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Notice of Funding Opportunity

Title: Department of Energy – Materials and Chemical Sciences Research for Direct Air Capture of Carbon Dioxide

Website: <https://www.grants.gov/web/grants/view-opportunity.html?oppld=331910>

Funding: Total: \$24,000,000. Maximum awards: \$200K-\$1.2M per year, depending on project.

Dates: Pre-Application Deadline: March 30, 2021
Application Submission Deadline: May 18, 2021

Summary: The DOE SC program in Basic Energy Sciences (BES) announces its interest in receiving applications from single investigators and from teams for support of experimental and theoretical efforts to advance fundamental understanding of the capture of carbon dioxide (CO₂) from dilute sources including combined capture and chemical conversion of CO₂. Although direct air capture of carbon dioxide (DAC) generally refers to the capture of CO₂ from ambient air, this FOA also considers the removal of CO₂ from partially concentrated air (e.g., building HVAC exhaust) and from natural fluids (e.g., the ocean and surface waters) that received their CO₂ directly from ambient air. Enhanced understanding of scientific phenomena and approaches for DAC would accelerate progress and strengthen the foundation for applications that deliver economic benefit and/or energy security.

Project Topic Areas:

1. Energy Transfer Mechanisms: Novel Energy Transfer Mechanisms for Regeneration of and Mass Transport in Direct Air Capture Systems.

Processes for DAC separations are governed by interdependent molecular and energy transfer mechanisms. Most contemporary DAC approaches utilize energy poorly, as evident by second-law efficiencies for CO₂ separation of 1 to 9 percent (for comparison, post-combustion capture from coal exhaust attains second-law efficiencies greater than 20 percent). Hence, hypothesis-driven, fundamental research is sought to discover and elucidate novel mechanisms for efficient energy and mass transfer in DAC. These mechanisms are normally affected by intermolecular attractions and repulsions, phase transitions, reversible- or irreversible-reaction chemistry, electron excitation or transfer, molecular diffusivities, and external forces. Applications focused on this topic must address one or both of the following categories:

- a. Mechanisms for highly selective energy delivery to natural or synthetic chemical separations systems containing captured carbon dioxide or its immediate derivative species and reaction intermediates. Exemplary mechanisms may employ reactive, electrochemical, magnetic, photo-induced steps or a synergistic confluence of such steps. Research focused solely on thermal mechanisms will not be supported.
- b. Mechanisms for preserving or redirecting heats of adsorption or solvation in a way that assists molecular transport or system regeneration after transport has occurred. Concepts that combine exothermic and endothermic stages to exchange thermal flux across a barrier are discouraged.

Appropriate fundamental chemical and materials sciences research for this topic must address one or both of the above categories and may consider the following related areas of interest: (i) how classical tradeoffs can be avoided (e.g., the correlation of selectivity and heat of regeneration), or replaced by more acceptable tradeoffs, based on understanding of factors that affect CO₂ release and system regeneration, or of factors that may eliminate thermal regeneration; (ii) how fundamental phenomena in separation systems can be balanced in order to approach the theoretical mass transfer limit in the CO₂ source phase.

2. Temporal Changes: Understanding Temporal Changes That Occur during Separations.

Materials and chemical processes involved in DAC can undergo chemical, physical, and/or structural changes over their operating lifetimes, for example due to unwanted chemical reactions and the accumulation of byproducts or impurities. Other factors include the evolution of separations media or materials from a nonequilibrium or metastable state toward an equilibrium state. Such changes can significantly affect the selectivity, efficiency, and rate of separation of a DAC system. Hence, proposed research should yield a better understanding of the fundamental mechanisms of these changes, to provide a scientific foundation for more robust DAC systems that operate in complex and challenging environments.

3. Science-driven Synthesis and Assembly: Science-driven Synthesis and Assembly of Innovative Materials for Direct Air Capture.

