Abstract Submitted
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Structure of a bottlebrush melt JAROSLAW PATUREJ, Univ of NC - Chapel Hill, USA and Institute of Physics, Univ of Szczecin, Szczecin, Poland, SERGEI SHEIKO, Univ of NC - Chapel Hill, USA, SERGEY PANYUKOV, P. N. Lebedev Physics Institute, Russian Academy of Sciences, Moscow, Russia, MICHAEL RUBINSTEIN, Univ of NC - Chapel Hill, USA — A bottlebrush polymer is a branched macromolecule composed of a linear chain (backbone) with side chains densely tethered to it. High grafting density of side chains gives rise to various unique structural properties, such as highly extended conformations of their backbones and tunable character of their stiffness and rheological properties with degree of polymerization of the side chains. We conducted coarse-grained molecular dynamics simulations to determine how the number of Kuhn segments in a bottlebrush backbone L and in the side chains N affect size, stiffness, and structure of these molecules. We found that the size (root-mean-squared radius of gyration and end-to-end distance) and persistence length of bottlebrushes in a melt state scales as $N^{1/2}$.

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