Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Phases of functionalized polymer-inorganic composites in solution studied via molecular dynamics[1] JOSHUA ANDERSON, RASTKO SKNEPNEK, ALEX TRAVESSET, Iowa State University and Ames Laboratory — Using self-assembling polymer systems to direct the formation of inorganic crystals, polymer-inorganic composite materials offer new opportunities in materials design. Molecular dynamics simulations allow for an exploration of the wide range of phases in these systems. Amphiphilic ABA triblocks with A hydrophilic, B hydrophobic, and functional ends with an affinity to inorganic particles are modeled to capture the minimum physics needed to describe polymer-inorganc systems currently being investigated by experiment. A number of phases are formed in solution as the attraction strength between the inorganic particles and the affinity of those particles to the functional end beads of the polymer are varied. Some of the phases found include hexagonal, square columnar, lamellar, perforated lamellar, and the gyroid. Polymer stretching plays an important role in each of the phases found, with a characteristic multi-modal behavior in the polymer end to end distance distribution. In the gyroid phase, for instance, the peaks correspond to the polymers being in two preferred conformations: v-shaped with a small end to end distance and fully extended in a line with the largest possible end to end distance. At high interaction strengths, inorganic particles are found to crystallize and form plate-like structures.

[1]This work is supported by DOE-BES through the Ames lab under contract no. DE-AC02-07CH11358

Joshua Anderson
Iowa State University and Ames Laboratory

Date submitted: 17 Nov 2008 Electronic form version 1.4