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Molecular dynamics simulations of interactions and friction between bottle-brush layers[1] DANIEL RUSSANO, JAN-MICHAEL CARRILLO, ANDREY DOBRYNIN, University of Connecticut — Experiments on tethered polyelectrolyte bottle-brush-like macromolecules consisting of glycoproteins display fascinatingly low friction properties of biological tissues such as cartilage. To understand the role of the electrostatic interactions in lubricating properties of brush layers we have performed MD simulations of charged and neutral bottle-brush macromolecules tethered to substrates. In the case of charged bottle-brush layers the compression force per unit area F between two brush layers in salt-free solutions increases with decreasing the distance D between substrates as $F \propto D^{-2}$. A stronger dependence of the compression force F on the surface separation D was observed for neutral bottle-brushes, $F \propto D^{-4.7}$, in the same interval of compression forces. This strong dependence of the compression force F on the distance D is due to excluded volume interactions between monomers belonging to two overlapping bottle-brush layers. The weaker dependence observed in polyelectrolyte bottle-brushes is due to interaction between counterion clouds surrounding the bottle-brush layers. The charged bottle-brush layers have lower friction coefficient than neutral layers at the same interval of the compression and shear forces.

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