# Electronic Supplementary Information

# Photo-responsive Anti-Fouling Polyzwitterionic Brushes: A Mesoscopic Simulation

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**Content**

**Table S1** Repulsive parameters $a_{ij}$ between different beads of TFC film and protein (blue: the polar amino acid; orange: the moderate polar amino acid; red: the hydrophobic amino acid)

| Type $a_{ij}$ | A | Average | B | Average | C | Average | C2 | Average | F | Average |
|---|---|---|---|---|---|---|---|---|---|---|
| ASP | 101.74 | 102.45 | 110.13 | 109.62 | 103.36 | 100.17 | 129.49 | 136.12 | 104.41 | 106.94 |
| GLU | 99.59 | | 108.91 | | 90.89 | | 145.16 | | 107.83 | |
| LYS | 111.97 | | 106.62 | | 98.05 | | 147.68 | | 114.01 | |
| ARG | 101.81 | | 106.84 | | 114.26 | | 123.58 | | 103.02 | |
| SER | 114.80 | | 123.07 | | 119.07 | | 132.18 | | 118.27 | |
| THR | 86.15 | | 97.28 | | 98.69 | | 144.82 | | 111.02 | |
| PRO | 100.97 | | 110.85 | | 98.42 | | 124.38 | | 106.87 | |
| ASN | 99.62 | | 106.83 | | 94.42 | | 138.08 | | 105.19 | |
| GLN | 105.42 | | 116.01 | | 84.41 | | 139.74 | | 91.83 | |
| ALA | 91.61 | 95.09 | 102.27 | 102.22 | 107.12 | 98.17 | 152.79 | 137.87 | 114.57 | 109.32 |
| GLY | 94.25 | | 107.19 | | 105.27 | | 128.20 | | 115.19 | |
| CYS | 77.01 | | 87.08 | | 96.36 | | 134.51 | | 110.71 | |
| HIS | 107.11 | | 109.95 | | 90.19 | | 137.53 | | 96.24 | |
| TYR | 105.48 | | 104.62 | | 91.90 | | 136.34 | | 109.91 | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ILE | 101.92 | 102.72 | 110.88 | 108.53 | 97.00 | 92.71 | 128.93 | 140.84 | 106.92 | 107.09 |
| LEU | 97.21 | | 110.36 | | 93.74 | | 155.11 | | 106.78 | |
| VAL | 110.13 | | 113.98 | | 102.19 | | 146.20 | | 98.78 | |
| PHE | 102.11 | | 106.52 | | 87.88 | | 145.56 | | 108.92 | |
| MET | 94.79 | | 104.81 | | 85.60 | | 142.06 | | 110.44 | |
| TRP | 110.19 | | 104.62 | | 89.86 | | 127.19 | | 110.70 | |

**Table S2 (a)** The dielectric constants of the systems with D = 0.160, R = 0.136, L = 4 / 7

| type / $\varepsilon_r$ | SP-form | MC-form |
|---|---|---|
| $A_{63}B_{10}C_{40}$ | 2.501 | 29.061 |
| $A_{63}B_{10}C_{70}$ | 2.397 | 39.225 |

**Table S2 (b)** The dielectric constants of the systems with D = 0.230, R = 0.068, 0.136, 0.205, L = 4 / 7

| type / $\varepsilon_r$ | SP-form | MC-form |
|---|---|---|
| $A_{68}B_5C_{20}$ | 2.424 | 18.592 |
| $A_{68}B_5C_{35}$ | 2.366 | 26.766 |

| | | |
|---|---|---|
| $A_{63}B_{10}C_{40}$ | 2.349 | 29.013 |
| $A_{63}B_{10}C_{70}$ | 2.277 | 39.218 |
| $A_{58}B_{15}C_{60}$ | 2.297 | 36.324 |
| $A_{58}B_{15}C_{105}$ | 2.223 | 46.801 |

**Table S2 (c)** The dielectric constants of the systems with D = 0.314, R = 0.136, L = 4 / 7

| type / $\varepsilon_r$ | SP-form | MC-form |
|---|---|---|
| $A_{63}B_{10}C_{40}$ | 2.257 | 28.984 |
| $A_{63}B_{10}C_{70}$ | 2.204 | 39.214 |

According to the work of Yang *et al.*[1], the dielectric constants were listed in Table S2. To reflect $\varepsilon_r$ in P(ACN-*r*-BBEM)-*g*-SPMA and BSA systems, there was a reasonable approximation to estimate it according to molecular structure. Namely, $\varepsilon_r$ is related to the number of hydrophobic and hydrophilic beads in the coarse-grained model. The hydrophobic beads are mainly composed of alkanes with $\varepsilon_r$ about 2.0. The hydrophilic beads are soluble in water surrounded by water beads, therefore, $\varepsilon_r$ can be set as 78.0 (dielectric constant of water at the room temperature). Thus, the system $\varepsilon_r$ can be expressed as:

$$\varepsilon_r = \frac{n_{hydrophilic} * 78.0 + n_{hydrophobic} * 2}{n_{hydrophilic} + n_{hydrophobic}}$$

where $n_{hydrophilic}$ means the total number of hydrophilic beads of polymers in the system, and $n_{hydrophobic}$ means the total number of hydrophobic beads of polymers in the system.

