Supplementary Materials for

"Distinct Antifouling Mechanisms on Different Chain Densities of Zwitterionic Polymers"

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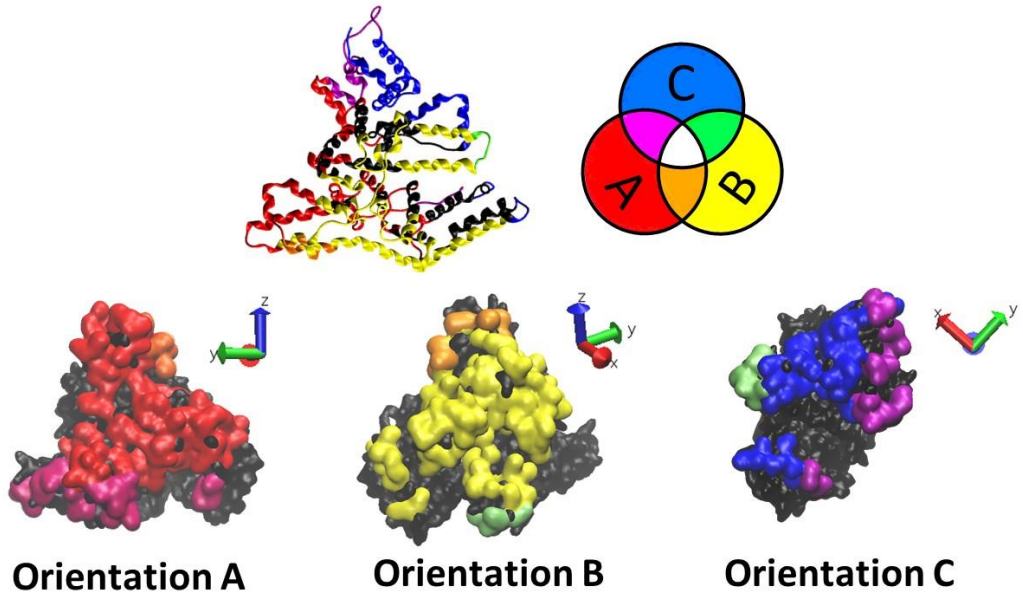

Figure S1. Three surface areas/orientations that are defined in BSA protein: A (color: red), B (color: yellow), and C (color: blue). The structure of the BSA protein is based on X-ray crystallography (PDB id code: 3V03). (Majorek, K.A., Porebski, P.J., Dayal, A., Zimmerman, M.D., Jablonska, K., Stewart, A.J., Chruszcz, M., Minor, W. *Mol Immunol* 52, 174–82 (2012)).

