SUPPORTING INFORMATION:

Anisotropic Three-Particle Interactions Between Spherical Polymer-Grafted Nanoparticles in a Polymer Matrix

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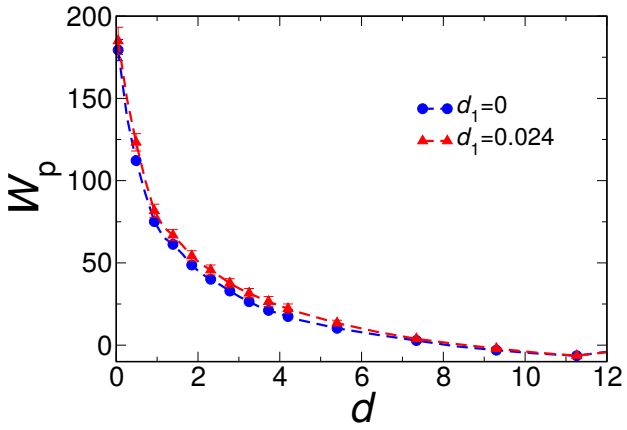

Figure S1: Comparison of the polymer-mediated PMF $W_{\rm p}(d)$ computed with dimer NPs fixed at a separation distance of $d_1 = 0$ apart (as done in all simulations) versus dimers fixed at their most favorable separation distance of $d_1 = 0.024$. The comparison is plotted for the representative NP-polymer system with $L_{\rm g} = 20$, $\Gamma_{\rm g} = 0.4$, and $L_{\rm m} = 40$ along the $\mathbf{x}'_{90^\circ}$.

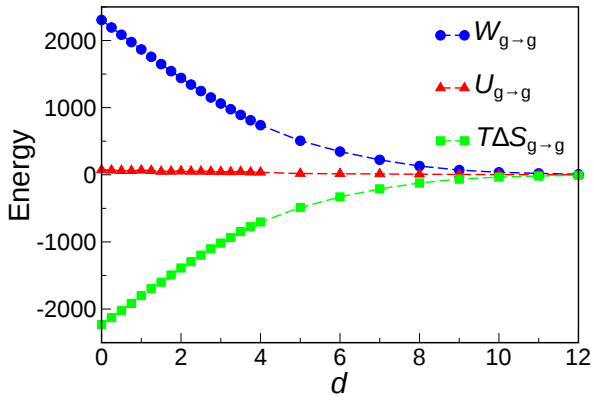

Figure S2: Decomposition of graft-graft repulsion $W_{g\to g}$ into its energetic $U_{g\to g}$ and entropic contributions $T\Delta S_{g\to g}$ as a function of separation distance d. The error bars are not shown as they are all smaller than the size of the symbols. $U_{g\to g}$ was calculated as the ensemble average of the potential energy arising graft-graft interactions computed from MD simulations at various fixed distances d while $T\Delta S(d)$ was calculated from the first law of thermodynamics: $T\Delta S(d) = U(d) - W(d)$

