U.S. DEPARTMENT OF ENERGY | Office of Science

Office of Science Overview

Briefing to NASEM Committee on Carbon Utilization Infrastructure, Markets, Research and Development

January 11, 2022

Todd Anderson, Office of Biological and Environmental Research

Bruce Garrett, Office of Basic Energy Sciences

DOE's Office of Science: World Leading Science
To Meet the Nation's Challenges Today and into the 21st Century

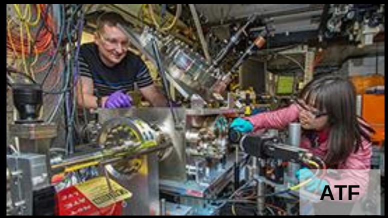
- The DOE Office of Science (SC) mission is the delivery of scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States.
- **Advancing the frontiers of science**
  - Providing largest Federal support in the physical sciences
  - Supporting nearly 28,000 Ph.D.s, graduate students, undergraduates, engineers, and support staff at more than 300 universities and at all 17 DOE laboratories
- **Advancing DOE missions**
  - Supporting energy and environmental research including Energy Frontier Research Centers, Energy Innovation Hubs, Bioenergy Research Centers, and High Performance and Leadership Computing Facilities
- **Serving the Nation's scientists**
  - Providing world-leading scientific user facilities to nearly 36,000 users per year

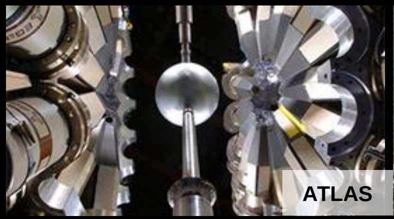
The Office of Science Research Portfolio

Advanced Scientific Computing Research	• Delivering world leading computational and networking capabilities to extend the frontiers of science and technology
Basic Energy Sciences	• Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels
Biological and Environmental Research	• Understanding complex biological, earth, and environmental systems
Fusion Energy Sciences	• Building the scientific foundations for a fusion energy source
High Energy Physics	• Understanding how the universe works at its most fundamental level
Nuclear Physics	• Discovering, exploring, and understanding all forms of nuclear matter
Isotope R&D and Production	• Supporting National Preparedness for isotope production and distribution during national crisis
Accelerator R&D and Production	• Supporting new technologies for use in SC's scientific facilities and in commercial products

Note: Isotope R&D and Production Program operates under Nuclear Physics in FY 2021. Accelerator R&D and Production operates under High Energy Physics in FY 2021.

28 Scientific User Facilities ~36,000 users (pre-pandemic)





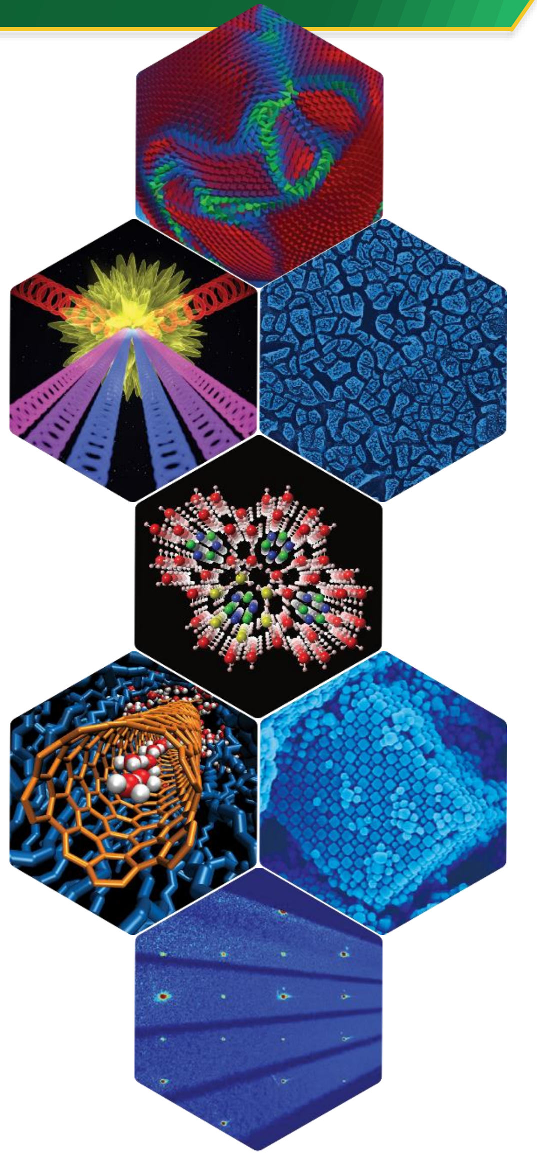
U.S. DEPARTMENT OF
ENERGY
Office of Science

Basic Energy Sciences Mission

To understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels

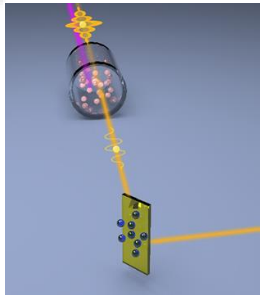
BES fulfills its mission through:

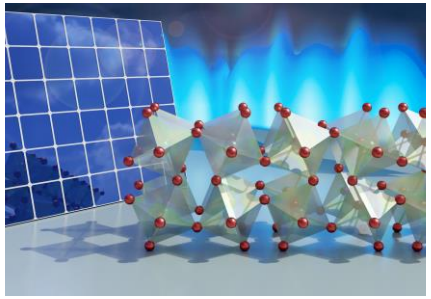
- Supporting basic research to discover new materials and design new chemical processes that underpin a broad range of energy technologies
  - **Critical role in clean energy research**
- Operating **world-class** scientific user facilities in x-ray, neutron, and electron beam scattering as well as in nanoscale research
- Managing construction and upgrade projects to maintain **world-leading** scientific user facilities

