

## **579b Structure and Properties of Alkane-Functionalized POSS Hybrid Materials**

*Jinhua Zhou and John Kieffer*

The self-assembly behavior of POSS-based nano-structured hybrid materials was investigated, using molecular dynamics simulations based on a reactive force field. POSS molecules were functionalized with hydrocarbon chains of different lengths, which can be considered as simple models for chainlike organic groups. By functionalizing only one of the cube corners, and by terminating the remaining corners with hydrogen, a certain amphiphilic character was introduced into the structural building block, which gave rise to a variety of assembly behaviors. Equilibrium structures and dynamics of these composite systems were analyzed as a function of temperature. In particular, this analysis was geared towards identifying the mechanical reinforcement effect that POSS has on the polymeric matrix. The effect of POSS/polymer ratio on the final materials performance is well understood through this study.