Basic Energy Sciences Research for Direct Capture of Carbon Dioxide

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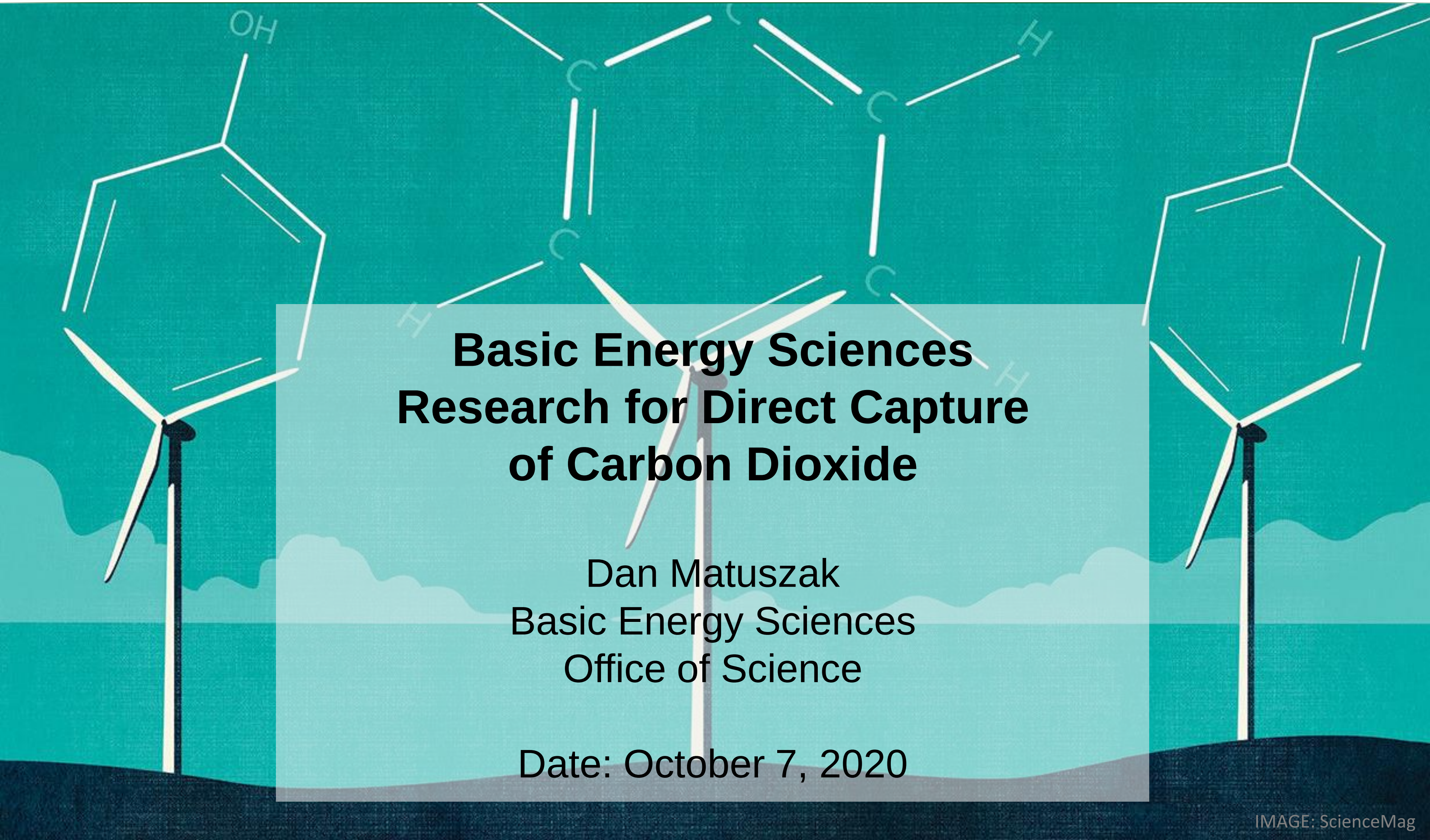
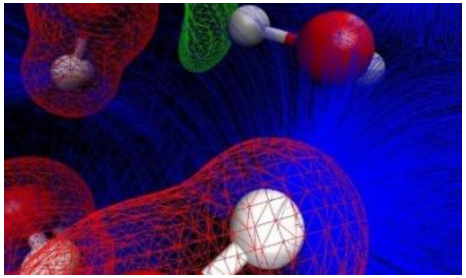


