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Supplementary Information

Self-Assembled Films from Chitosan and Poly(Vinyl Sulfonic Acid) on Nafion® for Direct Methanol Fuel Cell

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Table S1. Cartesian coordinates of the (2*S*,3*S*,4*R*,5*R*,6*S*)-5-amino-3,6-dimethoxytetrahydro-2*H*-pyran-2,4-diol / ethenesulfonic acid complex

S	3.12075	–0.32259	–0.35501
O	2.43833	0.99551	–0.29888
O	4.18154	–0.45927	–1.35037
O	2.08115	–1.42840	–0.44044
C	3.86870	–0.59183	1.22643
C	3.86458	0.33415	2.17675
C	–3.37524	0.04273	–0.05757
O	–3.86799	0.54709	1.16346
O	–2.67277	1.01614	–0.77934
C	–1.50738	1.51552	–0.14705
O	–0.97987	2.39963	–1.07677
C	–0.03279	3.31299	–0.53560
C	–0.54568	0.37161	0.15873
C	–1.22292	–0.72846	0.98829
O	–1.46888	–0.27407	2.29499
H	–2.31874	0.19811	2.28608
H	–0.52652	–1.57139	1.06932
C	–2.52111	–1.17735	0.29873
O	–2.27688	–1.85165	–0.92132
C	–1.94412	–3.22039	–0.76843
N	–0.05102	–0.16901	–1.12796
H	4.34723	–1.56238	1.32504
H	4.34874	0.16292	3.13439
H	3.38005	1.29192	2.01085
H	–4.18870	–0.25890	–0.72637
H	–4.38863	1.33990	0.96713
H	–1.76751	2.03796	0.78799
H	0.17027	4.03662	–1.32666
H	0.90246	2.81383	–0.25626
H	–0.45313	3.83900	0.33299
H	0.33359	0.73975	0.69314
H	–3.09566	–1.81418	0.98628
H	–1.85221	–3.63264	–1.77505
H	–2.73869	–3.75445	–0.23066
H	–0.99367	–3.36103	–0.23827
H	0.84325	–0.77970	–0.92940
H	0.23295	0.61666	–1.71950
H	–0.79112	–0.71123	–1.58749

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Table S2. Cartesian coordinates of the (2*S*,3*S*,4*R*,5*R*,6*S*)-5-amino-3,6-dimethoxytetrahydro-2*H*-pyran-2,4-diol / ethenesulfonic acid / methanol complex

O	3.243327	–0.165617	–0.332285
O	2.471604	1.081642	–0.104805
O	4.175056	–0.159943	–1.462748
O	2.284807	–1.347871	–0.385711
C	4.209503	–0.469903	1.121649
C	4.245302	0.382716	2.140177
C	–3.463685	0.061336	–0.187174
O	–4.069292	0.553482	0.989469
O	–2.705015	1.047572	–0.832611
C	–1.602052	1.547249	–0.100063
O	–0.995609	2.437278	–0.974798
C	–0.138575	3.386743	–0.351806
C	–0.662014	0.406947	0.289018
O	–1.406035	–0.706194	1.044388
O	–1.756251	–0.272351	2.336503
H	–2.610963	0.188779	2.287520
H	–0.723255	–1.554116	1.174280
C	–2.633782	–1.154437	0.235746
O	–2.248604	–1.806387	–0.956423
C	–1.994903	–3.195429	–0.813922
N	–0.034212	–0.119217	–0.942211
H	4.779280	–1.394475	1.076319
H	4.864520	0.187439	3.011938
H	3.660561	1.298387	2.118108
H	–4.211705	–0.236669	–0.928613
H	–4.636495	1.304025	0.758119
H	–1.946031	2.069085	0.807284
H	0.133951	4.099741	–1.131489
H	0.773572	2.918623	0.037278
H	–0.667685	3.915278	0. 453417
H	0.148320	0.787434	0.917399
H	–3.264932	–1.807414	0.855399
H	–1.600186	–3.537106	–1.771580
H	–2.923916	–3.729865	–0.573768
H	–1.247054	–3.396709	–0.036434
H	0.853413	–0.653313	–0.711344
H	0.243686	0.664207	–1.541660
H	–0.663862	–0.741829	–1.465538
O	0.994739	–2.255910	–2.636649
H	1.605674	–2.427435	–3.898774
H	1.691737	–2.124520	–1.961972
H	0.810775	–2.428242	–4.650488
H	2.145009	–3.383272	–3.963436
H	2.306278	–1.612736	–4.126706

Energy for methanol binding to the (2*S*,3*S*,4*R*,5*R*,6*S*)-5-amino-3,6-dimethoxytetrahydro-2*H*-pyran-2,4-diol/ethenesulfonic acid ionic pair

Geometries were optimized at the PBE0/6-31G* level. Single-point calculations were carried out at the PBE-D level[1-2] with the TZV(2d,2p) basis set.[3-5] As suggested by Grimme,[1,2] DFT-D calculations with the triple-zeta basis set include, in a sense, dispersion and BSSE corrections. Single-point calculations were performed with ORCA v2.6rev35.[6]

Table S3. Energies at the PBE-D/TZV(2d,2p) level for the (2*S*,3*S*,4*R*,5*R*,6*S*)-5-amino-3,6-dimethoxytetrahydro-2*H*-pyran-2,4-diol / ethenesulfonic acid ionic pair (E_1), methanol molecule (E_2) and (2*S*,3*S*,4*R*,5*R*,6*S*)-5-amino-3,6-dimethoxytetrahydro-2*H*-pyran-2,4-diol / ethenesulfonic acid / methanol complex (E_3) (energies in ha)

Structure	Ionic pair (E_1)	Methanol (E_2)	Complex (E_3)
Energy / ha	–1408.187629513	–115.630027852	–1523.839762685

$\Delta E = E_3 - (E_2 + E_1) = -0.02210532$ ha = –13.87 kcal mol^{-1}

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