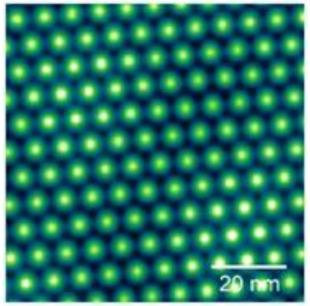


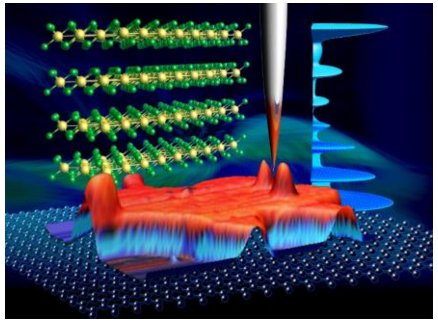
Materials Sciences and Engineering (MSE) Research

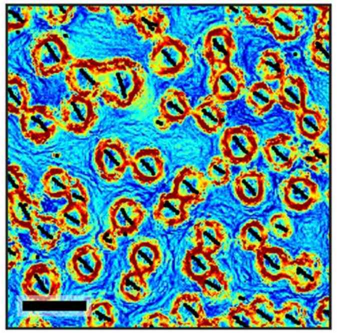
Broad Portfolio of Grand Challenge and Energy Use-Inspired Fundamental Research

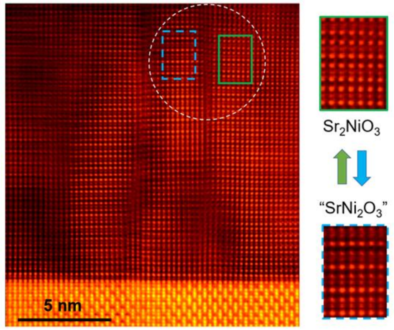












Scattering and Instrumentation Sciences:

Photon, neutron, and electron interactions with matter to characterize structures, dynamics, and functionality

Condensed Matter and Materials Physics:

Research on phenomena, including quantum, and response to stimuli in energy-related environments

Materials Discovery, Design, and Synthesis:

Synthesis and materials dynamics for discovery and design via innovative physical, chemical, and bio-molecular routes

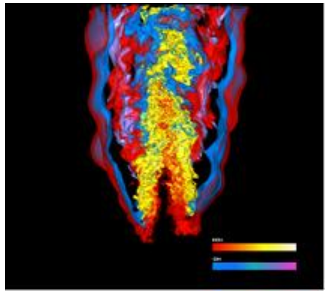
Division-wide Themes:

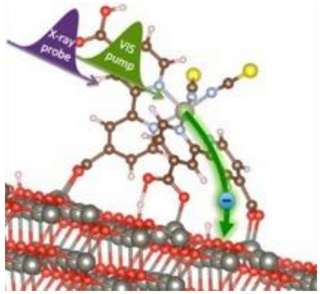
Clean energy; Quantum; Synthesis;
Theory, computation, data; Non-equilibrium dynamics;
Operando and multi-modal characterization

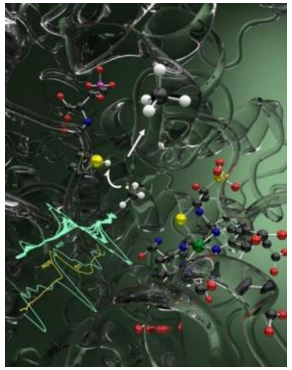
https://science.osti.gov/bes/mse

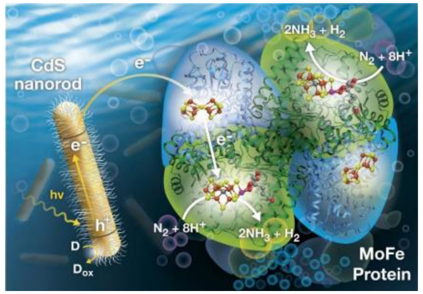
Chemical Sciences, Geosciences & Biosciences (CSGB) Research

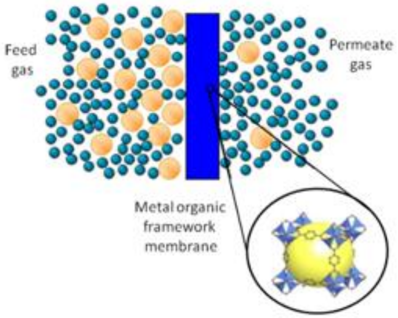
Broad Portfolio of Grand Challenge and Energy Use-Inspired Fundamental Research

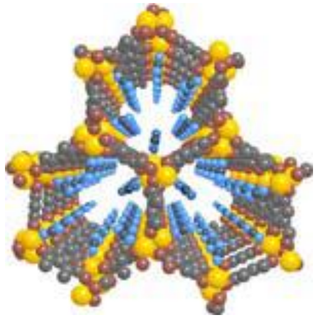












Fundamental Interactions:

Control chemical reactivity and dynamics in gas phase, condensed phases, and interfacial systems

Photochemistry and Biochemistry:

Molecular mechanisms of light energy capture and its conversion into chemical and electrical energy

Chemical Transformations:

Chemical synthesis, conversion, stabilization, and transport processes, from nano to geologic scales

Division-wide Themes:

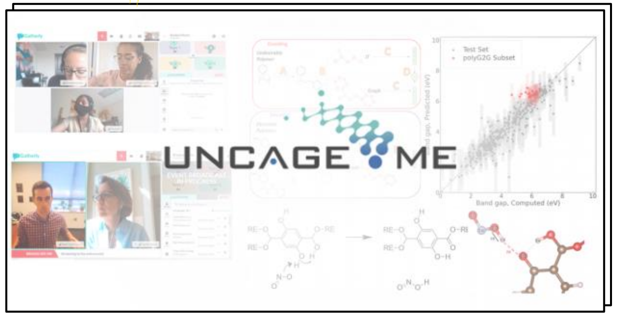
Clean Energy; Ultrafast Chemistry; Complex Interfaces; Charge Transport and Reactivity; Reaction Pathways; Aqueous Environments

https://science.osti.gov/bes/csgb

BES programs advancing carbon capture and conversions

- Fuels from Sunlight Energy Innovation Hub program (multi-institution, multidisciplinary; Total Hub funding – \$20M/year)
  - Goal: Build the scientific foundation for a scalable technology that converts carbon dioxide into renewable transportation fuels with only solar added energy. https://science.osti.gov/bes/Research/DOE-Energy-Innovation-Hubs

