Molecular Dynamics Simulations of Proton Transport in 3M and Nafion Perfluorosulfonic Acid Membranes

Ying-Lung Steve Tse[a,d,†], Andrew M. Herring[a,b], Kwiseon Kim[c], Gregory A. Voth[d,*]

[a]Renewable Energy Materials Research Science and Engineering Center, Colorado School of Mines, Golden, CO 80401, USA

[b]Department of Chemical and Biological Engineering, Colorado School of Mines, Golden, CO 80401, USA

[c]Computational Science Center, National Renewable Energy Laboratory, Golden, CO 80401, USA

[d]Department of Chemistry, James Franck Institute, and Computation Institute, the University of Chicago, Chicago, IL 60637, USA

Supporting Information

Table S1: Densities (g/cm^3) of Nafion and 3M with F3C or SPC/Fw water at different temperatures and hydration levels (λ). The external pressure was set at 1 atm.

λ	Nafion 300 K SPC/Fw	Nafion 300 K F3C	Nafion 353 K SPC/Fw	Nafion 353 K F3C	3M 300 K SPC/Fw	3M 300 K F3C	3M 353 K SPC/Fw	3M 353 K F3C
5	1.73	1.76	1.68	1.69	1.75	1.79	1.73	1.74
9	1.68	1.65	1.63	1.65	1.67	1.69	1.63	1.65
14	1.58	1.57	1.56	1.56	1.58	1.60	1.54	1.54

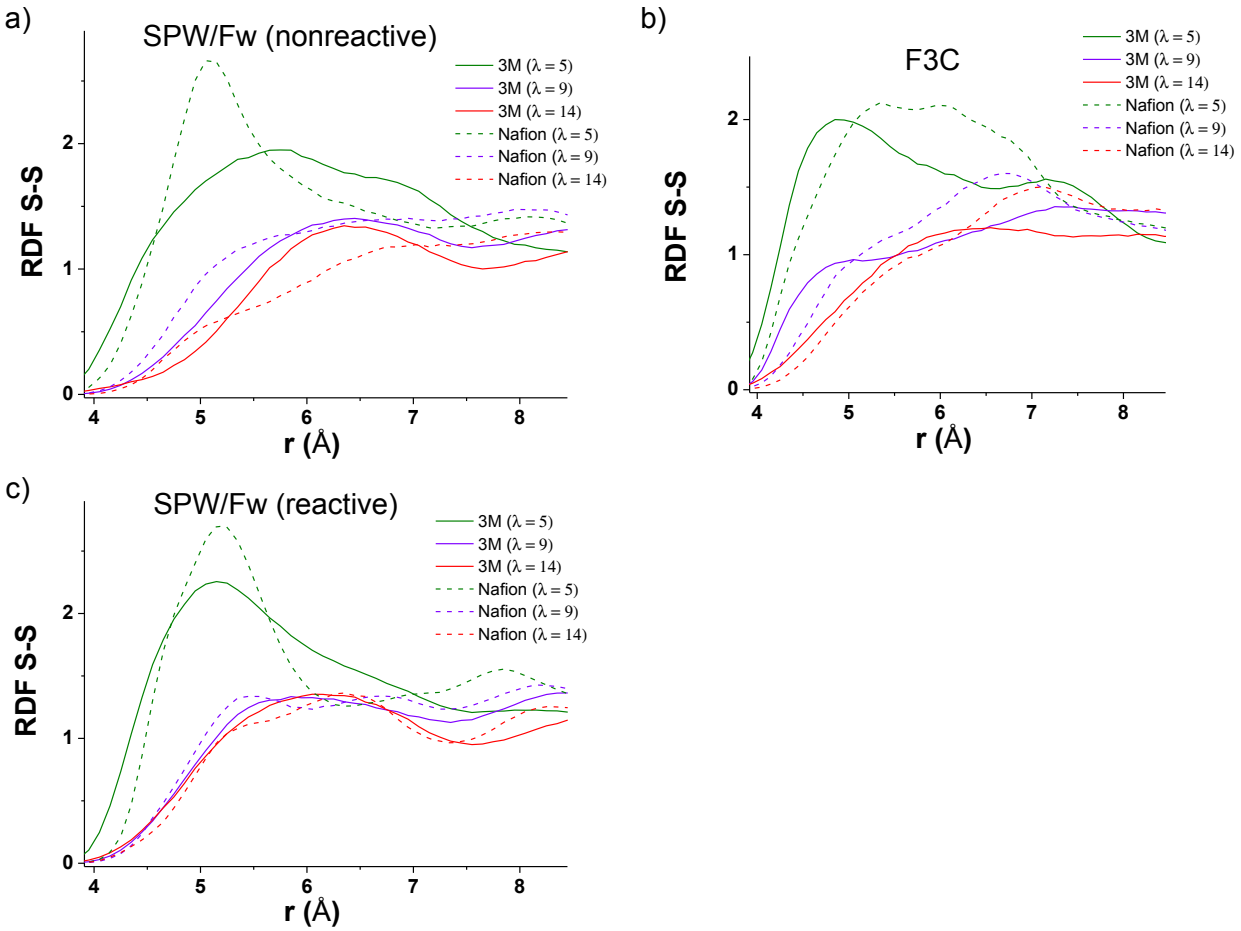

Figure S1. RDFs between the sulfonates as a function of hydration levels for the SPC/Fw water with nonreactive dynamics. The solid and dash lines are for 3M and Nafion respectively. The temperature is 300 K. b) For the F3C water (nonreactive) model. c) for SPC/Fw with reactive dynamics (MS-EVB).

Table S2: The coordination numbers for F3C water and hydronium in the first solvation shell around a sulfonate sulfur which is defined to between 0 and 4.25 Å.

λ	No. of hydronium oxygens in the range of 0 to 4.25 Å from sulfonate sulfur. F3C				No. of F3C water in the range of 0 to 4.25 Å			
	3M 300 K	3M 353 K	Nafion 300 K	Nafion 353 K	3M 300 K	3M 353 K	Nafion 300 K	Nafion 353 K
5	1.46	1.55	1.64	1.72	3.64	3.30	3.56	3.39
9	0.83	0.88	1.06	1.09	4.78	4.57	4.65	4.66
14	0.56	0.61	0.80	0.81	5.31	5.07	5.23	5.06