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Molecular Dynamics Simulations of Cubic Phases in Pluronics Systems and Their Role in Templating Nanoparticles[1] JOSHUA ANDERSON, ALEX TRAVESSET, CHRIS LORENZ, Iowa State University — We discuss molecular dynamics simulations aimed at predicting phase diagrams in Pluronic systems. Crystalline phases with cubic symmetries are particularly challenging to simulate. A general method that is able to obtain these phases is presented. As an example, we show our results for a system of ABA triblock polymers where each hydrophilic A block contains 10 beads and the hydrophobic block B contains 7 beads. These values match the ratio of PEO to PPO in Pluronic F127. Numerous simulation runs are carried out with differing initial conditions, which consistently produce textbook bcc and fcc lattices of micelles along with two other distorted bcc lattices. We find that the formation of a lattice is sensitive to the system's preparation and depends mainly on the kinetic temperature and equilibration time. Examination of the distorted lattices shows that they are related to the finite size of the simulation box. We conclude with some discussion on using these crystals as a template for nanoparticles or biomineralization.

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