

Supporting Information for

Molecular dynamics study on properties of hydration layers above

polymer antifouling membranes

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Table S1 21-step MD compression and relaxation schemes

Step	Simulation details	Simulation time (ps)
1,2	NVT 600 K, NVT 300 K	50,50
3	NPT 0.02P _{max} bar, 300 K	50
4,5	NVT 600 K, NVT 300 K	50,100
6	NPT 0.6 P _{max} bar, 300 K	50
7,8	NVT 600 K, NVT 300 K	50,100
9	NPT P _{max} bar, 300 K	50
10,11	NVT 600 K, NVT 300 K	50,100
12	NPT 0.5 P _{max} bar, 300 K	5
13,14	NVT 600 K, NVT 300 K	5,10
15	NPT 0.1 P _{max} bar, 300 K	5
16,17	NVT 600 K, NVT 300 K	5,10
18	NPT 0.01 P _{max} bar, 300 K	5
19,20	NVT 600 K, NVT 300 K	5,10
21	NPT 1 bar, 300 K	50000

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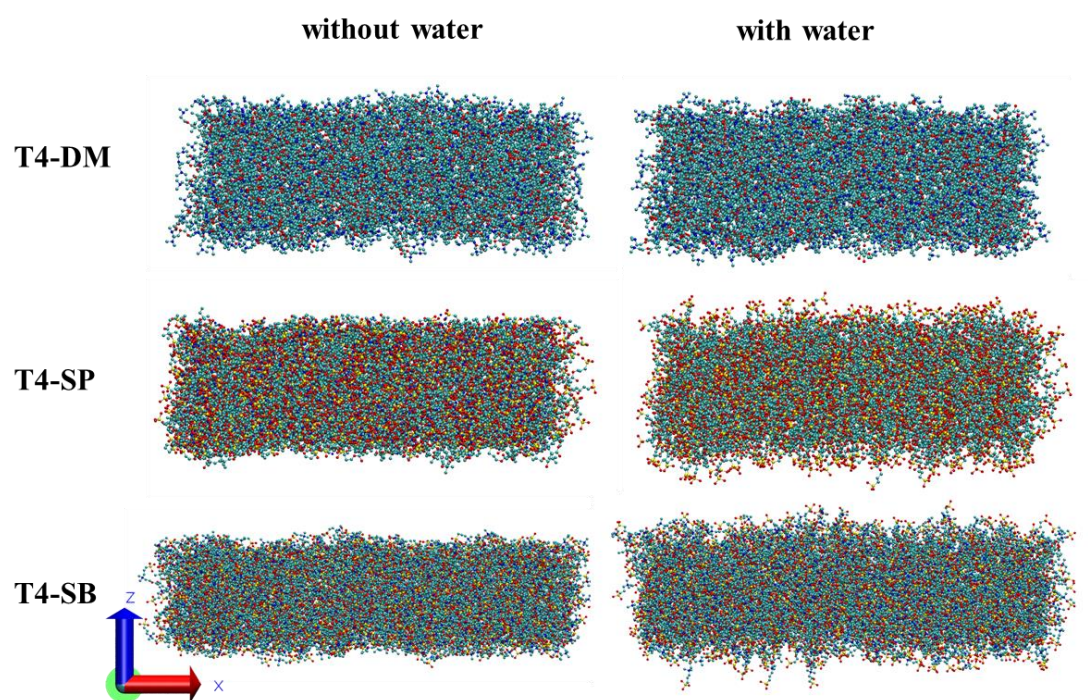


Figure S1 Final simulation configuration of three antifouling membranes under dry and hydrated states. Water molecules were not shown for clarity.