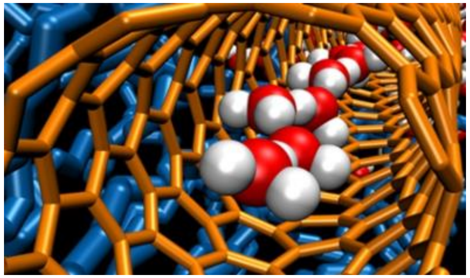
IMAGE: ScienceMag

About BES

MISSION: to support fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels in order to provide the foundations for new energy technologies and to support DOE missions in energy, environment, and national security.

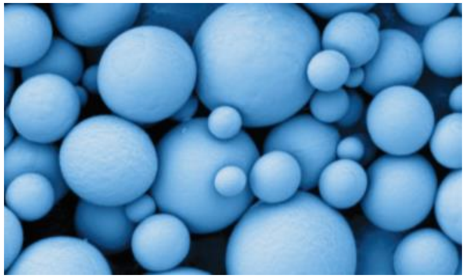


Chemical Sciences, Geosciences, and Biosciences (CSGB)

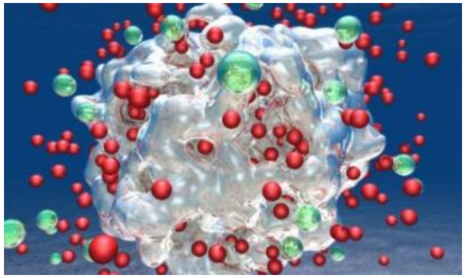


Materials Sciences and Engineering (MSE)

Scientific User Facilities (SUF)



Energy Frontier Research Centers (EFRCs)



Computational Materials Sciences, Computational Chemical Sciences

Energy Innovation Hubs

Origins of DAC Research at BES

Carbon Dioxide Research Division
(today in BER)

Office of Energy Research
(Office of Science, since 1998)

Materials and Chemical Sciences Research for Direct Air Capture of Carbon Dioxide
(FY2020, BES: *LAB 20-2303*)

1980-85 | 85-90 | 90-95 | 95-00 | 2000-05 | 05-10 | 10-15 | 15-20

Catalytic Conversion of CO_2
(within BES)

Separations

Fuels from Sunlight Hub

Energy Frontier Research Centers

CGS (Center for Gas Separations)
UNCAGE-ME (Center for Understanding and Control of Acid Gas-Induced Evolution of Materials for Energy)

Recent BES Support for DAC

BES Lab Announcement LAB 20-2303 focused is on fundamental materials and chemical sciences research topics applicable to DAC:

- Designing High Selectivity, Capacity, and Throughput Separations
- Data Science Driven Synthesis and Assembly of Materials for Direct Air Capture
- Understanding Temporal Changes That Occur During Separations

Results Three awards totaling $13.5 million over three years, with $4.5 million in FY2020 dollars and outyear funding contingent on congressional appropriations.

Lab Awarded	Research Area
Pacific Northwest National Laboratory	electrochemical approaches
Argonne National Laboratory	photochemical methods
Lawrence Livermore Laboratory	degradation processes in chemical absorption