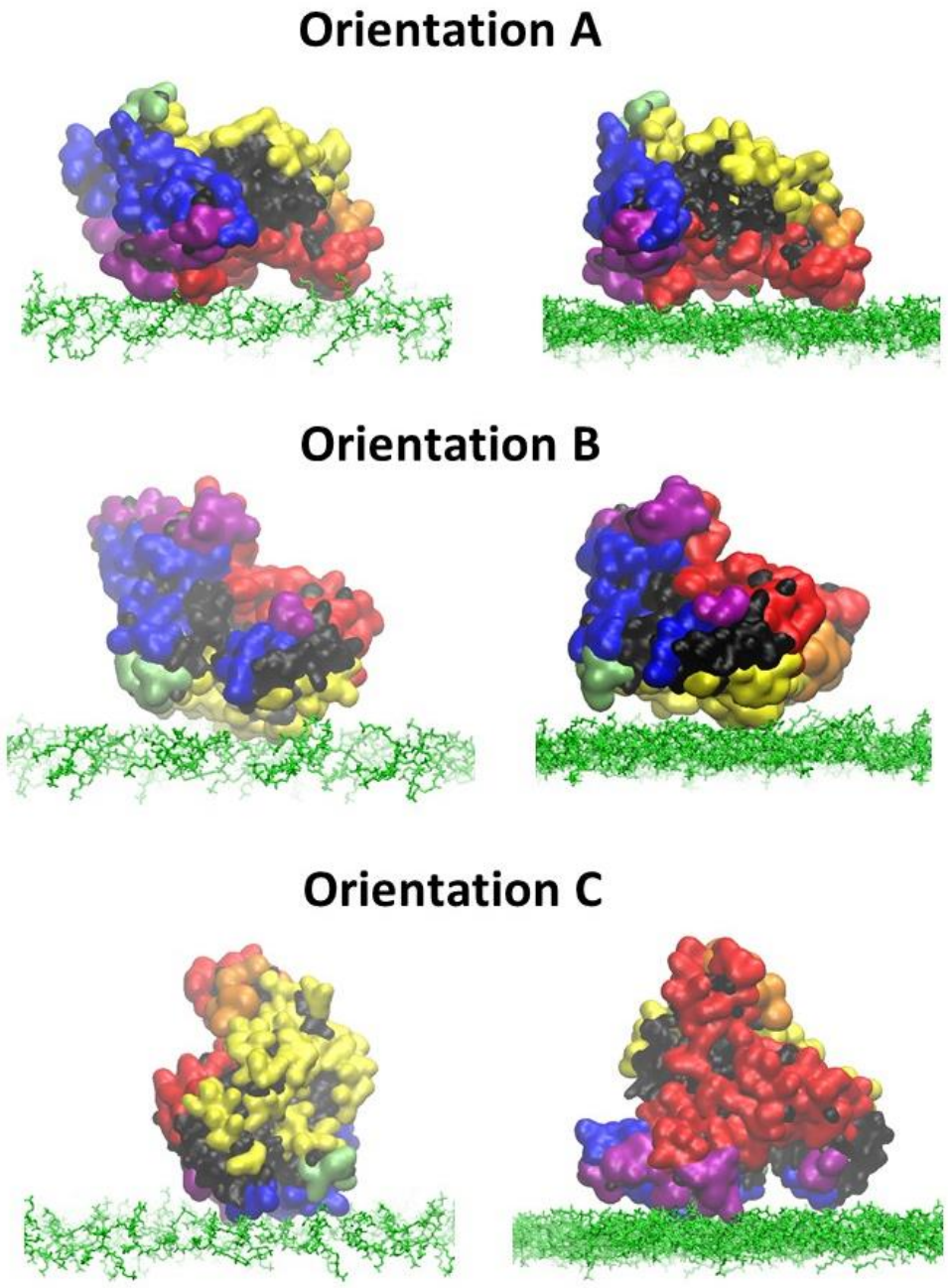

Figure S2. Initial constructed models by which BSA is placed on poly(SPE) surfaces at three different orientations, at low-density (left) and at high-density (right) surfaces: models LA, LB, and LC (left, from top to bottom), and models HA, HB, and HC (right, from top to bottom).

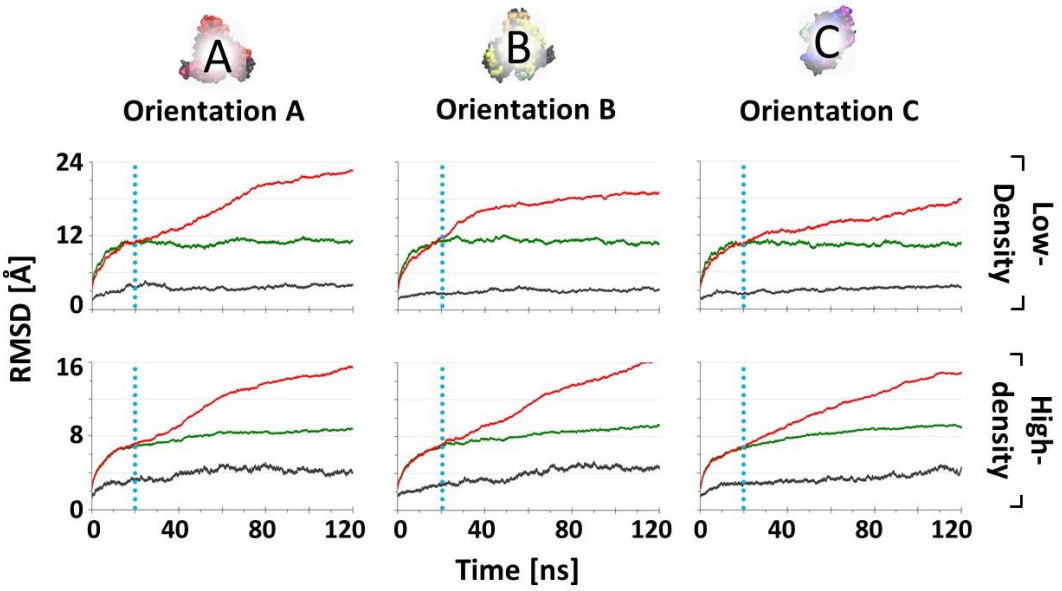

Figure S3. The root-mean-square-deviations (RMSDs) for models LA, LB, and LC at low-density surface (top, from left to right) and for models HA, HB, and HC at high-density surface (bottom, from left to right). The RMSD values were computed separately for bovine serum albumin (BSA) protein (color: black), for the poly(SPE) grafted surface (color: green), and for the combined BSA – poly(SPE) surface model (color: red).

