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Langevin dynamics simulations of PEO brushes in aqueous solutions FANG YIN, DMITRY BEDROV, GRANT SMITH, University of Utah — We have conducted extensive equilibrium and non-equilibrium simulations of poly(ethylene oxide) brushes in aqueous solutions using coarse-grain implicit solvent model. In equilibrium simulation we focused on studying a repulsive force between two brushes as a function of surface coverage and chain length. In the non-equilibrium simulation we attempted to mimic the conditions of the quartz crystal microbalance with dissipation (QCM-D) technique frequently used to analyze the mass change and viscoelasticity of an absorbate. To obtain an understanding of energy dissipation mechanism of PEO brush from a molecular level, we use Langevin dynamics method to study the viscoelasticity of the PEO chains attached on the surface under the oscillation, matching the dissipation shift part measured in QCM-D. We study the effect of frequency and amplitude of the oscillation impacted on the attached surface, grafting density, and grafting pattern (singly-bound and doubly-bound) on both loss tangent and dynamic moduli of PEO brush. Normal mode of PEO brush is also compared with that of PEO solution with equivalent volume fraction.

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