APPENDICES

APPENDIC A

ATOM TYPES AND FORCE FIELD LIBRARY FILES OF NAFION SIDE CHAIN FOR CHAPTER 2

Atom types file of Nafion side chain

- First, second and last columns are atom name, atom type and particle charge each of atom by respectively.

This is a remark line

molecule.res

UNK INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.522	111.1	.0	.00000
4	O2	O	M	3	2	1	1.540	111.208	180.000	-0.565313
5	S1	SO	M	4	3	2	1.483	72.290	131.671	0.957791
6	O3	O	E	5	4	3	1.479	115.066	-155.196	-0.568003
7	O4	O	E	5	4	3	1.477	115.798	-15.532	-0.563128
8	C5	CT	M	5	4	3	1.887	102.403	94.060	0.143303
9	F6	F	E	8	5	4	1.362	109.682	-66.914	-0.156160
10	F7	F	E	8	5	4	1.362	109.875	174.800	-0.154226

11	C8	CT	M	8	5	4	1.545	117.041	52.917	0.464168
12	F9	F	E	11	8	5	1.367	109.554	178.417	-0.171362
13	F10	F	E	11	8	5	1.344	110.967	-64.321	-0.163274
14	O11	OS	M	14	11	8	1.382	122.426	-167.285	0.271330
16	C13	CT	3	15	14	11	1.554	106.515	-128.317	0.338076
17	F1	F	E	16	15	14	1.341	108.872	65.971	-0.115090
18	F15	F	E	16	15	14	1.336	111.785	-54.258	-0.115941
19	F16	F	E	16	15	14	1.347	110.835	-175.344	-0.142704
20	F17	F	E	15	14	11	1.368	114.273	-11.689	-0.141405
21	C18	CT	M	15	14	11	1.560	109.591	108.800	0.353715
22	F19	F	E	21	15	14	1.348	109.696	66.316	-0.111988
23	F20	F	E	21	15	14	1.362	108.906	-176.783	-0.162546
24	O21	OS	M	21	15	14	1.370	107.941	-56.954	-0.224090
25	C22	CT	M	24	21	15	1.382	120.416	159.669	0.493847
26	F24	F	E	25	24	21	1.321	112.890	-71.026	-0.104389
27	F25	F	E	25	24	21	1.354	110.756	50.204	-0.160713
28	F23	F	M	25	24	21	1.326	106.550	167.845	-0.113053

LOOP

IMPROPER

DONE

STOP

Force field library file of Nafion side chain

remark goes here

MASS

O 16.000	0.434	same as o
SO 32.060	2.900	ATTN, need revision
CT 12.010	0.878	same as c3
F 19.000	0.320	same as f
OS 16.000	0.465	same as os

BOND

O -SO	330.70	1.600	ATTN, need revision
SO-CT	226.40	1.820	ATTN, need revision
CT-F	363.80	1.344	same as c3-f
CT-CT	303.10	1.535	same as c3-c3
CT-OS	301.50	1.439	same as c3-os

ANGLE

O -SO-O	68.000	116.170	ATTN, need revision
O -SO-CT	63.800	106.820	ATTN, need revision
SO-CT-F	55.185	108.950	ATTN, need revision
SO-CT-CT	50.000	114.700	ATTN, need revision
CT-CT-F	66.200	109.410	same as c3-c3-f
CT-CT-OS	67.800	108.420	same as c3-c3-os
F -CT-F	71.300	107.160	same as f -c3-f

CT-OS-CT	62.100	113.410	same as c3-os-c3
F -CT-OS	70.168	108.700	Calculated with empirical approach
CT-CT-CT	63.200	110.630	same as c3-c3-c3

DIHE

O -SO-CT-F	1	0.333	0.000	3.000	ATTN, need revision
O -SO-CT-CT	1	0.333	0.000	3.000	ATTN, need revision
SO-CT-CT-F	1	0.156	0.000	3.000	ATTN, need revision
SO-CT-CT-OS	1	0.156	0.000	3.000	ATTN, need revision
CT-CT-OS-CT	1	0.383	0.000	3.000	same as X -c3-os-X
F -CT-CT-F	1	0.156	0.000	3.000	same as X -c3-c3-X
F -CT-CT-OS	1	0.156	0.000	3.000	same as X -c3-c3-X
CT-OS-CT-F	1	0.383	0.000	3.000	same as X -c3-os-X
OS-CT-CT-OS	1	0.156	0.000	3.000	same as X -c3-c3-X
CT-CT-CT-F	1	0.156	0.000	3.000	same as X -c3-c3-X
CT-CT-CT-OS	1	0.156	0.000	3.000	same as X -c3-c3-X

