Addressing Challenges in Energy: Floating Wind in a Changing Climate (ACE-FWICC)

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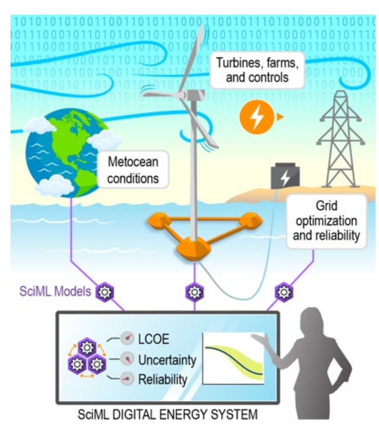
The challenges presented by the widespread and rapid deployment of floating offshore wind are complex and interdisciplinary. An integrated approach is required for floating offshore wind energy to reach cost and schedule goals that cannot be effectively met with siloed research focused on a subset of scientific gaps. The Center will develop a digital energy system using scientific machine learning (SciML) that links the key components of floating offshore wind driving the cost of power in a changing climate. These components of our Center's SciML Digital Energy System include the wind resource, wind, and wave (metocean) conditions, wind plant design and control, and integration of wind energy onto the power grid. In today's computational environment, it is impossible to practically use the existing suite of models to examine the cost of energy associated with the large-scale deployment of floating offshore wind turbines (FOWTs). The digital energy system will be constructed using SciML techniques, leveraging the domain-specific models and the Center's computational expertise. The primary advantage of the digital energy system is its ability to model FOWTs, wind farms, and wind power distribution in a coherent and computationally efficient way, enabling the development of new strategies to reduce energy costs in current and future climates. The Center's research falls into four themes: Metocean, Turbine and Farm, Grid, and SciML Digital Energy System. The Center has four objectives that map to the four research themes:

- <u>Objective 1</u>: Determine how the wind resource and metocean environment (including the impact of extreme events) will change on time scales ranging from weeks to decades.
- <u>Objective 2</u>: Enable levelized cost of energy (LCOE) reduction via improved control of FOWTs and wind farms—considering turbine lifetime, wake interactions, and grid integration—in current and future metocean environments.
- <u>Objective 3</u>: Determine optimal system designs for economic and reliable operation of the grid and efficient transport of power from offshore floating wind turbines in present and future climates.



- Objective 4: Develop a digital energy system model using SciML to test and evaluate the impact of uncertain changes in the wind resource and metocean conditions on FOWTs, wind farms, and the reliable and optimized integration of wind energy in the grid.

The Center will support the Earthshot goal of reducing LCOE and will integrate research across four themes. First, research in the Metocean Theme will improve estimates of the wind resource and metocean conditions on time scales ranging from days to decades, as well as add a treatment of farm-to-farm wakes. Second, work in the Turbine and Farm Theme will improve wind plant controls, leading to decreased maintenance costs, increased turbine lifetime, and better accounting for turbine-to-turbine wakes using realistic conditions delivered from the Metocean Theme. Third, research in the Grid Theme will improve planning and operation of the grid, accounting for the variability and intermittency of FOWTs. The results of these three themes will inform each other and will provide the basis for the SciML Digital Energy System Theme.

This research was selected for funding by the Office of Science.

Center for Coupled Chemo-Mechanics of Cementitious Composites for EGS (C^4M)

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Geothermal energy is renewable, has a small footprint, and, unlike other green energies, is available around-the-clock. Geothermal energy development requires access to the subsurface through wells that circulate fluids to extract thermal energy. In Enhanced Geothermal Systems (EGS), hydraulic stimulations increase energy recovery by increasing permeability and improving heat exchange. EGS wells are subjected to higher temperatures and more aggressive environments and thermo-mechanical stresses than oil or gas wells. Since they are integral to power-plant installations, they are also required to last decades.

