Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Characterization of Chain Conformations in Perfluorosulfonic Acid Membranes using Electron Energy Loss Spectroscopy

Chen Wang [a], Gerd Duscher [b,c*] and Stephen J. Paddison [a *]

[a] Department of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN 37996,USA

[b] Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN, 37996, USA

[c] Oak Ridge National Laboratory, Material Science & Technology Division, Oak Ridge, TN, 35763, USA

[*] Correspondence may be addressed to either: gduscher@utk.edu or spaddison@utk.edu

S.1 Definition of repeat units

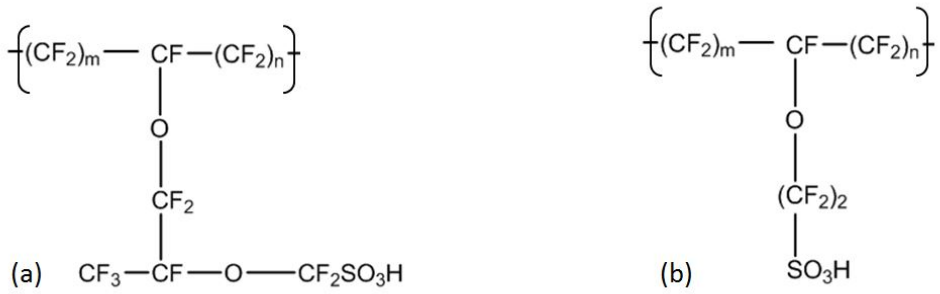

Fig. S.1 The structures of repeat units of: (a) Nafion EW=1244 and (b) Aquivion EW=828. The EW is determined by the selection of m and n, where m = 8 and n= 7.

S.2 Optimized structures of the repeat units

S.2.1 Coordinates of Nafion with defected helical conformation

Atom	X (Å)	Y (Å)	Z (Å)
C	-0.21900800	-0.30371000	0.07641900
C	0.42549700	0.25883600	1.37908200
C	-0.26677500	-0.18722800	2.70783700
C	0.58027000	0.10255800	3.99308100
C	-0.22814100	-0.00590200	5.33420600
C	0.69055600	-0.12392500	6.60197300
C	-0.04557400	0.16705200	7.95653400
C	0.71798400	-0.33183800	9.25059600
C	0.03897800	0.19670700	10.57898500
C	0.62595800	-0.34030900	11.93130600
C	-0.25651900	-0.00758000	13.19018500
C	0.53320000	-0.12286600	14.54148600
C	-0.38075700	-0.22777100	15.81049200
C	0.37279600	0.08129300	17.14982700
C	-0.36153600	-0.42548000	18.43207700
C	0.17149700	0.19141400	19.76188500
F	-1.51869800	0.00280500	0.02709600
F	-0.07749600	-1.62679800	-0.00000300
F	1.71679200	-0.14576200	1.39968800
F	0.37834600	1.60730500	1.30192200
F	-1.44864900	0.46584000	2.80523100
F	-0.49889300	-1.51886500	2.64675300
F	1.59799900	-0.78755400	4.03097600
F	1.08048500	1.35568700	3.90535300
F	-1.00034300	1.09781400	5.45300200
F	-1.01859700	-1.10185800	5.28049800
F	1.19070800	-1.37980400	6.63504500
F	1.70112200	0.76551800	6.47637600
F	-0.24472100	1.49904000	8.03909700
F	-1.24268000	-0.46475800	7.92509200
F	0.66403900	-1.68657900	9.24078800

F	0.15518200	1.54142000	10.59709600
F	-1.27301600	-0.14431600	10.54013500
F	0.74957700	-1.68336800	11.86993100
F	1.84664100	0.22160700	12.10772600
F	-0.73138900	1.25340500	13.08964800
F	-1.29430100	-0.87444000	13.21523200
F	1.31323900	-1.22716000	14.49685300
F	1.31431300	0.97513800	14.66303600
F	-1.40057900	0.65228700	15.68899900
F	-0.87824700	-1.48409300	15.86969600
F	1.59209600	-0.50466600	17.11059700
F	0.52596000	1.42274100	17.24643300
F	-1.67812300	-0.12462300	18.33599500
F	-0.21305300	-1.76525000	18.51045700
F	1.50570200	0.13109500	19.80650400
F	-0.21410100	1.46139600	19.88410200
F	0.38885800	0.21560900	-0.99005100
F	-0.30586300	-0.48125900	20.81288600
C	4.36221300	0.31453200	9.65612900
O	2.03614900	0.16946100	9.19493700
C	5.58119500	-0.46670100	10.27225100
C	3.14998500	-0.62456700	9.35020100
F	6.69671700	0.25576500	10.11615300
F	3.96533800	1.19141600	10.60802800
F	5.74860200	-1.66549100	9.70158500
F	3.40323200	-1.34535200	8.23679800
F	5.36562000	-0.64778000	11.57883700
F	3.01943000	-1.49817500	10.37364900
O	4.70588800	1.13893900	8.57138900
C	5.28121300	0.75120100	7.38238800
F	6.04041700	-0.35160200	7.49576400
C	6.17290500	1.93522200	6.91809200
F	4.34319000	0.51493000	6.44354400
S	6.79249600	1.74329000	5.15243700