IMPROPER

NONBON

O	1.6612	0.2100	same as o
SO	2.0000	0.2500	ATTN, need revision
CT	1.9080	0.1094	same as c3
F	1.7500	0.0610	same as f
OS	1.6837	0.1700	same as os

APPENDIC B

ATOM TYPE AND FORCE FIELD LIBRARY FILES OF HYDRONIUM ION FOR CHAPTER 2

Atom types file of hydronium ion

```
This is a remark line
molecule.res
H3O    INT  0
CORRECT     OMIT DU   BEG
  0.0000
   1  DUMM DU    M    0  -1  -2     0.000     .0          .0         .00000
   2  DUMM DU    M    1   0  -1     1.449     .0          .0         .00000
   3  DUMM DU    M    2   1   0     1.522   111.1         .0         .00000
   4  O1         OH   M    3   2   1     1.540   111.208   180.000  -0.567033
   5  H2         HO   E    4   3   2     0.989   163.123    90.000    0.521665
   6  H3         HO   E    4   3   2     0.988    61.408   160.688    0.522684
   7  H4         HO   E    4   3   2     0.988    61.408    19.312    0.522684
LOOP
IMPROPER
DONE
STOP
```

Force field library files of hydronium ion

remark goes here

MASS

OH	16.000	0.465	same as oh
HO	1.008	0.135	same as ho

BOND

OH-HO	369.60	0.974	same as ho-oh

ANGLE

HO-OH-HO	41.900	104.800	same as ho-oh-ho

DIHE

IMPROPER

NONBON

OH	1.7210	0.2104	same as oh
HO	0.0000	0.0000	same as ho

APPENDIC C

ATOM TYPE AND FORCE FIELD LIBRARY FILES OF KRYTOX-SILICA FOR CHAPTER 2

Atom types file of Krytox-Silica

This is a remark line

molecule.res

MOL INT 0

CORRECT OMIT DU BEG

0.0000

1	DUMM	DU	M	0	-1	-2	0.000	.0	.0	.00000
2	DUMM	DU	M	1	0	-1	1.449	.0	.0	.00000
3	DUMM	DU	M	2	1	0	1.522	111.100	.0	.00000
4	F3	F	M	3	2	1	1.540	111.208	180.000	-0.26000
5	C2	CT	M	4	3	2	1.312	71.097	105.324	0.78000
6	F4	F	E	5	4	3	1.311	108.787	-123.190	-0.26000
7	F5	F	E	5	4	3	1.312	108.928	118.258	-0.26000
8	C1	CT	M	5	4	3	1.535	110.796	-3.798	0.52000
9	F2	F	E	8	5	4	1.324	107.674	-175.432	-0.26000
10	F11	F	E	8	5	4	1.326	107.469	-57.586	-0.26000
11	C3	CT	M	8	5	4	1.535	115.635	63.500	0.68000
12	F1	F	E	11	8	5	1.322	109.541	-55.327	-0.26000
13	F6	F	E	11	8	5	1.326	109.788	62.278	-0.26000

