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Molecular Dynamics Simulation of Polyelectrolyte Brushes: From Hemispherical Micelles to Maze-like Aggregates. JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, Institute of Materials Science, University of Connecticut — We present results of the molecular dynamics simulations of the effects of solvent quality, strength of the electrostatic interactions, chain degree of polymerization and grafting density on the conformations of planar polyelectrolyte brushes in salt-free solutions. The polyelectrolyte brush could form: (1) hemispherical micelle aggregates, (2) vertically oriented cylindrical micelles, (3) maze-like aggregate structures, or (4) thin polymeric layer uniformly covering the substrate. These different brush structures appear as a result of the fine interplay between electrostatic and monomer-monomer attractive interactions. The brush thickness depends nonmonotonically on the value of the Bjerrum length. This nonmonotonic dependence is due to counterion condensing inside the brush.

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