Supplementary Information (SI) for Nanoscale Advances.
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Supplementary Information

Polystyrene Nanoplastics as PFAS Carriers and Their Interactions with Zwitterionic Phospholipid Membranes

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Table of Contents

Table S1. Adsorption of PFAS on the 3.1 nm and 6.7 nm NPs in water and on the POPC surface. 1

Figure S1. (a) PFOA, (b) PFOS, and (c) PTFE coated 6.7-nm NP in bulk water. Note: For each system of PFOA and PFOS, there are total 10 refillings (for total 1.0 μs). For the system of PTFE, there are total 12 refillings.....1

Figure S2. (a) PFOA, (b) PFOS, and (c) PTFE coated 3.1-nm NP in bulk water after 10 refillings for each system. 1

Figure S3. Interactions between the large NP and (a) PFOA, (b) PFOS, and (c) PTFE; and between the small NP and (d) PFOA, (e) PFOS, and (f) PTFE. Here the black/red line stands for the Coulomb/Lennard-Jones interactions, respectively. All the interactions were calculated up to a distance of 1.2 nm, which is the cutoff distance for short-range interactions in the simulations. 2

Figure S4. Minimum distance and interaction energies (LJ and electrostatic) between the POPC membrane and the 6.7-nm NP as a function of simulation time t and representative snapshots in pure water. 2

Figure S5. Minimum distance and interaction energies (LJ and electrostatic) between the POPC membrane and the 3.1-nm NP (a) and PTFE-coated NP (b) as a function of simulation time t and representative snapshots in 0.1 M KCl. 3

Figure S6. Temporal profiles of interaction energies (LJ and electrostatic) between $-SO_3^-$ group of PFOS and $-N^+(CH_3)_3$ group of POPC lipid membrane. 3

Figure S7. Minimum distance between the POPC membrane and the PFOS coated NP as a function of simulation time t and representative snapshots in 0.1 M KCl. 4

Figure S8. Snapshots of the PFOS-coated NPs adsorbed on the POPC lipid surface (left) and the zoomed-in view of the $–SO_3^-$ group of the adsorbed PFOS molecules interacting with the $–N^+(CH_3)_3$ group of the POPC surface (right) in 0.1 M KCl at t = 210. 4

Figure S9. Time evolution of number of PFOA molecules detached from NP. Note: two red arrows indicate two times when the PFOA-coated NP contacts the lipid surface.....5

Figure S10. The final snapshots for PFOA-coated NP system in pure water (a) and 0.1 M KCl (b).....5

Figure S11. Temporal profiles of interaction energies (LJ and electrostatic) of PFOA molecules with POPC lipid layers and the NP (bottom).....6

Figure S12. Snapshots of the PFOS-coated NPs adsorbed on the POPC lipid surface (left panel) and the zoomed-in view of the adsorbed PFOS molecules and corresponding POPC surface (right panel) in pure water (a) and 0.1 M KCl (b). 6

Table S1. Adsorption of PFAS on the 3.1 nm and 6.7 nm NPs in water and on the POPC surface.

System	NP size (nm)	PFAS type	Adsorption amount (g/g)	# of adsorbed molecules	Total molecule #
Bulk water	6.7	PFOA	0.78	177	200
		PFOS	1.03	193	200
		PTFE	1.12	240	240
Bulk water	3.1	PFOA	1.77	40	40
		PFOS	2.13	40	40
		PTFE	2.24	48	48
POPC	3.1	PFOA	1.28	29	40
		PFOS	1.97	37	40
		PTFE	2.24	48	48