14	O1	OS	M	11	8	5	1.352	107.798	-176.031	-0.32000
15	C4	CT	M	14	11		1.377	121.142	-157.026	0.42000
16	C5	CT	3	15	14	11	1.535	105.261	-165.005	0.78000
17	F7	F	E	16	15	14	1.315	108.991	-176.280	-0.26000
18	F8	F	E	16	15	14	1.315	111.266	-56.363	-0.26000
19	F9	F	E	16	15	14	1.308	110.189	64.283	-0.26000
20	F10	F	E	15	14	11	1.349	110.241	-51.033	-0.26000
21	C6	C	M	15	14	11	1.547	112.547	73.519	0.45000
22	O2	O	E	21	15	14	1.195	117.641	46.968	-0.45000
23	N1	N	M	21	15	14	1.332	115.057	-135.124	-0.57400
24	H2	H	E	23	21	15	0.994	118.413	3.599	0.35100
25	C7	CT	M	23	21	15	1.458	123.377	-177.093	0.11700
26	H1	H1	E	25	23	21	1.084	108.243	-121.679	0.05300
27	H13	H1	E	25	23	21	1.080	107.045	-5.701	0.05300
28	C8	CT	M	25	23	21	1.529	112.511	116.352	-0.10600
29	H14	HC	E	28	25	23	1.088	109.166	59.297	0.05300
30	H15	HC	E	28	25	23	1.086	107.605	174.234	0.05300
31	C9	CT	M	28	25	23	1.534	113.478	-63.861	-0.10600
32	Si2	Si	3	31	28	25	1.865	115.308	177.964	0.22980
33	O3	OH	S	32	31	28	1.636	113.078	-54.025	-0.48660
34	H3	HO	E	33	32	31	0.952	116.882	-105.752	0.41000
35	O4	OH	S	32	31	28	1.631	107.769	67.092	-0.48660
36	H4	HO	E	35	32	31	0.947	117.787	-167.271	0.41000
37	O5	OS	S	32	31	28	1.644	108.550	-173.086	-0.15320

38	Si1	Si	3	37	32	31	1.609	138.417	87.754	0.30640
39	O6	OH	S	38	37	32	1.633	110.975	-87.322	-0.48660
40	H5	HO	E	39	38	37	0.954	118.725	-63.963	0.41000
41	O7	OH	S	38	37	32	1.632	107.360	30.713	-0.48660
42	H6	HO	E	41	38	37	0.951	116.092	151.518	0.41000
43	O8	OS	S	38	37	32	1.625	109.994	151.157	-0.15320
44	Si3	Si	3	43	38	37	1.619	135.042	-162.512	0.30640
45	O9	OH	S	44	43	38	1.633	105.512	25.496	-0.48660
46	H7	HO	E	45	44	43	0.952	116.200	-158.272	0.41000
47	O10	OH	S	44	43	38	1.621	111.356	145.262	-0.48660
48	H8	HO	E	47	44	43	0.947	118.647	78.585	0.41000
49	O11	OS	S	44	43	38	1.627	109.620	-93.098	-0.15320
50	Si4	Si	3	49	44	43	1.617	138.426	132.458	0.30640
51	O12	OH	S	50	49	44	1.638	104.296	13.827	-0.48660
52	H9	HO	E	51	50	49	0.947	117.779	162.220	0.41000
53	O13	OH	S	50	49	44	1.620	113.114	133.083	-0.48660
54	H10	HO	E	53	50	49	0.951	116.620	105.525	0.41000
55	O14	OS	S	50	49	44	1.624	109.210	-105.358	-0.15320
56	Si5	Si	3	55	50	49	1.617	142.570	-122.451	0.30640
57	O15	OS	S	56	55	50	1.611	110.089	133.201	-0.15320
58	Si6	Si	3	57	56	55	1.623	147.497	21.297	0.30640
59	O18	OH	S	58	57	56	1.647	109.497	-82.032	-0.48660
60	H18	HO	E	59	58	57	0.948	117.932	-65.791	0.41000
61	O19	OH	S	58	57	56	1.615	112.270	35.993	-0.48660

62	H19	HO	E	61	58	57	0.955	118.183	-102.310	0.41000
63	O20	OH	S	58	57	56	1.621	104.936	157.348	-0.48660
64	H20	HO	E	63	58	57	0.947	116.969	-165.911	0.41000
65	O16	OH	S	56	55	50	1.625	112.715	-103.993	-0.48660
66	H11	HO	E	65	56	55	0.947	118.364	-91.817	0.41000
67	O17	OH	S	56	55	50	1.636	104.532	12.731	-0.48660
68	H12	HO	E	67	56	55	0.948	117.845	-166.898	0.41000
69	H16	HC	E	31	28	25	1.089	109.773	-59.650	0.05300
70	H17	HC	E	31	28	25	1.088	109.962	56.566	0.05300