The mission of C^4M is to help the United States exploit its abundant geothermal energy by elucidating and controlling the chemical transformations and mechanical properties of sustainable cement-like composite materials used to construct these wells. Specifically, its objectives are 1) to understand chemical changes in those materials under high temperature and pressure in order to design reliable and durable composites; 2) to quantify the effects of these changes on materials' performance; and 3) to control the solidification and transformations of the materials for successful and economic well construction and operation. Cost-effective cementitious composites to be designed for long-term operation under very high temperatures and pressures and chemically aggressive environments will have mineral or waste-product precursors with zero-net CO_2 release. To ensure well durability, materials with geologically stable mineral phases will be targeted, and inorganic coatings resistant to high temperatures and aggressive environments will be investigated.

To achieve its objectives, the Center has assembled a multi-disciplinary team of leading researchers including a minority-serving institution. The Center's experimental and modeling capabilities complement each other to elucidate and predict the performance of cementitious materials from the atomic to the macroscopic scale and for a time span ranging from seconds to years. Artificial intelligence and high-performance computing make possible the design of advanced materials with long durability under extreme conditions. In addition to their own capabilities, the C^4M groups take advantage of the unique user facilities housed in the partner national laboratories, including advanced light sources and nanoscience centers. Operationally, the Center is organized with a simple and agile structure that facilitates decision-making and reduces bureaucratic burdens to achieve the goal of cutting the cost of enhanced geothermal systems by 90% by 2035.

This research was selected for funding by the Office of Science.

Center for Ionomer-based Water Electrolysis (CIWE)

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To meet the Hydrogen Shot goals, one needs to uncover and understand the structure, evolution, and chemistry of the ion-conduction polymers (ionomers) in water electrolyzers. Such knowledge enables the design and optimization of these materials for improved efficiency, performance, and lifetime. The challenge stems from the dynamic and complex roles of the ionomers, which act as both a membrane separator and as a conductive binder. Understanding these dual roles requires filling critical knowledge gaps about *i*) the structure of the materials and how they change during operation at high currents, *ii*) the transport and activity of the reactant and product species through the ionomer and their impact on catalyst reactivity and degradation, and *iii*) design rules for making durable, high-performing catalyst/ionomer and ionomer/ionomer interfaces. CIWE will address these gaps through the use of physical and digital (i.e., representative physics-based mathematical models of real structures) twins that provide increased knowledge and overcome the "small-data" problem (*i.e.*, the fact that experiments are time and effort intensive and so cannot fully explore the parameter space in detail) that exists for these highly complex interfaces. Advanced data analysis and assessment including artificial intelligence and machine learning and exploration of coupled mechanical and electrochemical phenomena will be used to enhance understanding. Discoveries made by CIWE will impact basic DOE research and the electrolysis community. CIWE will also be a convening authority that links fundamental science activities around low-temperature hydrogen generation via water electrolysis to applied R&D to realize the Hydrogen Shot.

This research was selected for funding by the Office of Science.

Center for RESTORation of soil Carbon by precision biological strategies (RESTOR-C)

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Soil carbon represents a vast global carbon reservoir that has become depleted through human activities. To harness this natural carbon sink and advance toward the cost and scale goals of the DOE Carbon Negative Shot, RESTOR-C will develop plant- and microbe-based strategies to increase accumulation of persistent carbon in soil. These strategies are designed to increase the amount of atmospheric carbon fixed by plants and increase the amount of the fixed carbon that is channeled belowground as soil persistent carbon.

To accomplish this goal, the Center will apply cutting-edge molecular and computational methods to overcome key obstacles to persistent carbon storage across four Divisions: The *Soil Division* will explore the chemical, biological and environmental factors that govern the persistence of carbon in soils, to enable the development of stable, long-term carbon storage solutions with a focus on arid and marginal lands. The *Plant Division* will design plant genotypes that efficiently capture and sequester carbon, through a combination of increased photosynthetic efficiency and optimized root characteristics. These efforts will focus on sorghum, a stress-tolerant bioenergy crop that can grow in a range of soils and climates with minimal nutrient inputs. The *Microbial Division* will identify and optimize microbial communities to promote carbon retention in soil using advanced genomic technologies and artificial intelligence-guided high-throughput experiments. Finally, the *Scaling and Impact Division* will model, predict, evaluate, and optimize cost and scale of soil carbon sequestration approaches. This work will build and connect multi-scale models of carbon dynamics and economic feasibility to predict the impact of carbon sequestration approaches, evaluate strategies, and test approaches at the field level.