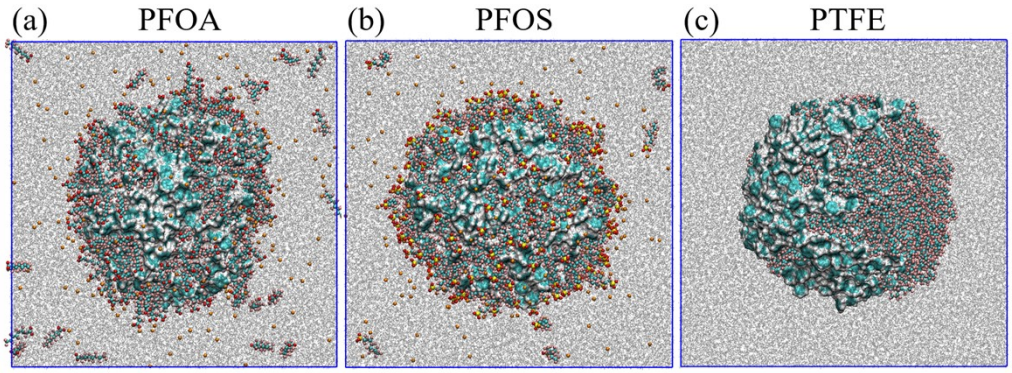


Figure S1. (a) PFOA, (b) PFOS, and (c) PTFE coated 6.7-nm NP in bulk water. Note: For each system of PFOA and PFOS, there are total 10 refillings (for total 1.0 μs). For the system of PTFE, there are total 12 refillings.

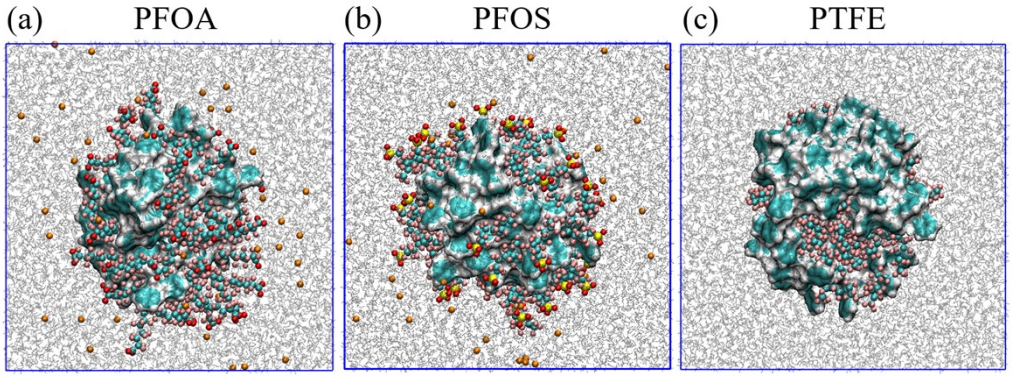


Figure S2. (a) PFOA, (b) PFOS, and (c) PTFE coated 3.1-nm NP in bulk water after 10 refillings for each system.

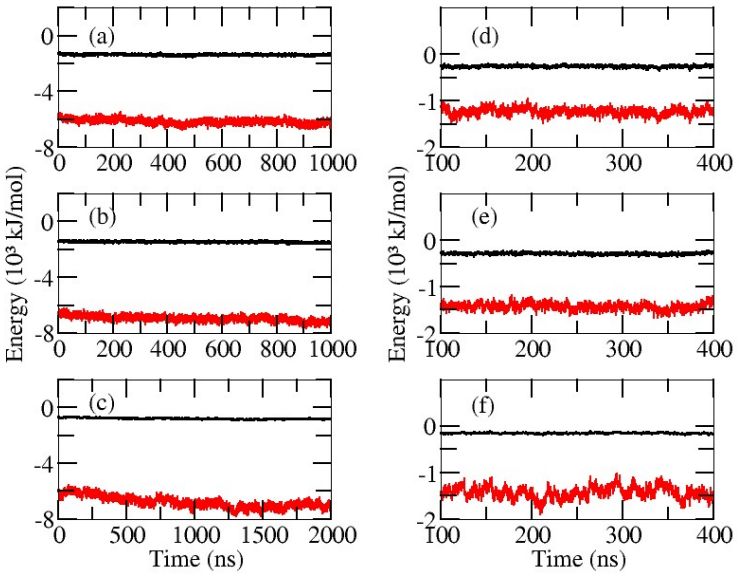


Figure S3. Interactions between the large NP and (a) PFOA, (b) PFOS, and (c) PTFE; and between the small NP and (d) PFOA, (e) PFOS, and (f) PTFE. Here the black/red line stands for the Coulomb/Lennard-Jones interactions, respectively. All the interactions were calculated up to a distance of 1.2 nm, which is the cutoff distance for short-range interactions in the simulations.