LOOP

IMPROPER

C4 N1 C6 O2

C6 C7 N1 H2

DONE

STOP

Force field library files of Krytox-Silica

remark goes here

MASS

F 19.000	0.320	same as f
CT 12.010	0.878	same as c3
OS 16.000	0.465	same as os
C 12.010	0.616	same as c
O 16.000	0.434	same as o
N 14.010	0.530	same as n
H 1.008	0.161	same as hn
H1 1.008	0.135	same as hc
HC 1.008	0.135	same as hc
Si 28.086	1.100	ATTN, need revision
OH 16.000	0.465	same as oh
HO 1.008	0.135	same as ho

BOND

F -CT	363.80	1.344	same as c3-f
CT-CT	303.10	1.535	same as c3-c3
CT-OS	301.50	1.439	same as c3-os
CT-C	328.30	1.508	same as c -c3
C -O	648.00	1.214	same as c -o
C -N	478.20	1.345	same as c -n
N -H	410.20	1.009	same as hn-n

N -CT	330.60	1.460	same as c3-n
CT-H1	337.30	1.092	same as c3-hc
CT-HC	337.30	1.092	same as c3-hc
CT-Si	238.00	1.809	ATTN, need revision
Si-OH	392.80	1.665	ATTN, need revision
Si-OS	392.80	1.665	ATTN, need revision
OH-HO	369.60	0.974	same as ho-oh

ANGLE

F -CT-F	71.300	107.160	same as f -c3-f
F -CT-CT	66.200	109.410	same as c3-c3-f
CT-CT-CT	63.200	110.630	same as c3-c3-c3
CT-CT-OS	67.800	108.420	same as c3-c3-os
CT-OS-CT	62.100	113.410	same as c3-os-c3
F -CT-OS	70.168	108.700	Calculated with empirical approach
OS-CT-C	68.000	109.820	same as c -c3-os
CT-C -O	68.000	123.110	same as c3-c -o
CT-C -N	67.900	115.150	same as c3-c -n
CT-CT-C	63.800	110.530	same as c -c3-c3
F -CT-C	63.719	110.055	Calculated with empirical approach
C -N -H	49.200	118.460	same as c -n -hn
C -N -CT	63.900	121.350	same as c -n -c3
O -C -N	75.800	122.030	same as n -c -o
N -CT-H1	49.800	109.500	same as hc-c3-n

N -CT-CT	65.900	112.130	same as c3-c3-n
H -N -CT	46.000	116.780	same as c3-n -hn
CT-CT-HC	46.400	110.050	same as c3-c3-hc
H1-CT-H1	39.400	108.350	same as hc-c3-hc
H1-CT-CT	33.235	109.490	Calculated with empirical approach
CT-CT-Si	44.400	113.500	ATTN, need revision
HC-CT-HC	39.400	108.350	same as hc-c3-hc
CT-Si-OH	44.400	113.500	ATTN, need revision
CT-Si-OS	44.400	113.500	ATTN, need revision
Si-CT-HC	34.500	112.300	ATTN, need revision
Si-OH-HO	56.400	124.100	ATTN, need revision
Si-OS-Si	31.100	149.800	ATTN, need revision
OH-Si-OH	42.300	113.100	ATTN, need revision
OH-Si-OS	42.300	113.100	ATTN, need revision
OS-Si-OS	42.300	113.100	ATTN, need revision

DIHE

F -CT-CT-F	1	0.156	0.000	3.000	same as X -c3-c3-X
F -CT-CT-CT	1	0.156	0.000	3.000	same as X -c3-c3-X
CT-CT-CT-OS	1	0.156	0.000	3.000	same as X -c3-c3-X
CT-CT-OS-CT	1	0.383	0.000	3.000	same as X -c3-os-X
F -CT-CT-OS	1	0.156	0.000	3.000	same as X -c3-c3-X
CT-OS-CT-F	1	0.383	0.000	3.000	same as X -c3-os-X
CT-OS-CT-C	1	0.383	0.000	3.000	same as X -c3-os-X