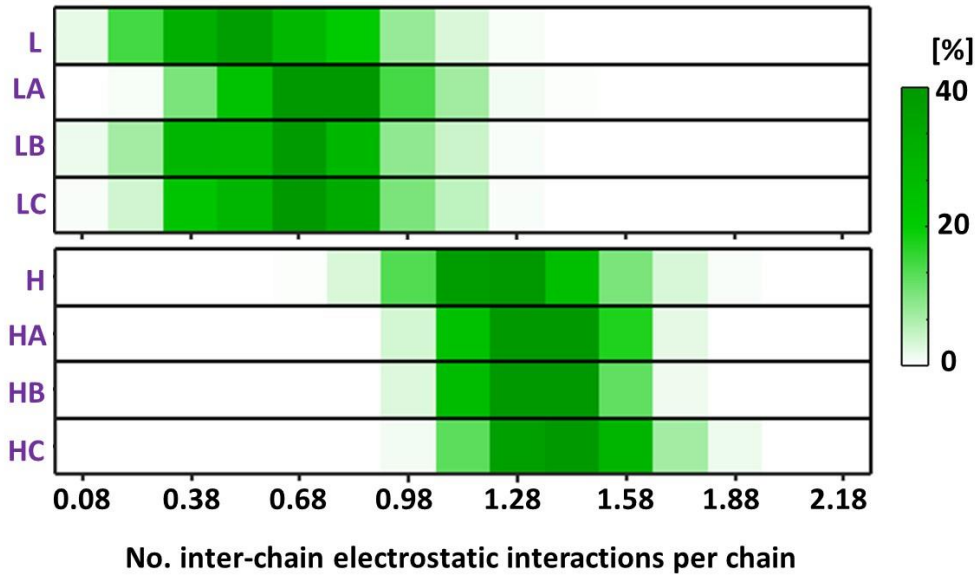

Figure S4. The averaged percentage distribution of the number of inter-chain electrostatic interactions within the poly(SPE) zwitterionic side-groups, in absence and in presence of BSA, at low- and high-density surfaces.

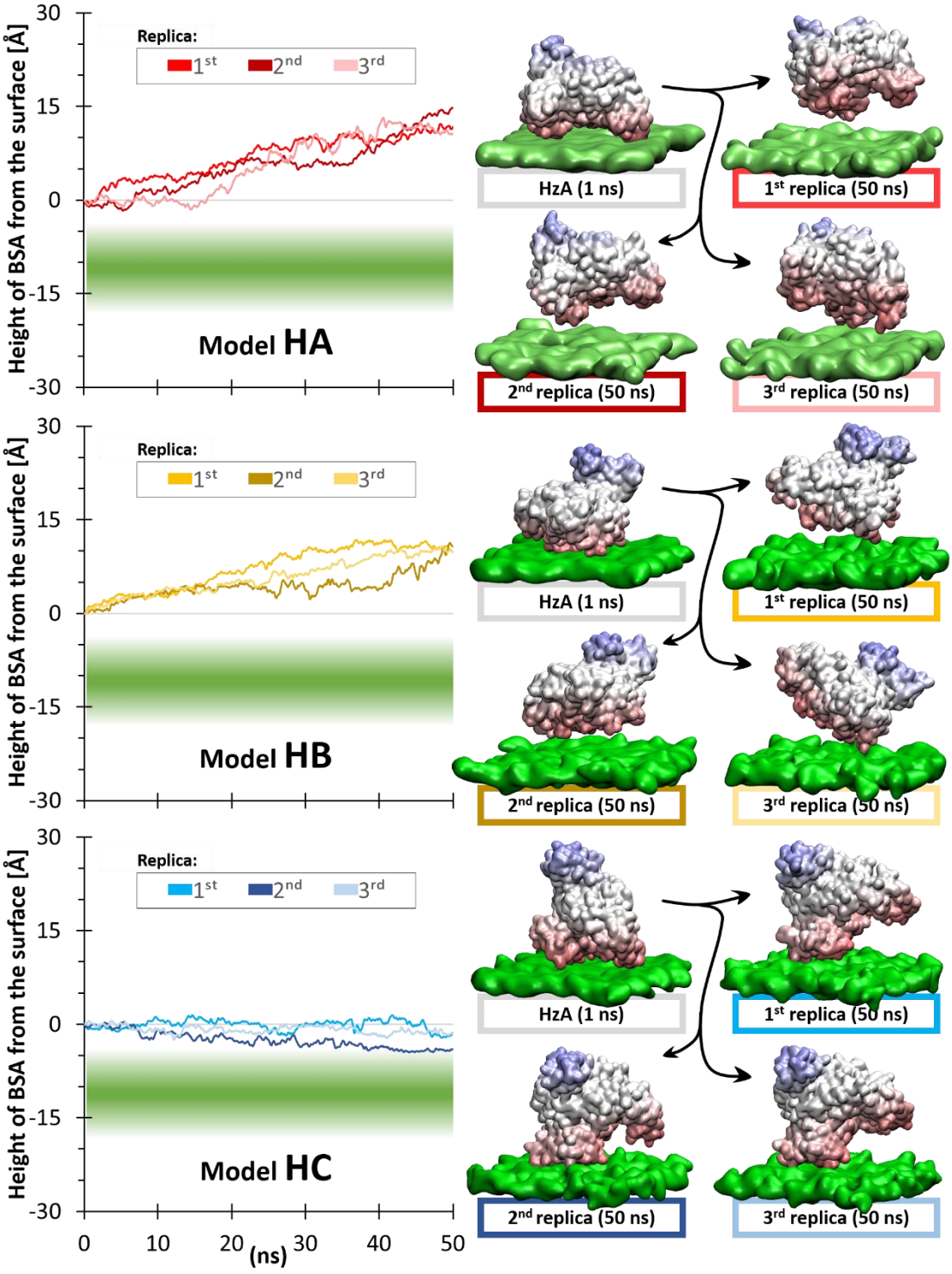

Figure S5. Snapshots of the detachment and anchoring of BSA simulated models at high-density surface for the three trajectories/replicas (right). Initial models are described in Fig. S2. The height values of the BSA from the surface were measured along the Z-component axis for the Cα atoms of amino acids (left). The values presented in the graphs are taken from the lowest Cα atom of the protein. The green bands represent the averaged positions of the polymer chains.

