

**Enhanced Hydronium Ion Diffusion in Proton Exchange Membranes
Reinforced with Multilayer Graphene Oxide: New Insights on Water
Retention and Ion Mobility using Molecular Dynamics Simulation**

Sachin Kumar Varshney¹, Poornesh Kumar Koorata^{1*}

*¹Electrochemical Energy System Design Lab, Department of Mechanical Engineering,
National Institute of Technology Karnataka, Surathkal, Mangalore - 575 025, India*

Tel.: +91-824-247-3890

Fax: +91-824-247-4033

*Corresponding Author: kpkoorata@nitk.edu.in

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1. Dreiding Force Field parameters

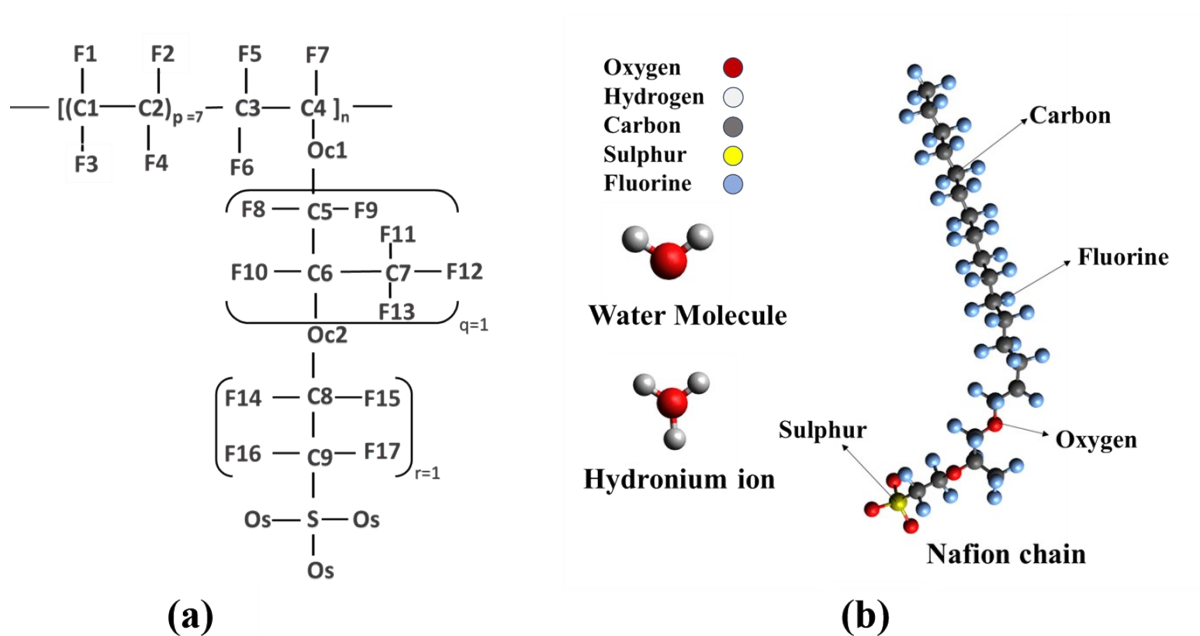


Figure S1: (a) The molecular composition of Nafion[®], where $p = 7$ and $q = r = 1$, (b) The atom models depicted in the figure consist of Hydronium ion, Water molecules, and Nafion[®] chain.

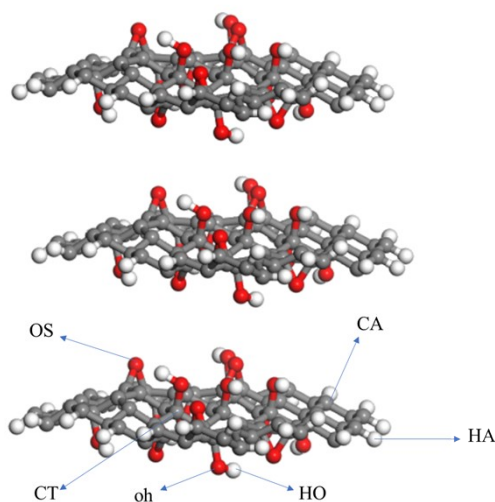


Figure S2: Detail of multilayer GO atoms.