OS-CT-C -O	1	0.000	180.000	2.000	same as X -c -c3-X
OS-CT-C -N	1	0.000	180.000	2.000	same as X -c -c3-X
CT-C -N -H	1	2.500	180.000	2.000	same as X -c -n -X
CT-C -N -CT	1	2.500	180.000	2.000	same as X -c -n -X
CT-CT-C -O	1	0.000	180.000	2.000	same as X -c -c3-X
CT-CT-C -N	1	0.000	180.000	2.000	same as X -c -c3-X
F -CT-CT-C	1	0.156	0.000	3.000	same as X -c3-c3-X
F -CT-C -O	1	0.000	180.000	2.000	same as X -c -c3-X
F -CT-C -N	1	0.000	180.000	2.000	same as X -c -c3-X
C -N -CT-H1	1	0.000	0.000	2.000	same as X -c3-n -X
C -N -CT-CT	1	0.000	0.000	2.000	same as X -c3-n -X
O -C -N -H	1	2.500	180.000	2.000	same as X -c -n -X
O -C -N -CT	1	2.500	180.000	2.000	same as X -c -n -X
N -CT-CT-HC	1	0.156	0.000	3.000	same as X -c3-c3-X
N -CT-CT-CT	1	0.156	0.000	3.000	same as X -c3-c3-X
H -N -CT-H1	1	0.000	0.000	2.000	same as X -c3-n -X
H -N -CT-CT	1	0.000	0.000	2.000	same as X -c3-n -X
CT-CT-CT-Si	1	2.000	0.000	3.000	ATTN, need revision
CT-CT-CT-HC	1	0.156	0.000	3.000	same as X -c3-c3-X
H1-CT-CT-HC	1	0.156	0.000	3.000	same as X -c3-c3-X
H1-CT-CT-CT	1	0.156	0.000	3.000	same as X -c3-c3-X
CT-CT-Si-OH	1	-0.200	0.000	3.000	ATTN, need revision
CT-CT-Si-OS	1	-0.200	0.000	3.000	ATTN, need revision
HC-CT-CT-Si	1	2.000	0.000	3.000	ATTN, need revision

HC-CT-CT-HC	1	0.156	0.000	3.000	same as X -c3-c3-X
CT-Si-OH-HO	1	0.667	0.000	3.000	ATTN, need revision
CT-Si-OS-Si	1	0.800	0.000	3.000	ATTN, need revision
Si-OS-Si-OH	1	0.600	0.000	3.000	ATTN, need revision
Si-OS-Si-OS	1	0.600	0.000	3.000	ATTN, need revision
OH-Si-CT-HC	1	-0.200	0.000	3.000	ATTN, need revision
OH-Si-OH-HO	1	0.667	0.000	3.000	ATTN, need revision
HO-OH-Si-OS	1	0.667	0.000	3.000	ATTN, need revision
OS-Si-CT-HC	1	-0.200	0.000	3.000	ATTN, need revision