This research will break new ground in multidisciplinary research, leveraging unique expertise at two national laboratories and four university partners, including two minority serving institutions, to integrate recent developments and make scientific breakthroughs spanning the biological, ecological, chemical, and computing sciences. At the end of the four-year period, the Center will have validated plant-microbe strategies to increase carbon at target field sites in California and New Mexico, as well as a dramatically expanded knowledge base and set of capabilities to rapidly extend these approaches to other locations and crops. In the long term, these methods have the potential to restore carbon in US agricultural lands, forging the way toward a carbon negative future.

This research was selected for funding by the Office of Science.

Center for the Science of Plasma-Enhanced Hydrogen Production (PEHPr)

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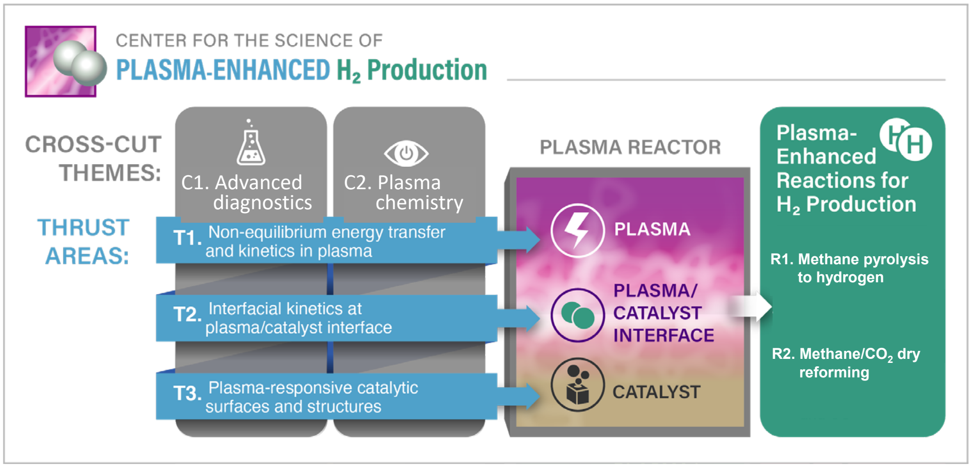

Low-cost, energy-efficient hydrogen (H_2) production with net-zero carbon emissions is critical for meeting U.S. 2050 climate targets. However, today's H_2 production from fossil fuels via steam reforming is energy inefficient and produces large amounts of carbon dioxide (CO_2). A game-changing approach is to produce H_2 and high-value carbon from methane and CO_2 by using non-equilibrium (NE) plasma created with renewable electricity to increase energy efficiency, reduce cost, and enable concurrent carbon capture, conversion, and storage, as well as distributed chemical synthesis. Plasmas are ionized gases with excited species and radicals that can lead to enhanced reactivity and thus, new chemical reaction pathways and high energy efficiency compared to traditional fossil fuel based H_2 and chemical production via thermal processes.

