

Molecular Dynamics Study of the Morphology of Hydrated Perfluorosulfonic Acid Polymer Membranes

An-Tsung Kuo, Wataru Shinoda⁺, and Susumu Okazaki[‡]

Department of Applied Chemistry, Nagoya University, Nagoya 464-8603, Japan

⁺Corresponding author. Tel: (+) 81-52-789-5288 Fax (+) 81-52-789-5118.

Email: w.shinoda@apchem.nagoya-u.ac.jp

[‡]Corresponding author. Tel: (+) 81-52-789-5229 Fax (+) 81-52-789-5118.

Email: okazaki@apchem.nagoya-u.ac.jp

SUPPORTING INFORMATION

Table S1. Diffusion coefficients of water molecule in hydrated PFSA membranes.

λ	<i>EW 844</i>		<i>EW 1144</i>	
	small	medium	small	medium
3	0.013 ± 0.004	0.013 ± 0.005	0.012 ± 0.007	0.011 ± 0.005
6	0.153 ± 0.027	0.151 ± 0.019	0.104 ± 0.030	0.126 ± 0.021
9	0.384 ± 0.034	0.388 ± 0.036	0.306 ± 0.034	0.287 ± 0.038
12	0.591 ± 0.029	0.630 ± 0.041	0.479 ± 0.046	0.486 ± 0.058
15	0.862 ± 0.037	0.865 ± 0.043	0.608 ± 0.066	0.674 ± 0.102
20	1.141 ± 0.020	1.136 ± 0.034	0.958 ± 0.052	1.017 ± 0.100

Table S2. Diffusion coefficients of hydronium ion in hydrated PFSA membranes.

λ	<i>EW 844</i>		<i>EW 1144</i>	
	small	medium	small	medium
3	0.0004 ± 0.0001	0.0004 ± 0.0003	0.0004 ± 0.0004	0.0005 ± 0.0002
6	0.024 ± 0.006	0.021 ± 0.005	0.017 ± 0.005	0.019 ± 0.008
9	0.083 ± 0.013	0.083 ± 0.016	0.064 ± 0.017	0.067 ± 0.017
12	0.158 ± 0.022	0.168 ± 0.019	0.133 ± 0.018	0.130 ± 0.023
15	0.254 ± 0.024	0.250 ± 0.018	0.188 ± 0.037	0.196 ± 0.014
20	0.392 ± 0.017	0.363 ± 0.029	0.300 ± 0.051	0.283 ± 0.027

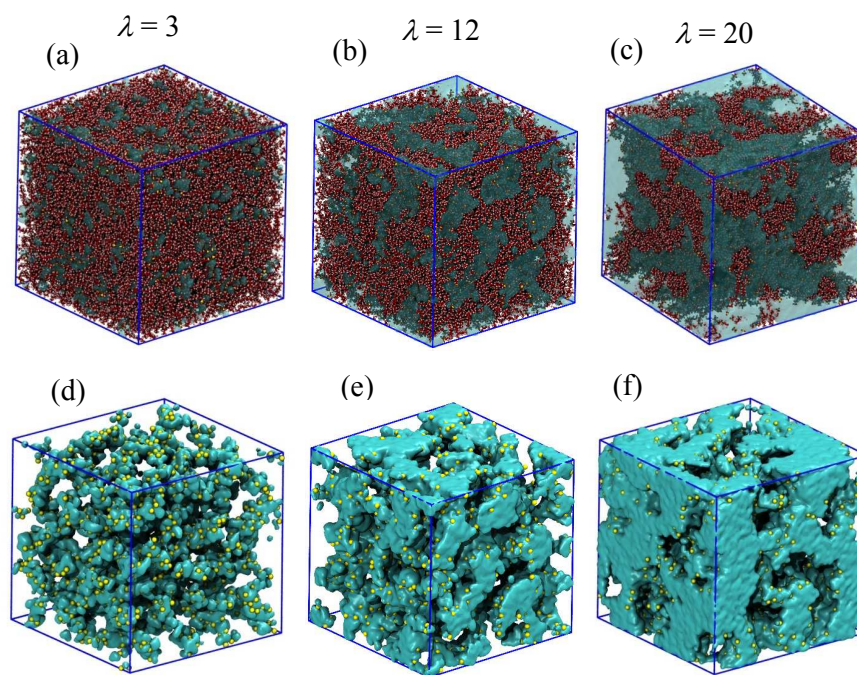


Figure S1. Snapshots from the MD simulations of medium-size models of *EW* 1144 PFSA membranes (upper panels) and isosurface representations of water domains including sulfonic groups (lower panels); (a, d): $\lambda = 3$, (b, e): $\lambda = 12$, and (c, f): $\lambda = 20$. Polymer chains are shown as dark red particles, sulfur atoms are represented as yellow particles, and the water region is drawn as a cyan solid contour.

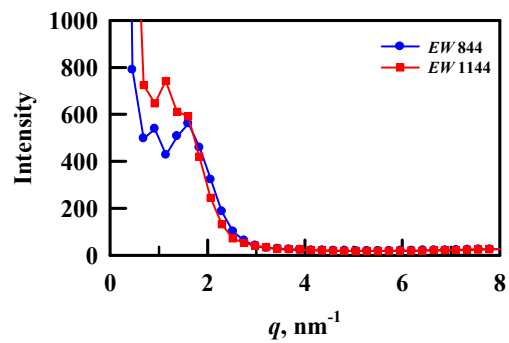


Figure S2. Structure factor of the *EW* 844 and *EW* 1144 PFSA membranes at $\lambda = 20$ obtained from the MD simulations of the large systems.