- Energy Frontier Research Centers (multi-PI, often multi-institution; \$2-4M/yr)
  - Goal: Tackle the toughest scientific challenges preventing advances in energy technologies in many areas including separations and catalysis. https://science.osti.gov/bes/efrc/Centers



CHASE

LiSA LIQUID SUNLIGHT ALLIANCE

ICDC INORGANOMETALLIC CATALYST DESIGN CENTER

- Core Research Programs (single-PI and small groups)

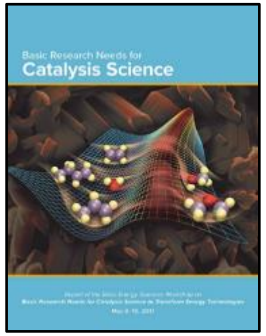
<u>Materials Sciences and Engineering</u>
- Materials Chemistry
- Synthesis and Processing Science
- Physical Behavior of Materials

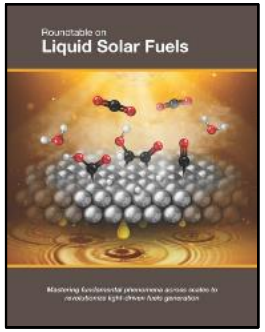
<u>Chemical Sciences, Geosciences, and Biosciences</u>
- Catalysis Science
- Separation Science
- Geosciences
- Solar Photochemistry
- Photosynthetic Systems
- Physical Biosciences

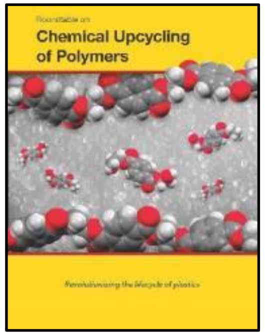
Strategic Planning Workshops and Roundtables identify priority research directions relevant to carbon utilization

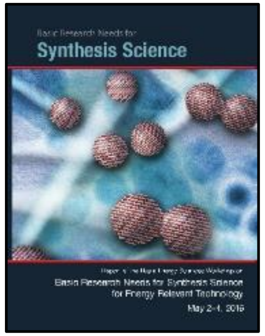
Energy Topics

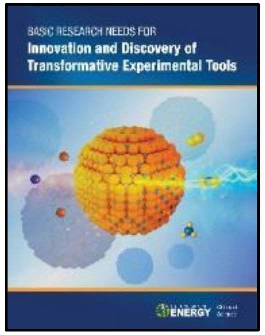
Synthesis and Characterization

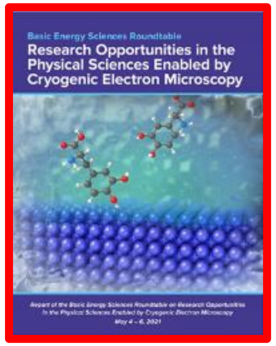










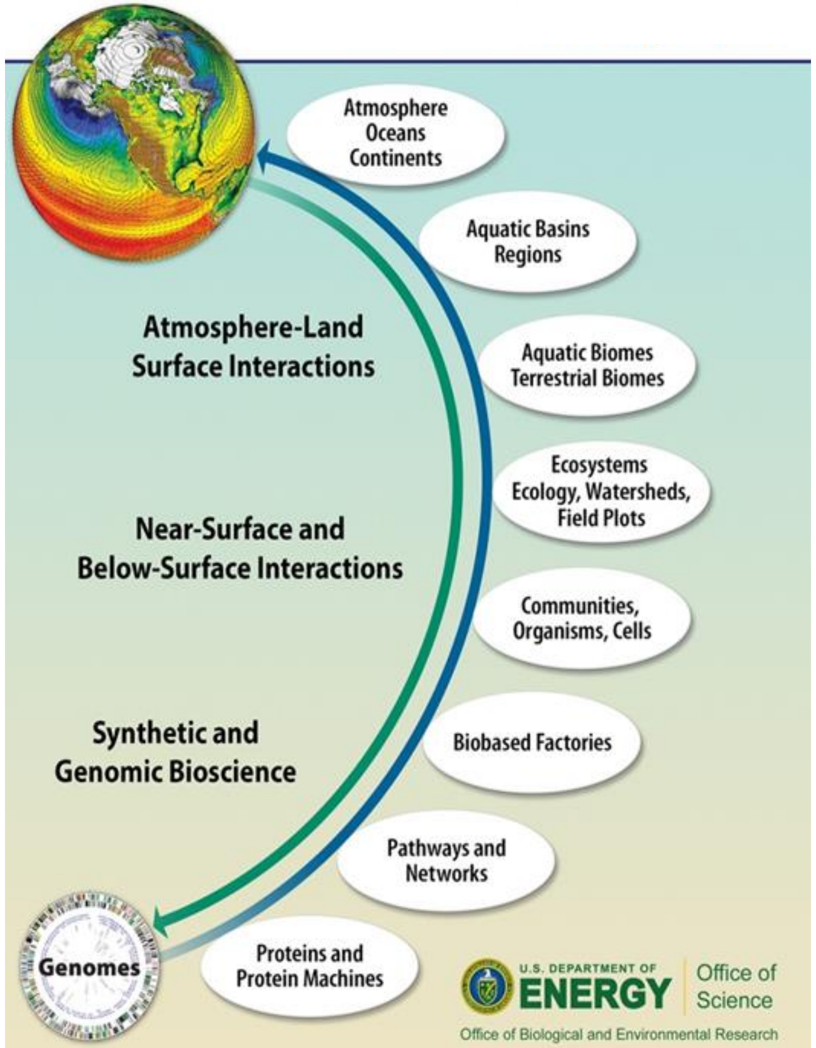


https://science.osti.gov/bes/Community-Resources/Reports

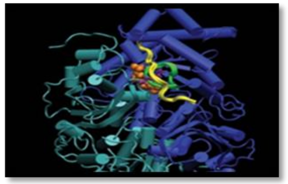
Upcoming Roundtable on Foundational Science for Carbon Dioxide Removal Technologies (early March 2022; report in summer 2022)

