Mesoscale Priority Research Direction

(Gas Transport in Mesoporous Inorganic-Organic Hybrids)

Opportunity

Designed combination of the unique properties of both "hard" inorganic nanocrystals and "soft" polymeric materials into hybrid structures of both basic and applied interest. Hybrid materials can be designed with 1-D, 2-D, or 3-D mesoscale structure, and enable crafting of unique gaseous transport paths using tools of directed assembly. Phenomena include CO_2 capture, H_2 storage, and gas separations.

Approach

Hybrid assembly of nanocrystals and polymers encompasses various architectures, including alternating laminae, polymer-infiltrated nanocrystal superlattices, and nanocrystal channels in polymers. These provide a unique variety of geometries to study how morphology impacts gas transport/separation. New in-situ calorimetry tools enable quantification of binding enthalpies; new in-situ optical methods allow diffusion tracking during transport.

Meso Challenge

Currently, woefully little is known about the optimum architectures and bonding motifs desired for efficient gas transport/storage:

- What are the ideal pore sizes and connectivities needed across all length scales?
- What (glassy or periodic) assemblies of gas-binding motifs are optimum for these problems?

Impact

New polymer-nanocrystal hybrid materials with controlled nano- to mesoscale architectures represents a new form of matter that would enable unprecedented control over selective gas storage, separations, and transport. The broad range of gas-solubilities in polymers when combined with gas-specific binding modalities in nanocrystals enables targeted end-use design not possible today.

References: BES Workshop Report: Basic Research Needs for Carbon Capture: Beyond 2020

Contact: Jeff Urban (LBNL)