Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Controlling the Self-Assembly of ABCBA Pentablock Copolymer Gels in Water Solution by the Hydrophobic Effect[1] JOSHUA ANDERSON, ALEX TRAVESSET, Iowa State University — We characterize the phases of a system of non-ionic pentablock copolymers with an ABCBA structure in water solution, where the A and C blocks are hydrophobic and the B blocks are hydrophilic. Coarse-grained simulations are performed using molecular dynamics with the solvent modeled implicitly, and the interaction potential includes a parameter that controls the quality of the solvent. In a good solvent, spherical micelles form and assemble into a swollen gel. We examine the aggregation number, gyration radii, micelle superstructures and percolation at various concentrations for this phase. As the B blocks become less hydrophilic, which occurs for increasing temperature, the micelles move close to one another and expel water. There is a gradual phase transition from spherical micelles to cylindrical worm-like micelles. We model the further expelling of water by increasing the concentration of polymers in the simulation and find that a lamellar phase forms. We compare our simulations with experimental results on recently synthesized modified Pluronic systems.

[1]Work funded by the Department of Energy through the Ames Laboratory under contract W-7405-ENG-82.

Joshua Anderson
Iowa State University

Date submitted: 03 Dec 2005 Electronic form version 1.4