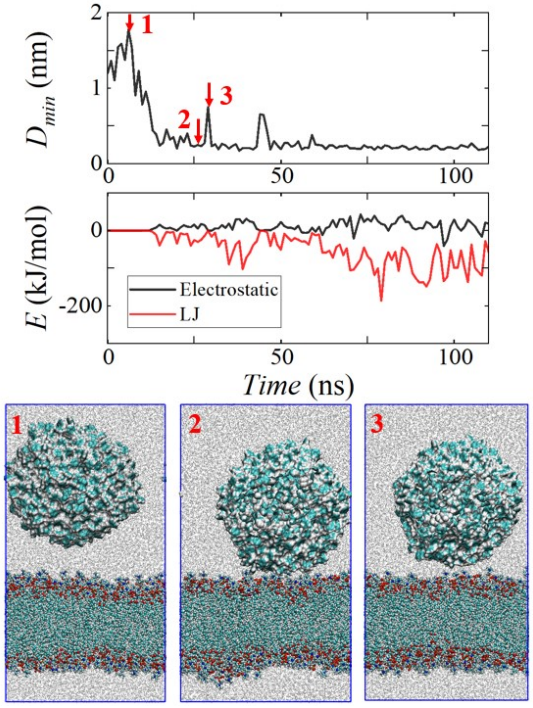


Figure S4. Minimum distance and interaction energies (LJ and electrostatic) between the POPC membrane and the 6.7-nm NP as a function of simulation time t and representative snapshots in pure water.

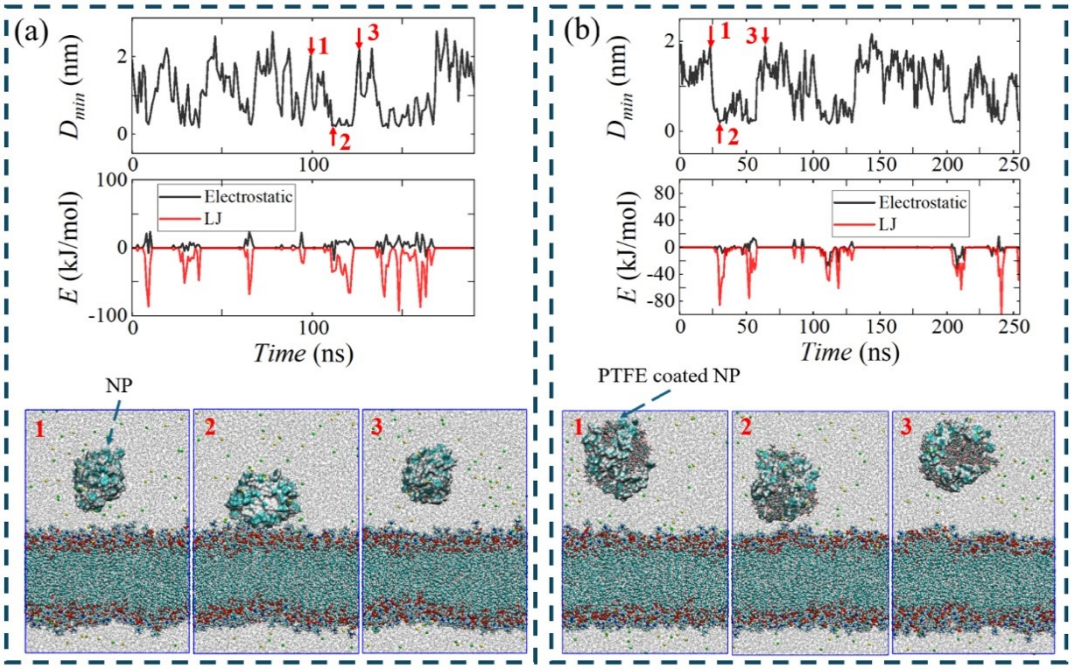


Figure S5. Minimum distance and interaction energies (LJ and electrostatic) between the POPC membrane and the 3.1-nm NP (a) and PTFE-coated NP (b) as a function of simulation time t and representative snapshots in 0.1 M KCl.

