Mesoscale Priority Research Direction

Designing Solution Self-Assembly Routes to Meso-Scale Materials

Opportunity

Discover and verify underpinning relationships between hierarchical structure, composition, and functional properties associated with materials derived through solution templating approaches.

Develop cost effective and green protocols for scalable materials processing.

Meso Challenge

Structure-directing molecular templates (surfactant, foldamer, block co-polymer) organize into hierarchical building blocks that self assemble into ever more complex structured materials over larger distances.

Modeling studies predict self-assembled structures (phase diagram) based upon the template and solution precursors.

Approach

Manipulate intra- and inter-molecular forces that act during solution self-assembly through rational design of molecular templates and selection/manipulation of solvent properties (pH, dielectric constant, ceramic precursor,…)

Invoke *in situ* characterization approaches to identify key formation mechanisms in these near energy neutral processes.

Impact

Project deliverable will be a general set of structural organization principles (a tool box) to drive hierarchical structural evolution across scales.

References:

Y Matsushita, K Hayashida, T Dotera, and A Takano, “Kaleidoscopic morphologies from ABC star-shaped terpolymers”, J. Phys. Condens. Matter 23 (2011) 284111.

N. González-Segredo and P. V. Coveney, “Self-assembly of the gyroid cubic mesophase: Lattice-Boltzmann simulations”, *Europhys. Lett.*, 65 (6), p. 795 (2004).

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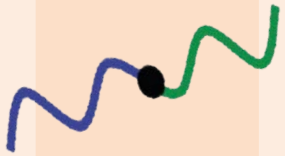
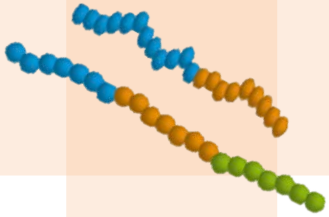
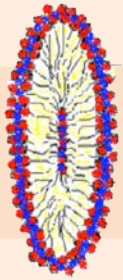
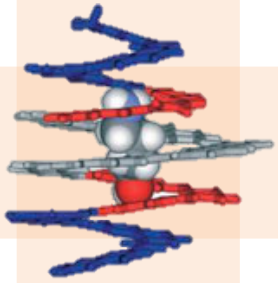
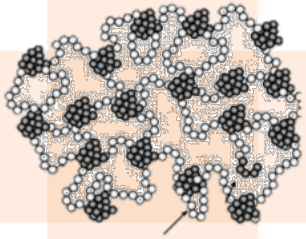
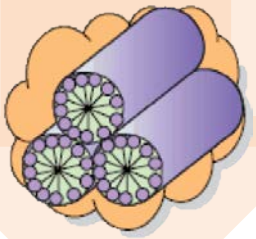
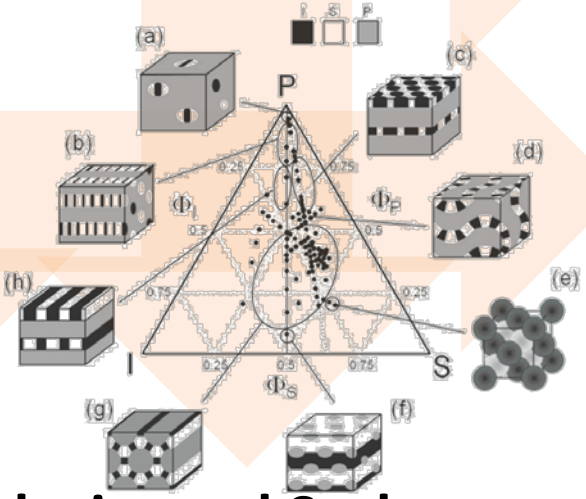
Integration of Theory and Experiment to Understand Parameters that Drive Solution Self-Assembly

Hierarchical Construction

	Surfactant Molecule	Foldamer Ionic + covalent	Di-, Tri-Block Co-polymer
Molecular Template			
Fundamental Building Unit			
Assembled Structure			

Modeling Challenges

- Molecule Design and Synthesis Protocols
- Molecular Forces that Manipulate Assembly
- Organization Principles that Drive Complex Structures

Increasing Level of Complexity and Scale