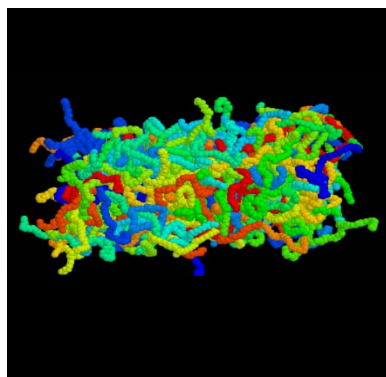


Molecular Simulations

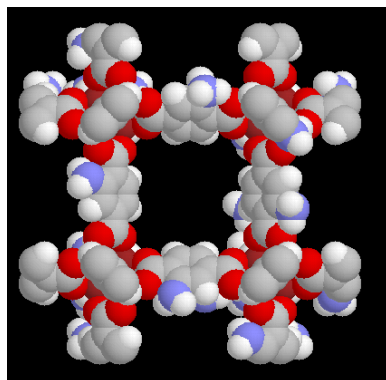
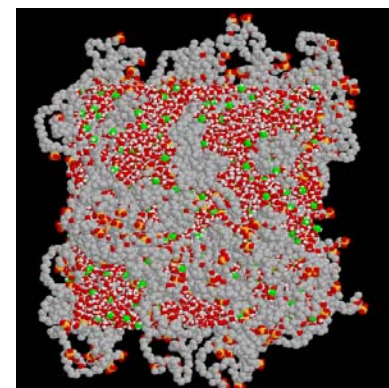
Deliver Structure/Property Relationships



polymeric materials

polymers at equilibrium and under flow (PE, PET)

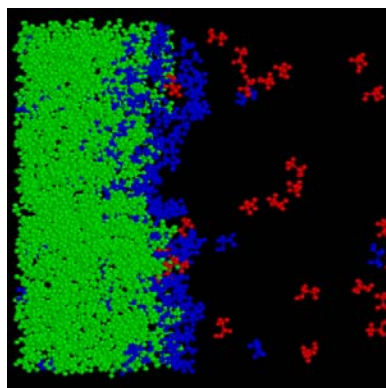
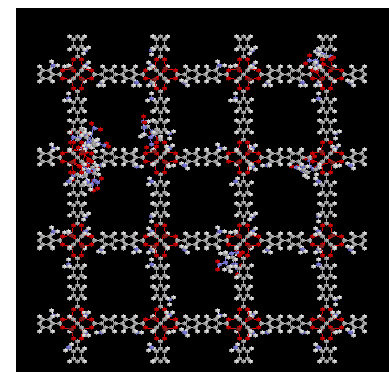
ion and molecular transport in polymer membranes



nanoporous materials

gas storage and separations in nanostructured adsorbents

Sensing of RDX, TATP and other explosives in MOFs



interfacial systems

near critical vapor-liquid interface structure

fuel cell electrode/electrolyte interface, catalyst layer

