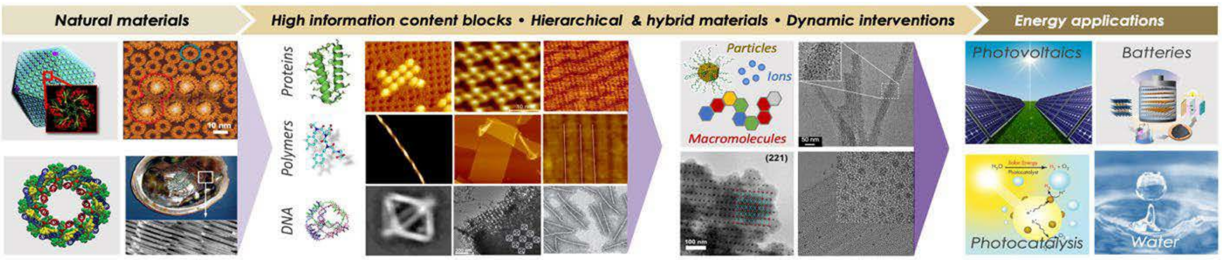
**The Center for the Science of Synthesis Across Scales (CSSAS)**
**EFRC Director: François Baneyx**
**Lead Institution: University of Washington**
**Class: 2018 – 2026**

***Mission Statement****: To harness the complex functionality of hierarchical materials by mastering the design of high-information-content macromolecular building blocks that predictively self-assemble into responsive, reconfigurable, self-healing materials, and direct the formation and organization of inorganic components for complex energy functions.*

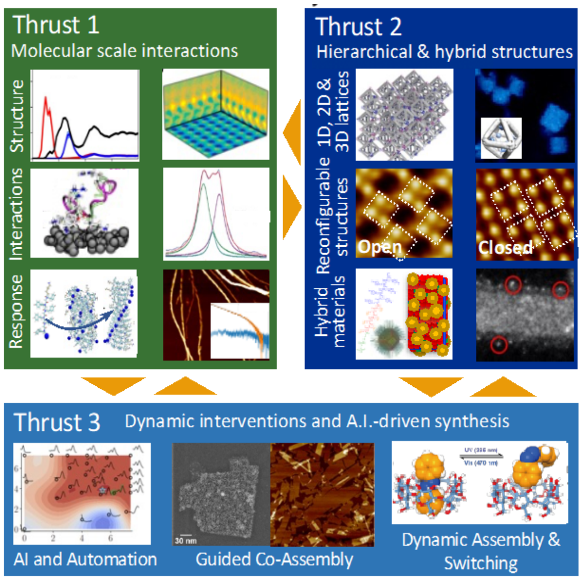



CSSAS: Predictive synthesis of hierarchical and hybrid materials to enable complex energy functions.

Hierarchical materials offer game-changing opportunities for energy technologies because they enable complex interconnected functions ranging from control of charge and mass transport, to dissipative response to external stimuli and the precise localization of sequential and parallel reactions. Nowhere is this more evident than in nature where hierarchical materials perform the stunning range of functions that has made life possible. While there have been many success stories in the quest to synthesize biomimetic and bioinspired materials with outstanding structure and function, efforts have not scratched the surface of what is possible because they have been driven by intuition and serendipity rather than by a deep predictive understanding of the fundamental rules underpinning hierarchical materials synthesis. We have created CSSAS to realize a shared vision: mastering the design of high-information-content macromolecular building blocks that predictively self-assemble into hierarchical materials. Currently, four major scientific gaps (SGs) stand between us and that vision:

1. While we have significantly grown the understanding of how building block sequence and chemistry translate into the molecular interactions and assembly dynamics by which order emerges (**SG1**), there are major opportunities to expand this knowledge.
2. While we have succeeded in connecting atomistic descriptions of intermolecular interactions with coarse grained (CG) models of building blocks to bridge the time and length scales required for predicting assembly outcomes of peptides and polymers (**SG2**), we cannot yet fully account for the crucial role of inorganic interfaces, solution conditions, and kinetics.
3. Although we understand many of the principles that underpin macromolecular assembly and inorganic morphogenesis by assembled scaffolds, we are still building an understanding of how the interplay of solvent, electrolytes, disparate building blocks, and dynamic processing conditions control energy landscapes across which assembly proceeds (**SG3**).
4. Finally, our ability to predict metastable states on the pathway to the final ordered state, or to encode a balance of forces that will, by design, create multi-well potentials for out-of-equilibrium switching in response to external stimuli (**SG4**) remains in its infancy.

With a highly synergistic team of internationally recognized thought-leaders from the University of Washington (lead institution), Pacific Northwest National Laboratory, the University of Chicago, the University of Tennessee Knoxville, the University of California San Diego, Columbia University, and North Carolina State University, CSSAS will fill these knowledge gaps by tackling three research goals:




CSSAS's thrusts integrate building block synthesis, *in situ* characterization, simulations, and AI to control order, hierarchy, and hybrid states of matter.

**1.** Determine the molecular-scale distribution and response of sidechains, solvent, and ions in the interfacial region of approaching building blocks, and atomic and nanoscale inorganic components targeted for assembly or directed nucleation. Understand how these distributions and responses give rise to the resulting interaction potentials that orchestrate materials formation at different scales.

**2.** Realize 2D and 3D hierarchical and hybrid materials by understanding how the interplay of interactions between disparate blocks, surfaces, solvent, and electrolytes determined in RG1 defines the energy landscapes across which hierarchy develops and inorganic nucleation proceeds.

**3.** Achieve adaptive control of synthetic outcomes and access non-equilibrium and metastable states of matter by integrating the tools of data science with *in situ* characterization and simulations, and by using external fields and localized changes in solution chemistry.

Our hypothesis-driven research starts by creating a set of systematically variable building blocks that span the scale of complexity – from large proteins to atomically- precise inorganic clusters. We accomplish the first goal by combining molecular-scale *in situ* observations with a hierarchy of simulation techniques that describe interactions and response dynamics. Our plan accomplishes the second goal by exploring the frontier of integration and hierarchical assembly of building blocks, while extending observations and simulations to length and timescales where hierarchy comes into full bloom. Finally, we address the third goal by exploiting the richness of *in situ* data and the predictive capacity of molecularly-informed coarse graining to harness the power of data-driven machine learning and AI-driven synthesis, where the full potential of real-time datasets is enlisted through data analytics applied to responsive building blocks. In doing so CSSAS will bridge the key knowledge gaps in the field biomolecular materials and create a lasting scientific foundation that advances BES's priority research directions, grand challenges and transformative opportunities.

| **The Center for the Science of Synthesis Across Scales (CSSAS)** | |
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