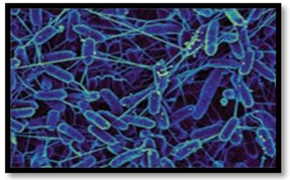
- **Organizers:** SC-BES (Lead), FECM, EERE, ARPA-E
- **Goal:** Identify the key underpinning science needs and priority research opportunities that will accelerate research, development, and deployment of CDR technologies
- **Roundtable Scope**: Consider areas for BES research to enable future, as well as advance current, CDR technologies:
  - CO_2 capture from dilute sources
  - Durable CO_2 storage in minerals and materials
  - Geological sequestration

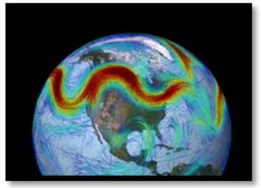
Biological and Environmental Research



Understanding complex biological, earth, and environmental systems







- Explore the frontiers of genome-enabled biology
- Understand interdependencies of physical and biogeochemical Earth processes
- Enable innovation and discovery through user facilities

Bioenergy Research

Goal: Provide the basic science needed to convert renewable biomass to a range of fuels chemicals, and other bioproducts in support of a burgeoning bioeconomy.

- *Plant Genomics*

Subgoal: *Gain a genome-level understanding of plant metabolism, physiology, and growth to develop new bioenergy feedstocks with traits tailored for bioenergy and bioproduct production.*

- *Microbial Conversion*

Subgoal: *Develop an understanding of microbial and fungal metabolism necessary to design new strains, communities, or enzymes capable of converting plant biomass components into fuels, chemicals, and bioproducts.*

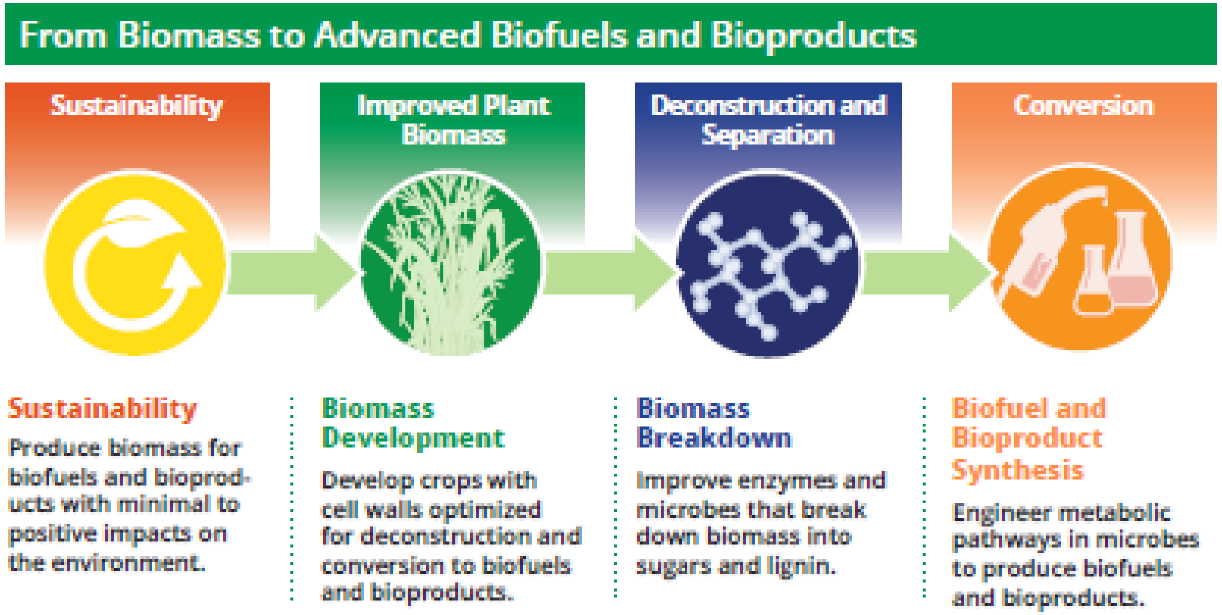
- *Sustainable Bioenergy*

Subgoal: *Understand the genomic properties of plants, microbes, and their interactions to enable the development of new approaches that improve the efficacy of bioenergy crop production on marginal lands with few or no agricultural inputs, while minimizing ecological impacts.*

Conversion of Lignocellulosic Biomass to Fuels, Chemicals and Products Currently produced from Petroleum

Bioenergy Research Centers (BRCs)

- **Great Lakes Bioenergy Research Center (GLBRC)**
  University of Wisconsin, Michigan State University
  (https://www.glbrc.org/)
- **Joint BioEnergy Institute (JBEI)**
  Lawrence Berkeley National Laboratory
  (https://www.jbei.org/)
- **Center for Bioenergy Innovation (CBI)**
  Oak Ridge National Laboratory (https://cbi.ornl.gov/)
- **Center for Advanced Bioenergy and Bioproducts Innovation (CABBI)**
  University of Illinois (UIUC) (https://cabbi.bio/)



GREAT LAKES BIOENERGY RESEARCH CENTER

JBEI Joint BioEnergy Institute

cbi THE CENTER FOR BIOENERGY INNOVATION

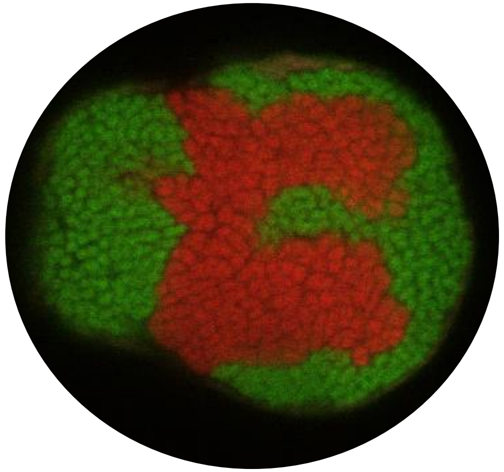
CABBI Center for Advanced Bioenergy and Bioproducts Innovation