F	7.23873400	2.01841600	7.72777600
F	5.47247100	3.08167100	6.96589700
O	5.70759100	2.09291200	4.24689300
O	7.53252700	0.50060100	5.08261400
O	7.87581500	2.96575200	5.15217000
H	7.46075400	3.72945900	4.70555200

S.2.2 Coordinates of Nafion with H136 helical conformation

Atom	X (Å)	Y (Å)	Z (Å)
C	0.74820100	0.02745000	7.88231000
C	0.50182200	0.47539700	5.28754400
C	0.19682300	0.67615800	2.68742900
C	0.05330300	0.43911200	0.00001500
C	0.09112400	0.41927100	14.41804400
C	0.02803500	0.35167100	11.81951400
C	-0.05929900	0.16887100	9.22455400
C	-0.21611600	0.12687700	6.63678100
C	-0.32732800	0.05996900	4.03366300
C	-0.16514100	-0.19263500	1.45524300
C	0.05329100	-0.43910200	15.74419200
C	0.48048900	-0.36963400	13.12881300
C	0.72205400	-0.19047000	10.52687300
F	1.63487400	1.05188000	7.82801200
F	0.71793400	1.80967200	5.25554700
F	-0.33886500	1.91003100	2.54850100
F	-0.93960100	1.34609700	-0.08700300
F	-1.11272000	0.98517100	14.20283700
F	-1.30889100	0.19174000	11.69043500
F	-1.14648400	-0.63052600	9.15035100
F	-0.85714800	-1.05510800	6.50957400
F	-0.28174400	-1.29040400	3.95271000
F	0.60276200	-1.31078800	1.51095900
F	1.23440300	-1.08210000	15.65890300
F	1.82427400	-0.52853300	13.09447700

F	1.96169700	0.34933400	10.45410600
F	1.69061900	-0.16857800	5.22865600
F	1.54600000	0.78729000	2.74792100
F	1.23440100	1.08209900	0.08529800
F	1.01215200	1.39810200	14.62259900
F	0.31754900	1.66884800	11.93018200
F	-0.44910000	1.46231600	9.32884300
F	-1.13089400	1.09774800	6.86038100
F	-1.61032500	0.45209300	4.20582400
F	-1.47260800	-0.55519600	1.55249300
F	-0.93959700	-1.34611700	15.83119300
F	-0.11238700	-1.58523200	13.17222800
F	0.81816900	-1.53531800	10.61509300
O	1.34500900	-1.24759400	7.82409300
C	2.87228300	-2.89519400	7.07329300
C	4.37644800	-3.20370500	6.73033200
C	2.69200300	-1.53119600	7.81695900
F	4.52244800	-4.51753400	6.51980800
F	2.23355800	-2.78721500	5.88405700
F	5.20460400	-2.82286900	7.71004900
F	3.17392800	-1.63378100	9.07580300
F	4.71447800	-2.54870800	5.61516600
F	3.43365900	-0.60741200	7.17534200
O	2.21540900	-3.96742100	7.70159800
C	2.51358800	-4.50441800	8.93118700
F	3.81473000	-4.39488800	9.25356800
C	2.13540200	-6.00883500	8.86040000
F	1.79081200	-3.91667600	9.90621600
S	2.17841900	-6.86112500	10.53646100
F	3.00128800	-6.63703300	8.05188700
F	0.88499200	-6.14465100	8.38493200
O	0.98771700	-6.47195900	11.27799700
O	3.52544300	-6.74197200	11.05426400
O	1.98223200	-8.39773000	10.01797500

H	1.04122800	-8.63301900	10.13667400

S.2.3 Coordinates of Aquivion with defected helical conformation

Atom	X (Å)	Y (Å)	Z (Å)
C	-0.21900500	-0.30371200	0.07641500
C	0.43901600	0.23909100	1.38050000
C	-0.35206400	-0.06965400	2.69381200
C	0.52913700	0.01836800	3.98518200
C	-0.28777500	0.17919800	5.31399000
C	0.54787400	-0.20353000	6.59349200
C	-0.00024900	0.41185500	7.93061500
C	0.72683000	-0.06787100	9.25035800
C	-0.10677800	0.28398700	10.56039400
C	0.63966800	0.04250800	11.91948700
C	-0.30833400	-0.03597900	13.16979000
C	0.45486800	0.12635900	14.53088600
C	-0.37983300	-0.27448200	15.79639600
C	0.26545500	0.20526300	17.14215300
C	-0.34479300	-0.43412300	18.42998700
C	0.17149600	0.19141100	19.76188900
F	-1.51869900	0.00280500	0.02709600
F	-0.07749700	-1.62679700	-0.00000200
F	1.67212500	-0.31601200	1.46442800
F	0.56113700	1.57835300	1.26156400
F	-1.37013900	0.81586500	2.78702500
F	-0.85923900	-1.32187200	2.61522000
F	1.26776700	-1.11262800	4.05862400
F	1.35226700	1.08716900	3.87446500
F	-0.69983600	1.46285400	5.39512900
F	-1.36957300	-0.63089000	5.26711200
F	0.54176300	-1.54936900	6.67982100
F	1.82270000	0.22345300	6.41988600
F	0.12093500	1.75708700	7.85854500
F	-1.31275800	0.08732400	8.00731600

