

Supporting Information

On the Relationship Between Polymer Electrolyte Structure and Hydrated Morphology of Perfluorosulfonic Acid Membranes

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TABLE S.1: Coordination number of each sulfur evaluated from the $S(SO_3^-)-S(SO_3^-)$ PCFs within the distance 0-8 Å at various water contents λ

λ	SSC with different EW				Nafion with different EW			
	678	778	878	978	744	844	944	1144
3	3.74	3.55	3.46	3.19	3.95	3.86	3.71	3.35
6	3.02	2.88	2.80	2.72	3.09	2.98	2.95	2.78
9	2.32	2.18	2.10	2.11	2.32	2.26	2.28	2.16
15	1.62	1.65	1.49	1.50	1.62	1.64	1.57	1.59
22	1.27	1.24	1.22	1.23	1.34	1.28	1.27	1.40

TABLE S.2: Hydration number of each sulfur evaluated from the $S(SO_3^-) - O(H_2O)$ PCFs within the distance 0-4.8 Å at various water contents λ

λ	SSC with different EW				Nafion with different EW			
	678	778	878	978	744	844	944	1144
3	3.30	3.25	3.22	3.13	3.53	3.57	3.65	3.40
6	6.27	6.09	6.11	5.94	6.58	6.45	6.57	6.46
9	7.41	7.31	7.20	7.18	7.40	7.33	7.42	7.38
15	8.18	8.12	8.02	8.03	7.93	7.93	8.02	7.84
22	8.50	8.50	8.39	8.36	8.17	8.18	8.17	8.12

TABLE S.3: Hydronium ion coordination number of each sulfur evaluated from the $S(SO_3^-) - O(H_3O^+)$ PCFs within the distance 0-4.8 Å at various water contents λ

λ	SSC with different EW				Nafion with different EW			
	678	778	878	978	744	844	944	1144
3	2.05	2.03	2.03	1.94	1.99	2.00	1.96	1.93
6	1.16	1.20	1.17	1.19	0.98	0.99	1.00	0.97
9	0.82	0.79	0.77	0.80	0.70	0.69	0.72	0.69
15	0.56	0.58	0.56	0.56	0.50	0.49	0.50	0.52
22	0.44	0.45	0.46	0.46	0.40	0.40	0.41	0.43

TABLE S.4: Water coordination number of each hydronium ion evaluated from the $O(H_2O) - O(H_3O^+)$ PCFs within the distance 0-3.2 Å at various water contents λ

λ	SSC with different EW				Nafion with different EW			
	678	778	878	978	744	844	944	1144
3	1.63	1.62	1.61	1.63	1.81	1.81	1.82	1.78
6	2.81	2.73	2.76	2.72	3.12	3.08	3.10	3.07
9	3.23	3.21	3.19	3.16	3.44	3.43	3.42	3.42
15	3.52	3.47	3.47	3.46	3.67	3.66	3.66	3.60
22	3.65	3.63	3.58	3.59	3.77	3.77	3.74	3.70

TABLE S.5: Coordination number of each water molecule evaluated from the $O(H_2O) - O(H_2O)$ PCFs within the distance 0-5.2 Å at various water contents λ

λ	SSC with different EW				Nafion with different EW			
	678	778	878	978	744	844	944	1144
3	2.97	2.92	2.78	2.57	2.97	3.02	2.97	2.77
6	6.91	6.94	6.67	6.59	7.20	7.21	7.34	7.12
9	9.62	9.35	9.11	9.10	10.17	10.11	10.10	9.88
15	12.38	12.57	12.23	12.31	13.05	13.13	13.08	12.96
22	14.01	14.18	14.05	14.00	14.66	14.53	14.64	14.70

