# Industrial Decarbonization Research in Office of Science

Gail McLean

Director, Chemical Sciences, Geosciences and Biosciences Division Office of Basic Energy Sciences US DOE Office of Science



https://science.osti.gov/bes



### **U.S. DEPARTMENT OF ENERGY** Science

#### **Our Mission:**

Deliver scientific discoveries and major scientific tools to transform our understanding of nature and advance the energy, economic, and national security of the United States.

Office of

More than **34,000 r**esearchers supported at more than **300** institutions and **17** DOE national laboratories

Steward **10** of the 17 DOE national laboratories

FUNDING

More than **37,000** users of 28 Office of Science scientific user facilities

\$8.1B (FY 2023 enacted)

Energy.gov/science



### **Office of Science Research Portfolio**

Advanced Scientific Computing Research	<ul> <li>Delivering world leading computational and networking capabilities to extend the frontiers of science and technology</li> </ul>
Basic Energy Sciences	<ul> <li>Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels</li> </ul>
Biological and Environmental Research	<ul> <li>Understanding complex biological, earth, and environmental systems</li> </ul>
Fusion Energy Sciences	<ul> <li>Supporting the development of a fusion energy source and supporting research in plasma science</li> </ul>
High Energy Physics	<ul> <li>Understanding how the universe works at its most fundamental level</li> </ul>
Nuclear Physics	<ul> <li>Discovering, exploring, and understanding all forms of nuclear matter</li> </ul>
Isotope R&D and Production	<ul> <li>Supporting isotope research, development, production, processing and distribution to meet the needs of the Nation</li> </ul>
Accelerator R&D and Production	<ul> <li>Supporting new technologies for use in SC's scientific facilities and in commercial products</li> </ul>



### **Office of Science**

- Supports fundamental research, for instance in computational sciences, chemistry, materials sciences, biochemistry, and systems biology, that could advance industrial decarbonization.
- Research at SC-supported user facilities, such as the Nanoscale Science Research Centers and High End Computing facilities, can address large scale, complex R&D challenges relevant to industrial decarbonization.



Viewing the transition state of a photochemical reaction

 Center efforts with potential relevance for industrial decarbonization include Energy Frontier Research Centers (EFRCs), Bioenergy Research Centers (BRCs), Energy Innovation Hubs, and Energy Earthshot Research Centers (EERCs).



#### **SC Energy Earthshots Initiative**

Joint initiative between BES, ASCR, and BER to address key basic research challenges in support of the DOE Energy Earthshots stretch goals for the first 6 DOE Energy Earthshots.

Two complementary programs:





Energy Earthshot Research Centers (EERCs): Multi-disciplinary, multi-institutional teams led by DOE laboratories focused on fundamental research that addresses key research challenges for the Energy Earthshots.

Scientific Foundations for Energy Earthshots: Small group awards led by academic or private sector institutions focused on use-inspired foundational science addressing knowledge gaps limiting achievement of Earthshot goals.

SC announced 29 awards in FY 2023, 11 EERCs (recommended ~\$4.8 M/yr/EERC) and 18 scientific foundations grants (~\$2-5 M/award over 3 years).



### **EERC Awards Relevant to Industrial Decarbonization**

# **C-STEEL - Center for Steel Electrification by Electrosynthesis**, Argonne National Laboratory, Brian J Ingram

Partners - Case Western Reserve Univ, ORNL, Univ of Illinois Chicago, Northern Illinois Univ, Purdue Univ Investigates an electrodeposition process that uses electricity to initiate a reaction and deposit a usable iron metal at much lower temperatures than existing processes.