A team of renowned experts with expertise in plasma physics, chemistry, catalysis, materials science, and diagnostics have assembled to address key challenges in understanding and manipulating the NE energy transfer and kinetics associated with plasma pyrolysis of methane to form H_2 and plasma-assisted catalysis of CO_2 dry reforming of methane to form syngas (H_2 + CO), which inhibit advances in this potential pathway to clean H_2 production. The objectives of the research are to: (1) advance understanding of NE plasma energy transfer and chemistry involving excited molecules and free radicals, including plasma-particle and plasma-surface interactions; (2) control plasma NE, electron energy distributions, and reactivity; and (3) develop new diagnostic methods and kinetics models, novel NE plasma pyrolysis methods, and new catalysts with optimal performance in the presence of plasma. Achieving these goals will help to bring forth energy-efficient plasma-mediated processes for low-cost electrified H_2 production. These advances could lead to a paradigm shift in clean H_2 production with carbon capture and help to achieve the DOE Hydrogen Shot goal of $1/kg H_2 in a decade, which will promote U.S. leadership in clean H_2 production and climate change mitigation. This Center will promote diversity and develop leadership skills of early career researchers in energy sciences and electrified non-equilibrium H_2 production. The Center's research will inspire students to study energy sciences, inform the public about new clean-energy technologies, and accelerate knowledge transfer among academic institutions, government laboratories, and industry.

This research was selected for funding by the Office of Science.

Center for Steel Electrification by Electrosynthesis (C-STEEL)

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Today, producing iron from ores is an energy-intensive process that requires temperatures greater than 2500 °F and accounts for 1% of all industrial carbon emissions in the United States. C-STEEL envisions a future that harnesses the inherent efficiency of electrochemical processes that require low (or no) heat input to enable scalable, sustainable, and low-cost industrial iron manufacturing. Electrodeposition uses electricity to drive the production of purified products (e.g., iron metal/alloys) from a liquid electrolyte. This transformative approach will provide a pathway to reduce greenhouse gas emissions from industrial process heating by developing an alternative to using blast furnaces for producing iron for steelmaking. Fundamental scientific challenges to the controlled electrochemical deposition of iron remain, however. For instance, today there are comparatively few chemical design strategies, particularly at metal interfaces, to mitigate undesirable side reactions such as hydrogen evolution, corrosion, or passivation. C-STEEL will develop a set of atomic-level chemical design rules to tailor iron coordination environments in electrolytes and enable selective use of electrons for energy-efficient iron production. Design of these atomic-level interactions will enable precise control over both the structure and alloy composition of the metal products for subsequent use in steel manufacturing. To achieve this mission, the Center will integrate three research areas to probe the mechanisms that control iron coordination in both low-temperature water-based systems and intermediate-temperature ionic liquid-based systems and subsequent control of deposit structure and composition. State-of-the-art capabilities in chemistry, physical characterization, electrochemical behavior, simulation, and modeling will be combined with an integrated data and computation infrastructure. An artificial intelligence-based, model-driven experiment (MODEX) framework will lead to predictive control of iron coordination and intelligent designed electrolytes with targeted properties. C-STEEL will promote a new generation of scientists and engineers who will realize and implement the transformational decarbonization technologies. C-STEEL intends to create inclusive and rigorous personal development opportunities through collaborative partnerships, targeted career growth opportunities, outreach programs that build scientific awareness in future scientists, and investment in mentorship and leadership opportunities. These commitments are guided by the Center-wide plans for diverse and equitable hiring, creation of safe and inclusive work environments, and mentoring support for students and postdocs.

This research was selected for funding by the Office of Science.

Center for Understanding Subsurface Signals and Permeability (CUSSP)