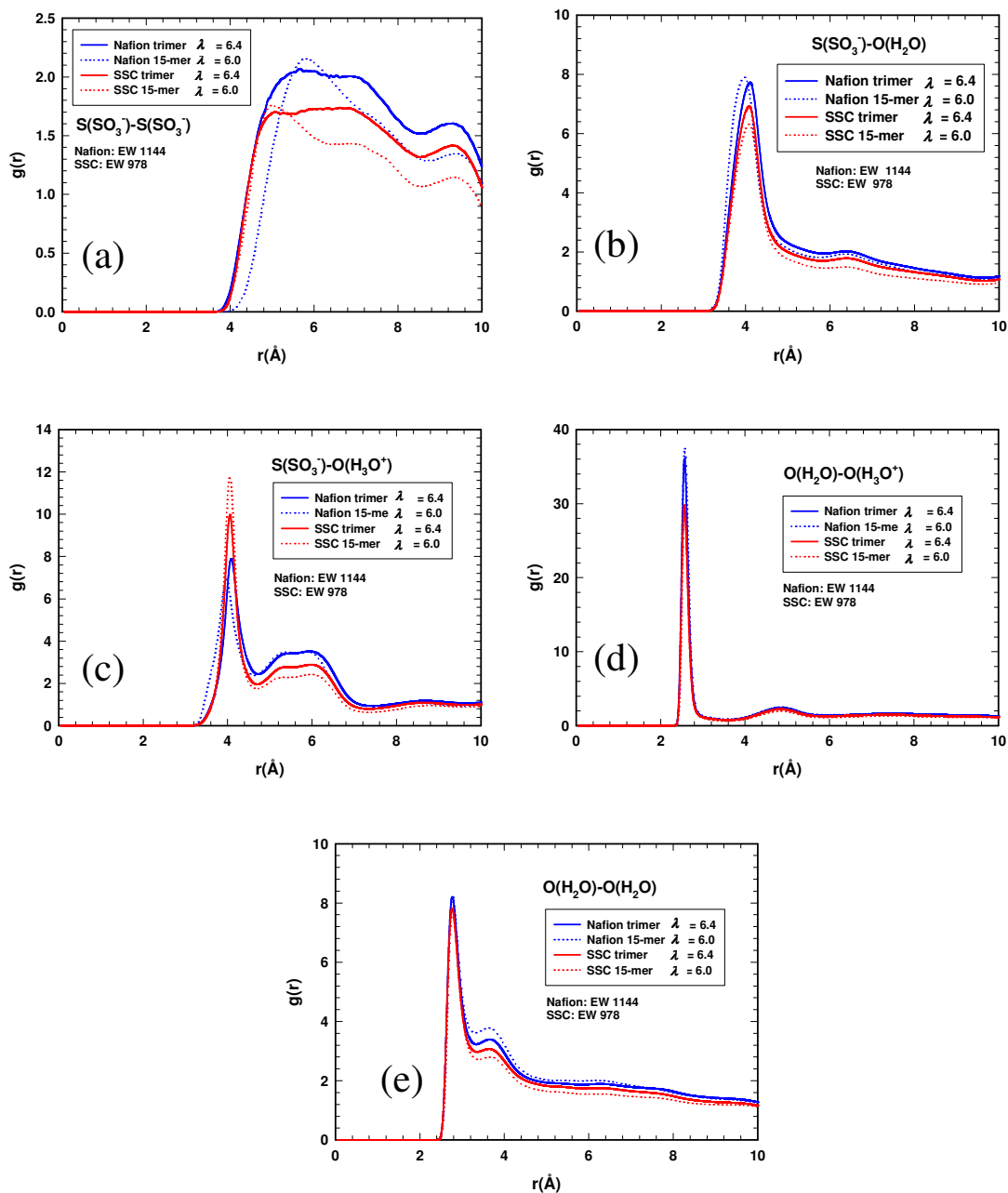


Figure S.1. Comparison of pair correlation functions for hydrated membranes composed of three and 15 monomers. (a) Sulfur-sulfur; (b) Sulfur-water (oxygen atom of water molecule); (c) Sulfur-hydronium ion (oxygen atom); (d) water-hydronium ion; and (e) water-water.

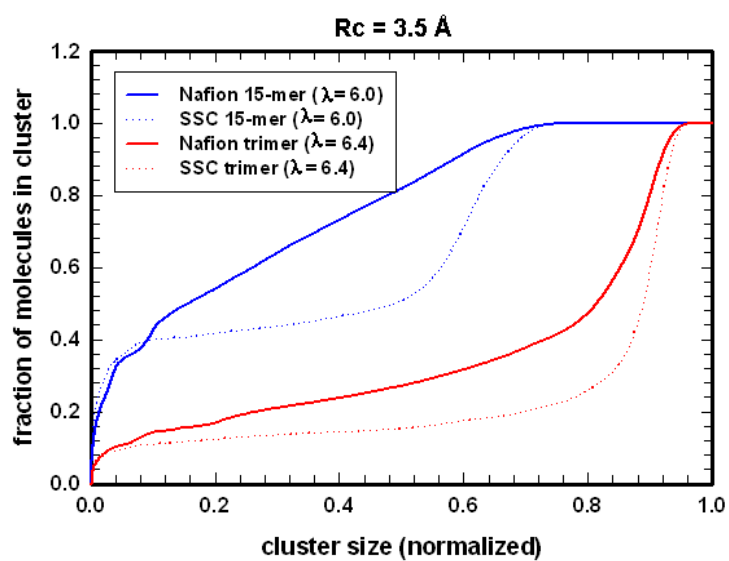


Figure S.2. Cumulative probability distribution functions for number of water molecules in a cluster for a cut-off distance of 3.5 Å at intermediate water contents: Comparison as a function of molecular weight.