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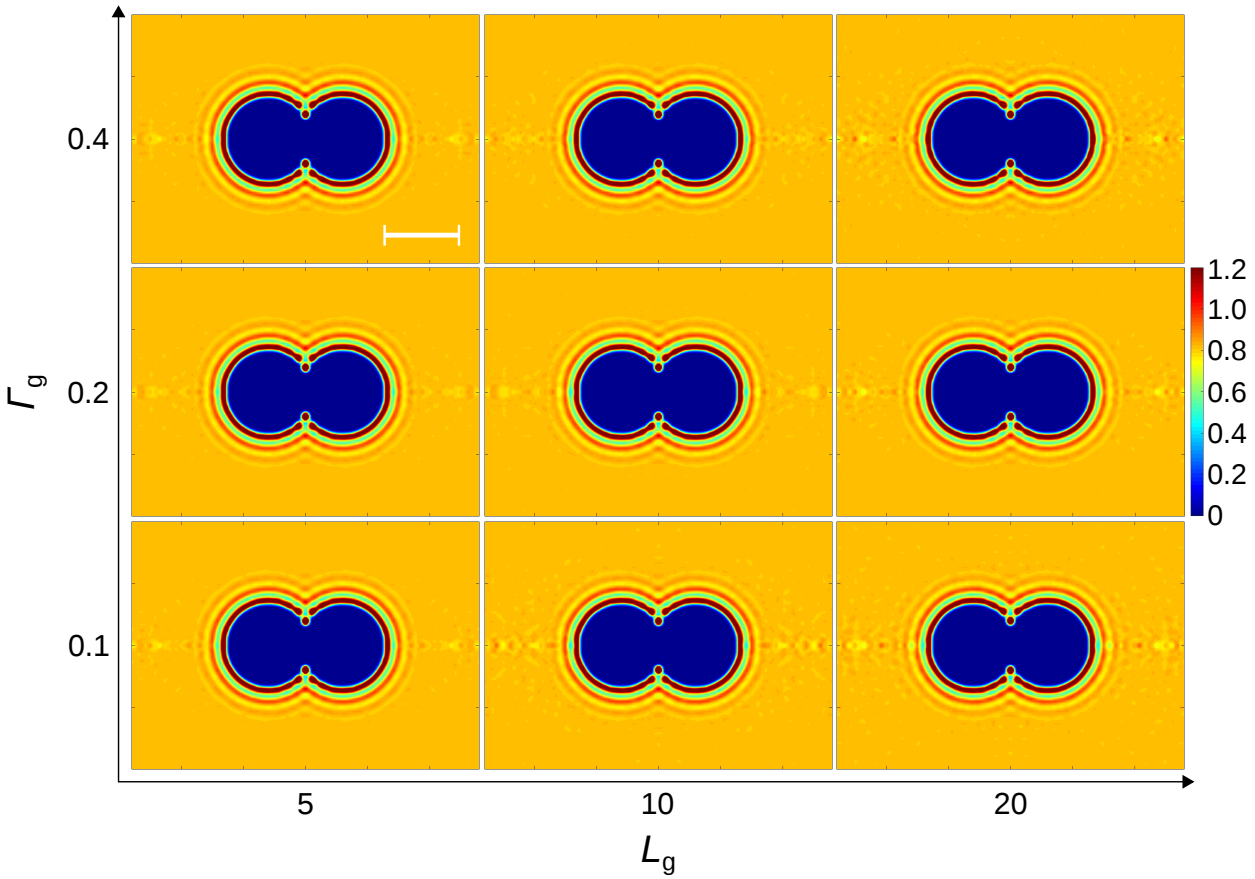

Figure S3: 2D contour maps of the overall monomer density $\rho_{g+m}(x, r)$ corresponding to nine distinct NP-polymer systems differing in graft length (L_g = 5, 10, 20) or grafting density (Γ_g = 0.1, 0.2, 0.4). Color bar denotes the magnitude of this density in units of beads/σ^3. Scale bar denotes the size of the NP core, $D_c = 6$.