Table S1: Details of partial charge

Atom type	Partial charge
C1, C2	0.54
C3	0.50
C4	0.46
C5	0.84
C6	0.41
C7	0.84
C8	0.84
C9	0.31
F1, F2, F3, F4	0.27
F5, F6	-0.25
F7	-0.22
F8, F9	-0.24
F10	-0.27
F11, F12, F13	-0.28
F14, F15	-0.24
F16, F17	-0.31
Oc1	-0.50
Oc2	-0.54
S	1.08
O _s	-0.61
O (Oxygen of Water molecule)	-0.82
O _h (Oxygen of Hydronium molecule)	-0.3818
H	0.41
H _h	0.4606

Table S2: Bond parameters for Dreiding Force Field

S.No.	Species	$K_b(\text{kcal/mol } \text{\AA}^2)$	$R_o(\text{\AA})$
1.	C1-C1	429.320	1.4982
2.	C1-C2	700.0	1.53
3.	C2-C2	700.0	1.53
4.	C-F	605.259	1.336
5.	C2-O	700.0	1.42
6.	S-O	700.0	1.48
7.	S-C2	700.0	1.80
8.	H _h -O _h	1085.96	0.982
9.	H _w -O _w	500.0	1.00
10.	CT-CT	700	1.53
11.	CA-CA	1400	1.39
12.	CA-CT	700	1.39
13.	CA-HA	700	1.02
14.	HO-oh	700	0.98

Table S3: Angle parameters for Dreiding Force Field

S.No.	Species	$K_a(\text{kcal/mol rad}^2)$	$\Theta(\text{degrees})$
1.	O-S-O	350.0	115.50
2.	O-S-C2	350.0	109.47
3.	S-C2-F	100.0	109.47
4.	X-C-X	100.0	109.47
5.	C-C-C	106.27	122.55
6.	C-C-F	100.34	118.32

7.	F-C-F	108.24	121.50
8.	H _h -O _h -H _h	79.03	113.40
9.	H _w -O _w -H _w	120.0	109.47
10.	X-CA-X	120	100
11.	X-CT-X	109.471	100
12.	CT-OS-CT	104.51	100
13.	CT-oh-HO	104.51	100

Table S4: Dihedral parameters for Dreiding Force Field

S.No.	Species	K _Φ	d	n
1	X-C-C-X	1.0000	-1	3
2	C1-C1-C1-C1	3.2171	1	3
3	F-C1-C1-C1	4.1222	1	3
4	F-C1-C1-F	4.0424	-1	3
5	X-C-O-X	1.0000	-1	3
6	X-C-S-X	1.0000	-1	3
7	X-CA-CT-X	1	1	3
8	CA-CA-CA-CA	12.5	1	3
9	X-CT-CT-X	0.5	1	3

Table S5: Lennard-Jones potential for Dreiding Force Field

S.No.	Atom type	epsilon(kcal/mol)	sigma(Å)
1.	S	0.344	4.03
2.	O	0.0957	3.4046
3.	C1	0.0844	3.8837
4.	C2	0.0951	3.8983
5.	F	0.0496	3.3953
6.	O _h , O _w	0.1848	3.1655

7.	H_h, H_w	0.01	0.8018
8.	CT	0.0951	3.8983
9.	CA	0.0951	3.8983
10.	oh	0.0957	3.4046
11.	OS	0.0957	3.4046
12.	HA	0.0152	3.195
13.	HO	0.0152	3.195

Table S6: Diffusion coefficient of hydronium ion (D_h) ($\times 10^{-5}$ cm²/s) at 300K.

Hydration Level(λ)	Nafion ($\times 10^{-5}$ cm ² /s)	Nafion/GO-multilayer ($\times 10^{-5}$ cm ² /s)
3.5	0.0059	0.0035
7	0.04591	0.02437
10	0.10066	0.23417
13	0.24602	0.29018
16	0.3067	0.36915
20	0.40232	0.52272

Table S7: Diffusion coefficient of hydronium ion (D_h) ($\times 10^{-5} \text{ cm}^2/\text{s}$) at 350K.

Hydration Level(λ)	Nafion ($\times 10^{-5} \text{ cm}^2/\text{s}$)	Nafion/GO-multilayer ($\times 10^{-5} \text{ cm}^2/\text{s}$)
3.5	0.00864	0.00575
7	0.10934	0.0646
10	0.21115	0.36604
13	0.4004	0.43507
16	0.61525	0.68235
20	0.7945	0.89183