Supplementary Material for PCCP

Supplementary Information: The force field parameters

TABLE 1: Partial Charges on the PPFSA and Hydronium Ion, the atom numbers for Nafion-117 are illustrated in Figure 1.

	Atom type	Atom number	Partial Charges
PPFSA	C	1,1,1	0.2164
		2,2	0.1983
		3,3	0.3065
		4	0.3246
		5	-0.0805
	F	1	-0.1082
	O	1,1	-0.1802
	S		1.0559
	O_S		-0.5863
hydronium	H_h		0.416
	O_h		-0.248

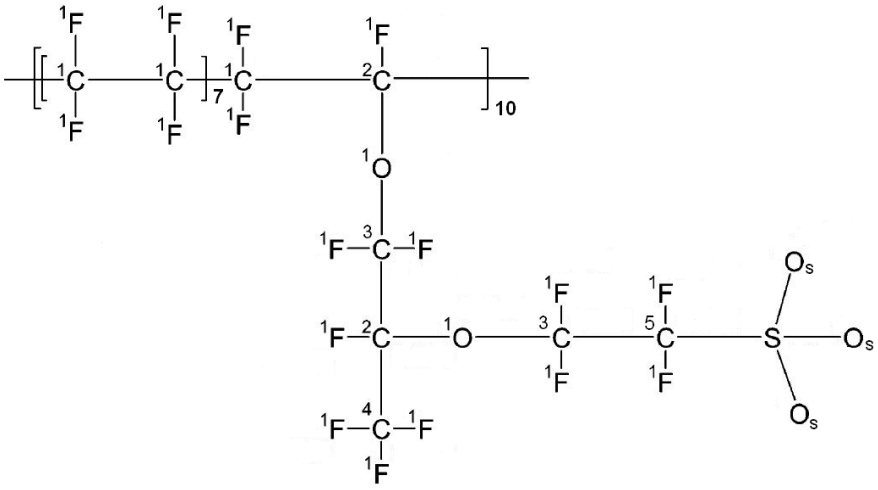

Fig. 1 The atom types and atom numbers in Nafion-117

TABLE 2: Force Field Parameters for the PPFSA and Hydronium Ion

Bond type	r_0 (Å)	k_b (kcal/mol/ Å^2)
C-C	1.5356	276.0580
C-S	1.8545	176.4593
C-F	1.3485	338.8046
C-O_E	1.3622	297.7457
O_S-S	1.4800	587.9230
H_h-O_h	0.9820	543.0000
Angle type	θ (degree)	k_θ(kcal/mol/rad^2)
C-C-C	109.0639	44.4644
C-C-S	115.2954	18.3324
C-C-O_E	110.7657	43.5794
C-S-O_S	112.0818	62.4607
O_S-S-O_S	125.8476	98.8656
F-C-C	106.7816	60.7610
F-C-O_E	108.9077	63.9312
F-C-F	107.9771	85.7607
F-C-S	109.7797	33.5332
C-O_E -C	120.6078	117.1048
H_h-O_h-H_h	113.0000	79.0263

Dihedral type	n=1, φ_0=0	n=2, φ_0=π	n=3, φ_0=0
	k_φ(kcal/mol/rad^2)	k_φ(kcal/mol/rad^2)	k_φ(kcal/mol/rad^2)
C-C-C-F	0	0	0.1570
F-C-C-F	0	0	-0.0490
C-C-C-C	0.4	-0.1980	0.1390
C-C-C-O_E	0	3.8543	-0.9799
F-C-C-O_E	0	4.5948	0.1692
C-O_E-C-F	0	1.7199	0.0824
C-C-O_E-C	0	1.7706	0.4405
O_E-C-C-S	0	0.5035	0.6250
F-C-C-S	0	-3.3082	-0.0612
C-C-S-O_S	0	2.4770	-0.1478
F-C-S-O_S	0	2.9759	0.1545
O_E-C-C- O_E	0	7.5972	1.2930

Van der Waals	ε (kcal/mol)	R (Å)
C	0.0660	3.9286
F	0.0530	3.3113
S	0.2500	3.9847
O_E	0.1400	3.2551
O_S	0.1700	3.3225
O_h	0.1848	3.5532