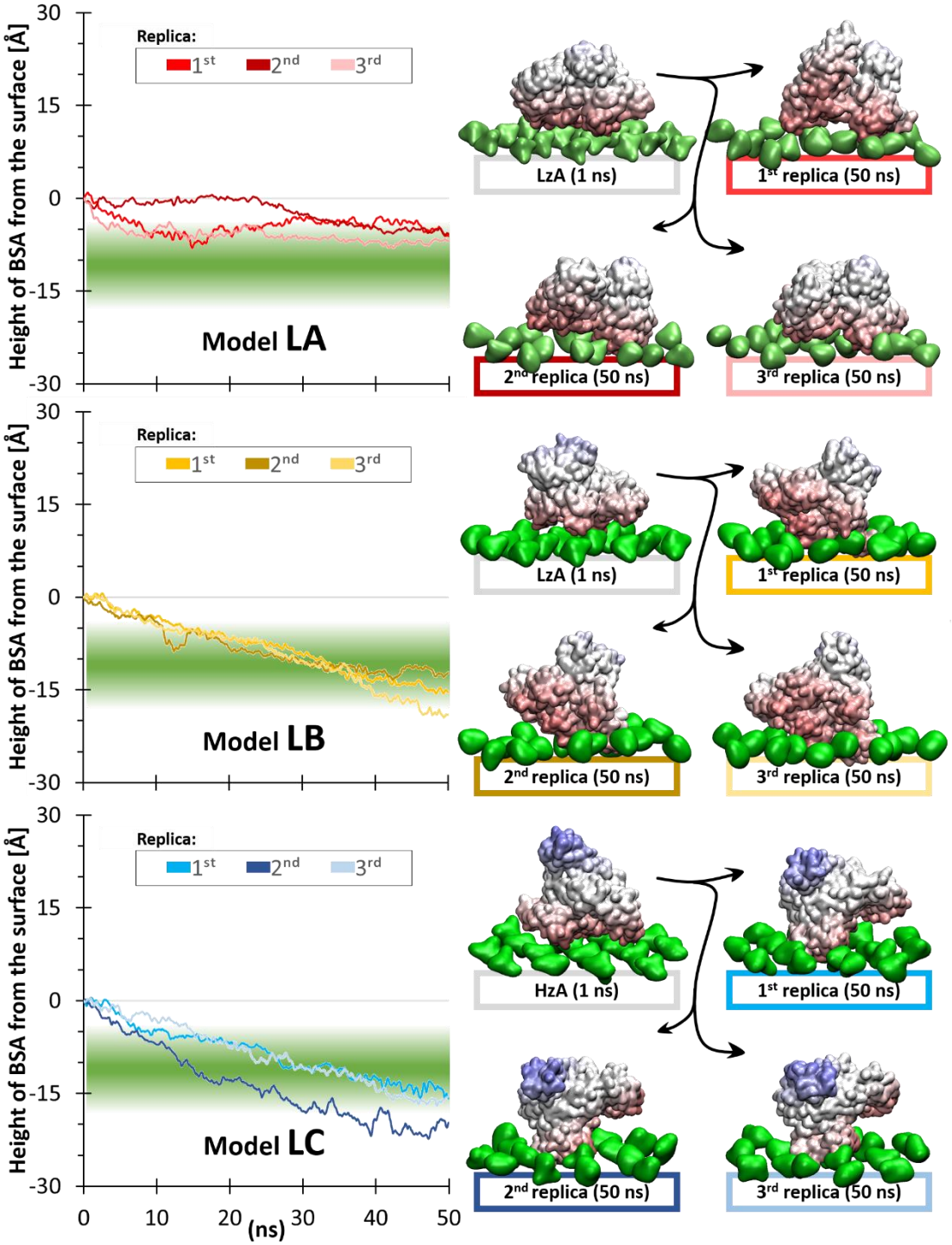

Figure S6: Snapshots of anchoring and penetrating of BSA simulated models at low-density surface for the three trajectories/replicas (right). Initial models are described in Fig. S2. The height values of the BSA from the surface were measured along the Z-component axis for the Cα atoms of amino acids (left). The values presented in the graphs are taken from the lowest Cα atom of the protein. The green bands represent the averaged positions of the polymer chains.

