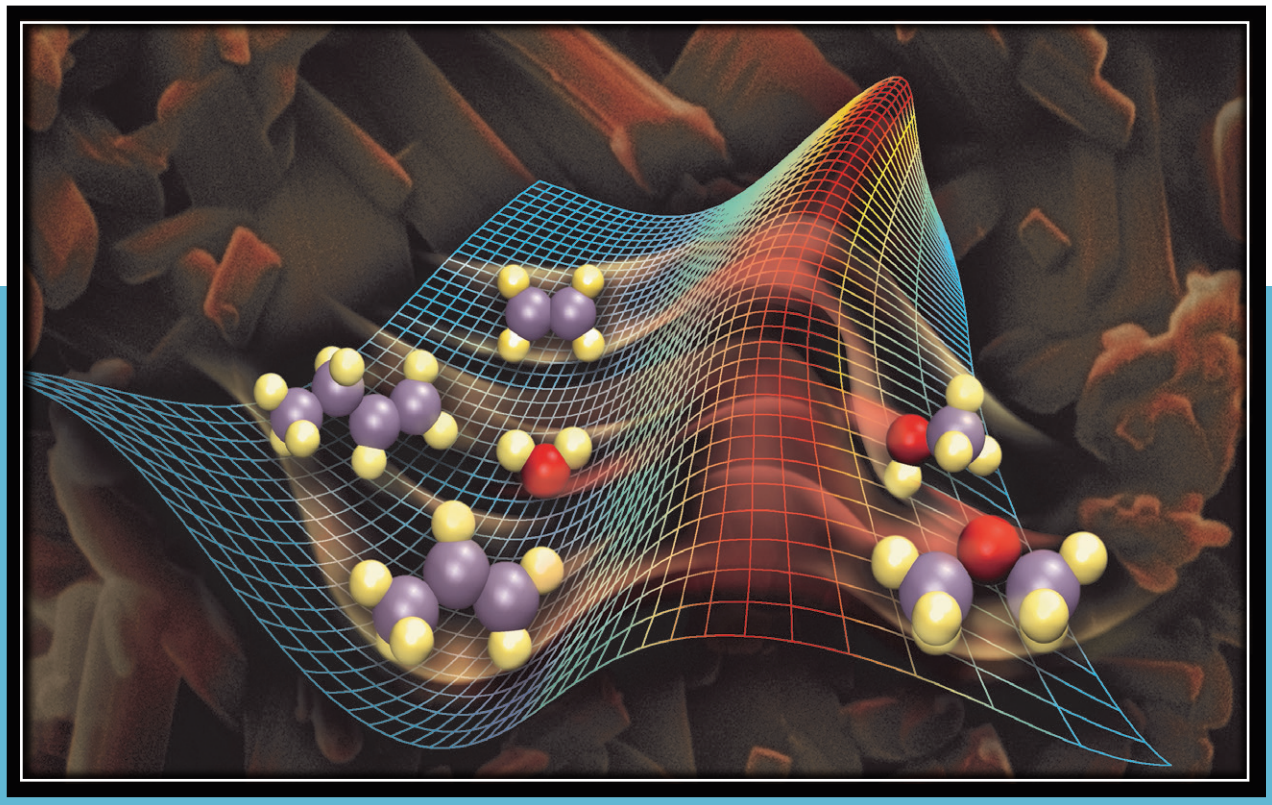
- **Drive new catalyst discoveries by coupling data science, theory, and experiment**

  Key questions: *How do we augment hypothesis-based catalyst discovery with data-science tools, including machine and deep learning, to extract new knowledge from highly diverse datasets? How can we use this approach to predict effective combinations of catalytic functions, structural components, reaction environments, and reaction mechanisms for complex systems?*

  The complex coupling of many variables that govern catalyst reactivity and evolution make it challenging to determine relationships between catalyst structure/composition and performance. Data science can reveal important patterns in such high-dimensional data, providing insights for predicting performance, designing critical validation experiments, and discovering new catalysts.

Summary

Catalysts are ubiquitous in energy systems, chemical production, and many other industrial processes. Catalysis science promises to revolutionize how new catalysts and catalytic processes are designed to enable the continued introduction of new energy resources and economical and sustainable synthesis of chemicals and energy carriers, including novel approaches to chemical energy storage. The design of new catalytic processes with higher efficiencies and longer catalyst lifetimes requires significant advances in our understanding and control of complex catalyst architectures, their dynamic evolution, and the resulting chemical transformation networks. These advances will require advanced characterization and analysis methods, precise synthesis techniques, multiscale theory and modeling, strategic use of the tools of data science, and integration of these activities across disciplines. The five Priority Research Directions outlined in this brochure identify the most important activities that should be undertaken to ensure the discovery and successful implementation of new catalytic approaches, to optimize the use of all of our energy resources, and to enable long-term economic prosperity.



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