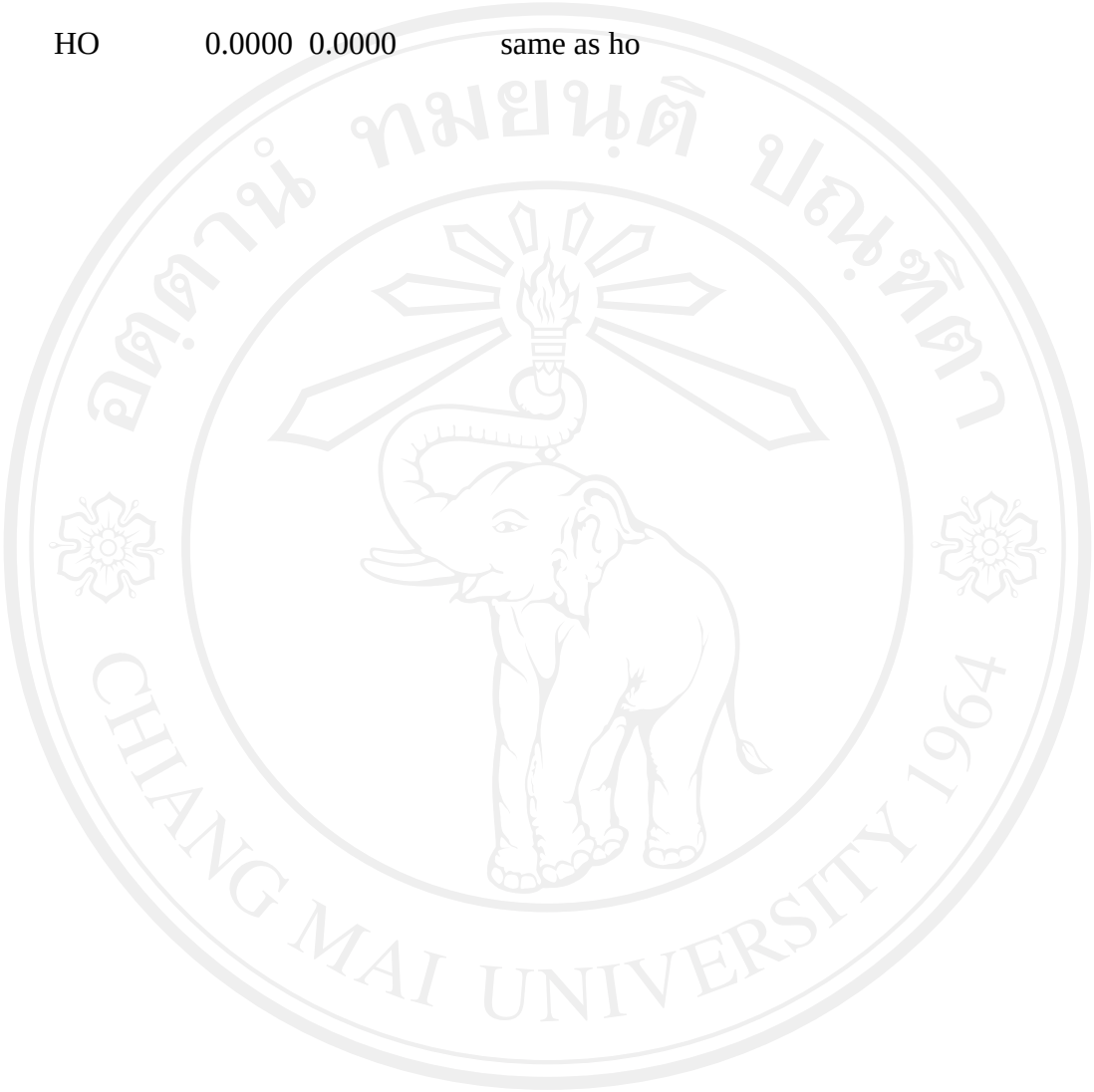
IMPROPER

CT-N -C -O	1.1	180.0	2.0	Using default value
C -CT-N -H	1.1	180.0	2.0	Using default value

NONBON

F	1.7500	0.0610	same as f
CT	1.9080	0.1094	same as c3
OS	1.6837	0.1700	same as os
C	1.9080	0.0860	same as c
O	1.6612	0.2100	same as o
N	1.8240	0.1700	same as n
H	0.6000	0.0157	same as hn
H1	1.4870	0.0157	same as hc
HC	1.4870	0.0157	same as hc

Si	3.1492	0.0710	ATTN, need revision
OH	1.7210	0.2104	same as oh
HO	0.0000	0.0000	same as ho



APPENDIC D

CALCULATION OF KRYTOX-SILICA STRUCTURE NUMBER FOR 5% WT KRYTOX-SILICA IN NAFION SYSTEM FOR CHAPTER 2

Molecular weigh of Krytox-Silic model

$(CF_3(CF_2)_2OCF(CF)_3CONH(CH_2)_2Si(OH)_2(OSi(OH)_2)_4OSi(OH)_3$

$= 839.6$ g/mol

Thus $= \dfrac{839.6 g/mol}{6.62\times10^{23} molecule/mol} = \dfrac{839.6g}{6.62\times10^{23} molecule}$

5% wt of Krytox-Silica $= \dfrac{5}{100} = \dfrac{Krytox-Silica(g)}{Nafion(g)}$

When add 1 Krytox-Silica molecule $= \dfrac{5}{100} = \dfrac{\frac{839.6}{6.62\times10^{23}}}{Nafion(g)}$

Molecular weigh of Nafion $= 1100$ g/mol

$= \dfrac{1100 g/mol}{6.62\times10^{23} molecules/mol}$

$= \dfrac{1100g}{6.62\times10^{23} molecules}$

$\therefore$ Nafion $Nafion(g) = \dfrac{839.6\times100}{6.62\times10^{23}\times5}$ g $= \dfrac{\frac{839.6\times100}{6.62\times10^{23}\times5} g}{\frac{1100g}{6.62\times10^{23} molecules}}$

≈ 15 molecules

Because of 1 Nafion molecule has 1 SO_3^- group thus equal to 15 Nafion molecules.