Biosystems Design and Environmental Microbiome Research

Biosystems Design

***Goal:** Advance fundamental understanding of genome biology and develop the genome-scale engineering technologies needed to design, build, and control plants and microbes for desired beneficial purposes.*

Environmental Microbiome Research



***Goal:** Develop a process-level understanding of microbiome function and be able to predict ecosystem impacts on the cycling of materials (carbon, nutrients, and contaminants) in the environment.*

Enabling Capabilities and User Facilities

Enabling Capabilities

Goal: *Support the development of computational and instrumental platforms to enable broader integration and analysis of large-scale complex data.*

Computational Biology: Integrated Computational Platforms

Biomolecular Characterization and Imaging Science

nmdc National Microbiome Data Collaborative

KBase PREDICTIVE BIOLOGY

DOE Systems Biology Knowledgebase

User Facility Integration

Goal: *Build unique, best-in-class capabilities within Office of Science user facilities (including JGI, EMSL, and DOE's light and neutron sources) to enhance the multidisciplinary research*

JGI JOINT GENOME INSTITUTE DEPARTMENT OF ENERGY

EMSL

Synchrotron Light and Neutron Sources
Nanoscience Centers
(operated by SC-BES)

NERSC

Strategic Planning and Workshops that Direct the Portfolio

[NAS- Safeguarding the Bioeconomy]

[Bioenergy Research Brochure]

[BER Virtual Laboratory report - BERAC]

[BER Genome Eng. for Mat. Synthesis]

[NAS-Research at the Interface]

[NAS Study: Industrialization of Biology]

[Breaking the Bottleneck of Genomes]

[BES-Challenges at the Frontiers - BESAC]

SC expectations for NASEM study

- Assess research efforts underway to address barriers in approaches to carbon utilization and identify gaps in research effort:
  - Include areas where fundamental chemical, materials and biological research can provide needed foundational knowledge to advance current carbon utilization approaches;
  - As appropriate, identify areas where fundamental chemical, materials and biological research indicates opportunities to advance new approaches for carbon utilization.
- Update the 2019 National Academies comprehensive research agenda on needs and opportunities for carbon utilization technology RD&D:
  - Include consideration of new opportunities for carbon utilization to contribute to a net zero carbon future.

Contact information

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Highlights

Direct Coupled Electrochemical System for Capture and Conversion of Carbon Dioxide from Ocean Water

Scientific Achievement

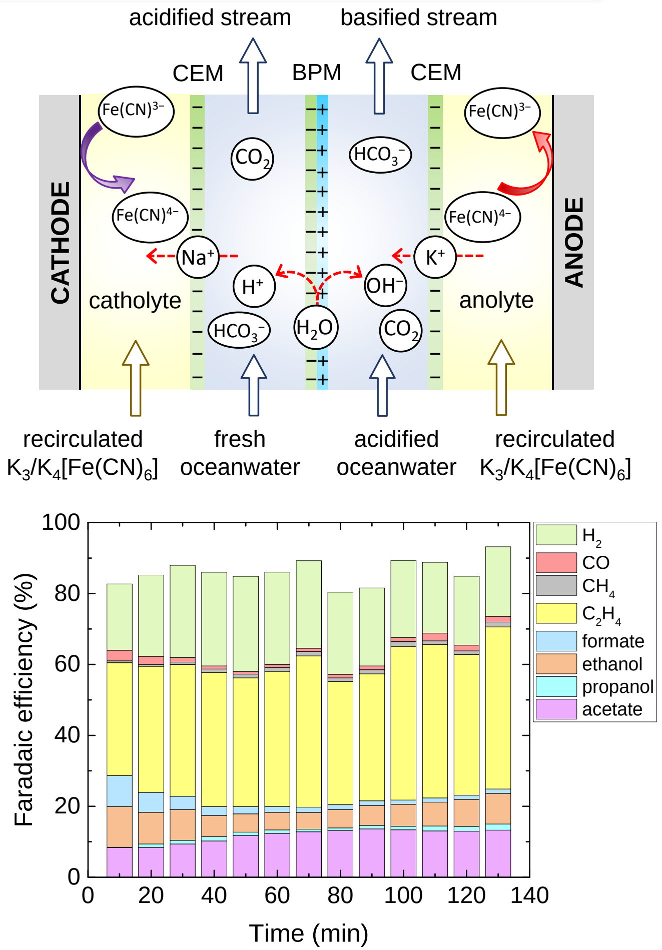
A direct coupled system captures CO_2 from ocean water using electrochemical energy of 0.98 kWh/kg CO_2 and converts CO_2 to CO at a Faradaic efficiency of up to 95% in vapor-fed cells.

Significance and Impact

The bipolar membrane (BPM) electrodialysis cell replaces the commonly used water splitting reaction with a one-electron redox couple at the electrodes, significantly lowering the electrochemical energy consumption. Tandem vapor-fed cells were used to eliminate O_2 and convert CO_2 at high Faradaic yields.

Research Details

- Parasitic losses due to water splitting reaction is eliminated by using a one-electron redox couple at the electrodes of the electrodialysis cell.
- Electrochemical energy for CO_2 capture from ocean water as low as 0.98 kWh/kg CO_2 with ~70% efficiency; gas output composition >90% CO_2
- Ag-based vapor-fed cell converts CO_2 to CO with up to 95% Faradaic efficiency; Cu-based vapor-fed cell converts CO_2 to conversion to fuels and chemicals with up to 73% Faradaic efficiency.



