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Structural and conformational properties of bottlebrush polyelectrolyte solutions

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Bottlebrush polyelectrolyte solutions have great significance in biology, e.g. aggrecan is a major proteoglycan in articular cartilage, and exhibit great potential in various applications (e.g., drug delivery), however, there is little theoretical understanding of their behavior compared to their linear polyelectrolyte solutions. We made a comparative investigation of linear and bottlebrush polyelectrolyte solutions with the use of molecular dynamics simulations. In particular, we utilize a previously developed polyelectrolyte coarse-grained bead-spring model that includes an explicit treatment of the charged species and solvent to probe the conformational properties of polyelectrolyte linear and bottlebrush polyelectrolytes at different polymer and salt concentrations. Specifically, we calculate the polymer hydrodynamic radius and radius of gyration along with its eigenvalues. Moreover, we calculate the structure factor and determine the scaling of the location of the polyelectrolyte peak with polymer concentration. Overall, our findings are in agreement with small angle neutron scattering (SANS), dynamic light scattering (DLS) and osmotic pressure measurements made on model systems. These complementary experimental and computational techniques probe different length and time scales providing a comprehensive picture of the essential properties of bottlebrush polyelectrolytes.