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Geothermal systems can be harnessed to generate electricity when water flowing through hot underground rocks captures and brings up enough heat to power turbines. Although natural geothermal systems exist, the same subsurface heat is much more widely available in rocks that are not permeable enough for fluid flow. Enhanced geothermal systems (EGS) overcome this obstacle by stimulating and enhancing existing fractures in the rock to establish a fluid flow circuit – one in which cold water pumped down one well returns to the surface superheated in another. As currently demonstrated by worldwide pilot projects, EGS holds great promise as an abundant, always-on source of clean energy. However, broad deployment of EGS relies not just on the ability to create a permeable fracture flow network in hot dense rock, but also on the ability to maintain fluid flow and heat productivity for many years. CUSSP is focused on the latter problem – which depends on the ability to reliably predict the long-term flow behavior for a given set of conditions. The flow of pressurized fluid through hot fractured rock can change over time in ways that are currently difficult to predict. Chemical and physical responses of the rock to fluids and changes in temperature and pressure distribution can open unproductive flow channels or close productive ones, with complex feedbacks that make long-term flow rates and heat production uncertain. While geophysical sensing tools can detect changes in the properties of EGS reservoirs, linking those signals to underlying processes is currently challenging. CUSSP recognizes the importance of learning how to convert data-rich sensing signals directly into process understanding, to ultimately replace assumptions in simulators with accurate process knowledge that can be monitored remotely. Using a highly instrumented EGS testbed site at the Sanford Underground Research Facility (South Dakota, USA), CUSSP takes advantage of the ability to simultaneously collect multiple complementary geophysical sensing signals to monitor the distribution of temperature, strain, electrical resistivity, and seismic activity under controlled fluid flow conditions. Laboratory-based fracture flow experiments with rocks from the site will be used to understand and constrain rates of coupled chemical and physical responses, and to train deep neural network machine learning (ML) models. Using exascale supercomputing, joint inversions of sensing data streams constrained by the ML models will demonstrate a method for linking signals to process knowledge for the first time. Success of CUSSP will help the DOE achieve its EGS Earthshot objectives by providing an innovative foundation for the development of future modeling approaches and technologies that couple high-precision observation and high-accuracy prediction of EGS reservoirs.

This research was selected for funding by the Office of Science.

DEGradation Reactions in Electrothermal Energy Storage (DEGREES)

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A resilient, flexible, and decarbonized electric grid needs large-scale clean energy storage with power output of hundreds of megawatts and more than 10 hours of storage duration—i.e., long duration energy storage. One potential technology is thermal energy storage (such as used for concentrating solar power and being considered for nuclear reactors), but it has a high cost because of operating and maintenance expenses, and downtime from replacing degraded materials and systems. These materials must also function at extremely high temperatures (up to 1,200°C) so they can discharge high-quality heat and accommodate clean electric power generation on a grid scale. To fill this gap for cost-effective and high-performing thermal energy storage materials, DEGREES is an Energy Earthshot Research Center that will provide fundamental understanding of the science behind complex degradation mechanisms and instabilities that impact performance. Understanding the degradation process at an atomic and molecular level can help predict and ultimately control the materials' performance in a way that can be scaled to practical, grid-scale systems.

A variety of phase change materials (e.g., metals, alloys, and salts) and thermochemical materials (e.g., carbonates, oxides, and hydroxides) will be considered in this research. The work will involve crosscutting theory, modeling, and experimental work performed by a diverse group of researchers at national laboratories and universities. The DEGREES research is organized into three interrelated scientific pushes: (1) *understand* degradation mechanisms in complex phase change and thermochemical materials, (2) *mitigate* degradation through thermodynamic and kinetic insight, and (3) *discover and synthesize* high-performing and durable materials using the scientific insight gained. DEGREES will also prioritize the use of inexpensive, Earth-abundant raw materials in the design of environmentally friendly and sustainable materials. Because degradation of thermal storage materials is a major roadblock preventing the contribution of this technology to the clean energy transition, the breakthroughs resulting from this work represent a game-changer when it comes to large-scale deployment of renewable energy.

This research was selected for funding by the Office of Science.