Integrated data science and experimental research efforts with a clear scientific focus are sought to address the particular materials challenges of direct capture of CO₂ from dilute sources (e.g., ambient air, ocean and surface waters) and accelerate science-based synthesis and assembly of transformative materials with multiple properties

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designed for this purpose. Applications must emphasize hypothesis-driven synthesis and assembly science to create innovative, robust materials that selectively capture CO₂ and either release or convert it into a useful material, fuel or chemical via non-thermal, low-energy processes. Because fundamental understanding and spatial and temporal control of synthesis, assembly, and related chemical pathways is essential to achieving this goal, proposed research also must incorporate in-situ and/or operando characterizations and high-fidelity determinations of structure dynamics and chemical processes. Proposed research that does not emphasize fundamental understanding and control of synthesis and assembly pathways and non-thermal, low-energy CO₂ separation, capture, release, or conversion mechanisms via an approach that integrates data science techniques and advanced in-situ and/or operando characterizations is outside the scope of this FOA and maybe declined. Proposed research that focuses on optimization of material properties via the use of high-throughput synthesis, test and evaluation processes or on optimization of existing direct air capture processes also is outside the scope of this FOA and maybe declined.

Funding:

DOE anticipates that, subject to the availability of future year appropriations, a total of up to \$24 million in current and future fiscal year funds will be used to support awards under this FOA. Award ceiling is \$1,200,000 per year, and award floor is \$500,000 per year for applications led by DOE/NNSA National Laboratories and \$200,000 per year for applications led by other eligible applicants. Applications requesting more or less than this amount of support may be declined without further review. Cost sharing for basic and fundamental research is not required pursuant to an exclusion from the requirements of Section 988 of the Energy Policy Act of 2005. The exact number of awards and award size will depend on the number of meritorious applications and the availability of appropriated funds. DOE anticipates making awards with a project period of three (3) years. DOE anticipates awarding grants, interagency agreements, and National Laboratory authorizations under this FOA. Multi-institutional teams must apply using a prime and subaward model with one application submitted by the lead institution.

Project Requirements:

A pre-application is required and must be submitted by the date indicated on the cover of the FOA. Pre-applications will be reviewed for responsiveness of the proposed work to the research topics identified in this FOA. DOE will send a response by email to each applicant encouraging or discouraging the submission of an application by the date indicated on the cover of the FOA. Applicants who have not received a response regarding the status of their pre-application by this date are responsible for contacting the program to confirm this status. Applications that have not been encouraged by DOE may be declined without merit review.

This FOA does not support an applicant's commercial activity. Applications from for-profit organizations that propose a scientific scope of work related to current business activity or uses are considered to be commercial activity and will be declined. Applications containing a scientific scope of work that is or has been supported by or proposed to a Federal Small Business Innovative Research or Small Business Technology Transfer (SBIR / STTR) program are considered to be commercial activity and may be declined without merit review. All for-profit applicants must include a description, not to exceed 200 words, of how their proposed work will advance scientific understanding of a basic and fundamental nature as an appendix to the research narrative.

Eligible Applicants:

All types of domestic applicants are eligible to apply, except nonprofit organizations described in section 501(c)(4) of the Internal Revenue Code of 1986 that engaged in lobbying activities after December 31, 1995. DOE/NNSA National Laboratories are eligible to submit applications under this FOA and may be proposed as subawardees under another organization's application. If recommended for funding as a lead applicant, funding will be provided through the DOE Field-Work Proposal System and work will be conducted under the laboratory's contract with DOE. No administrative provisions of this FOA will apply to the laboratory or any laboratory subcontractor. If recommended for funding as a proposed subawardee, the value of the proposed subaward will be removed from the prime applicant's award and will be provided to the laboratory through the DOE Field-Work Proposal System and work will be conducted under the laboratory's contract with DOE. Non-DOE/NNSA FFRDCs are not eligible to submit applications under this FOA but may be proposed as subawardees under another organization's application. If recommended for funding as a proposed subawardee, the value of the proposed subaward may be removed from the prime applicant's award and will be provided through an Inter-Agency Award to the FFRDC's sponsoring Federal Agency. Other Federal Agencies are not eligible to submit applications under this FOA but may be proposed as subawardees under another organization's application. If recommended for funding as a proposed subawardee, the value of the proposed subaward may be removed from the prime applicant's award and will be provided through an Inter-Agency Award.