Center for Hierarchical Waste Form Materials (CHWM)
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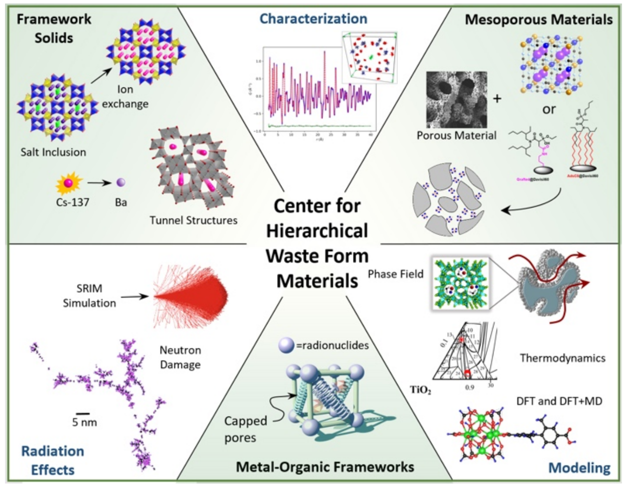
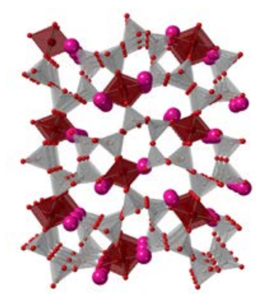
Lead Institution: University of South Carolina
Class: 2016 – 2024

Mission Statement*: To develop the chemical understanding and hierarchical structure motifs needed to create materials for effectively immobilizing nuclear waste species in persistent architectures.*



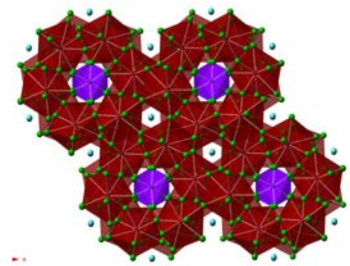
The Center for Hierarchical Waste Form Materials (CHWM) is organized as an integrated, multi-disciplinary team to develop the fundamental science from which advanced waste forms for extreme and dynamic conditions can emerge. A simple and practical definition of a hierarchical structure is that it contains a small-scale structural motif within a larger-scale structure or framework. Conceptually, our hierarchical structures consist of porous structures, either repeating (crystallographically ordered) or non-repeating (disordered), whose cavities are occupied by crystalline or non-crystalline fillers. Examples of materials in this work include crystalline salt inclusion materials (SIMs), metal-organic frameworks (MOFs), porous silica (including Prussian-blue and silver salt functionalized versions), and hollandite mineral structures with molecular tunnels. The CHWM will apply the unique understanding and predictive capabilities developed over the previous four years to make the new discoveries and advances needed to design waste forms with superior stability and performance across extremes in time and environment. The synthesis of such hierarchical structures will be achieved by exploiting previously underutilized or unrealized chemistries.

Hierarchical materials can be tailored from the molecular/crystal lattice through higher scales, offering opportunities to immobilize specific radionuclides in an optimized matrix. Accomplishing such goals requires a fundamental understanding sufficient for effective design of hierarchical materials with tailored properties. Such hierarchical materials can conceivably isolate targeted radionuclides, such as the transuranic elements plutonium, neptunium and americium, more effectively by tolerating higher waste atom content together with lower treatment cost and more rapid processing. Through advances in integrated experiment and modeling, the CHWM, during its first four years, made significant discoveries across a spectrum of hierarchical materials that may provide the foundational science from which researchers can design, manipulate, and ultimately control such materials functionality.



Structure of a new plutonium containing waste form: $Cs_2PuSi_6O_{15}$, Pu (cyan) Si (grey) O (red) Cs (purple).

Novel waste forms are likely to have a transformative impact in reducing the environmental and financial costs of remediation for specific classes of waste. These include the by-products and secondary waste streams that are a result of inefficiencies in current parent processes (e.g., volatile species, poorly retained elements.) and also smaller volume wastes that do not warrant the resources to develop industrially-scalable processes. In addition, there are wastes that are troublesome for known technologies (e.g., those with low solubilities, limited chemical stability.). Fortunately, recent technological advances in materials synthesis, computational modeling, and advanced characterization now provide tools with which to efficiently pursue innovative waste form development that was previously not possible or prohibitively costly. Hierarchical materials are one of the most promising classes of materials that have the potential to complete the suite of technical approaches that will provide for cost-effective stewardship of the nation's processed nuclear waste.



Structure of $Na_3AlPu_6F_{30}$ composed of a $Pu_6F_{30}^{6-}$ framework (red) MF_6 (purple), F^- (green) Na^+ (blue), exhibiting high waste atom content.

The development of new classes of materials to meet current and future Environmental Management challenges that lie beyond the capability of conventional waste forms requires a fundamental understanding of their synthesis, stability, and the transport phenomena occurring within them. Those advances can only be achieved through collaborative efforts among integrated teams such as those present in the CHWM, applying and developing cutting edge materials science. The CHWM is uniquely positioned for this task, benefitting from our established synthetic techniques integrated with the means for structural and compositional modifications, characterization and property measurements, and advanced theory and modeling across multiple length scales. This successful core team, now with the addition of international leaders in radiation effects in materials, will enable advances in the fundamental understanding of novel hierarchical material systems, ultimately leading to structural motifs that can effectively immobilize select nuclear waste species in persistent architectures.

The CHWM will target three research directions to achieve new waste forms: 1. Model, synthesize, and demonstrate the stability of transuranic-containing hierarchical materials; 2. develop direct and indirect synthetic routes for element specific structure motifs; and 3. understand transport in multi-scale porous and hierarchical materials

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