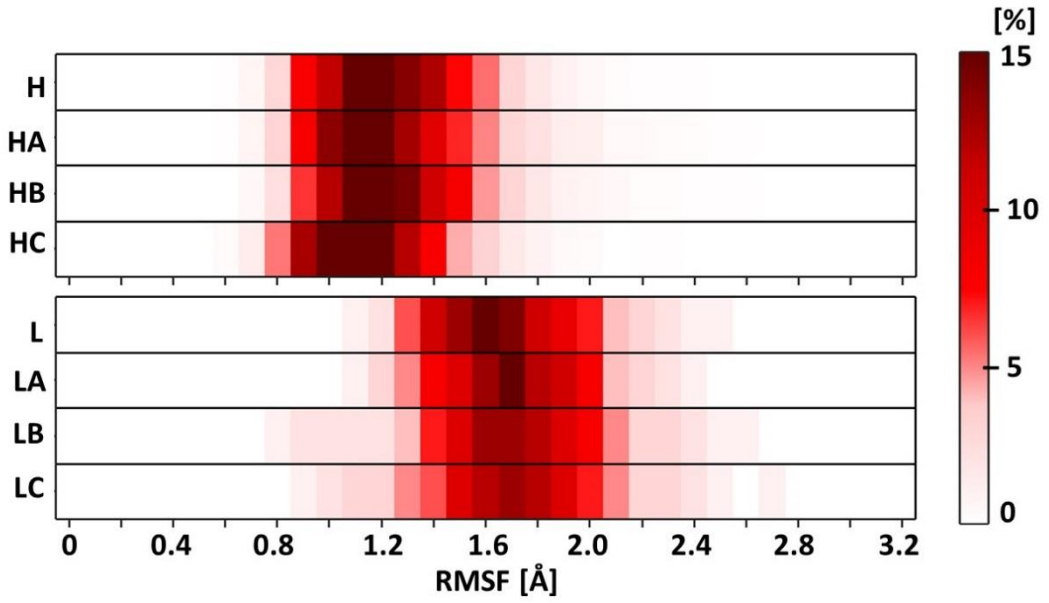

Figure S7. The averaged percentage distribution of the root-mean-square fluctuations (RMSFs) for the polymer chains for the models in the absence of BSA – model H, and in presence with BSA models HA, HB, and HC at high-density (top), and for the models in the absence of BSA – model L, and in presence with BSA models LA, LB, and LC at low-density (bottom).

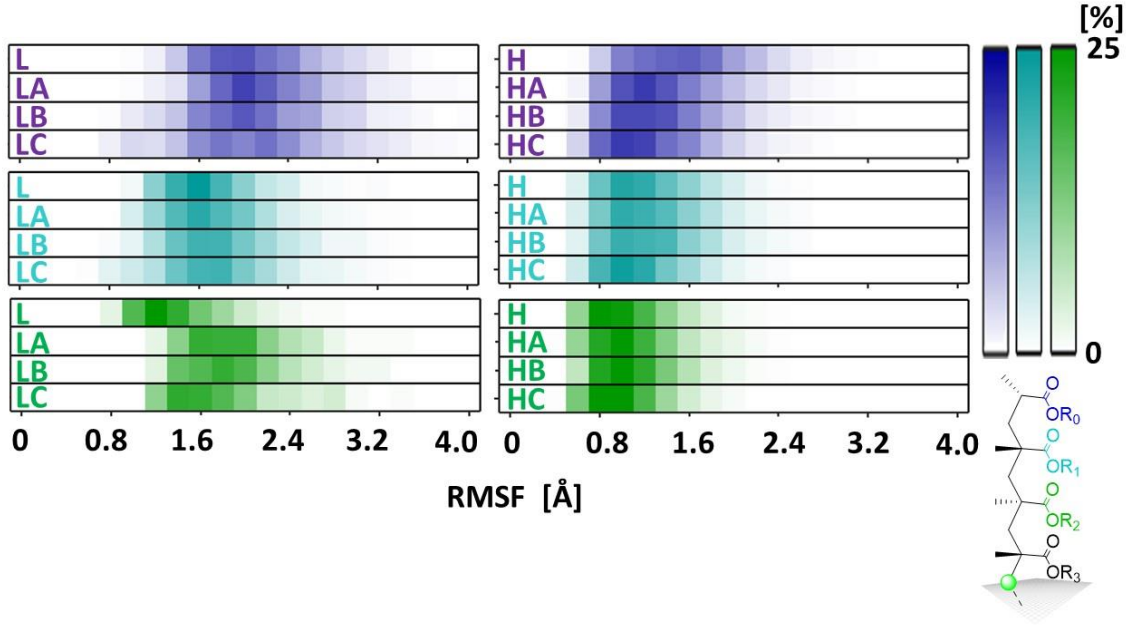

Figure S8. The averaged percentage distribution of the root-mean-square fluctuations (RMSFs) for the each of the three-polymer side chains R_0 (color: purple), R_1 (color: light blue), and R_2 (color: green) for the models in the absence of BSA – model L, and in presence with BSA models LA, LB, and LC at low-density (left), and for the models in the absence of BSA – model H, and in presence with BSA models HA, HB, and HC at high-density (right).

