

The physics of dendrimer-like DNAs: simulation and experiment

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Dendrimers are synthetic macromolecules, characterized by a highly branched and regular internal architecture. Recently, dendrimer-like DNAs (DL-DNAs) were synthesized via enzymatic ligation of Y-shaped DNA building blocks. These charged dendrimers represent a novel macromolecular aggregate, which holds high promise in bringing about targeted self-assembly of soft-matter systems in the bulk and at interfaces.

We present a joint simulation-experimental study of these novel macromolecules. Based on a bead-spring model for the DL-DNAs (of varying generation numbers) we perform large-scale simulations to determine the equilibrium properties and the conformational characteristics of these macromolecules. The obtained results are compared to light scattering experiments [1]. The simulation data provide a broad variety of additional information about the internal molecular structure of DL-DNAs by varying the generation number and the salinity of the solvent. In an effort to simulate concentrated solutions of DL-DNAs, we extract an effective, coarse-grained potential, based on Widom's particle-insertion method. With this potential at hand, we investigate the bulk behaviour of DL-DNAs. These findings are essential to investigate if these macromolecules are a viable candidate for the experimental realization of cluster crystals with multiple site occupancy in the bulk [2].

The study of these charged dendrimer systems represents a relevant field of research in the area of soft matter due to their potential role for various interdisciplinary applications, ranging from molecular cages for drug delivery to the development of dendrimer- and dendron-based ultra-thin films in the area of nanotechnology [3].

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