F	0.77368700	-1.42254000	9.22155800
F	-0.53119400	1.56304600	10.51422400
F	-1.18750200	-0.53419100	10.54932500
F	1.32784100	-1.11657400	11.83506200
F	1.50416200	1.06528900	12.11749000
F	-1.22948200	0.94952500	13.07747900
F	-0.92999900	-1.23587300	13.16166300
F	1.55996000	-0.65365700	14.49149100
F	0.82085700	1.42223900	14.65587100
F	-1.61124400	0.27630900	15.69623500
F	-0.49324000	-1.62142200	15.82206300
F	1.58638100	-0.09079600	17.11390700
F	0.10993600	1.54669300	17.22825700
F	-1.68999200	-0.29160600	18.39219000
F	-0.03284000	-1.74860400	18.45691000
F	1.50570200	0.13109600	19.80650300
F	-0.21410000	1.46139700	19.88410100
F	0.38885700	0.21560900	-0.99004900
F	-0.30586300	-0.48125800	20.81288400
O	2.08420800	0.31211300	9.23599400
C	2.67529900	1.53925100	9.48725800
F	1.79976800	2.49614000	9.82103800
C	3.49304500	2.01830200	8.24947700
F	3.54989300	1.36925800	10.49966700
S	4.79693100	3.30169800	8.70616300
F	2.67181000	2.58212900	7.35224500
F	4.14096000	0.98125400	7.69450600
O	5.95654700	2.61334300	9.25436200
O	4.11400000	4.39205300	9.37165000
O	5.16851700	3.79949800	7.19478300
H	6.00629800	3.36593200	6.93969600

S.2.4 Coordinates of Aquivion with H136 helical conformation

Atom	X (Å)	Y (Å)	Z (Å)

C	0.61918800	0.11822200	7.88231700
C	0.41887500	0.57771700	5.29281500
C	0.17810800	0.69639200	2.68303400
C	0.05330400	0.43912000	0.00002600
C	0.09324400	0.42051300	14.41850500
C	-0.01971000	0.35705000	11.82406800
C	-0.18267400	0.20752500	9.23411100
C	-0.33052100	0.22871000	6.63297900
C	-0.35188300	0.09101200	4.02909700
C	-0.16309000	-0.18854600	1.45585300
C	0.05328300	-0.43910300	15.74418400
C	0.44989700	-0.37341300	13.12189000
C	0.63266600	-0.18522100	10.51123200
F	1.43100600	1.20595400	7.84000900
F	0.56188100	1.92023900	5.22972100
F	-0.36898400	1.92353000	2.52733500
F	-0.93960300	1.34609600	-0.08700500
F	-1.09976300	1.01361800	14.21901400
F	-1.36145100	0.21435400	11.72528200
F	-1.26625000	-0.59699800	9.15893700
F	-1.02735300	-0.92243700	6.49370000
F	-0.24846200	-1.25701700	3.98414600
F	0.62100500	-1.29396400	1.52349200
F	1.23440500	-1.08210000	15.65890700
F	1.79081600	-0.54937800	13.06321300
F	1.88293600	0.31903300	10.41483800
F	1.64366800	0.00541000	5.29456300
F	1.52522500	0.82203900	2.75750300
F	1.23440100	1.08209600	0.08529700
F	1.03806500	1.37853200	14.61341200
F	0.29167400	1.66940000	11.93377100
F	-0.58811400	1.49064500	9.38367000
F	-1.21110700	1.22679900	6.86900400
F	-1.65414700	0.43660000	4.16222000

F	-1.46545700	-0.57039900	1.54810900
F	-0.93959600	-1.34612800	15.83118900
F	-0.15547100	-1.58269900	13.17404100
F	0.69856800	-1.53526100	10.58428900
O	1.50662400	-0.97928500	7.88328800
C	1.22576600	-2.28516400	7.55894500
F	0.12445400	-2.74697200	8.17478700
C	2.46027000	-3.11579200	8.01042500
F	1.06549500	-2.45879200	6.22791800
S	2.41951700	-4.88646400	7.37018700
F	2.50794800	-3.16233000	9.34830100
F	3.58487400	-2.55464800	7.53314700
O	2.81499200	-4.87820400	5.96924500
O	1.20497300	-5.50233200	7.86238800
O	3.66459100	-5.47427600	8.24986200
H	4.45101800	-5.49703600	7.67027100