FLOWMAS: Floating Offshore Wind Modeling and Simulation

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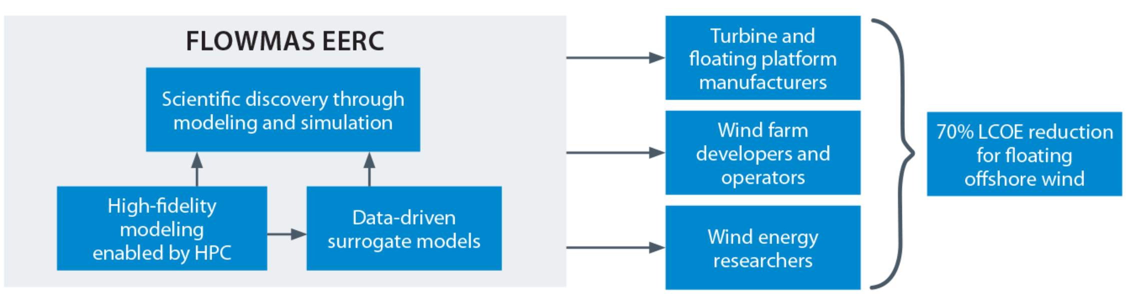
As part of a larger effort to decarbonize the electric grid, the U.S. Department of Energy's (DOE's) Floating Offshore Wind Shot seeks to reduce the levelized cost of energy (LCOE) of floating offshore wind energy 70% by 2035. The FLOWMAS Energy Earthshot Research Center (EERC) will deliver the fundamental research necessary to enable breakthroughs on this aggressive timeline. Knowledge of, and models for, the conditions, loads, and dynamics of floating offshore wind turbines in the meteorological-ocean environment are sorely lacking, especially in extreme conditions. One cannot fully optimize a system that is poorly understood and for which adequate models do not exist. FLOWMAS integrates researchers from mathematical-, computational-, and atmospheric-science backgrounds to better model and better understand the dynamics ranging from climate scales to wind turbine floating platforms and blades that are needed to achieve the Wind Shot. Building on DOE investments in high-fidelity models for climate and land-based wind energy that can exploit exascale-class computing, FLOWMAS researchers will create a suite of high-fidelity codes for floating offshore wind energy that incorporates the microscale (i.e., wind turbines, floating platforms, and mooring systems), mesoscale (i.e., regional weather dynamics), and global/climate scales. Researchers will use results from high-fidelity simulations and ongoing DOE-supported field campaigns to create data-driven surrogate models that are computationally efficient and can explore many system conditions and for long time durations not accessible with computationally expensive high-fidelity models. Finally, the developed models will leverage exascale-computing power to create a new understanding of the floating offshore wind energy system, including how climate change will impact offshore wind energy resources, the physics of floating wind farm and turbine wake dynamics, and the loads and dynamics of floating wind turbines during operational and extreme events.



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Non-Equilibrium Energy Transfer for Efficient Reactions (NEETER)

Dr. David Sholl, Director of the Transformational Decarbonization Initiative[1]

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Production of chemicals and petroleum refining are two of the most greenhouse gas (GHG) intense sectors of US industry, accounting for more than 500 million tons of CO_2 emissions and 39% of industrial energy consumption in 2020. Because of their economic significance and GHG intensity, delivering GHG-free process heat in the chemicals and refining sectors is a key focus for DOE's Industrial Heat Earthshot. Development of alternative heat delivery methods suitable for broad classes of chemical processes and reactions, especially endothermic reactions using renewable electrical energy, has the potential to radically reduce industrial GHG emissions and directly address the Earthshot goal. This EERC focuses on replacing steady-state, bulk heating with electrified processes that deliver spatially and temporally localized pulses of heat for catalytic processes. The overarching goal of this Center is to leverage transient temperature and pressure conditions in non-equilibrium (NE) chemical processes to allow unconventional reaction pathways with high energy and atom efficiency, allowing electrification of processes that currently generate large GHG emissions due to heating. These NE processes will not only allow electrification of heating that today relies on fossil fuel combustion but also make it possible to achieve desirable chemical transformations that cannot be achieved using standard thermal catalysis. This EERC will focus on two rapidly emerging NE approaches to achieving electrified heterogeneous catalysis, namely, programmable Joule heating and mechanochemistry. Both methods involve localized delivery of heat and/or pressure in an intense, non-steady state manner, offering exceptional opportunities to move beyond the constraints of traditional catalysis. Studying Joule heating and mechanochemistry together will address foundational questions about these methods in ways that are not possible by considering them in isolation, reinforcing the strength of framing these issues within an EERC. To advance these non-traditional heating approaches, NEETER will study carefully selected prototypical endothermic reactions involving C-H and C-C bonds in hydrocarbons with different molecular weights, namely dehydrogenation of light alkanes and deconstruction of polymers such as polypropylene and polyethylene. NEETER's research will be driven by using multimodal *in-situ/operando* tools, including neutron, X-ray, microscopy and ultrafast laser spectroscopy, multiscale modeling, AI/ML and data analytics. NEETER will take advantage of major DOE user facilities at ORNL and SLAC, including the Oak Ridge Leadership Computing Facility (OLCF), the Spallation Neutron Source (SNS), the High Flux Isotope Reactor (HFIR), the Center for Nanophase Materials Sciences (CNMS), and the SLAC National Accelerator Lab.