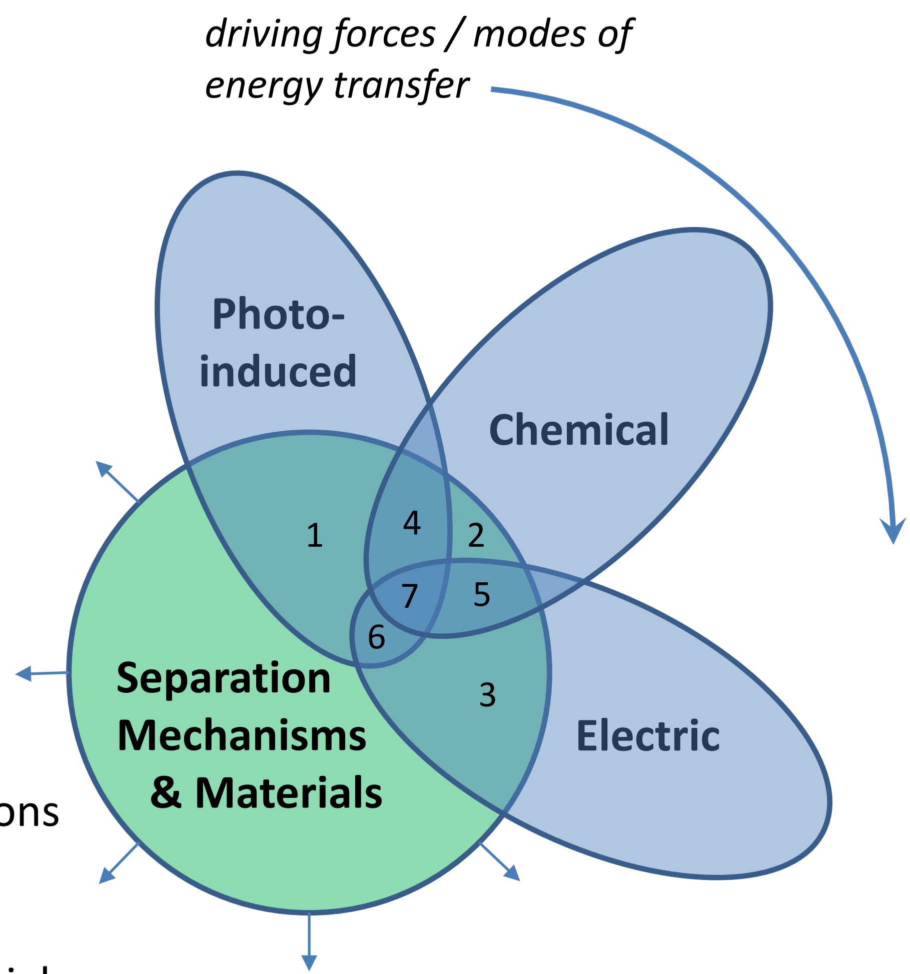
Opportunities for BES Research in DAC

<u>**Major Challenges**</u>

Regeneration leads to a large energy penalty
- Penalty is associated with dH_{ads}
- Thermal energy transfer is unselective

Driving force for a physical separation is low
- Mechanical energy transfer is unselective

Temporal changes in separation systems



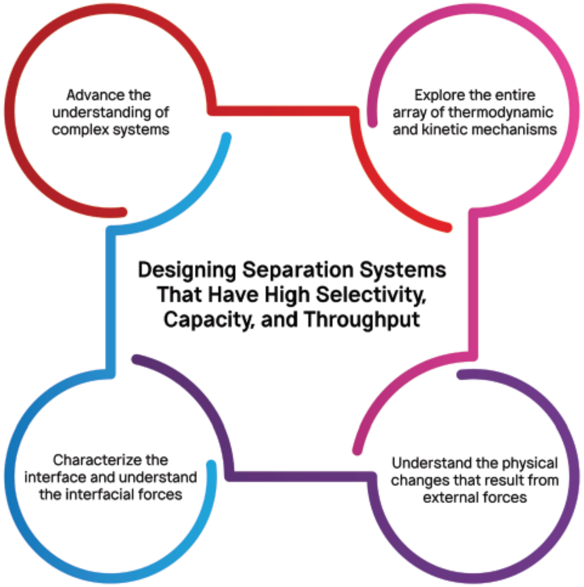
<u>**Strategic Research Areas**</u>

Improve Energy Delivery
- photoinduced, chemical, electric, *etc*.

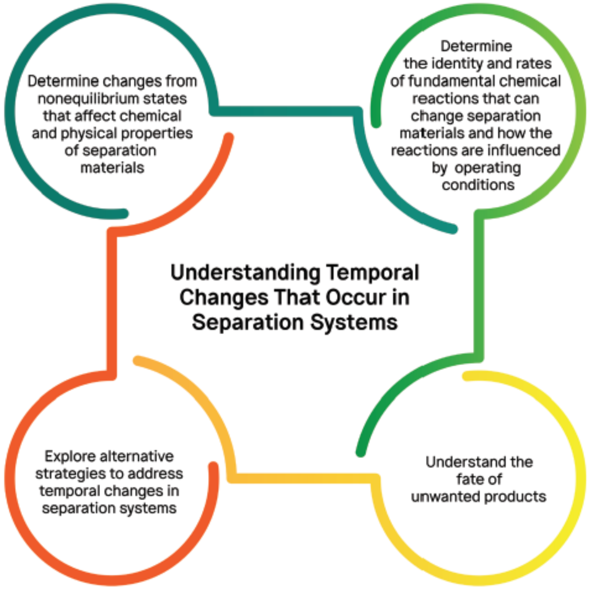
Leverage Alternative & Multi-modal Separations
- thermodynamic, kinetic, transport