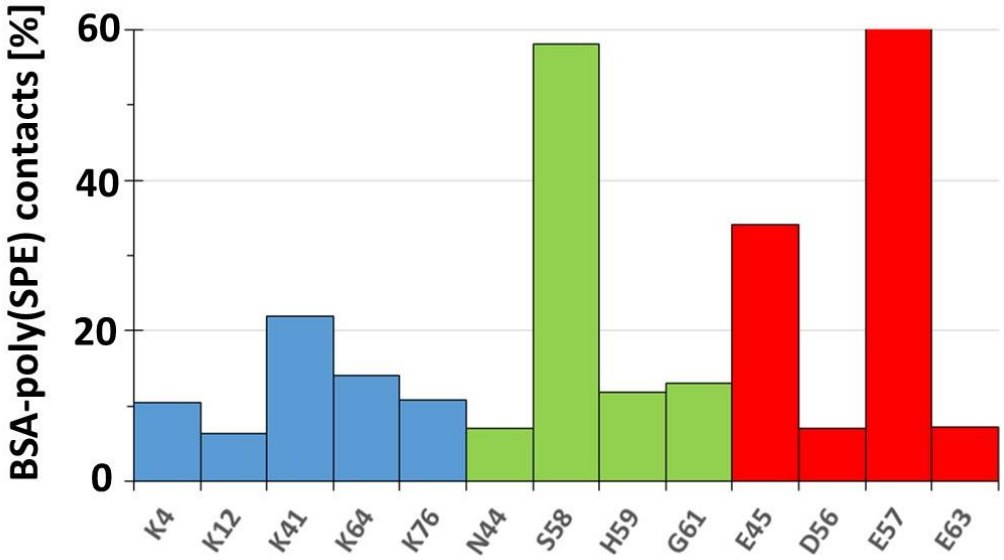

Figure S9. The percentage interactions that were computed for model HC. The percentage electrostatic interactions between positively charged amino acids (color: blue), negatively charged amino acids (color: red) within the BSA and the polymer chains. The percentage hydrogen bond interactions between uncharged amino acids within the BSA and the polymer chains (color: green).

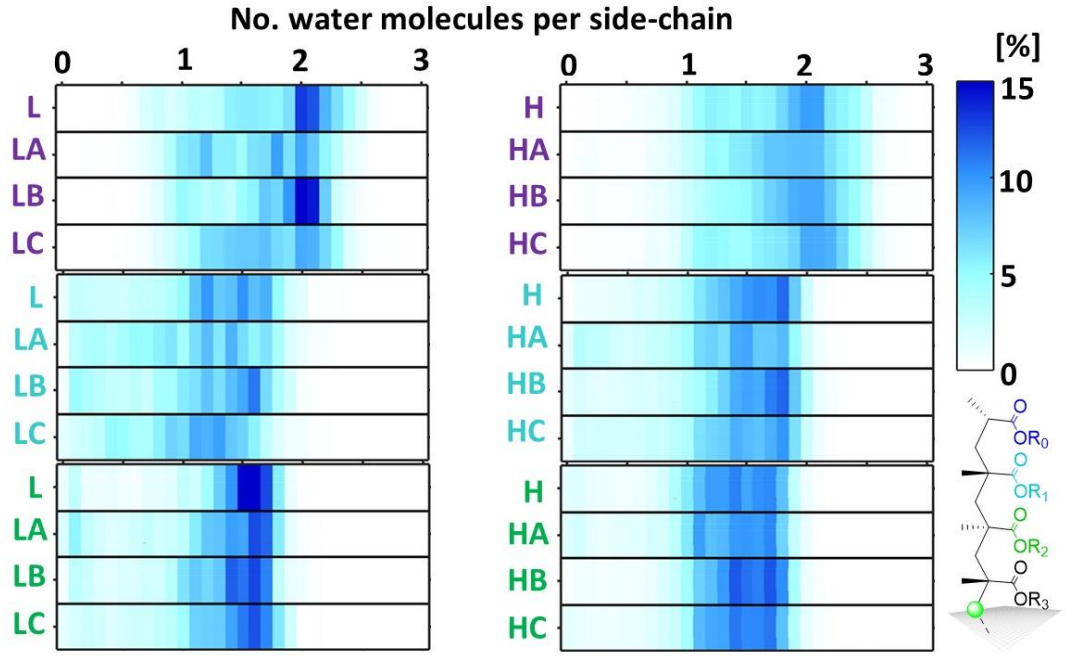

Figure S10. The averaged percentage distribution of the number of water molecules per side chain R_0, R_1, and R_2.

