Phases of functionalized polymer-inorganic composites in solution studied via molecular dynamics\textsuperscript{1} JOSHUA ANDERSON, RASTKO SKNEPE-NEK, 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-inorganic 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.

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