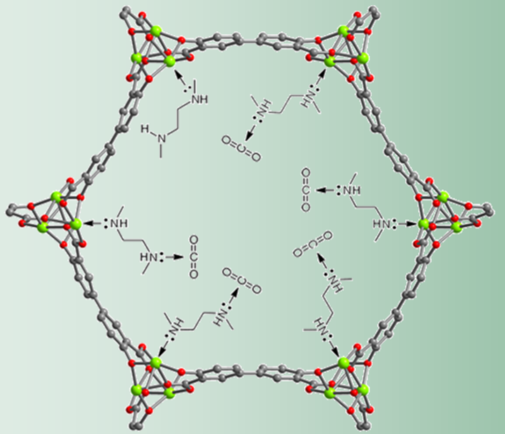
Schematic illustration of the BPM electrodialysis cell, and gas/liquid product distribution of converted CO_2 from ocean water..

Digdaya, Sullivan, Lin, Han, Cheng, Atwater, Xiang, *Nat. Commun.* **2020**, *11*, 4412

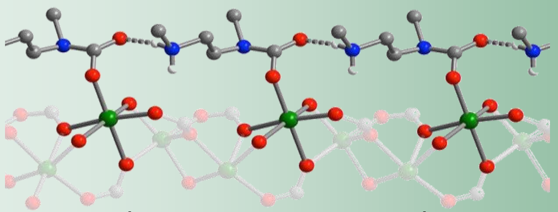
Metal-Organic Frameworks for Low-Energy Carbon Capture

BES Basic Science

Energy Frontier Research Center



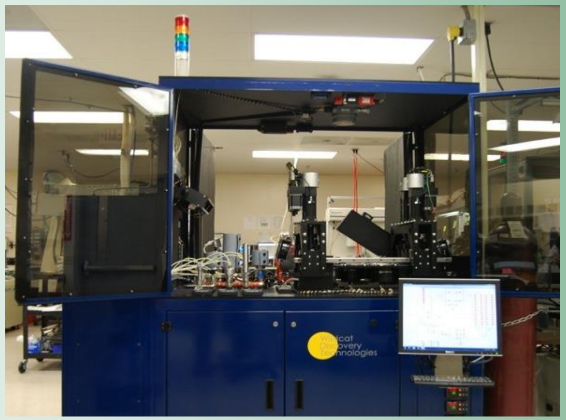
Unprecedented mechanism was discovered for cooperative CO_2 binding to diamines appended to magnesium surface sites in a metal organic framework. This mechanism enables low-energy, reversible CO_2 capture that can be chemically tuned.



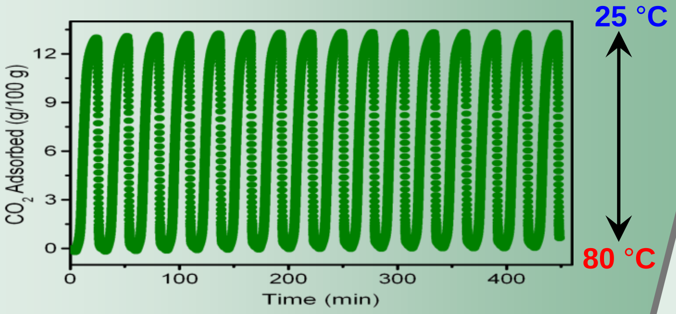
(*Nature* **2015**, *519*, 303)

Center for Gas Separations
Relevant to Clean Energy Technologies

ARPA-E Applied R&D



New high-throughput technology enabled rapid screening to chemically tune the MOF metal sites and diamines to enhance CO_2 capture (>10% at 25ºC) with low-temperature cycling



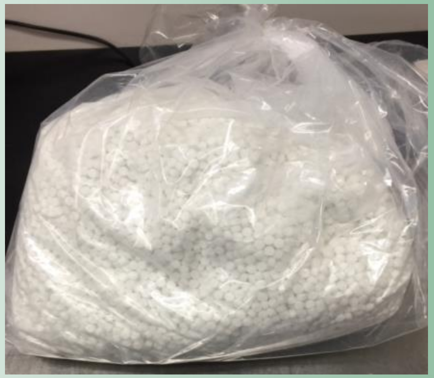
Manufacturing/ Commercialization

Start-up

mosaic

Revolutionizing chemical separations

LBNL inventors created a company for the scale-up and testing of structured MOF forms



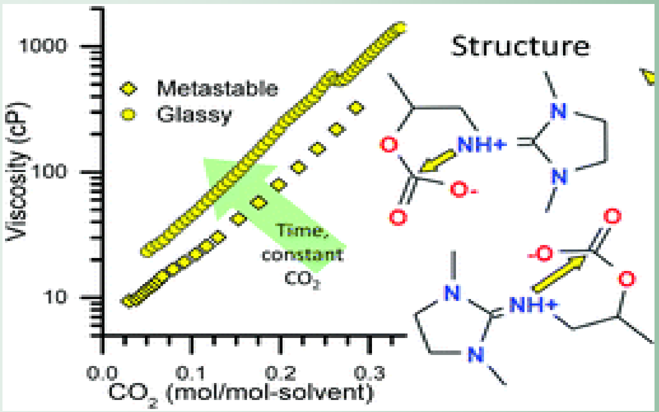
1 mm-diameter pellets of a MOF that can endure the strain from cycling carbon dioxide adsorption

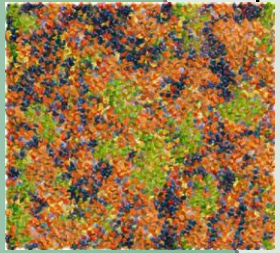
First company to join Cyclotron Road incubator at Lawrence Berkeley National Laboratory (LBNL)

BERKELEY LAB

Reimagining Solvent-Based Carbon Capture: Integrated multidisciplinary team (theoreticians, chemists, chemical engineers)

BES Basic Science



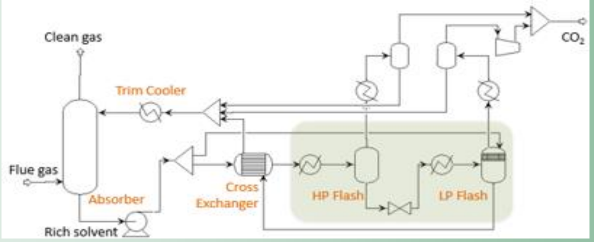


Combined theory and experiment effort uncovered a transformation of capture solvents into a glassy phase after CO_2 absorption and subsequent aging at operating temperatures. The approach was used to provide a molecular-level understanding of properties such as acid-base equilibria and mesoscopic ordering of CO_2-rich solvents to enable the design of solvents that mitigate hydrolysis while also reducing viscosity.