Expand the Radius of Mechanisms and Materials

2019 NAS Study Identified a Research Agenda for Transforming Separation Science



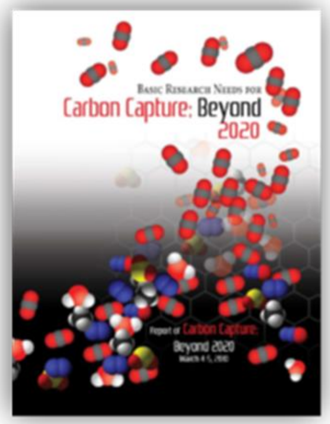
- Explore the entire array of thermodynamic and kinetic mechanisms
- Characterize the interface and understand interfacial forces
- Understand the physical changes that result from external forces

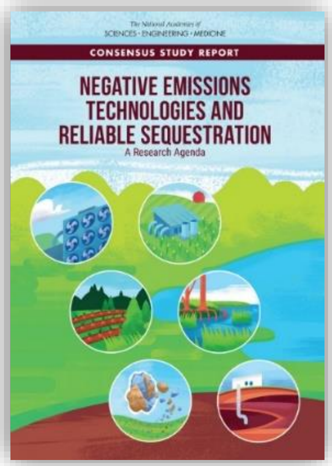


- Understand temporal changes occurring in separation systems
- Determine changes from nonequilibrium states that affect the chemical and physical properties of separation materials
- Understand the fate of unwanted products
- Explore strategies to address temporal changes

There is a Need for Basic Science in the Capture of Gaseous Carbon Species

Advancing the **basic sciences** that underpin CO_2 separation and capture processes is a critical and urgent need.





Future negative emissions technologies for dilute gases, such as direct air capture, will become feasible and economical at large-scale, by

- Better understanding and controlling dynamic atomic-level and molecular-level interactions of the targeted species with the separation media
- Designing new materials with tuned structures and functionalities for optimum separation selectivity and energetics
- Implementing separations with multiple physical driving forces (electromagnetic, thermal, mechanical, etc.)
- Introducing new concepts of reactive separations (chemical driving forces)

Leveraging National Scientific User Facilities

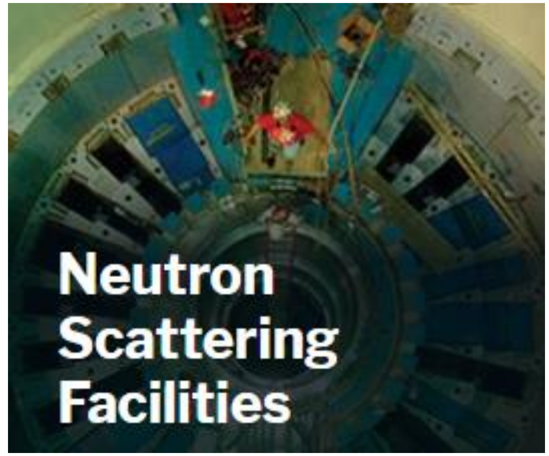
Stanford Synchrotron Radiation Light Source (SSRL)

National Synchrotron Light Source II (NSLS-II)

Linac Coherent Light Source (LCLS)

Advanced Photon Source (APS)

Advanced Light Source (ALS)



High Flux Isotope Reactor (HFIR)

Spallation Neutron Source (SNS)

Center for Nanophase Materials Sciences (CNMS)

Center for Integrated Nanotechnologies (CINT)

Center for Functional Nanomaterials (CFN)

The Molecular Foundry (TMF)

Center for Nanoscale Materials (CNM)

Thank you