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Multiscale Simulations of Pluronic Micelles GRANT SMITH, DMITRY BEDROV, University of Utah — Poly(ethylene oxide)/poly(propylene oxide)/poly(ethylene oxide) triblock copolymers (Pluronics®) self-assemble in aqueous solution to form (roughly) spherical micelles. With increasing polymer concentration and temperature, these nanoscale micellar polymer building blocks begin to interact resulting in formation of particle gels and micellar crystalline phases. The structure of Pluronic solutions has been probed extensively via small angle neutron scattering (SANS). Interpretation of SANS measurements relies on models of various degrees of sophistication for both the single micelle form factor F(q) and the micelle-micelle structure factor S(q). Information regarding single micelle structure and micelle-micelle interactions gleaned from SANS measurements depends sensitively on the model used. A key assumption in modeling of SANS data for these solutions is that the micelles are perfectly spherical, allowing for representation of the q-dependent scattering intensity as a product of F(q) and S(q). We have carried out multiscale molecular simulation studies of Pluronic micelle solutions in order to better understand the structure of these important nanoscale polymer particles, their interaction in aqueous solution, and the validity of the various models utilized in interpreting SANS measurements. Our simulations reveal that the micelles exhibit significant anisotropic character that strongly influences their interaction and the structure of the micellar solution.

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