# **NEETER - Non-Equilibrium Energy Transfer for Efficient Reactions,** Oak Ridge National Laboratory, David Sholl

Partners - Delaware State Univ, Georgia Institute of Technology, PPPL, Princeton Univ, SLAC National Accelerator Laboratory, Univ of Houston, Univ of Maryland College Park

Focuses on replacing bulk steady-state heating with electrified processes that deliver spatially and temporally localized pulses of heat for catalytic chemical processes, using mechanocatalysis or Joule heating

#### C4M · Center for Coupled Chemo-Mechanics of Cementitious Composites for EGS, Brookhaven National Laboratory, Tatiana Pyatina

Partners: SNL, LLNL, LBNL, LANL, UIUC, Princeton Univ, Cornell Univ, Univ of Texas at Austin Aims to understand and control the chemical transformations and mechanical properties of sustainable composite materials for enhanced geothermal systems



#### **Science Foundations Awards Relevant to Industrial Decarbonization**

#### **Fundamental studies of hydrogen arc plasmas for highefficiency and carbon-free steelmaking**, Arizona State University, Sridhar Seetharaman

Partners: Navajo Technical University; NREL; University of Texas, Austin Conducts laboratory scale experiments at extreme conditions to understand the basic science behind hydrogen-plasma-smelting-reduction of iron ore and develop theoretical models coupling physics for iron ore reduction



**Understanding Thermo-Chemo-Mechanical Transformations in Thermal Energy Storage Materials and Composites**, Georgia Institute of Technology, Akanksha Krishnakumar Menon Partner: LBNL

Studies how material composition, structure and mechanical stress co-evolve in thermal energy storage materials, informing development of multifunctional materials that maximize storage capacity and minimize degradation.



#### **Science Foundations Awards Relevant to Industrial Decarbonization**

# Harnessing Electrostatics for the Conversion of Organics, Water and Air: Driving Redox on Particulate Liquids Earthshot (DROPLETS), University of Illinois, Urbana-Champaign,

#### Joaquín Rodríguez López

Partners: ANL; Georgia Institute of Technology; Northern Arizona Univ; Texas State Univ Investigates the chemistry of redox reactions within aqueous water droplets to harness the unique reactivity of microdroplets in processes involving redox reactions, such as CO<sub>2</sub> capture, and the electrosynthesis of molecules

#### Biological Routes for Synthesizing the Industrial Platform Chemical, Propylene, from Deconstructed Lignin Waste And Captured Carbon Dioxide Produced during Lignin Valorization into Bio-oil, Ohio State University, Justin North

Partners: Florida Institute of Technology; PNNL

Focuses on metabolic pathway design to minimize CO<sub>2</sub> and heat use and efficiently use water through an integrated process of lignin hydrolysis and conversion to propylene hydrocarbons.



#### **Science Foundations Awards Relevant to Industrial Decarbonization**

## Unleashing Photosynthesis and Nitrogen Fixation for Carbon Neutral Production of N-Rich Compounds, Washington University in Saint Louis, Himadri Pakrasi

Partners: NREL; Alabama State University

Focuses on biologically-derived ammonia and other nitrogen-rich compounds to significantly reduce the energy and CO2 emissions resulting from the production of chemicals and synthetic fertilizers.



### **BES EFRCs Relevant to Industrial Decarbonization**

**Center for Programmable Energy Catalysis (CPEC),** University of Minnesota, Paul Dauenhauer Understand how electrons rearrange on metal and metal oxide surfaces such that they can be programmed to optimally control catalytic reactions and accelerate surface reactions beyond kinetic limitations

**Catalysis Design for Decarbonization Center (CD4DC),** University of Chicago, Laura Gagliardi Discover and develop reticular metal-organic framework materials as catalysts for the decarbonization energy transition and to optimize the key catalytic reactions involved.

**Center for Closing the Carbon Cycle (4C),** University of California, Irvine, Jenny Yang Advance synergistic capture and conversion of carbon dioxide from dilute streams into useful products through the convergent study of sorbents and catalysts

Understanding and Controlling Accelerated and Gradual Evolution of Materials for Energy (UNCAGE-ME), Georgia Institute of Technology, Ryan Lively

Develop knowledge in the characterization, prediction, and control of materials evolution in the presence of realistic contaminants, processes, and mixtures to accelerate materials discovery for sustainable production and utilization of H<sub>2</sub> and CO<sub>2</sub>.



# THANK YOU!



https://science.osti.gov/bes

11 Energy.gov/science