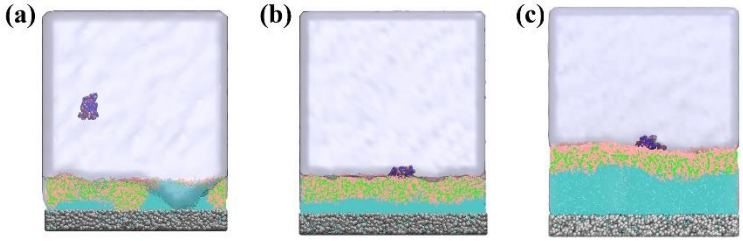


**Fig. S1** Water distribution in the simulation box of $A_{63}B_{10}C_{40}$ systems under *vis* light exposure, with D = 0.160 **(a)**, 0.230 **(b)**, 0.314 **(c)**, respectively.

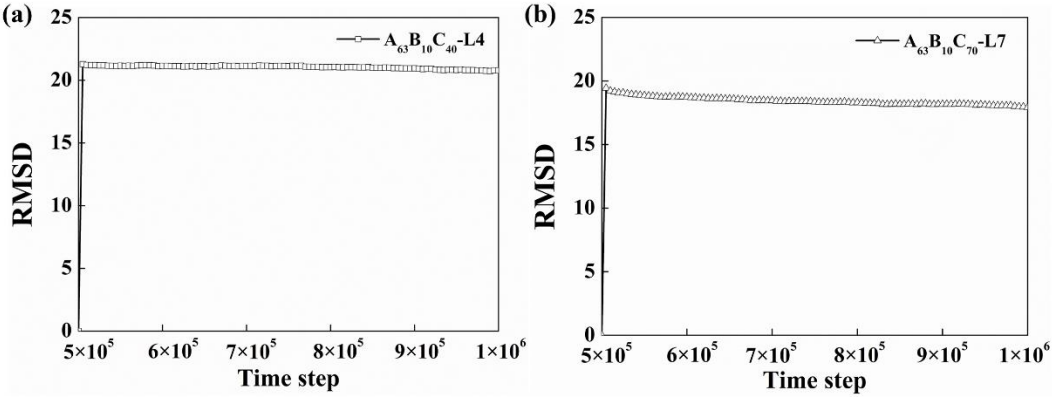


**Fig. S2** RMSD profiles of brushes from *vis* light exposure to UV exposure with D = 0.230, in $A_{63}B_{10}C_{40}$ system **(a)** and $A_{63}B_{10}C_{70}$ system **(b)**.

In Fig. S2, RMSD data of brushes from the SP form to the MC form in system of $A_{63}B_{10}C_{40}$ are shown. As light switches from *vis* to UV, in the first $1\times10^5$ steps, the RMSD curve rises sharply, namely, the conformation of brushes changes obviously. Under *vis* exposure, the chain with SP form is in a shrank state and the size is smaller; when

experiencing UV radiation, the chain swells apparently and the size increases obviously. Those results confirm the reasonability of the $R_g^2$ data of system $A_{63}B_{10}C_{40}$, as well as explain the thickening of the selective layer. Namely, the swelling hydrophilic selective layer can supply a strong mechanical push to remove the foulant. Fig. S2b displays the RMSD data of $A_{63}B_{10}C_{70}$ system. Although the RMSD curve also rises sharply in the first $1\times10^5$ steps, the equilibrium value is slightly less than that of $A_{63}B_{10}C_{40}$ system. That is, the conformation stability of chain in $A_{63}B_{10}C_{70}$ system is higher than that of $A_{63}B_{10}C_{40}$ system. The longer brush-hair causes a stronger steric-hindrance effect to limit the deformation of brushes and creates a tighter hydration layer when experiencing UV radiation. Therefore, the $R_g^2$ values in $A_{63}B_{10}C_{70}$ system shows opposite change trend compared with those in $A_{63}B_{10}C_{40}$ system. While the antifouling ability of the system become enhanced.

REFERENCE

1. Yang, S. C.; Zhu, Y. L.; Qian, H. L.; Lü, Z. Y. Molecular dynamics simulation of antipolyelectrolyte effect and solubility of polyzwitterions. *Chem Res Chinese U* **2017,** 33 (2), 261-267 DOI: 10.1007/s40242-017-6354-0.