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Formation of micelles in homopolymer-copolymer mixtures MARCUS MÜLLER, Institut fur Theoretische Physik, Georg-August Universitat, Gottingen, Germany, ANNA CAVALLO, Institut Charles Sadron, Strasbourg, France, KURT BINDER, Institut fur Physik, WA331, Johannes-Gutenberg Universitat, Mainz, Germany — Using Monte Carlo (MC) simulations of the bond fluctuation model and self-consistent field (SCF) calculations, we study the formation of micelles in a mixture of homopolymers and asymmetric AB-diblock copolymers with composition, $f_A = 1/8$. We work in the semi–grandcanonical ensemble, *i.e.*, we fix the monomer density and incompatibility, $\chi N \simeq 100$, and control the composition of the mixture via the exchange chemical potential, $\delta\mu$ between the copolymer and homopolymer solvent. The MC simulation comprises moves that allow homopolymers to mutate into AB-diblock copolymers and *vice versa*. These moves are very efficient in equilibrating the configurations. We accurately locate the critical micelle concentration, study the micellar size distribution and characterize the shape of the micelles by the tensor of gyration and radial density profiles. The simulation results are *quantitatively* compared to predictions of the SCF theory in the grandcanonical ensemble without adjustable parameter. Only in the limit of high molecular weight the simulation results gradually approach the theoretical predictions. The structure and phase behavior of mixed micelles is investigated by SCF calculations.

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