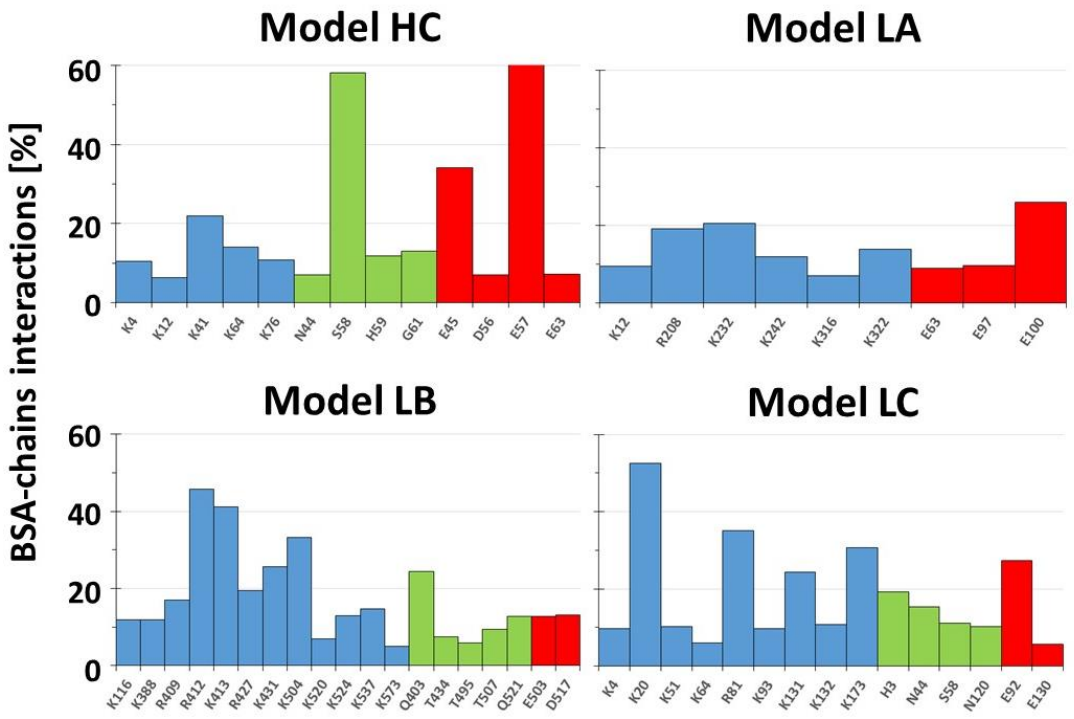

Figure S11. The percentage electrostatic interactions between positively charged amino acids (color: blue), negatively charged amino acids (color: red) within the BSA and the polymer chains. The percentage hydrogen bond interactions between uncharged amino acids within the BSA and the polymer chains (color: green). The interactions were computed for the models by which shown these interactions.

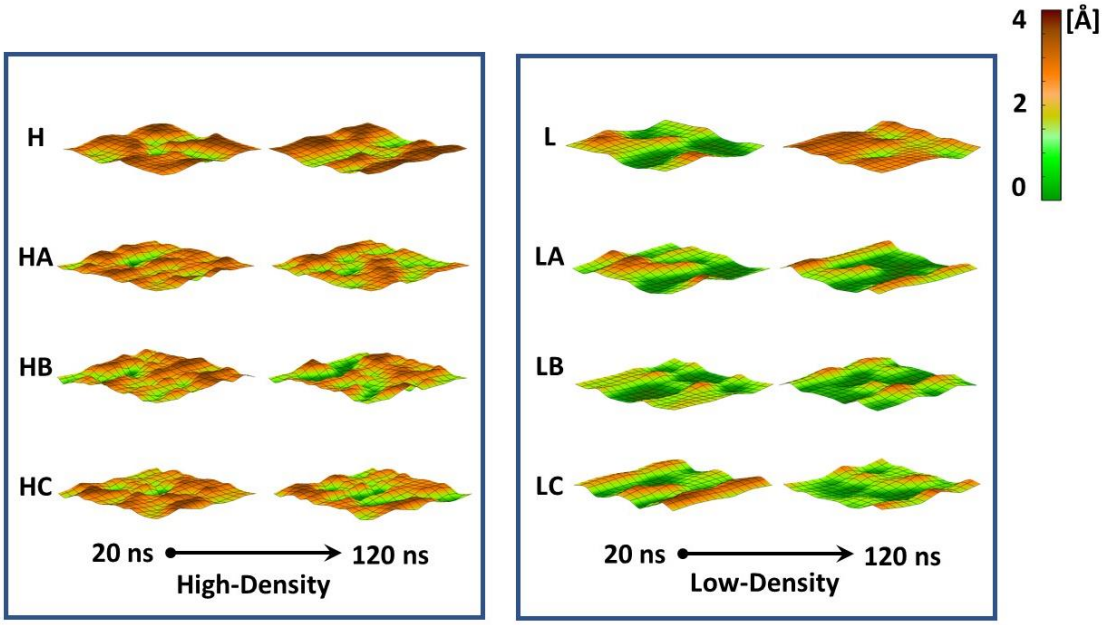

Figure S12. The topology heights of the polymer chains on the surfaces at snapshots of 20 ns and 120 ns of the MD simulations, for the models in the absence of BSA – model H, and in presence with BSA models HA, HB, and HC at high-density (left), and for the models in the absence of BSA – model L, and in presence with BSA models LA, LB, and LC at low-density (right).

