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Brownian Dynamics Simulation of Multiblock Copolymers in Selective Solvents¹ YONGSHENG LIU, HUIFEN NIE, RAMA BANSIL, Boston University — In this talk we will present results of Brownian dynamics simulation on triblock (ABA, BAB), penta-block (ABABA, BABAB) and hepta-blocks (ABABABABA or BABABAB) in selective solvents for the A blocks to study the effect of varying the number of blocks, solvent selectivity, concentration and temperature on the association behavior of multi-blocks. Structure factors and percolation analysis of the clusters was used to characterize the resulting structure. At a concentration of 20% we obtained micellar clusters arranged in a BCC lattice, in agreement with scattering experiments. The ratio of number of loops to bridges decreases as the number of blocks in the copolymer increases, as does the polydispersity. The size of the clusters was larger when the outermost block was in the poor solvent condition. Our results imply that as the number of blocks increases it is favorable to form bridges instead of loops. This leads to a larger number of smaller clusters with more bridges.

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