Hence, this system has 1 Krytox-Silica and 15 Nafion molecules.

APPENDIC E

PUBLICATIONS AND PRESENTATIONS

BY AUTHOR

Publications:

1. **Yana, J**.; Nimmanpipug, P.; Chirachanchai, S.; Gosalawit, R.; Dokmaisrijan, S.; Vannarat, S.; Vilaithong, T.; Lee, V.S.; "Molecular Dynamics Simulations of Krytox-Silica–Nafion Composite for high temperature fuel cell electrolyte membranes" *Polymer* **2010**, 51, 4632-4638. (impact factor = 3.828 source : Journal Citation Reports, 2010)
2. **Yana, J.**; Lee, V. S.; Nimmanpipug, P.; Aukkaravittayapun, S.; Vilaithong, T. "Dry and Wet Molecular Dynamics Simulations of Nafion® Polymer Electrolyte Fuel Cell Membrane" *Journal of Solid Mechanics and Materials Engineering* **2007**, 1, 556-563. (impact factor = 0.343 source : Journal Citation Reports, 2005)
3. **Yana, J.**; Lee, V.S.; Rattanachai, Y.; Songsiriritthigul, P.; Medhisuwakul, M.; Vannarat, S.; Dokmaisrijan, S.; Vilaithong, T.; Nimmanpipug, P.; "Computational and Experimental Study of Low Energy Ar^+ Bombardment on Nafion" *Surface and Coatings Technology* **2012**, (Accepted)

Presentations:

1. **Yana, J**.; Lee V. S. ; Vannarat, S.; Dokmaisrijan, S.; Medhisuwakul, M.; Vilaithong, T.; Nimmanpipug, P. “Molecular Simulations of Ion Sputter Coating on Nafion and Carbon Models as Alternative Catalyst in PEMFC Application” The Pure and Applied Chemistry Conference 2012 (PACCON2012), Chiang Mai University, Chiang Mai, Thailand, January 11-13, 2012. (Poster presentation)
2. **Yana, J**.; Lee V. S. ; Vannarat, S.; Dokmaisrijan, S.; Medhisuwakul, M.; Vilaithong, T.; Nimmanpipug, P. “Molecular Simulations of Ion Bombardment and Plasma Sputter Coating for Fuel Cell Application” 15th International Annual Symposium on Computational Science and Engineering (ANSCSE15)**,** Bangkok University, Bangkok, Thailand, March 29 – May 2, 2011. (Oral presentation)
3. **Yana, J**.; Lee V. S. ; Vannarat, S.; Dokmaisrijan, S.; Medhisuwakul, M.; Vilaithong, T.; Nimmanpipug, P. “Molecular Simulations of Ion Sputter Coating on Nafion and Carbon Models as Alternative Catalyst in PEMFC Application”, PERCH Congress VI, 4-7 May 2011, Jomtien Palm Beach Resort Pattaya, Thailand. (Oral presentation)
4. **Yana, J**.; Lee V. S. ; Songsiriritthigul, P.; Medhisuwakul, M.; Vannarat, S.; Dokmaisrijan, S.; Vilaithong, T.; Nimmanpipug, P. “Molecular Dynamics Simulation of Nafion Surface Modification by Ar^+ Beam Bombardment” 1st International Conference on Computation for Science and Technology (ICCST-I), Chiang Mai, Thailand, August 4-6, 2010. (Oral presentation)

