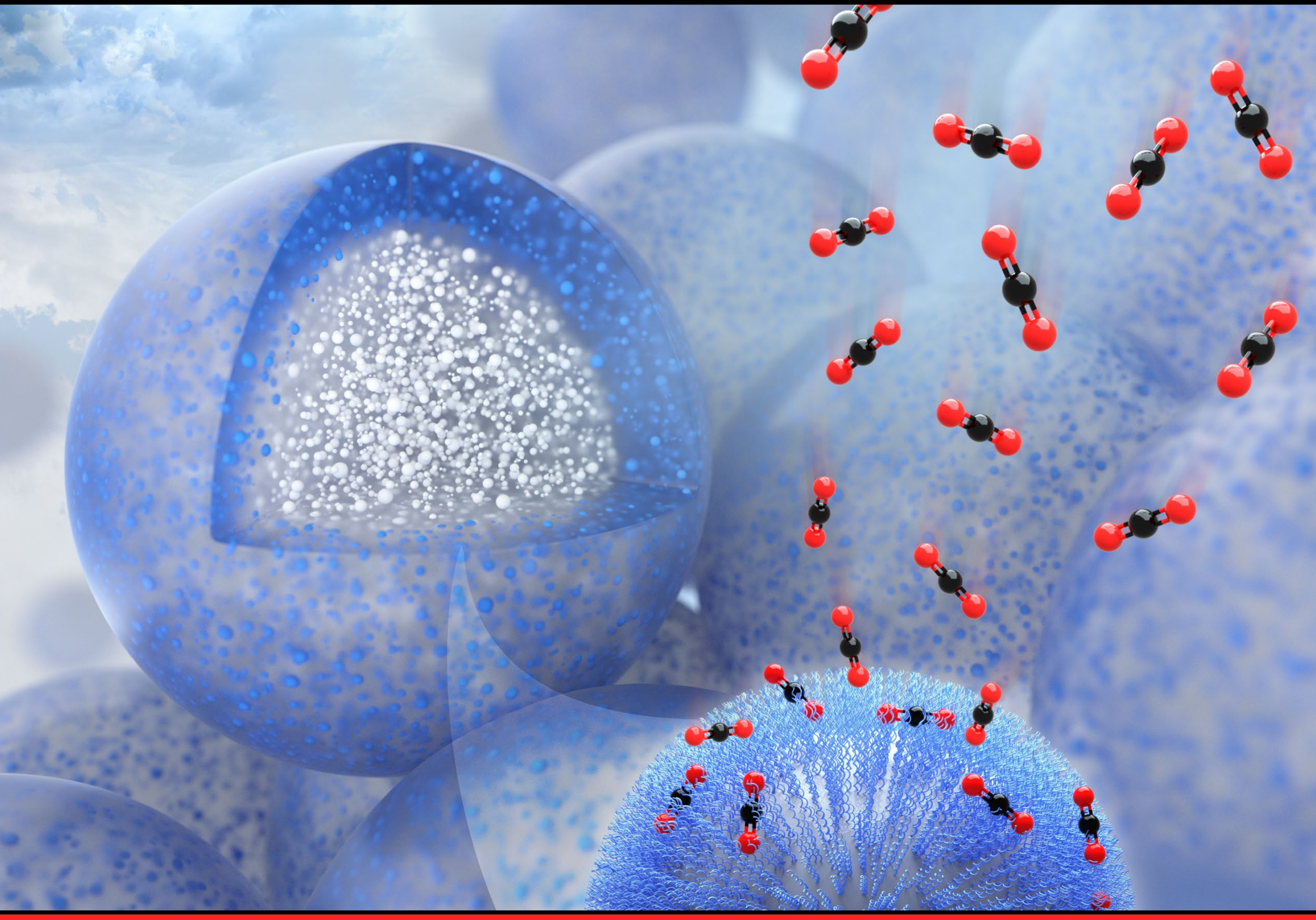
Basic Energy Sciences Roundtable

Foundational Science for Carbon Dioxide Removal Technologies



Science to revolutionize CO_2 removal and accelerate progress towards carbon-negative technologies

Foundational Science for Carbon Dioxide Removal Technologies

Globally, the frequency of extreme climate events is increasing – with the rising levels of CO_2 in the atmosphere due to human activity believed to be a major contributor. The international consensus is that net carbon emissions must be eliminated to avoid significant negative consequences. While reducing and capturing CO_2 at the source of generation is a critical strategy, recent reports from the Intergovernmental Panel on Climate Change conclude that carbon dioxide removal (CDR) from the environment will be essential to reducing CO_2 in the atmosphere. However, effective, economical, and secure methods for CO_2 removal on the massive scale that is required do not exist, nor does the foundational science needed for their development. Recognizing these challenges, the Department of Energy announced the Carbon Negative Energy Earthshot in 2021, setting the goal of removing CO_2 from the atmosphere and durably storing it at meaningful scales for less than $100/metric ton of CO_2-equivalent within a decade.

