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Interaction between Brush Layers of Bottle-Brush Polyelectrolytes: Molecular Dynamics Simulations[1] DANIEL RUSSANO, Boston University, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — Interactions between tethered layers composed of aggrecan (charged bottle-brush) macromolecules are responsible for the molecular origin of the cartilage biomechanical behavior. To elucidate the role of the electrostatic forces in interaction between bottle-brush layers we have performed molecular dynamics simulations of charged and neutral bottle-brush macromolecules tethered to substrates. In the case of charged bottle-brush layers the disjoining pressure P between two brush layers in salt-free solutions increases with decreasing the distance D between substrates as $P \propto D^{-1.8}$. A stronger dependence of the disjoining pressure P on the surface separation D was observed for neutral bottle-brushes,$P \propto D^{-4.6}$, in the same interval of the disjoining pressures. These scaling laws for dependence of the disjoining pressure P on the distance D are due to bending energy of the bottle-brush macromolecules within compressed brush layers. The weaker distance dependence observed in polyelectrolyte bottle-brushes is due to interaction between counterion clouds surrounding the bottle-brush macromolecules preventing strong brush overlap.

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Jan-Michael Carrillo
University of Connecticut

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