***Phys. Chem. Chem. Phys.* 2020**, *22, 19009.*

Fossil Energy and Carbon Management Applied Research

Further development of chemistries with custom infrastructure to measure solvent properties and efficiency
Incorporated projections of process performance and cost (AspenPlus).



***J. Phys. Chem. Lett.* 2016**, 7, 1646.
***ChemSusChem* 2020**, 13, 3429.
***Energy Environ. Sci.* 2020**, 13, 4106.
***IJGHGC* 2021**, in press.

Industrial Partnerships

Industry-led 0.5 MW demonstration at DOE's National Carbon Capture Center

Pacific Northwest
NATIONAL LABORATORY

Nationwide collaboration unlocks switchgrass genome

Objective

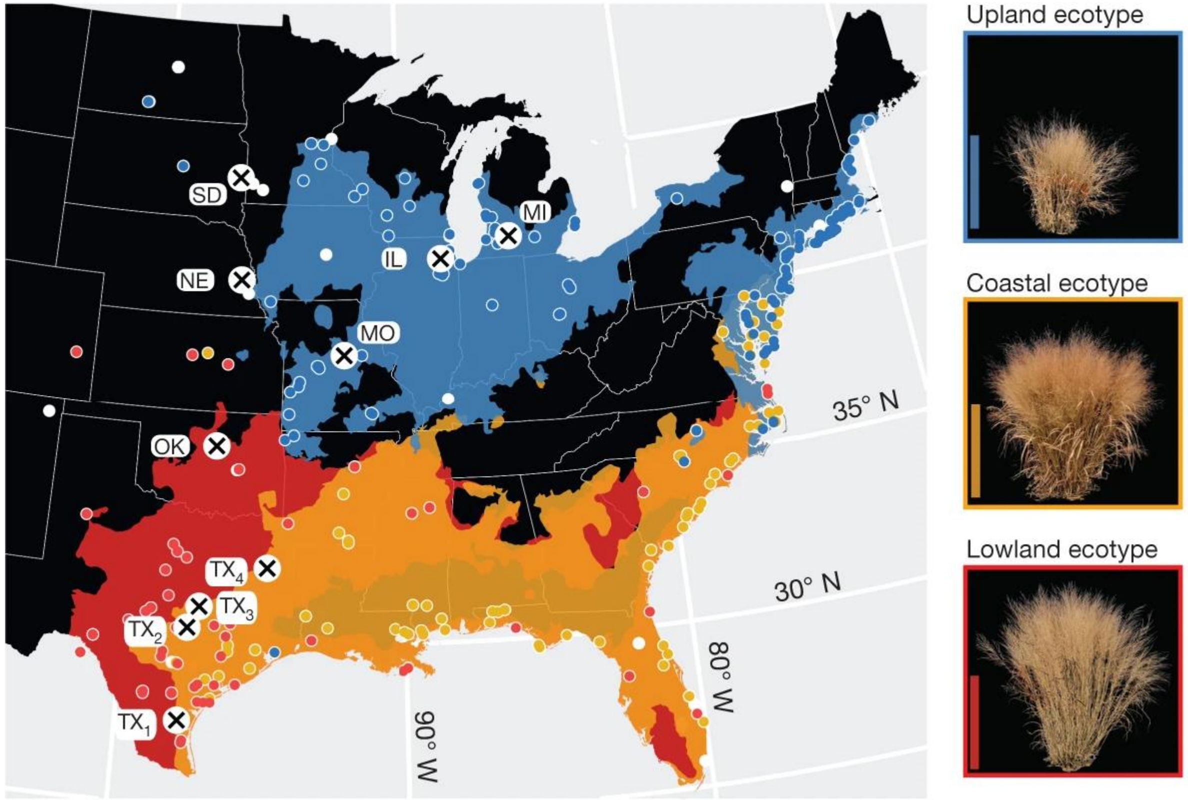
Produce a high-quality reference sequence of the complex switchgrass genome

Approach

- Ten common gardens spanning climate zones across eight states and 1,100 miles, each containing a propagated panel of 732 switchgrass genotypes.
- Sequence, assemble, and annotate the switchgrass genome.
- Analyze biomass and survival among genotypes for climate–gene–biomass associations.

Result/Impacts

- Affords the ability to assess genotype changes in expressed switchgrass phenotypes across climatic and geographic regions
- All four BRCs have expanded the network of common gardens and are exploring improvements to switchgrass through more targeted genome editing techniques to improve crop traits and customize the crop for additional end products.
- The work builds off of a BSSD Sustainability Award to (T. Juenger, UTexas) assessing switchgrass varieties across multiple field sites across the breadth of the U.S.

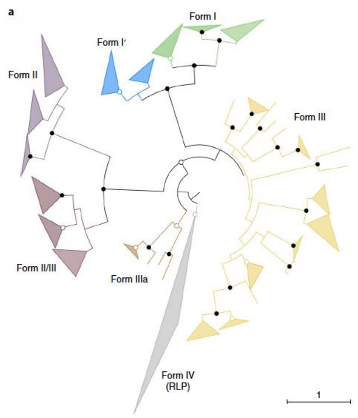


Geographic distribution of common gardens and plant collection locations, and spatial distribution models of each ecotype. The ecotype color legend accompanies the representative images of each ecotype to the right of the map.

