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Polymer Crowding in Confined Polymer-Nanoparticle Mixtures[1]

WYATT J. DAVIS, ALAN R. DENTON, Department of Physics, North Dakota State University — Crowding can influence the conformations and thus functionality of macromolecules in quasi-two-dimensional environments, such as DNA or proteins confined to a cell membrane. We explore such crowding within a model of polymers as penetrable ellipses, whose shapes are governed by the statistics of a 2D random walk. The principal radii of the polymers fluctuate according to probability distributions of the eigenvalues of the gyration tensor. Within this coarse-grained model, we perform Monte Carlo simulations of mixtures of polymers and hard nanodisks, including trial changes in polymer conformation (shape and orientation). Penetration of polymers by nanodisks is incorporated with a free energy cost predicted by polymer field theory. Over ranges of size ratio and nanodisk density, we analyze the influence of crowding on polymer shape by computing eigenvalue distributions, mean radius of gyration, and mean asphericity of the polymer. We compare results with predictions of free-volume theory and with corresponding results in three dimensions*. Our approach may help to interpret recent (and motivate future) experimental studies of biopolymers interacting with cell membranes, with relevance for drug delivery and gene therapy.

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