Supporting information

Morphology and Proton Transport in Sulfonated Poly(ether ether ketone) Membranes: A Molecular Dynamics and DFT Study

Shunguo Zhang[ab], Xusheng Cheng[ab] and Liwei Wang[*ab]

* Corresponding authors

a Institute of Refrigeration and Cryogenics, Key Laboratory of Power Machinery and Engineering of MOE, Shanghai Jiao Tong University, Shanghai 200240, China

Email:Lwwang@sjtu.edu.cn

b Shanghai Non-Carbon Energy Conversion and Utilization Institute, Shanghai 200240, China

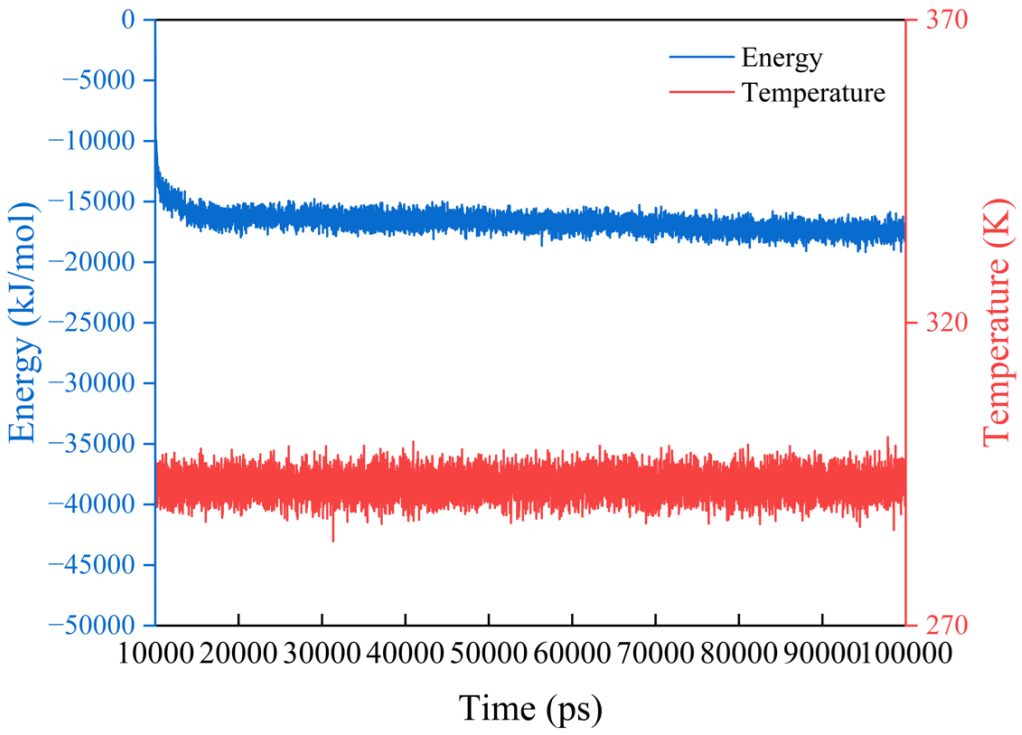

Fig. S1 Temperature and total potential energy variation (100ns) of the dynamic simulation system with *DS*=50%, λ=0 at room temperature.