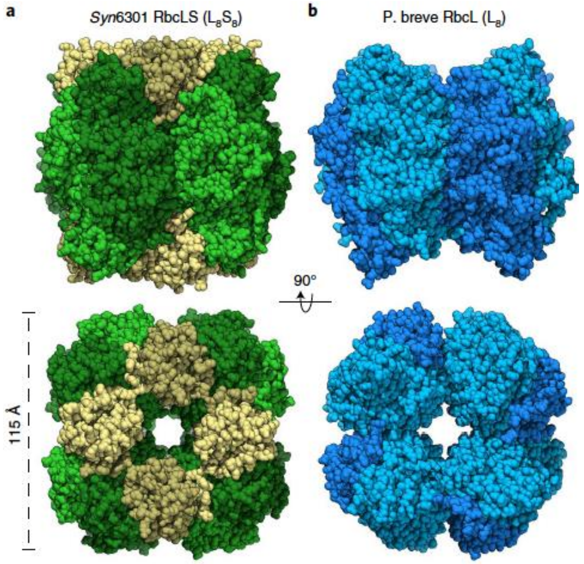
Lovell, J.T., *et al.* "Genomic mechanisms of climate adaptation in polyploid bioenergy switchgrass," ***Nature*** (2021). [DOI: 10.1038/s41586-020-03127-1]

Novel bacterial clade reveals origin of form I Rubisco

Objectives
- All plant biomass is sourced from the carbon fixing enzyme Rubisco
- Although there is significant interest in engineering Rubisco to improve overall plant productivity, there has been little progress in the field
- All plants contain Form I Rubisco, and all Form I Rubisco consist of both eight Large (RbcL) and eight Small (RbcS) subunits. No Form I Rubisco has previously been discovered to lack the small subunit, which would represent a key transition in Rubisco evolution
- Understanding how Rubisco evolved may provide unique insight into engineering Rubisco



Approach
- Used metagenomics to discover a previously uncharacterized clade of Rubisco that is the sister clade to Form I Rubisco, that we named Form I'
- Synthesized, expressed, purified, and biochemically characterized the novel enzyme
- Solved solution state and crystal structure of novel Form I' Rubisco



Results/Impacts
- Structural insight into how Form I Rubisco evolved will provide the basis for engineering Rubisco in bioenergy crops
- Demonstration of the utility of metagenomics to discover novel families of enzymes

Banda et al., (2020) Novel bacterial clade reveals origin of form I Rubisco, **Nature Plants**, doi.org/10.1038/s41477-020-00762-4

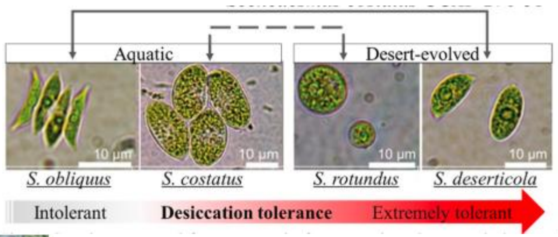
Algal Genome Sequencing Program at JGI

JGI JOINT GENOME INSTITUTE
A DOE OFFICE OF SCIENCE USER FACILITY

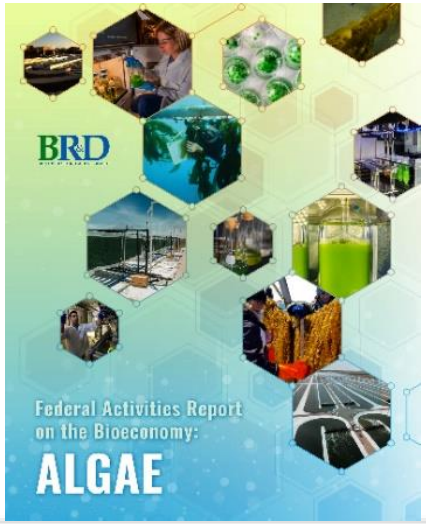
Five-Year Milestones: Produce 100 algal genomes. Initiate algal Grand Challenge Projects.

Coordinated with the JGI-LANL Algal Partnerships
At LANL co-funded by DOE Bioenergy Technology Office

Los Alamos
NATIONAL LABORATORY

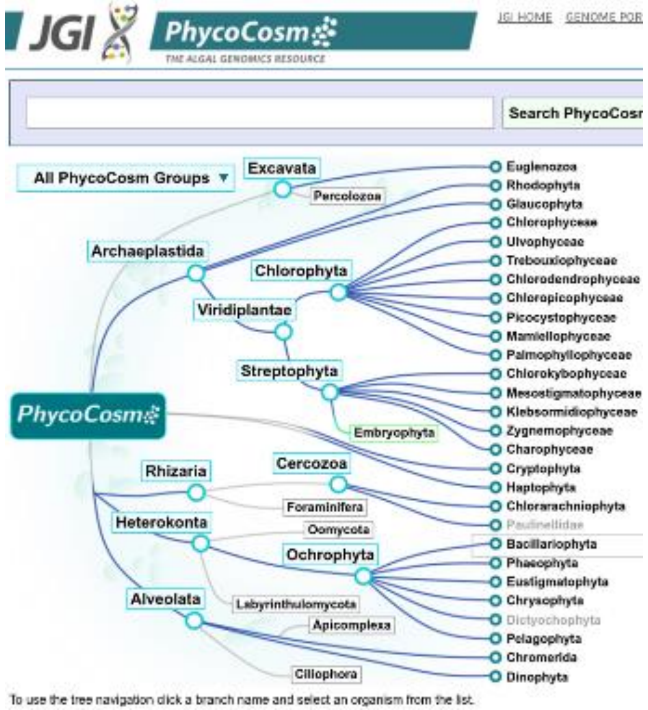


Interagency
Algal Working Group



JGI Algal Resources

1[st] release of Phycocosm: 100+ algal genomes



Nucleic Acids Research

PhycoCosm, a comparative algal genomics resource

Igor V. Grigoriev[1,2,3,*], Richard D. Hayes[1], Sara Calhoun[1,3], Bishoy Kamel[1,3], Alice Wang[1,2], Steven Ahrendt[1], Sergey Dusheyko[1], Roman Nikitin[1], Stephen J. Mondo[1], Asaf Salamov[1], Igor Shabalov[1] and Alan Kuo[1]

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