This research was selected for funding by the Office of Science.

Terraforming Soil EERC: Accelerating Soil-Based Carbon Drawdown Through Advanced Genomics and Geochemistry

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To reduce the United States' net carbon dioxide (CO_2) emissions to zero and limit the impacts of global warming, it is essential to actively remove CO_2 from the atmosphere. Soils store a vast amount of carbon in organic and inorganic forms—on the order of 3000 billion tons globally—this is more carbon than is found in the atmosphere and on land combined. While the United States' 166 million hectares of agricultural soils have lost a vast amount of carbon in the past century due to cultivation and erosion, there is clear potential to reverse this trend and actively manage agricultural lands with strategies that capture CO_2 from the atmosphere. The *Terraforming Soil* Energy Earthshot Research Center (EERC) will research new bio- and geo- engineered techniques to understand, predict, and accelerate scalable and affordable CO_2 drawdown in soils, via both organic and inorganic carbon cycle pathways. The Center's overarching goal is to advance the fundamental understanding of CO_2 drawdown in soils through both organic and inorganic pathways, measuring soil C storage capacity, durability, and regional variations that have bearing on land-management practices. In Objective 1, synthetic biology tools will be used to accelerate naturally occurring plant and microbial traits that shape CO_2 fixation processes, organic matter formation and mineral dissolution. Combined genome sequencing and isotope tracing approaches will be used to quantify the fundamental mechanisms of how organic matter accrues over time and the traits of plants and microorganisms that need to be better reflected in process models. In Objective 2, the Center will focus on positive interactions that can occur during the weathering of primary minerals and the formation of organic matter-mineral complexes—together, these have dramatic potential to accelerate soil CO_2 drawdown via combined organic and inorganic pathways. But currently, the interactions between soil weathering, soil biology, and organic matter cycling are poorly understood. The Center's field and laboratory-based studies will measure how soil management approaches can be 'stacked' together, to optimize total CO_2 drawdown via co-deployment of novel engineered crops or microbes, silicate minerals, or organic amendments. Research for Objective 3 will integrate new modeling capabilities and data exploration to enable better predictions of soil CO_2 drawdown in both space and time. Novel micro- and macro-scale simulation tools will be combined with advanced modeling, machine learning, and data science approaches, allowing the Center to better forecast the potential impacts of new soil CO_2 drawdown approaches at multiple scales. The *Terraforming Soil* EERC team includes world-class experts in soil carbon cycling, photosynthesis biochemistry, plant/microbial gene engineering and genomics, mineral geochemistry, machine learning, exascale modeling and computing, additive manufacturing, and *in situ* isotope-based characterization. Throughout the research program, the Center will bridge cutting-edge analytical and computational studies with a commitment to engage with community stakeholders, exploring the technical, social, and economic implications of engineered soil CO_2 drawdown. The Center will emphasize diverse training opportunities for students and early career scientists and amplify equity and inclusion throughout the research pipeline.

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