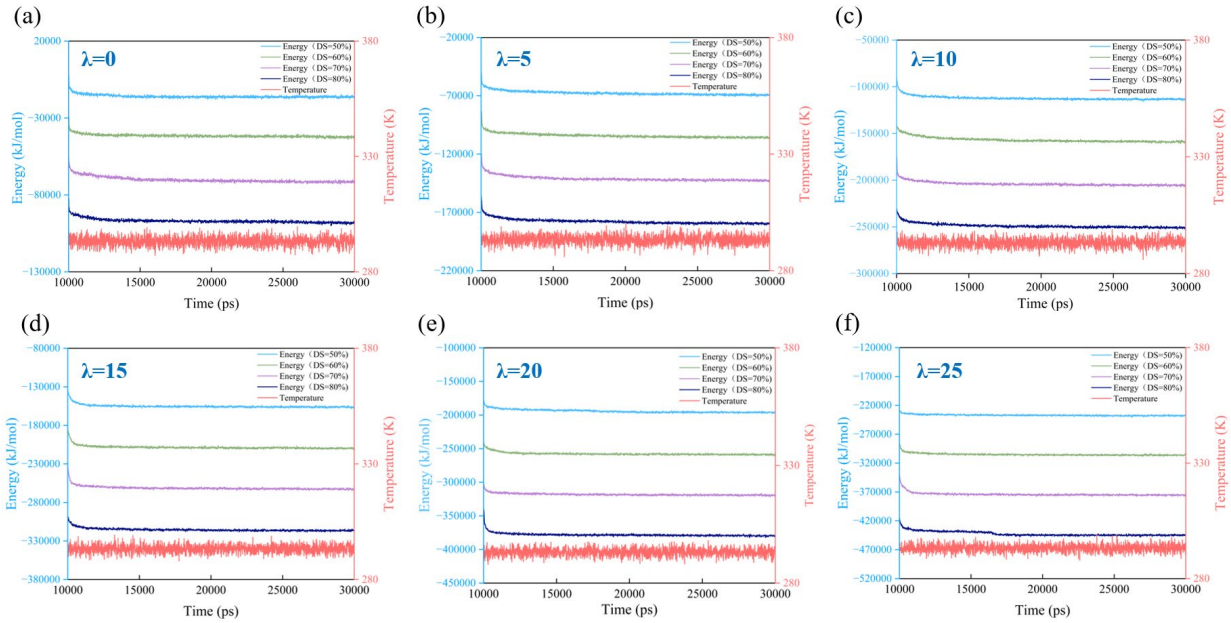

Fig. S2 Temperature and total potential energy variation of the dynamic simulation system with *DS*=50% to 80% under different water contents at room temperature.

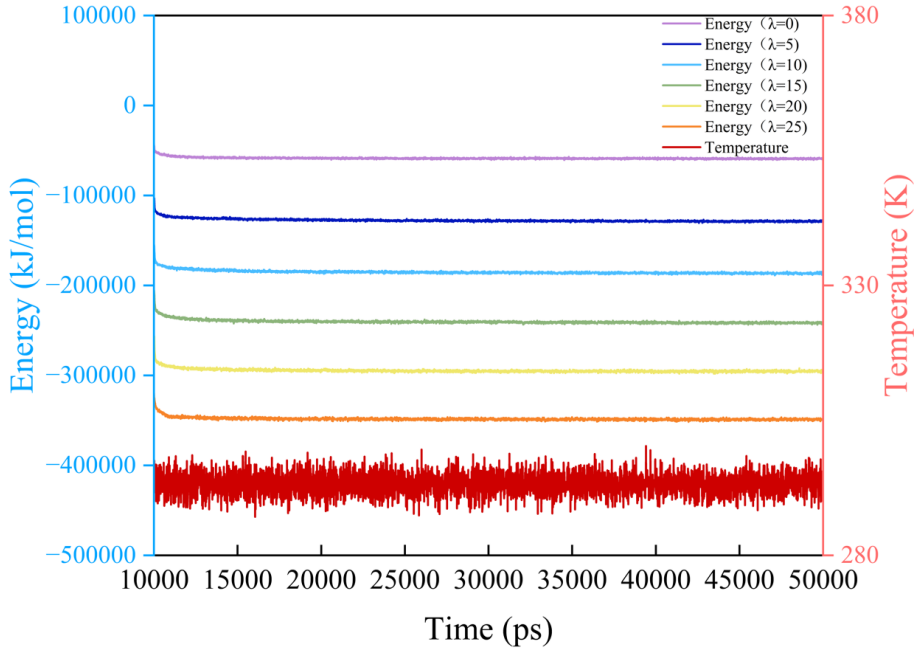

Fig. S3 Temperature and total potential energy variation of the dynamic simulation system with λ=0 to 25 under *DS*=66% at room temperature.