5. **Yana, J**.; Lee V. S. ; Vannarat, S.; Dokmaisrijan, S.; Medhisuwakul, M.; Vilaithong, T.; Nimmanpipug, P. “MD Simulation of Nafion Surface Modification by Ar^+ Bombardment” 14th International Annual Symposium on Computational Science and Engineering (ANSCSE14)**,** Mae Fah Luang University, Chiangrai, Thailand, March 23-26, 2010. (Oral presentation)
6. **Yana, J**.; Lee V. S. ; Dokmaisrijan, S.; Songsiriritthigul, P.; Medhisuwakul, M.; Vannarat, S.; Vilaithong, T.; Nimmanpipug, P. “Theoretical Study of Effect of Ar^+ Bombardment on Nafion Side Chain” 14th International Annual Symposium on Computational Science and Engineering (ANSCSE13), Kasetsart University, Bangkok, Thailand, March 25-27, 2009. (Oral presentation)
7. **Yana, J**.; Lee V. S. ; Songsiriritthigul, P. ; Medhisuwakul, M.; Vannarat, S. ; Vilaithong, T.; Nimmanpipug, P. “Molecular Dynamics Simulations of Ion Bombardment on Nafion Side Chain Cluster Model” The Pure and Applied Chemistry Conference 2009 (PACCON2009), Naresuan University, Phitsanulok, Thailand, Jan 14-16 , 2009. (Oral presentation)
8. **Yana, J.**; Nimmanpipug, P.; Chirachanchai, S.; Aukkaravittayapun, S.; Vilaithong, T.; Kungwan , N.; Lee, V. S. “Molecular Dynamic Simulations of Krytox-Silica-Nafion Polymer Composite Based Modification of Polymer Electrolyte Fuel Cell Membrane at High Temperature” The Pure and Applied Chemistry Conference 2008 Bangkok, Thailand, Jan 30- Feb 1, 2008. (Poster presentation)

9. **Yana, J.**; Nimmanpipug, P.; Dokmaisrijan, S.; Aukkaravittayapun, S.; Lee, V. S. “Molecular Dynamic Simulations Study on the Role of Water Effecting the Proton Diffusion in Nafion® Fuel Cell Membrane”, PERCH Congress V, 6-9 May 2007, Jomtien Palm Beach Resort Pattaya, Thailand. (Poster presentation)
10. **Yana, J.**; Nimmanpipug, P.; Dokmaisrijan, S.; Aukkaravittayapun, S.; Lee, V. S. “Molecular Dynamic Simulations of Water Effecting on Proton Diffusion in Nafion® Polymer Electrolyte Fuel Cell Membrane”, 3rd Colloquium on Postgraduate Research National Postgraduate Colloquium on Materials, Minerals and Polymers 2007 (MAMIP2007), Vistana Hotel, Penang, Malaysia, April 10-11, 2007. (Poster presentation)
11. **Yana, J.**; Lee, V. S.; Nimmanpipug, P.; Aukkaravittayapun, S.; Vilaithong, T. “Molecular Dynamic Simulations of Krytox-Silica-Nafion® Composite in an Aqueous System”, NSTDA Annual Conference Science and Technology for National Productivity and Happiness (NAC2007), Thailand science park, Bangkok, Thailand, March 28-30, 2007. (Poster presentation)
12. Lee, V.S.; **Yana, J.**; Nimmanpipug, P.; Jitonnom, J.; Komhoi, P. “Atomistic Simulation and Molecular Dynamics for Polyoxyethylene / Polyethylenimine Blends” Asian Workshop on Polymer Processing (AWPP) 2006, Bangkok, Thailand, December 6-8, 2006.
13. **Yana, J.**; Nimmanpipug, P.; Dokmaisrijan, S.; Aukkaravittayapun, S.; Lee, V. S. “Dry and Wet Molecular Dynamics Simulations of Nafion® Polymer Electrolyte Fuel Cell Membrane”, Asian Symposium on Materials and Processing 2006 (ASMP2006), Sofitel Central Plaza, Bangkok, Thailand, November 9-10, 2006. (Oral presentation)

14. **Yana, J.**; Nimmanpipug, P; Lee, V. S. “Molecular Dynamics Simulations of Nafion® Polymer Electrolyte Membrane Fuel Cell in Proton, Hydronium and Water System”, Proceeding of the 10th Annual National Symposium on Computational Science Engineering (ANSCSE10), Chiang Mai University, Thailand, March 22-24, 2006. (Oral presentation)
15. **Yana, J.**; Nimmanpipug, P; Lee, V. S. “Proton Transfer Modeling of Nafion® polymer membrane electrolyte side chain”, 31st Congress Sci. Tech. Thailand, Suranaree University of Technology, Nakhon Ratchasima, October 18-20,2005. (Oral presentation)
16. **Yana, J.**; Nimmanpipug, P; Lee, V. S. “Molecular Dynamics Simulations of Nafion® Pendant Chain in Fuel Cell Membrane”, Proceeding of the 9th Annual National Symposium on Computational Science Engineering (ANSCSE9), Mahidol University, Thailand, Mahidol University, Thailand, March 23-25, 2005,391-396.

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