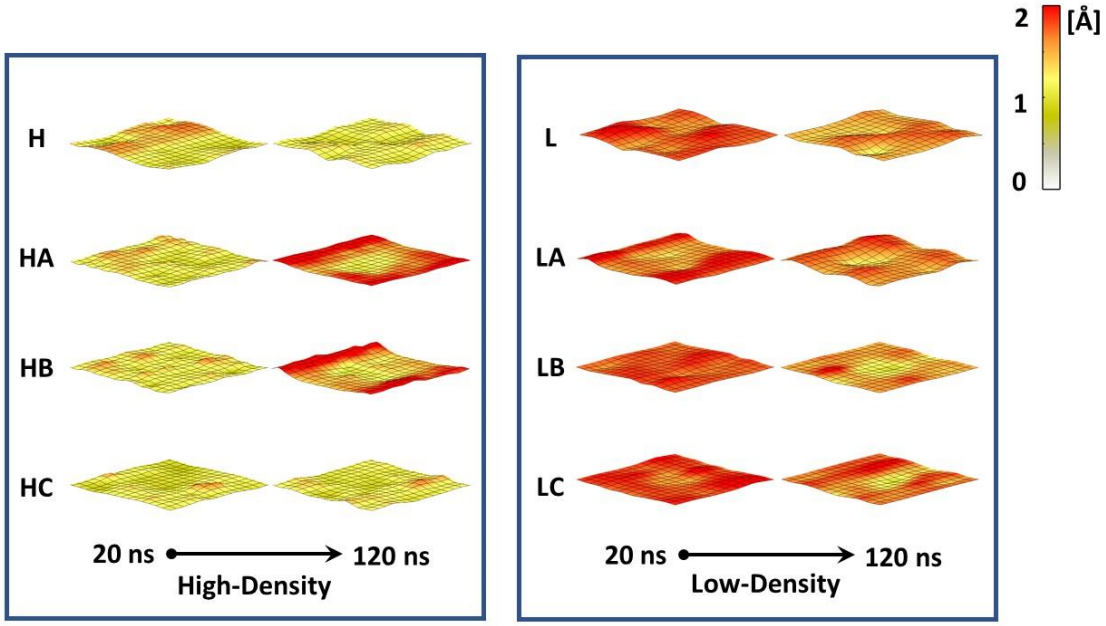

Figure S13. The topology of the RMSF of the polymer chains on the surfaces at snapshots of 20 ns and 120 ns of the MD simulations, for the models in the absence of BSA – model H, and in presence with BSA models HA, HB, and HC at high-density (left), and for the models in the absence of BSA – model L, and in presence with BSA models LA, LB, and LC at low-density (right).

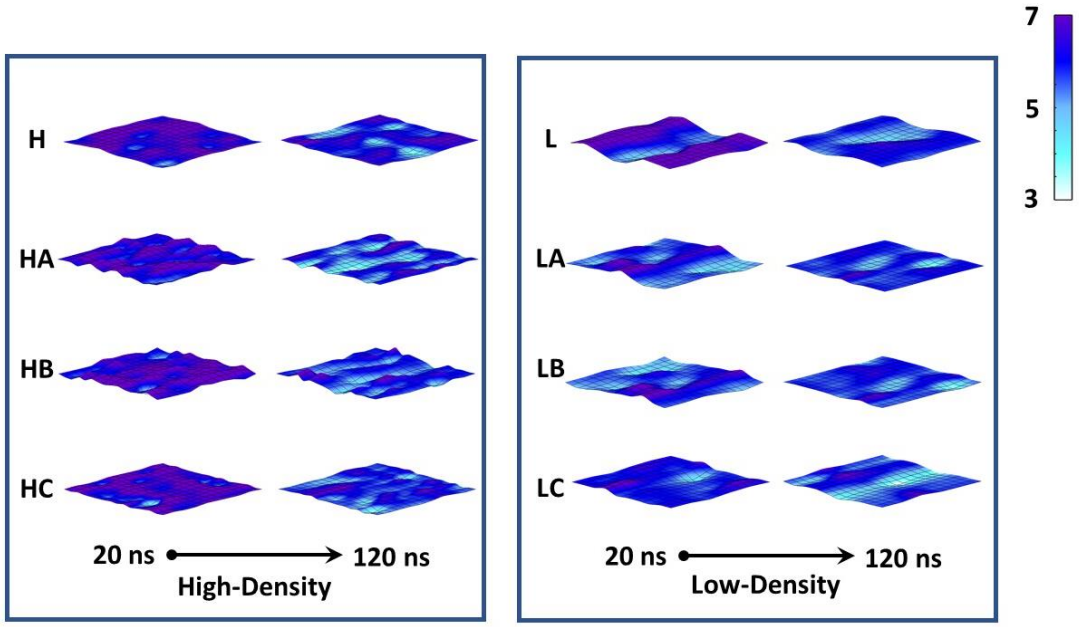

Figure S14. The topology of the water hydration of the polymer chains on the surfaces at snapshots of 20 ns and 120 ns of the MD simulations, for the models in the absence of BSA – model H, and in presence with BSA models HA, HB, and HC at high-density (left), and for the models in the absence of BSA – model L, and in presence with BSA models LA, LB, and LC at low-density (right).

Table S1. The residues and the total number of charged and uncharged residue within the BSA that face the poly(SPE) surface in each orientation.

Orientation	Residues within BSA facing the poly(SPE) surface	Number of positively charged residues	Number of uncharged H-Donor residues	Number of negatively charged residues
A	56 -111 199-213 240-251 307-330 347-378 411-420 458-505 532-539	31	51	38
B	158-189 216-227 264-283 290-311 330-342 368-403 432-452 540-558	23	44	31
C	1-92 120-139 168-174 500-511 560-565	17	35	29