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Multi-scale modeling of DNA-dendrimers in electrolyte solutions

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We have studied a novel class of macromolecules, the so-called DNA-based dendrimers. They have recently been synthesized from the enzymatic ligation of Y-shaped DNA building blocks. In order to describe such dendrimers of various generations we have performed MD simulations employing two independent models: a bead-spring model and the oxDNA model. The former one models each base-pair of double-stranded DNA as a single charged monomer and the interactions and interaction parameters in the model have been carefully chosen to mimic the structural properties of a single DNA chain. The system was immersed in water, which was modeled as a uniform dielectric and counterions were introduced in the system to preserve electroneutrality. Furthermore, we added salt, treating it explicitly, in order to investigate its influence on conformational characteristics of a single dendrimer molecule. On the other hand, the oxDNA model allowed us to take a closer look into the DNA structure, treating DNA as a string of rigid nucleotides which interact through potentials that depend on the position and orientation of the nucleotides. Equilibrium properties of a single dendrimer-like DNA molecule from the first to the sixth generations obtained from these two models have been investigated and the obtained simulation results have also been compared to the experiments. We have found an excellent agreement between the theoretical and experimental results, which has encouraged us to use the introduced models for theoretical analysis of novel self-assembled structures, such as cluster crystals in the bulk. The study of these charged dendrimer-systems is an important field of research in the area of soft matter due to their potential role in various interdisciplinary applications, ranging from molecular cages and carriers for drug and gene delivery in a living organism to the development of dendrimer-based ultra-thin films in the area of nanotechnology.