309f Development of Coarse-Grained Force Fields for Polymer-Tethered Silsesquioxanes

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Nanostructured polyhedral oligomeric silsesquioxane (POSS) molecules have a unique hybrid organic/inorganic composition that renders them attractive candidates for synthesizing novel materials with new or enhanced properties. Experiments and simulations demonstrate that POSS molecules functionalized with a single polymer tether self-assemble into higher-order structures, e.g., micelles in solution and lamellae in the melt state. Motivated by these observations, we developed a coarse-grained model of monotethered POSS in solution. Distribution functions (e.g., bond length, valence angle, and radial distribution functions) obtained from all-atom molecular dynamics simulations were used to parameterize the coarse-grained interaction potentials in the model. The results from simulations using the coarse-grained model were compared to data from all-atom simulations of monotethered POSS and available experimental data to validate the accuracy of the interaction potentials and assess the utility of our approach. Here we will discuss our efforts to develop these coarse-grained force fields. Our goal is to apply them in future simulations to study tethered POSS self-assembly at the mesoscale.