Center for Nanoscale Controls on Geologic CO_2 (NCGC)
EFRC Director: Donald J. DePaolo
Lead Institution: Lawrence Berkeley National Laboratory
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Mission Statement*: To enhance the performance and predictability of subsurface storage systems by understanding the molecular and nanoscale origins of CO_2 trapping processes, and developing computational tools to translate to larger-scale systems.*

The vision for the Center is to understand, predict, and enhance the performance of underground CO_2 storage systems. Specific goals are to produce (1) a next-generation understanding of the nanoscale-to-mesoscale chemical-mechanical behavior of shale - a critical material for a low-carbon energy future, (2) quantitative models for the efficiency of reservoir capillary trapping and its effect on solution and mineral trapping, (3) methods to predict mineralogical trapping, and (4) theory, experimental data, and computational tools to allow nanoscale effects to be translated to mesoscale and continuum scale model equations and parameters.

The NCGC consists of a team of highly qualified investigators with expertise in, and access to, the most advanced analytical and computing facilities available for furthering fundamental knowledge of the geochemical aspects of geologic carbon storage, in particular the chemistry of mineral-fluid interfaces and fluid-fluid interfaces that control the physics of fluid flow and chemical reactions. Experimental investigations will transition from simplified analogue materials to more realistic geologic materials. Newly developed characterization and experimental approaches will be integrated with mesoscale chemical-mechanical-hydrologic modeling and simulation to achieve a transformational predictive capability for stratigraphic- and reservoir CO_2 trapping efficiency and reliability.

Scientific gaps that the Center will address are:

1. The origin and evolution of wetting properties of complex, reactive fluids in contact with common minerals encountered in carbon storage
2. Reactivity between fluids and minerals in nanoporous to macroporous rocks
3. Long term-evolution of capillary-trapped CO_2
4. The response of fractured shale to intrusion of CO_2-containing mixed fluids
5. Theory and computational tools that allow the large scale and long-timescale evolution of fluid-rock systems to be simulated such that they reflect the nanoscale and mesoscale properties of geological materials at far-from equilibrium conditions.

The research of the NCGC is divided into three Thrust Areas that address (1) the sealing effectiveness of fractured shales, (2) reservoir processes that control secondary trapping (capillary, dissolution and mineral trapping) and (3) developing the computational tools and insight necessary to model mesoscale couplings and material properties and dynamics. Systems of study will include well-characterized natural rock and mineral samples, and synthetic materials fabricated by established methods and methods to be developed. A key aspect of our approach is to bring multiple characterization methods, and diverse complementary expertise, to bear on the same experiments, and to integrate modeling and simulation with experiments. The Center will leverage the characterization and computational facilities at LBNL (Advanced Light Source, Molecular Foundry, National Energy Research Scientific Computing Center), ORNL (Spallation Neutron Source, High Flux Isotope Reactor, Center for Nanomaterials Science) and other synchrotron facilities (Advanced Photon Source at Argonne Laboratory, Stanford Synchrotron Radiation Laboratory, and the National Synchrotron Light Source at Brookhaven Lab).

Stratigraphic Trapping by Fractured Shale: Thrust Area 1 aims to provide an understanding of the resilience of seals to CO_2 leakage, i.e.: "Is flow of brine-CO_2 mixtures along fractures a self-enhancing or a self-limiting phenomenon?" The answer to this question is challenging, because brine-CO_2 flow through fractures induces processes that promote fracture opening (mineral dissolution) but, also, processes that promote fracture closing or clogging (mineral precipitation, dissolution of asperities, alterations of fracture mechanics, generation of colloids). These processes are challenging to examine, because they involve couplings between different phenomena (surface chemistry, rock mechanics, multiphase flow, molecular diffusion) at multiple scales (nanometers to millimeters).

Reservoir Trapping Processes: Thrust Area 2 aims to provide a better understanding of the fundamental scientific questions that constrain the most uncertain components of reservoir trapping; the role of residual and mineral trapping, their corresponding rates & efficiencies, and their long term evolution in heterogeneous subsurface systems.

Modeling Approaches for the Mesoscale Challenge: Thrust Area 3 aims to build on the progress made in NCGC to address the mesoscale challenge from the DOE BES Basic Research Needs *report From Quanta to the Continuum: Opportunities for Mesoscale Science.* This Thrust is organized into three broader topics on 1) Mesoscale Reaction Rates: Upscaling Reaction Rates from Molecular to Pore Scale, 2) Mesoscale Fractures: Modeling Fracture Networks, and 3) Mesoscale Reactive Transport: Theoretical and Computational Approaches for Upscaling to the Mesoscale.

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