

Multiscale Simulation of Organic-Inorganic Polyhedral Nano-Materials

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Because of their unique organic/inorganic composition, polyhedral oligomeric silsesquioxane molecules (POSS) are considered promising building blocks for synthesizing novel hybrid nano-composites. A number of applications are being proposed for these materials. Recent experiments show that mono-tethered POSS monomers self-assemble into higher-order structures, e.g. micelles in solution and lamellae in the melt state. The molecular mechanisms that govern the assembly of these structures, as well as those that determine their thermodynamic properties, are, at present, not adequately understood.

All-atom molecular simulation is the ideal tool for investigating the thermodynamic properties of nano-particulate systems composed of only a few thousands atoms. Because of computer power limitations, it is necessary to employ coarse-grained (CG) models to investigate the self-assembly of systems that contain hundreds of POSS monomers. It is now widely recognized that in order to obtain reliable theoretical predictions, it is essential to derive the CG models consistently from all-atom simulation results.

Motivated by the availability of interesting experimental observations, as well as by the limits of state-of-the-art simulation procedures, we developed a CG model of mono-tethered POSS molecules consisting of one short alkane chain attached to one corner of the silsesquioxane cage. The monomers were dissolved in normal hexane. All-atom molecular dynamics simulations were performed at 300 and 400 K. From the simulation results (site-site radial distribution functions, valence bonds and angles, and dihedral angles), we implemented a CG model in which the hexane solvent is treated implicitly. We used the CG model to study the self-assembly of the POSS monomers, and to predict the properties of the hexane-POSS system as a function of composition. In this presentation, we will discuss the coarse-graining procedure and compare our simulation results to available experimental data.