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Influence of Crowding on Polymer Conformations in Polymer-Nanoparticle Mixtures: Monte Carlo Simulations[1] WEI KANG LIM, ALAN R. DENTON, Department of Physics, North Dakota State University — Within the cytoplasm and nucleoplasm of eukaryotic cells, a complex mixture of macromolecules (biopolymers, such as proteins and RNA) and smaller molecules share a tightly restricted space. In this crowded environment, hard nanoparticles exclude volume to softer biopolymer coils, restricting protein and RNA conformations and folding pathways. At sufficiently high concentrations, nanoparticle crowding also can affect phase stability, inducing aggregation or separation into polymer-rich and polymer-poor phases. Through Monte Carlo simulations, we explore the impact of crowding on polymer conformations and phase behavior in a coarse-grained model of polymer-nanoparticle mixtures. Neglecting polymer self-interactions, we exploit the random-walk geometry of ideal coils to model the polymers as effective ellipsoids whose shapes fluctuate according to the probability distribution of the gyration tensor. Accounting for penetration of polymers by smaller nanoparticles, we calculate the crowding-induced shift in the polymer shape distribution. We compare our results with predictions of a free-volume theory and available experimental data.

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Alan R. Denton
Department of Physics, North Dakota State University

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