A suite of concurrent technologies are projected that could provide significant contributions to CDR. One option is biologically focused -- removal and sequestration through growth of biomass with subsequent energy generation coupled to capture and sequestration. In addition, studies report three physical, chemical and geochemical approaches that could transform the technological landscape: 1) Direct capture of CO_2 from both ambient air and other dilute sources that concentrate CO_2 from ambient air, such as the oceans and other large bodies of water. 2) Durable storage of carbon through mineralization, which binds carbon dioxide as carbonates, as well as conversion through the synthesis of molecules and materials with useful functionality. 3) Sequestration in geologic formations deep underground.

Basic research to identify and understand the fundamental principles governing carbon dioxide removal processes of capture, conversion, and storage is essential for achieving "net zero" and "negative" carbon emissions. In March 2022, the US Department of Energy (DOE) Office of Basic Energy Sciences (BES)—in coordination with the DOE Technology Offices of Energy Efficiency and Renewable Energy, Fossil Energy and Carbon Management, and Advanced Research Projects Agency-Energy (ARPA-E)—held a roundtable titled "Foundational Science for Carbon Dioxide Removal Technologies," to discuss the scientific and technical barriers for CO_2 capture, conversion, and storage. Five priority research opportunities were identified to address these scientific and technical challenges and accelerate progress toward the realization of zero carbon emissions.

The full report will be posted at: https://science.osti.gov/bes/Community-Resources/Reports.

Priority Research Opportunities

- **Master Interfacial Processes of CO_2 Transport and Reactivity Across Multiple Length and Time Scales**

  Key question: *How can we exploit the coupling across interfaces between disparate phases to enhance CO_2 reactivity and mass and energy transport?*

  CO_2 molecules crossing gas-fluid-solid interfaces via coupled physical and chemical reactions underlie all CDR processes. The driving forces for CDR at interfaces (pH, gradients in reactive species) are diminished during operation, slowing capture kinetics, or worse, passivating surfaces of natural and synthetic materials. Incorporating a function that continuously regenerates reactivity could revolutionize efficacy of CDR media. Successful design and exploitation of next-generation CDR media that include regenerative capabilities requires an atomic- to macroscopic-level description of interfacial processes. Moreover, accurate descriptions of carbon capture and sequestration processes at interfaces must account for their inherent rough, multicomponent, and dynamic nature.

- **Create Materials that Simultaneously Exhibit Multiple Properties for CO_2 Capture and Release or Conversion**

  Key question: *What design principles and synthetic methods can generate materials that simultaneously exhibit high binding affinity, low energy barrier to release or chemical conversion, and durability?*

  Creating new high-performance materials is a key to reducing the energy required for capturing CO_2 from dilute sources and for converting CO_2 into valuable products with net-negative emissions. In particular, understanding the degradation and restoration pathways that impact function is essential to extending the lifetime of materials. At the same time, these materials need to be designed to respond rapidly to incoming CO_2 and to capture or convert it with high efficiency. The development of new synthetic approaches, in situ characterization tools, and computational methods will accelerate the discovery of materials with a transformative impact on CDR technologies.

- **Discover Unconventional Pathways and Materials for Energy-Efficient CO_2 Capture, Release, and Conversion**

  Key question: *How can unconventional thermodynamics and kinetics be exploited to drive CO_2 binding and release or reactivity with low energy consumption?*

  CO_2 sorbents commonly utilize enthalpically driven processes for capture and are regenerated using thermal energy derived from fossil resources. With the rapid deployment of renewable energy, there is a unique opportunity to explore unconventional mechanisms for both processes, including electrochemical, electromagnetic, acoustic, entropic, and other alternatives, that can enable selective, energy-efficient capture and regeneration. A key challenge is to understand how these approaches can be used to decouple the strong CO_2 binding affinity required for capture from the energy barrier to its subsequent release or conversion. To do so, new computational and experimental tools are needed to probe localized energy transfer and molecular reconfigurations at capture sites and across interfaces.

