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Response of Soft Colloids to Crowded Environments

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Soft colloids are microscopic particles that, when dispersed in a solvent, can adjust their size and shape in response to changes in local environment. Typical examples are microgels, made of loosely crosslinked networks of polymer chains, that respond to changes in concentration by deswelling and faceting. Practical applications of microgels include drug delivery, chemical and biosensors, and photonic crystals. Within a coarse-grained model of elastic particles that interact via a hertzian pair potential and swell according to the Flory-Rehner theory of polymer networks, we explore the response of microgels to two fundamental types of crowding. First, we investigate the influence of nanoparticle crowding on microgel swelling by extending the Flory-Rehner theory from binary to ternary mixtures and adapting polymer field theory to model the entropic cost of nanoparticle penetration. Second, we examine the impact of particle compressibility on liquid-solid phase transitions in microgel suspensions. In both studies, we perform Monte Carlo simulations to model equilibrium properties of single particles and bulk suspensions [1]. Novel trial moves include random changes in microgel size and shape and in nanoparticle concentration. Our results demonstrate that particle softness and penetrability can profoundly affect single-particle and bulk properties of soft colloids in crowded environments. In particular, we find that addition of nanoparticles can significantly modify microgel swelling and pair structure and that particle compressibility tends to suppress crystallization. Our conclusions have broad relevance for interpreting experiments on soft matter and guiding the design of smart, responsive materials.
[1] M. Urich and A. R. Denton, Soft Matter 12, 9086 (2016).
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