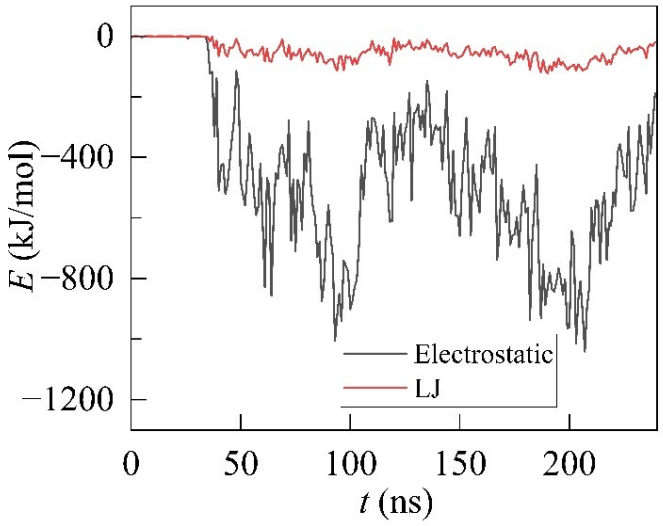


Figure S6. Temporal profiles of interaction energies (LJ and electrostatic) between $-SO_3^-$ group of PFOS and $-N^+(CH_3)_3$ group of POPC lipid membrane.

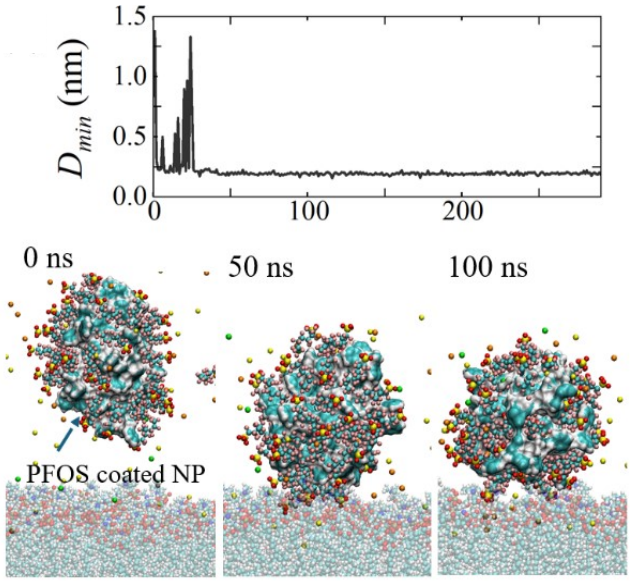


Figure S7. Minimum distance between the POPC membrane and the PFOS coated NP as a function of simulation time t and representative snapshots in 0.1 M KCl.

