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From Comb-like Polymers to Bottle-Brushes[1] HEYI LIANG, ZHEN CAO, ANDREY DOBRYNIN, University of Akron, SERGEI SHEIKO, University of North Carolina at Chapel Hill — We use a combination of the coarse-grained molecular dynamics simulations and scaling analysis to study conformations of bottle-brushes and comb-like polymers in a melt. Our analysis show that bottle-brushes and comb-like polymers can be in four different conformation regimes depending on the number of monomers between grafted side chains and side chain degree of polymerization. In loosely-grafted comb regime (LC) the degree of polymerization between side chains is longer than side chain degree of polymerization, such that the side chains belonging to the same macromolecule do not overlap. Crossover to a new densely-grafted comb regime (DC) takes place when side chains begin to overlap reducing interpenetration of side chains belonging to different macromolecules. In these two regimes both side-chains and backbone behave as unperturbed linear chains with the effective Kuhn length of the backbone being close to that of linear chain. Further decrease spacer degree of polymerization results in crossover to loosely-grafted bottle-brush regime (LB). In this regime, the bottle-brush backbone is stretched while the side-chains still maintain ideal chain conformation. Finally, for even shorter spacer between grafted side chains, which corresponds to densely-grafted bottle-brush regime (DB), the backbone adopts a fully extended chain conformation, and side-chains begin to stretch to maintain a constant monomer density.

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