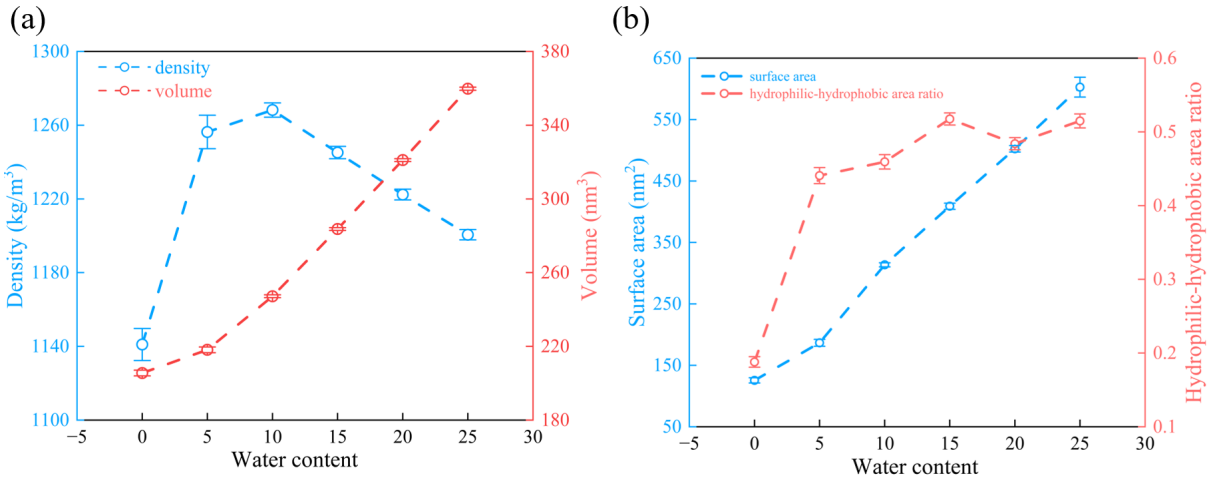

Fig. S4 Long-term evolution (>50 ns) of *DS*=66% SPEEK membranes properties with λ (a) density and volume, (b) surface area and hydrophilic-hydrophobic area ratio.

Table S1 Energy Statistics in Different Time Intervals with *DS*=50% and λ=0

Time intervals	Data (D)	Deviation (|(D-D(100ns))/D(100ns)|*100%)

15ns (average of14-16ns)	-16071.78	8.11%
30ns (average of29-30ns)	-16283.6	6.90%
50ns (average of49-51ns)	-16604.4	5.07%
100ns (average of98-100ns)	-17490.9	0

Table S2 Comparison of Baseline (B) vs. Extended (E) Simulation Time Characteristics

Characteristics	**λ=0**	**λ=5**	**λ=10**	**λ=15**	**λ=20**	**λ=25**
Density (B)	1128.26	1241.39	1264.15	1242.10	1221.90	1201.79
Density (E)	1141.01	1256.33	1268.23	1245.16	1222.38	1200.58
Deviation (B-E)/B*100%	-1.13%	-1.20%	-0.32%	-0.25%	-0.04%	0.10%
Volume (B)	207.86	220.73	247.99	284.18	321.20	359.43
Volume (E)	205.55	218.12	247.19	283.66	321.07	359.79
Deviation (B-E)/B*100%	1.11%	1.18%	0.32%	0.18%	0.04%	-0.10%
Surface area (B)	128.22	196.06	317.36	413.87	507.12	628.62
Surface area (E)	125.60	186.66	313.62	409.01	502.41	602.76
Deviation (B-E)/B*100%	2.04%	4.79%	1.18%	1.17%	0.93%	4.11%
H/H area ratio (B)	18.25%	44.10%	46.21%	50.05%	48.52%	52.06%
H/H area ratio (E)	18.79%	44.07%	45.94%	51.75%	48.40%	51.48%
Deviation (B-E)/B*100%	-2.97%	0.07%	0.59%	-3.40%	0.25%	1.12%

Table S3 Comparison of calculated model characteristics for different conformations (*DS*=66%, λ=10)

Characteristics	**1**	**2**	**3**	**4**	**5**	**RMSD**	**Deviation (%)** (RMSD/average) *100%
Density	1265.5	1267.66	1261.74	1262.47	1264.23	2.13	0.17
Volume	247.73	247.31	248.46	248.32	247.97	0.42	0.17
Surface area	334.63	338.02	328.56	335.85	330.76	3.44	1.03
H/H area raito	49.45%	46.79%	46.38%	46.17%	47.55%	0.012	2.51
Hydrogen bond count	332.88	327.23	322.29	336.72	333.36	5.11	1.55
$D_{H_3O^+}$	1.20E-08	1.28E-08	1.21E-08	1.15E-08	1.18E-08	4.21E-10	3.5