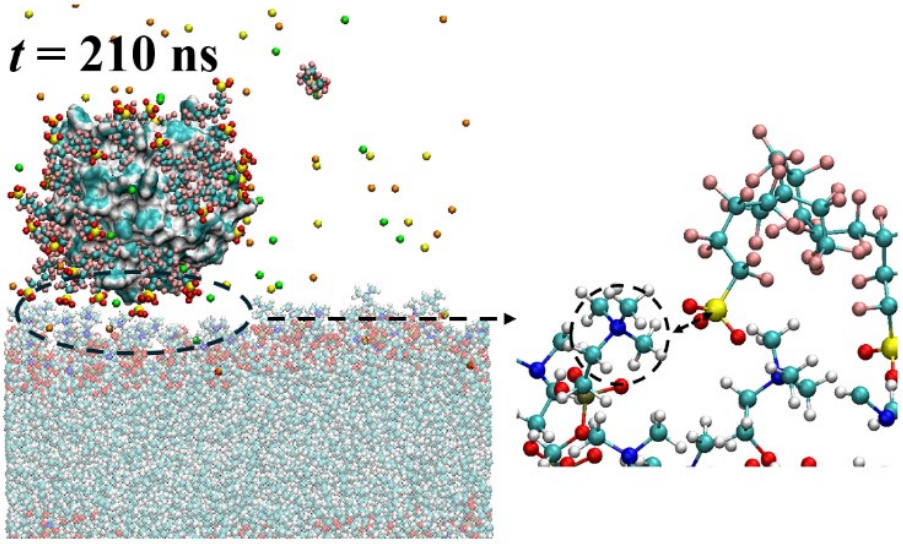


Figure S8. Snapshots of the PFOS-coated NPs adsorbed on the POPC lipid surface (left) and the zoomed-in view of the $–SO_3^-$ group of the adsorbed PFOS molecules interacting with the $–N^+(CH_3)_3$ group of the POPC surface (right) in 0.1 M KCl at t = 210.

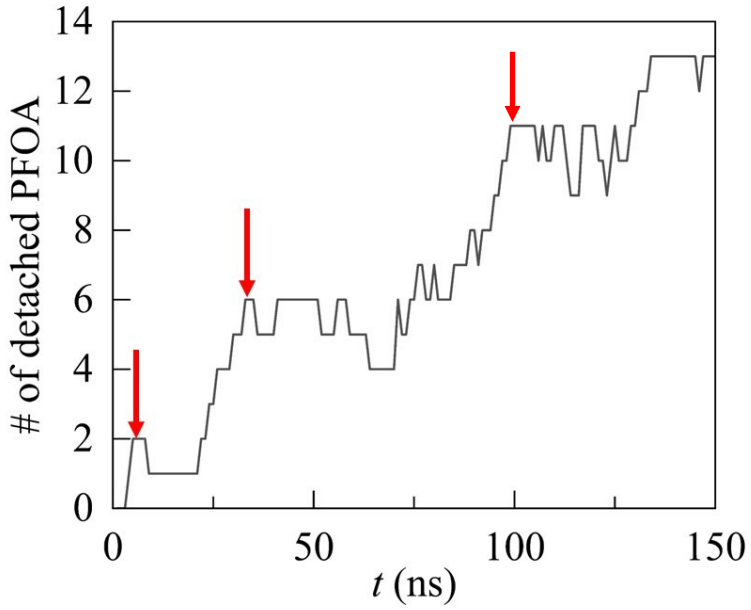


Figure S9. Time evolution of the number of PFOA molecules detached from the NP. Note: Red arrows indicate the times at which the PFOA-coated NP contacts the lipid surface.

