Multi-scale Fluid-Solid Interactions in Architected and Natural Materials (MUSE)
EFRC Director: Milind Deo
Lead Institution: University of Utah
Class: 2018 – 2024

Mission Statement*: To synthesize geo-inspired materials with repeatable hierarchical heterogeneity and develop an understanding of transport and interfacial properties of fluids confined within these materials.*

Today, energy recovery from the subsurface accounts for more than 80% of the global energy use according to the U. S. Department of Energy, Quadrennial Technology Review. More than 50 billion cubic meters of fresh water are consumed annually for energy production which is unsustainable. With this pressing need for next-generation technologies for a sustainable energy future, the central MUSE research mission of developing a fundamental knowledge of fluid behavior at complex solid interfaces is now as relevant as ever. Interactions of fluids at solid interfaces are key to understanding the thermodynamic, transport, mechanical, and electronic properties of fluids and materials in applications spanning energy storage and production, basic separations, catalysis and carbon capture. There is considerable evidence that the known laws of adsorption, reaction, phase transitions, and flow do not hold for fluids confined in porous materials at the nanometer scale. Thus, new or modified laws must be created based on sound experimental measurements to improve the predictive capability of fundamental models at multiple scales.

MUSE brings together a multi-disciplinary team to address these very challenges by establishing 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. The defining objective of the MUSE EFRC is to address key scientific knowledge gaps on the origins of anomalous flow, thermodynamic, reactivity, and mechanical behaviors of confined fluids in architected materials. Some of the most important challenges include the design of geo-inspired architected materials with precisely defined heterogeneity, detailed insights on the dynamic evolution of siliceous interfaces, the effect of pore and interfacial chemical controls on single and multi-phase flow and nanomechanics, a detailed knowledge of fluid phase behavior in confinement, and bridging measurement and computational scales to probe complex fluid interactions in nanoscale environments.

MUSE is organized into five distinct but highly interrelated research thrusts: (1) *Material Synthesis:* Develop robust geo-inspired architected materials with predictable, hierarchical porosity and surface chemistries; (2) *Properties Measurement:* Measure and understand anomalous thermodynamic, flow, reactivity and mechanical behaviors of confined fluids in hierarchical porous materials; (3) *Dynamic Measurements:* Elucidate the dynamic evolution of chemical structure and pore morphology of solid-fluid interfaces in geo-inspired materials using advanced national core facilities; (4) *Nano-Mechanics:* Probe anomalous deformation, chemo-mechanical coupling and material failure mechanisms due to surface interactions and heterogeneity; and (5) *Modeling and Simulation:* Create validated, atomistically-informed molecular dynamic simulations of materials and fluids at realistic conditions.

Figure 1 shows how these five thrusts are centered around exploring the origins of anomalous thermodynamics, flow, reactivity and mechanical behaviors arising from fluids confined in architected materials through the themes of *interface design*, *thermodynamics in confinement*, *reactivity and mechanics*, and *flow in confinement*. The thrusts and research themes allow rich collaboration between team members, as shown in Figure 2, by the example of ten recent experiments.

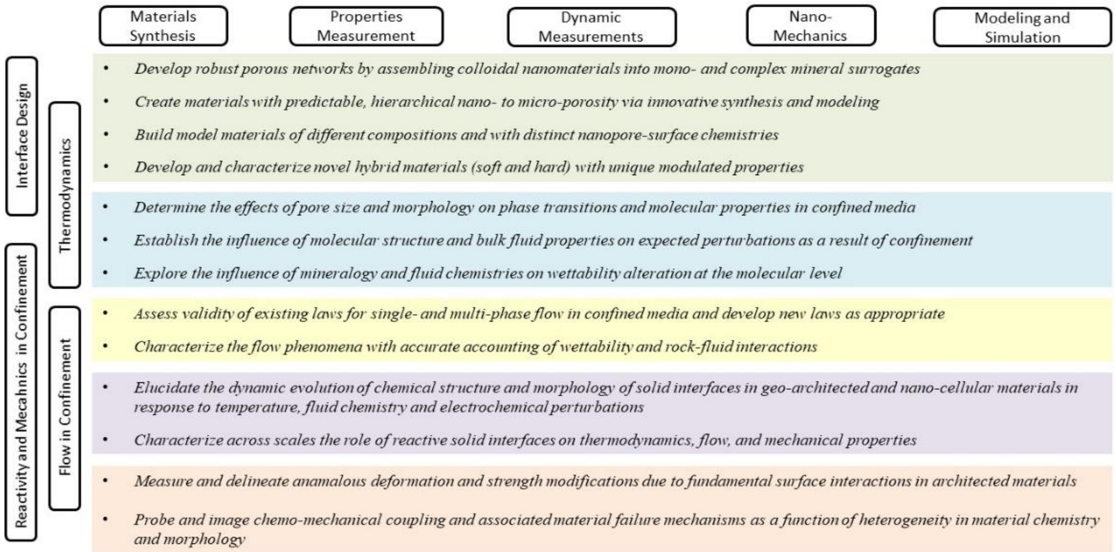

Figure 1. Design, Observations, Modeling and Simulations of Fluids in Architected Geo-Inspired Materials

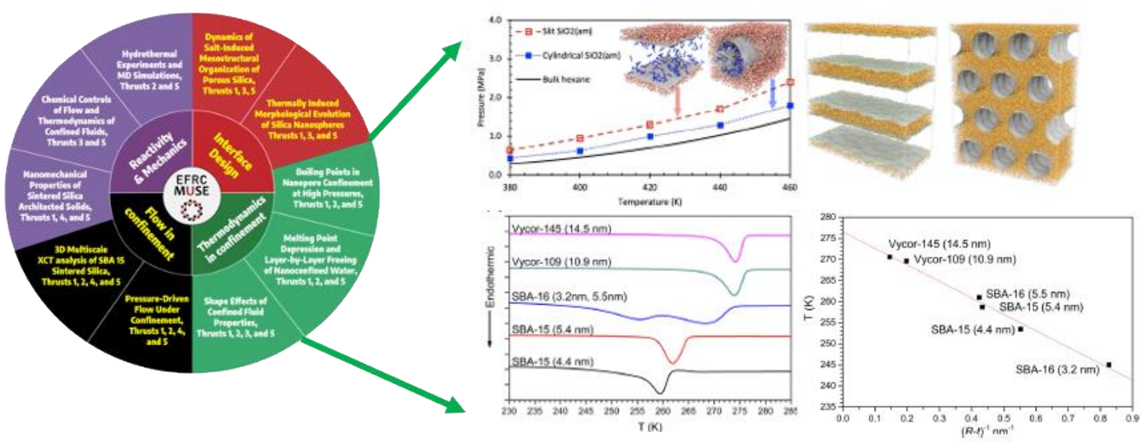

Figure 2. Experiments and Modeling Efforts span different thrusts, allowing rich collaborations.

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