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Polymer Crowding and Depletion-Induced Interactions in Polymer-Nanoparticle Mixtures[1] WEI KANG LIM, ALAN DENTON, Dept. of Physics, North Dakota State University — Macromolecules in crowded environments, such as biopolymers (DNA, RNA, proteins) in biological cells or synthetic polymers in nanocomposite materials, adopt conformations that can differ substantially from those in unconfined spaces. In mixtures of nanoparticles and nonadsorbing (free) polymers, depletion of polymers induces effective interactions between the nanoparticles. Depletion-induced interactions in turn affect the structure and thermodynamic phase behavior of polymer-nanoparticle mixtures. Such interactions can drive bulk demixing and may be involved in compartmentalization of macromolecules in the cell nucleus. Within a coarse-grained model of hard-sphere nanoparticles and ellipsoidal polymer, we perform Monte Carlo simulations to compute polymer shape distributions*, depletion-induced pair potentials, and pair distribution functions, and to explore demixing of polymer-nanoparticle mixtures in the protein limit. We compare our results with theoretical predictions and available experimental data.

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