

Abstract Submitted
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Molecular Dynamics Simulations of Grafted Layers of Bottle-Brush Polyelectrolytes¹ DANIEL RUSSANO, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Department of Physics, University of Connecticut — Using molecular dynamics simulations, we study the effect of the brush grafting density and degree of polymerization of the side chains on conformations of brush layers made of charged bottle-brush macromolecules. The thickness of the brush layer first decreases with increasing brush grafting density; then, it saturates and remains constant in the wide interval of the brush grafting densities. The brush layers consisting of the bottle-brush macromolecules with longer side chains have a larger layer thickness. The elongation of the side chains of the bottle-brush macromolecules decreases with increasing brush grafting density. This contraction of the side chains is due to counterion condensation inside the volume occupied by bottle-brushes. Our simulations showed that counterion condensation is a multiscale process reflecting different symmetries of the bottle-brush layer.

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