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Electronic supplementary information

Hydrogen bonding Induced Protein Adsorption on Polymer Brush: A Monte Carlo

Study

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Figure S1. Variation of the contact number between H monomers and substrate ($N_{\text{H-Substrate}}$) with grafting density (σ) in the case of short grafting chain, i.e., $le_p = 10$. Data are mean ± SD, n = 5. (a)-(c) showing the morphologies of the grafting polymers and the adsorbed proteins.



Figure S2. Morphological snapshots showing two typical adsorption processes of a single protein in the case of short polymer brush with low grafting density ($le_p = 10$ and $\sigma = 0.05$). (a₁)-(a₄) the adsorption process of one protein. (b₁)-(b₄) the adsorption process of the other protein. In order to clearly observe the morphological transition of the protein, the polymer brush is not drawn.



Figure S3. Morphological snapshots showing two typical adsorption processes of a single protein in the case of short polymer brush with high grafting density ($le_p = 10$ and $\sigma = 0.30$). (a₁)-(a₄) the adsorption process of one protein. (b₁)-(b₄) the adsorption process of the other protein.



Figure S4. Variations of H-H contact number between non-bonded nearest neighbor H monomers ($N_{\rm HH}$) with simulation time when the grafting density is $\sigma = 0.30$. The amount of proteins in the simulation box is 5. The grafting chain length is $le_{\rm p} = 10$. (a) and (b) showing the morphologies of the proteins and polymer brushes at corresponding simulation time.



Figure S5. Variation of the contact number between H monomers and substrate ($N_{\text{H-Substrate}}$) with grafting density (σ) in the case of long grafting chain, i.e., $le_p = 25$. Data are mean ± SD, n = 5. (a)-(c) showing the morphologies of the grafting polymers and the adsorbed proteins.



Figure S6. Variations of the mean square radius of gyration of the grafting chains projected onto the surface normal $(\langle S_{\perp}^2 \rangle)$ and the surface plane $(\langle S_{\parallel}^2 \rangle)$ with the hydrophilicity of grafting polymer chains $(-\varepsilon_{PW})$ in the case of $le_{P} = 25$, $\sigma = 0.15$.