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Modelling Soft Colloidal Particles in Crowded Environments

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Soft colloidal particles have inspired fundamental and practical interest recently for their rich and tunable properties, both on the single-particle level and collectively in bulk suspensions. Interdisciplinary research has led to applications in the chemical, biomedical, food, consumer care, and pharmaceutical industries. The simplest example of a soft colloid may be a linear polymer coil, which can be modeled as a deformable particle, whose size and shape respond to confinement. In biological cells, macromolecular crowding in the cytoplasm and nucleoplasm tightly constrains the conformations of biopolymers, such as proteins, DNA, and RNA. By combining Monte Carlo simulations with free-volume theory, we demonstrate that crowding by nanoparticles affects both the sizes and shapes of random-walk polymer coils, with implications for the structure and function of biopolymers.

Another class of soft colloids is comprised of microgels – microscopic porous networks of cross-linked polymers. When dispersed in water, microgels swell in size and can acquire charge through dissociation of counterions. The equilibrium size of a microgel particle is governed by a delicate balance of osmotic pressures, which can be tuned by varying single-particle properties and externally controlled conditions, such as temperature, pH, ionic strength, and concentration. Because of their tunable size and capacity to encapsulate dye or drug molecules, these soft colloidal particles have practical relevance for biosensing, drug delivery, carbon capture, and filtration. Combining molecular dynamics simulations with Poisson-Boltzmann and Flory theories for a model of elastic, compressible particles, we demonstrate that, with increasing concentration, ionic microgels can deswell due to a redistribution of counterions. In contrast, nonionic microgels respond mainly to steric interparticle forces. We further explore consequences of size polydispersity for the structure, thermodynamic phase behavior, and rheology of microgel suspensions.

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