Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

**Simulation of Organic-tethered Silesquioxane Nanocube Assemblies** XI ZHANG, Department of Materials Science and Engineering, University of Michigan, ELAINE CHAN, LIN HO, Department of Chemical Engineering, University of Michigan, SHARON GLOTZER, Department of Chemical Engineering and Materials Science and Engineering, University of Michigan — Polyhedral oligomeric silesquioxane (POSS) based materials are a class of organic/inorganic hybrid nanomaterials with superior properties. Recent experiments have demonstrated that the self-assembly of tethered POSS "nanocubes" is a promising route to synthesis novel materials with highly ordered and sophisticated nanostructures. We have developed a coarse-grained model and performed molecular simulations for organic-tethered POSS molecules, to complement the ongoing experimental studies and advance our understanding of the fundamental assembly principles. We systematically explore the parameters that control the assembly process and the resulting equilibrium structures, including concentration, temperature, tethered POSS molecule 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. Our computational methodology not only provides insight to the assembly process of existing structures, but also facilitates the rational design of novel POSS based organic/inorganic hybrid materials.

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Date submitted: 01 Dec 2004 Electronic form version 1.4