Multi-scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)
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***Mission Statement**: To synthesize geomaterials with repeatable hierarchical heterogeneity and develop an understanding of transport and interfacial properties of fluids confined within these materials.*

Successful operations of energy recovery and storage, sensor technologies, membranes for air and water purification, and catalytic processes require a fundamental understanding of the interactions of fluids at solid interfaces. There is considerable evidence that the known laws of adsorption, reaction, phase transitions, flow and mechanical strength are affected by the presence of fluids confined in porous geomaterials with nanometer-sized pores.

To accomplish transformational changes in energy science, MUSE will 1) develop a fundamental understanding of confinement and surface interactions in geomaterials on fluid phase behavior, reactivity, and multiphase flow properties; 2) examine the impact of mineralogy and material heterogeneity on chemo-mechanical properties; 3) determine *in-operando* cross-scale structural and microstructural material properties with fluids in confinement; and 4) develop validated multiscale and multi-physics models of mechanics, phase behavior, and flow that capture the observed chemo-morphological coupling.

MUSE is organized into four functional *Research Thrust Areas*: (1) Materials Architecture and Characterization, (2) Property Measurements, (3) Dynamic Characterization, and (4) Multiscale Multiphysics Modeling, and five, cross-cutting scientific areas as highlighted in Figure 1. Novel geo-architected materials developed in Thrust 1 are used as substrates for determining properties of multi-phase fluids in heterogeneous confined architectures in Thrust 2, and for dynamic *in-operando* determination of material and fluid properties in Thrust 3. These measurements are informing the development of *experimentally-validated*, *atomistically-informed* modeling tools and frameworks in Thrust 4.

The functional thrusts interact with members across the center to address scientific themes and technical challenges as summarized in Figure 1. Hierarchical nanostructured geomaterials with increasing levels of complexity are being created and characterized. Experiments with similarly–ordered, naturally occurring materials such as shales will also be performed for comparison. Phase behavior, flow and mechanical properties measurements will demonstrate chemo-mechanical interactions. These new phase transition measurements in architected geomaterials at realistic conditions provide confirmation of modeling findings. In-operando observation of such phenomena will generate enhanced understanding of how confinement and surface interactions are affecting these fluid properties.

The Dynamic Characterization focus area will develop *in situ (in-operando)* observation methods at system conditions. X-ray and neutron radiation provided by Basic Energy Sciences (BES) facilities allows the research team to probe the structure and dynamics of matter spanning from the molecular to the macro length scales. Detailed nonreactive and reactive molecular dynamics (MD) modeling, enhanced by first principles quantum mechanics calculations, will be applied to improve fundamental understandings of, 1) phase behaviors of multicomponent fluids confined in nanometer size pores, 2) heterogeneous adsorption of fluid molecules on the heterogeneous surfaces of organic and inorganic materials, and 3) diffusion of fluid molecules within nanopores, and 4) reaction-induced mechanical deformations of nanostructures.

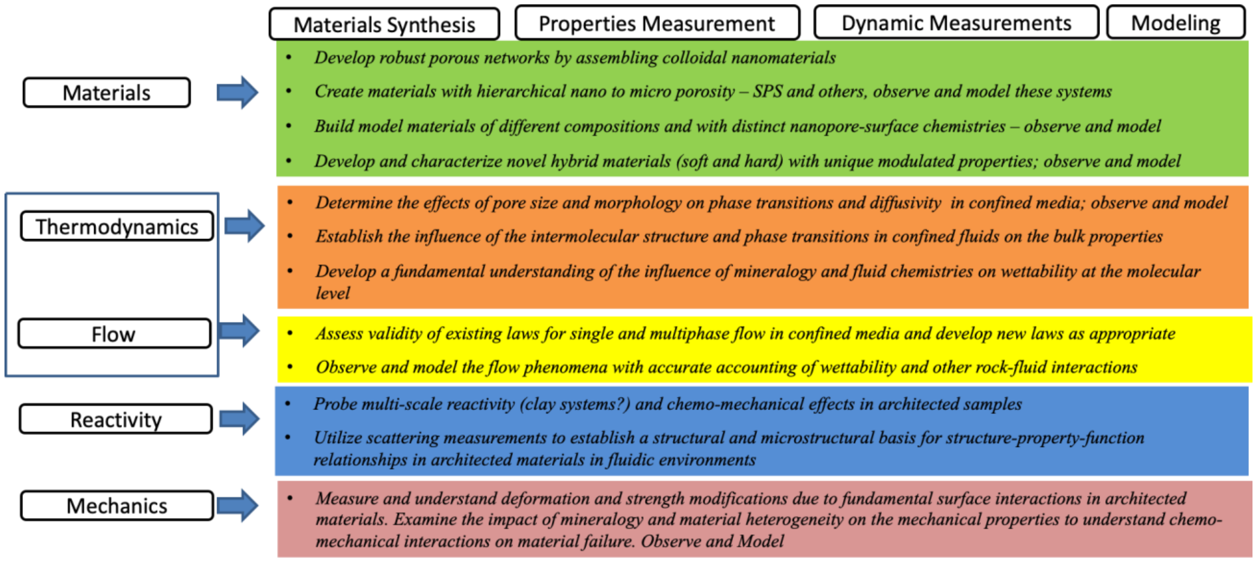

Figure 1: The four functional and scientific thrust areas of MUSE highlighting the major cross-cutting technical challenges that are being addressed.

The Center is generating new data and creating new models on phase transitions, flow characteristics, and multiphase properties in confined geomaterials. MUSE brings together a multi-disciplinary team to establish a multi-scale scientific basis for advancing energy technologies that are of critical importance to the current and future world energy security and environmental sustainability.

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