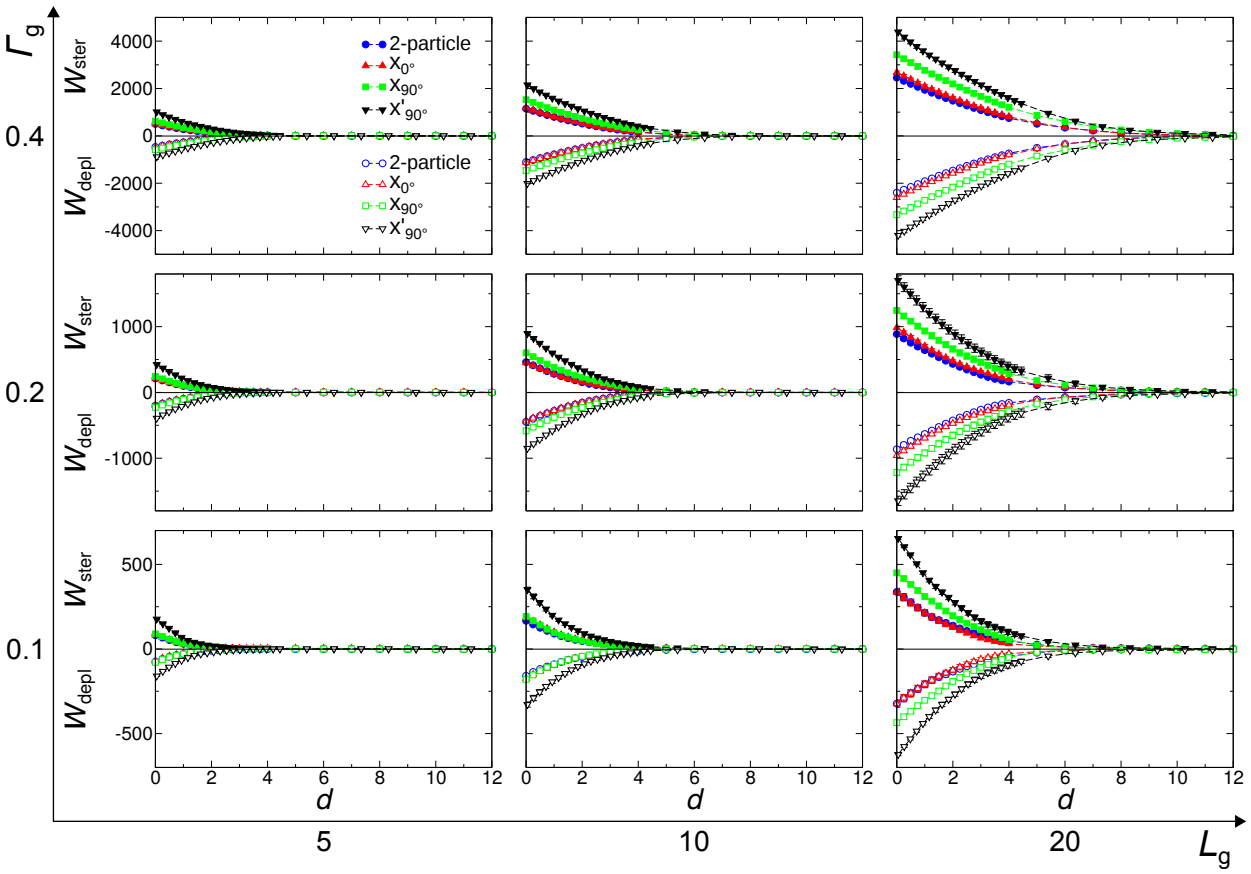

Figure S4: Comparison of the steric repulsion and depletion attraction profiles along 2- and 3-particle reaction coordinates for polymer-grafted NPs of size $D_c = 6$ grafted with polymer chains of different lengths ($L_g = 5$, 10, and 20) and at different grafting densities ($\Gamma_g = 0.1$, 0.2, and 0.4) in a polymer matrix of chain length $L_m = 40$.

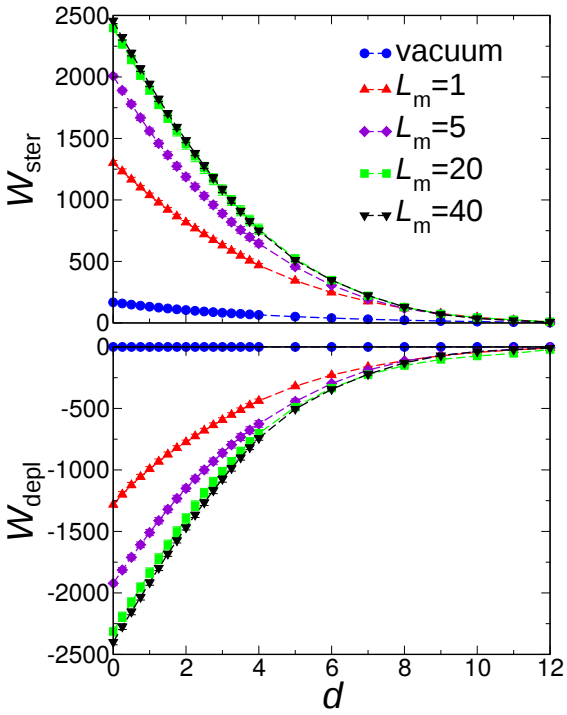

Figure S5: Comparison of 2-particle steric repulsion and depletion attraction profiles for NP cores of size $D_c = 6$ grafted with polymer chains of length $L_g = 20$ interacting across vacuum and across polymer matrices of lengths $L_m = 1$, 5, 20, and 40.

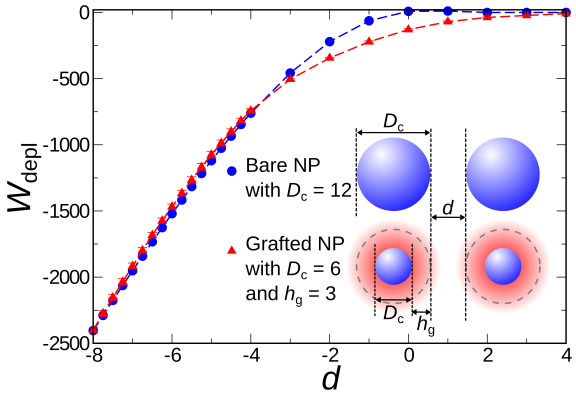

Figure S6: Comparison of depletion attraction computed from simulations of grafted NPs in a polymer matrix (system 1 with NP cores of size $D_c = 6$ but effective span of $D_c + 2h_g = 12$, where h_g is the average height of the polymer brush) against that computed from simulations of bare NPs of size $D_c = 12$ in the same polymer matrix.