Heterogeneous Functional Materials for Energy Systems (HeteroFoaM)
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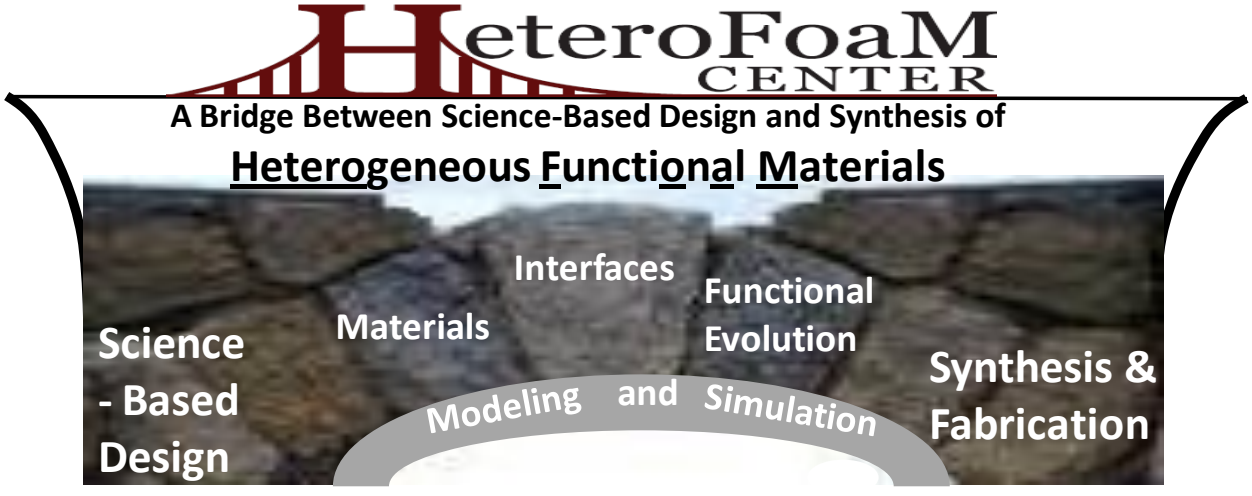
Lead Institution: University of South Carolina

***Mission Statement*:** *To create control science to build a bridge between synthesis and modeling by understanding, designing, and synthesizing heterogeneous functional materials from the atomistic to nano-scale to macro-scale for energy storage and conversion systems such as fuel cells, batteries, supercapacitors, electrolyzers, and solid membranes.*

Material systems consist of hetero-materials arranged in hierarchical architectures (from nano to macro) that significantly facilitate functional performance such as charge and mass transfer along surfaces and across interfaces for chemical and energy transformation processes. Examples include composite mixed-conductors, nano- or micro-structured heterogeneous materials, porous electrodes, nano-structured interfaces and heterostructures, and many other combinations that typically serve as the heart of devices such as fuel cells, electrolyzers, batteries, photovoltaics, catalytic fuel processing devices, and functional membranes and coatings. The functional behavior of these materials occurs at multiple scales of time and length.

For heterogeneous functional materials (left), the local morphology is a critical element of the material conception and design, and the material is not defined until the synthesis process is selected. **A diagram of our technical approach to these challenges appears in the schematic below.** The left hand side of the chart focuses on how to design the materials (including modeling of properties, performance, synthesis, and processing) and the right hand side of the chart focuses on how the heterogeneous functional systems are made. The backbone of our philosophy is to create a science bridge of relationships (the center of the chart) between how these special heterogeneous materials are made and how they work. Creation of the science bridge needed to do that is the responsibility of our teams of experts, which are focused in three areas, bulk materials design; surface, morphology, and structure design; and evolution of properties and morphology.



Functional materials interact with each other and with the applied electrical, chemical, thermal and mechanical fields applied to them. In that sense, they create material systems.

The special purview of the HeteroFoaM Center is exploitation of multi-scale geometry and arrangements of functional heterogeneous constituents to create material systems with a remarkable range of properties and functionality not bounded by the characteristics of the constituents. Insulating and conducting materials can be mixed together, for example, to create energy storage devices (capacitors) with a capacity increase of six orders of magnitude depending on the material system design, as we have shown. We have also demonstrated that the surfaces, interfaces, and particle sizes in porous electrodes for fuel cells can be designed to reduce energy losses during direct conversion of fuel to electricity by more than twelve orders of magnitude. Other examples are found in over 100 archival papers and 6 patent disclosures filed to date by the HeteroFoaM Team (c.f. **www.HeteroFoaM.com**).

The primary goal of this program is to build a predictive science bridge between how we design Heterogeneous Functional Materials (HeteroFoaMs) with multi-scale models and how we make them work in a prescriptive way. Only the beginning foundations of that bridge are present. We must build from both ends. We must use the breakthroughs in computer-driven additive (and other) synthesis methods to make the best materials we can conceive of, and use the best models we can develop to construct a science foundation for understanding those materials to inspire and support the advancement of new creative concepts. That same foundation must also predict the evolution of properties and performance that often controls implementation. And we must create materials design tools for HeteroFoaMs that enable creative, knowledge-based design for prescribed functionality without the expense and time lost by Edisonian methods. The Center structure of this program is essential to make this happen. We cannot build the bridge without the support of a strong integration of the science of materials, surfaces/interfaces, and property and morphology evolution. The present approach fully embraces the role of geometry at the nano-level. We require that field equations be developed for all aspects of the representations of functional behavior, so that computer-driven representations of multi-physics behavior at the local level can be used to design the nano-structure, specifically and precisely, as well as to eventually drive the synthesis processes. This is a major departure from homogeneous domain and chemical rate models that do not capture this critical micro-structure design element of heterogeneous materials. The present approach also recognizes that advances in synthesis and fabrication have brought us to the threshold of controlling local morphology over multiple scales. The HeteroFoaM Center will capture and exploit that new opportunity.

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