Maleimide: A Potential Building Block for the Design of Proton Exchange Membranes Studied by Ab Initio Molecular Dynamics Simulations

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Supplementary Information

Table S1 Atomic coordinates of the initial configuration (unit: Å)

Atoms	X	Y	Z
H1	4.489	7.030	8.818
H2	6.863	4.386	10.334
H3	-0.457	7.735	5.172
H4	2.910	11.372	12.668
H5	3.495	0.748	2.838
H6	-0.070	5.174	9.987
H7	6.476	6.947	5.519
H8	3.236	3.427	10.528
H9	3.168	8.694	4.978
H10	5.200	2.533	13.488
H11	1.205	9.587	2.018
H12	4.441	10.560	9.039
H13	1.964	1.561	6.467

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H14	1.966	7.000	7.023
H15	4.439	5.121	8.484
H16	1.276	4.334	13.939
H17	5.129	7.786	1.567
H18	5.865	0.825	11.940
H19	0.084	1.057	0.140
H20	3.784	8.458	10.065
H21	2.621	3.663	5.441
H22	1.198	8.712	8.550
H23	5.207	3.409	6.956
H24	1.983	6.409	12.915
H25	4.421	5.712	2.591
N26	6.565	3.762	10.878
N27	-0.159	8.358	4.628
N28	3.174	10.947	11.944
N29	3.231	1.173	3.562
N30	0.328	5.782	9.493
N31	6.077	6.338	6.013
N32	2.876	3.868	11.199
N33	3.528	8.253	4.307
O34	5.768	5.107	12.573
O35	0.637	7.014	2.933
O36	3.859	12.755	10.708

O37	2.546	-0.633	4.799
O38	1.183	4.414	7.837
O39	5.222	7.707	7.670
O40	2.062	2.089	12.439
O41	4.343	10.031	3.067
O42	7.134	1.899	9.669
O43	-0.728	10.221	5.837
O44	2.645	8.806	12.565
O45	3.760	3.314	2.941
O46	-0.130	7.634	10.780
O47	6.536	4.486	4.726
O48	3.389	6.014	10.540
O49	3.016	6.106	4.966
C50	5.954	3.983	12.097
C51	0.450	8.137	3.409
C52	3.705	11.553	10.857
C53	2.700	0.567	4.649
C54	1.015	5.529	8.335
C55	5.390	6.591	7.171
C56	2.226	3.283	12.288
C57	4.179	8.837	3.218
C58	5.621	2.684	12.650
C59	0.784	9.437	2.856

C60	4.042	10.456	9.896
C61	2.363	1.665	5.610
C62	1.468	6.853	7.818
C63	4.936	5.268	7.688
C64	1.766	4.411	13.128
C65	4.639	7.710	2.378
C66	5.991	1.758	11.815
C67	0.414	10.363	3.691
C68	3.681	9.316	10.458
C69	2.724	2.804	5.048
C70	1.059	7.778	8.654
C71	5.346	4.343	6.852
C72	2.152	5.543	12.565
C73	4.253	6.578	2.941
C74	6.632	2.376	10.649
C75	-0.226	9.745	4.857
C76	3.101	9.569	11.772
C77	3.304	2.552	3.734
C78	0.355	7.146	9.772
C79	6.050	4.974	5.734
C80	2.869	5.268	11.336
C81	3.536	6.852	4.170

Table S2 Energetic fluctuations during the CPMD simulation in NVT ensemble at five different temperatures (the corresponding standard deviations are shown in brackets)

Parameters	Run1	Run2	Run3	Run4	Run5
T	362.57	412.56	462. 90	511.10	564.14
	(31.49)	(35.20)	(39.42)	(43.56)	(46.82)
K_{el}	0.02002	0.02004	0.03002	0.03022	0.03502
	(9.3556×10^{-4})	(0.00102)	(0.00124)	(0.00135)	(0.00143)
K_{ion}	0.12598	0.07021	0.29256	0.14129	0.24299
	(0.01315)	(0.01475)	(0.01659)	(0.01957)	(0.01846)
E_{KS}	-531.42719	-531.40622	-531.38305	-531.35673	-531.36429
	(0.01343)	(0.01495)	(0.01695)	(0.01980)	(0.01898)
E_{class}	-531.30121	-531.33601	-531.09049	-531.21543	-531.12131
	(0.00126)	(0.00108)	(0.00138)	(0.00159)	(0.00164)
E_{tot}	-531.28119	-531.31597	-531.06047	-531.18541	-531.08629
	(8.47479×10^{-4})	(3.89866×10^{-4})	(6.4857×10^{-4})	(8.21703×10^{-4})	(8.5771×10^{-4})