579a Self-Assembled Morphologies of Monotethered Poss Nanocubes from Computer Simulation

Xi Zhang, Elaine R. Chan, Lin C. Ho, and Sharon C. Glotzer

Self-assembly of functionalized nano building blocks is a promising strategy for “bottom-up” materials design. Recent experiments have demonstrated that the self-assembly of tethered polyhedral oligomeric silsesquioxane (POSS) “nanocubes” can be utilized to synthesize novel materials with highly ordered, complex nanostructures. We have developed a simplified model and performed molecular simulations for organic-mono-tethered POSS nanocubes to investigate how the novel architecture of these hybrid organic/inorganic building blocks can be manipulated to achieve useful structures via self-assembly. We systematically explore the parameters that control the assembly process and the resulting equilibrium structures, including concentration, temperature, tethered cube topology, and solvent conditions. We report conventional lamellar and cylindrical structures that are typically found in block copolymer and surfactant systems, but with interesting modifications of the phase diagram caused by the bulkiness and cubic geometry of the POSS nanocubes.