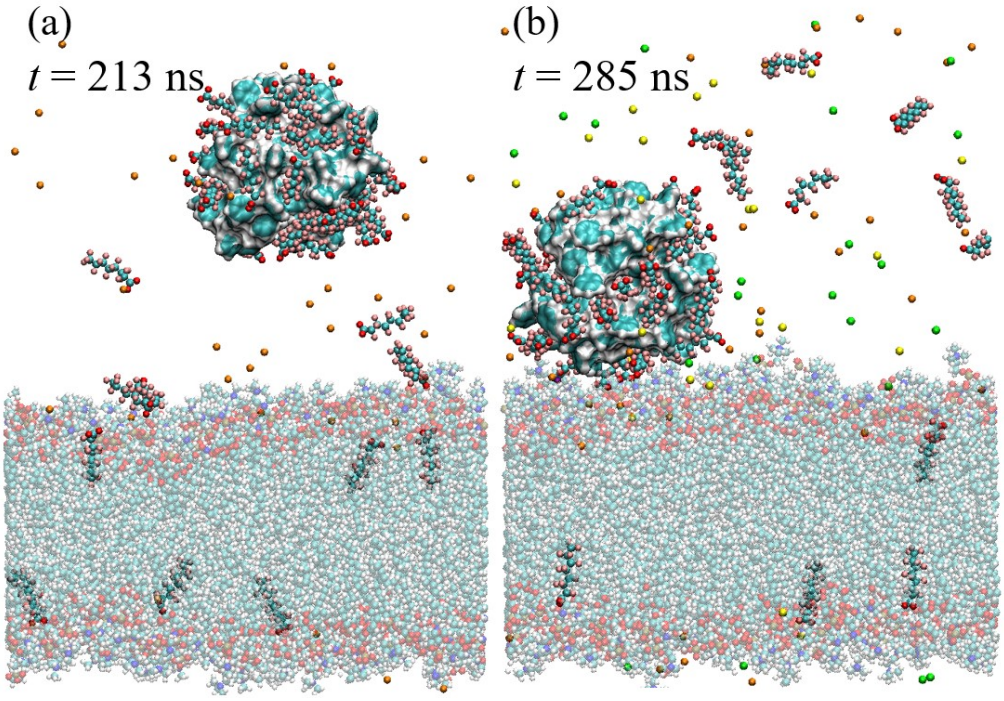


Figure S10. The final snapshots for PFOA-coated NP system in pure water (a) and 0.1 M KCl (b).

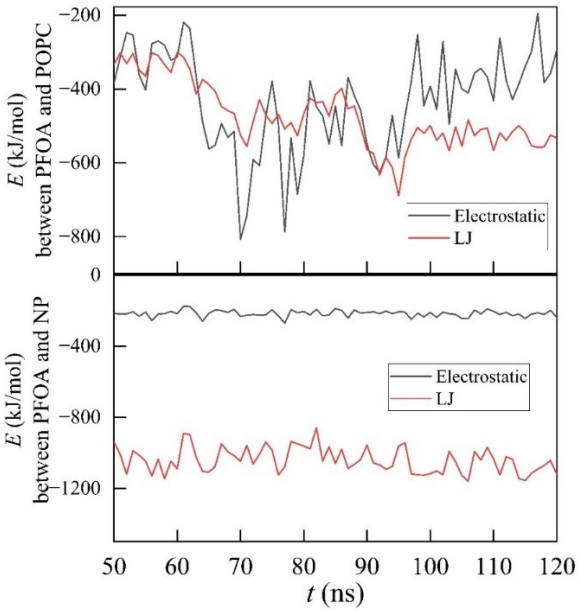
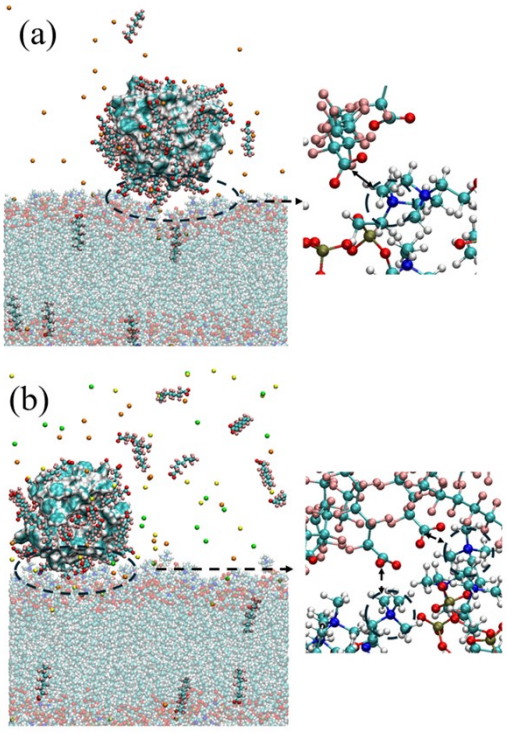


Figure S11. Temporal profiles of interaction energies (LJ and electrostatic) of PFOA molecules with POPC lipid layers and the NP (bottom).



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