POLYMER SPREADING ON UNIDIRECTIONALLY NANOTEXTURED SURFACES USING MOLECULAR DYNAMICS

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Supplementary material

Figure S1 depicts the potential function interactions that define the molecular dynamics simulations described in this work. The potentials are identified using arrows and numbers that correspond to the equations that describe the potentials, which are similar to validated potentials and parameters used in previous research.

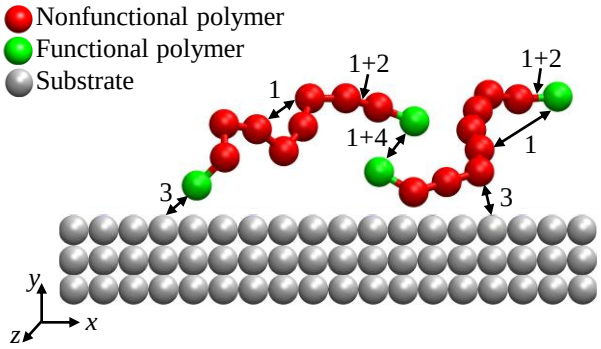

Figure S1. Schematic of energy potential function interactions where numbers refer to the corresponding equations.

A Lennard Jones potential U_{LJ} exists between all polymer beads, given by

$$U_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} - \left(\frac{\sigma}{r_c}\right)^{12} + \left(\frac{\sigma}{r_c}\right)^{6}\right], \quad (1)$$

where r is the distance between two beads, σ = 0.7 nm is the bead diameter, $r_c = 2.5\sigma$ is the cutoff distance within which interactions between neighboring beads are considered, and $\varepsilon = Tk_B$ is the potential well depth, where T = 300 K is the absolute temperature and k_B is the Boltzmann constant. A finitely extensible

nonlinear elastic (FENE) potential U_{FENE} acts as a spring to bond neighboring beads of the same molecule, *i.e.*,

$$U_{FENE}(l) = -\frac{1}{2}kR_0^2 \ln\left[1-\left(\frac{l-l_0}{R_0}\right)^2\right], \tag{2}$$

where l is the bond length, $l_0 = 1.3\sigma$ is the equilibrium bond length, $R_0 = 0.3\sigma$ indicates the maximum extensible range, and $k = 40\varepsilon/\sigma^2$ is the spring constant. The substrate interacts with the polymer via a dispersive van der Waals interaction U_{VDW}, described as

$$U_{VDW}(r) = 2\varepsilon\left[\frac{1}{2}\left(\frac{\sigma}{r}\right)^9 - \frac{3}{2}\left(\frac{\sigma}{r}\right)^3\right]. \tag{3}$$

We also use a short-range exponential potential U_{EXP} to model the attraction of functional end beads to each other, which represents the attraction of functional hydroxyl groups and is given by

$$U_{EXP}(r) = -2\varepsilon \exp\left(-\frac{r-r_c}{d}\right), \tag{4}$$

where $r_c = 1.0\sigma$ is the cutoff distance and $d = 0.3\sigma$ is the decay length.