Mesoscale Priority Research Direction

Theory & Computation for Self-Assembly

Opportunity

Scientific challenge: Understand the principles that give rise to emergent phenomena in directed- and self-assembly of materials with desired composition and structure. Scalable synthesis of materials using solution-phase processes involves many stage, or levels of description, including: quantum mechanics of electrons, molecular interactions, bulk phases such as solutions and interfaces (e.g., electrolytes and colloidal surfaces), small particles created by nucleation and growth of particles, and interactions of colloidal particles that are influenced by fluid flow. There are common concepts at individual stages such as transport (mass, energy, heat), flow, diffusion, transformation (chemical reactivity, phase, collective order), equilibria, and collective response.

Current state of understanding: Currently we do not know how to bridge these concepts across stages and the individual stages are treated as isolated or coupled only through parameterization.

Meso Challenge

What makes it meso?

The focus is on the connection between individual stages and the resulting emergent phenomena. There are opportunities to develop an understanding of the fundamental principles that connect stages, expanding techniques, language and descriptors.

Approach

What can be done to address the challenge?

Characterize the “mesoscale transitions” through the stages along the route to scalable synthesis.

What new computational tools and techniques need to be developed to address the challenge?

Efficient tools to couple statistical mechanics to electronic structure to extend these methods to understanding phenomena in complex solutions and at interfaces

Development of particle based flow and diffusion models that are consistent with detailed Newtonian based dynamics as well as grid based models of transport and flow that correctly predict behavior across different scales

Development of system reduction, sampling, filtering and projection techniques to bridge stages and consistently treat important processes

Impact

How will pursuit of the research direction, including the meso opportunity, impact the scientific challenge?

Detailed understanding leading to control of “mesoscale transitions” will enable the design of self-assembly processes to create new materials precisely, rapidly, inexpensively, efficiently and in meaningful quantities.

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Contact: Chris Mundy, Greg Schenter, Shawn Kathmann, Bruce Palmer and Bob Weber (Pacific Northwest National Lab)