- **Control Multiphase Interactions Required for CO_2 Conversion into Molecules, Minerals, and Materials**

  Key question: *What are the key multiphase interfacial structures, chemistries, and phenomena that control kinetics and mechanisms of CO_2 transformation into minerals and materials?*

  Rational tuning of multiphase physical and chemical interactions for CO_2 conversions into minerals and materials can enable scalable and durable CO_2 storage. Consideration of active sites, confinement, and mass transport is necessary to quantitatively determine, predict, and control the rates of catalytic transformations in chemically dynamic environments. Mineralization strategies require an understanding of the roles of polynuclear species, amorphous or dense liquid precursors, and ion desolvation on carbonate mineralization rates, as well as the ability of biomimetic approaches to enhance both processes.

- **Achieve Predictive Understanding of Coupled Processes in Complex Subsurface Geologic Systems for Secure Carbon Storage**

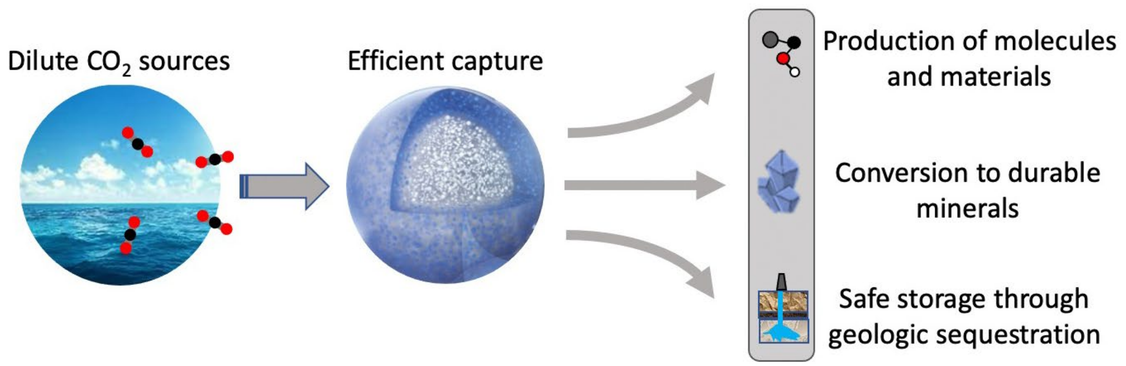
  Key question: *How can we integrate experimental and ambient data with physics-based modeling across time and length scales to understand and discover geochemical-geomechanical processes and create predictive models for long-term CO_2 storage security?*

  Subsurface geologic sequestration must store CO_2 for thousands of years in complex kilometer-scale formations that vary in lithology, groundwater chemistry, and structure. CO_2 storage will cause changes to the reservoirs that are currently not predictable; understanding the processes relevant to prediction of their long-term evolution requires data that capture this complexity. Field data provide an opportunity to validate experimental and computational methods that connect reservoir integrity to molecular-scale chemistry. Integration of geophysical signals with machine learning-driven simulations rooted in physics-based models can constrain the coupled geochemical-geomechanical processes, enabling more reliable forecasts of long-term reservoir performance.

Summary

The five priority research opportunities would address scientific and technical barriers associated with controlling CO_2 transport and reactivity at interfaces, making durable materials that efficiently capture and convert CO_2 into long-lived and useful products, and achieving secure underground CO_2 storage. These opportunities provide a cogent framework for greatly accelerating the design and development of materials and chemical processes required for atmospheric CO_2 reduction. These outcomes build upon and go well beyond research opportunities outlined in previous BES workshops and recent DOE reports; identify significant avenues for discovering and developing novel mechanisms, materials, and systems for capture, conversion, and storage; and can create a paradigm shift in the foundational science to enable innovative CDR technologies.

Advances can be realized by connecting a molecular-scale understanding of CO_2 at interfaces to outcomes in complex environments and by integrating novel operando experimental techniques, predictive theory and modeling, and analytical data science methods. Such progress can enable synthesis of innovative multi-functional materials, elucidation of degradation processes and pathways to their mitigation, control of CO_2 interactions with molecules, minerals, and materials, and prediction of the evolution of CO_2 and its products in complex geologic settings. Research based on the priorities outlined here can greatly advance the understanding of CO_2 capture, conversion, and storage, and provide the scientific foundation for effective, efficient, and safe CDR technologies.



Successful carbon dioxide reduction technologies will require advances along three axes:

1) Robust materials that efficiently capture and rapidly release CO_2 based on a molecular understanding of binding and an ability to exploit unconventional mechanisms.
2) Methods for converting CO_2 into molecules, materials and minerals rooted in an understanding of kinetics and thermodynamics of catalysis and crystallization.
3) A predictive understanding of the coupled mechanical and geochemical processes driven by CO_2 injected into the subsurface that accounts for the complexity of heterogeneities across length scales. All three depend on an understanding and control of interfacial dynamics in systems of disparate phases.

Cover figure courtesy of Ah-Hyung Park

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