Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Electronic supplementary information

Computational design of 2D functional covalent–organic framework membranes for water desalination

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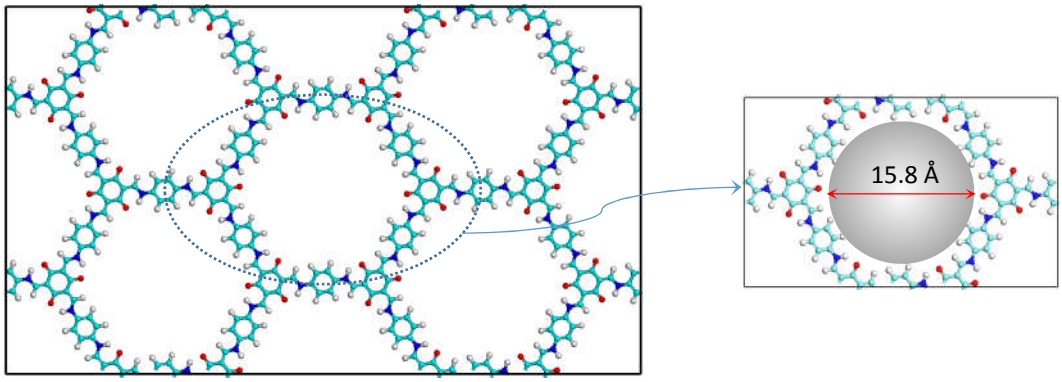

Fig. S1 Atomic structure of TpPa-1.

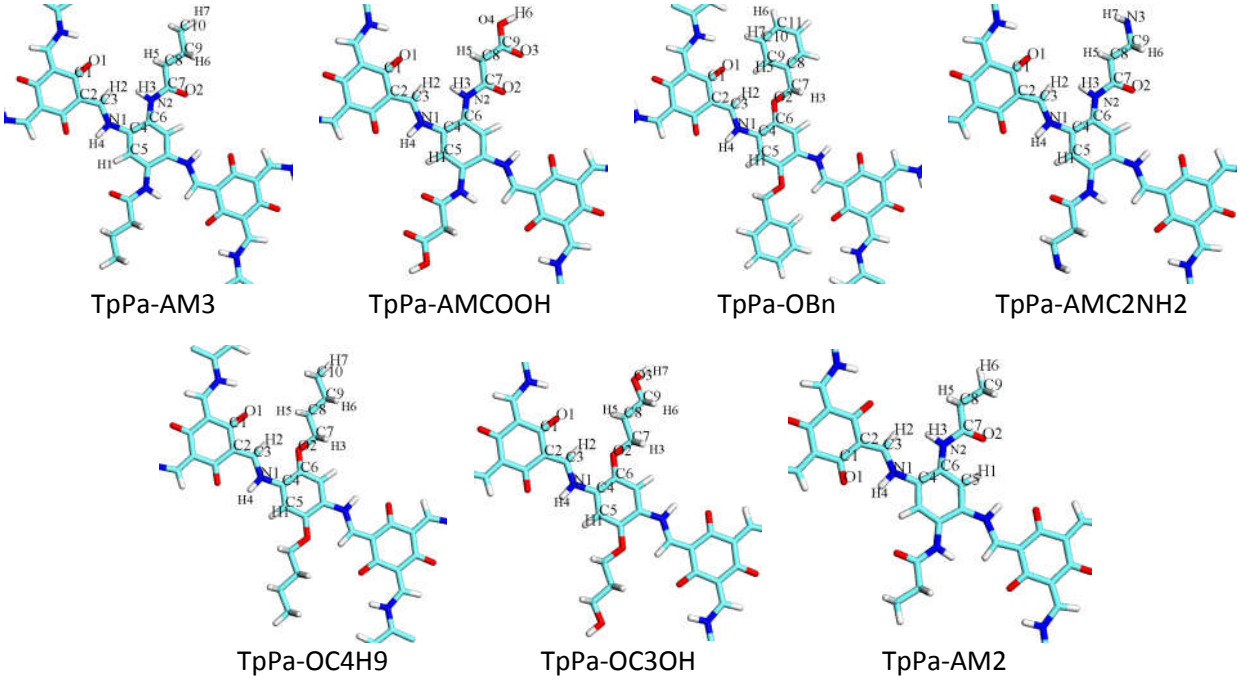

Fig. S2 Functional groups and atomic notations in TpPa-X.

Table S1 Force field parameters.

Atom	σ (Å)	ε/k_B (K)
O	3.118	30.166
N	3.261	34.691
C	3.431	52.790
H	2.571	22.122

Table S2 Atomic charges by the DDEC method.

TpPa-AM3		TpPa-AMCOOH		TpPa-OBn		TpPa-AMC2NH2	
Atom	Charges (*e*)	Atom	Charges (*e*)	Atom	Charges (*e*)	Atom	Charges (*e*)
H1	0.159	H1	0.159	H1	0.131	H1	0.159
H2	0.090	H2	0.089	H2	0.107	H2	0.089
H3	0.283	H3	0.282	H3	0.056	H3	0.285
H4	0.307	H4	0.307	H4	0.290	H4	0.306
H5	0.107	H5	0.158	H5	0.102	H5	0.108
H6	0.069	H6	0.392	H6	0.072	H6	0.076
H7	0.096	C1	0.454	H7	0.086	H7	0.269
C1	0.455	C2	–0.295	C1	0.451	C1	0.454
C2	–0.295	C3	0.127	C2	–0.303	C2	–0.294
C3	0.127	C4	0.113	C3	0.149	C3	0.127
C4	0.113	C5	–0.245	C4	0.144	C4	0.113
C5	–0.247	C6	0.187	C5	–0.310	C5	–0.247
C6	0.185	C7	0.613	C6	0.191	C6	0.184
C7	0.593	C8	–0.469	C7	0.074	C7	0.608
C8	–0.320	C9	0.709	C8	0.039	C8	–0.378
C9	–0.027	N1	–0.301	C9	–0.127	C9	0.108
C10	–0.315	N2	–0.466	C10	–0.070	N1	–0.301
N1	–0.302	O1	–0.491	C11	–0.107	N2	–0.454
N2	–0.452	O2	–0.444	N1	–0.303	N3	–0.665
O1	–0.495	O3	–0.485	O1	–0.475	O1	–0.495
O2	–0.498	O4	–0.552	O2	–0.246	O2	–0.506

TpPa-OC4H9		TpPa-OC3OH		TpPa-AM2	
Atom	Charges (*e*)	Atom	Charges (*e*)	Atom	Charges (*e*)
H1	0.134	H1	0.139	H1	0.159
H2	0.110	H2	0.110	H2	0.089
H3	0.042	H3	0.046	H3	0.284
H4	0.299	H4	0.301	H4	0.306
H5	0.097	H5	0.114	H5	0.099
H6	0.052	H6	0.015	H6	0.100
H7	0.089	H7	0.346	C1	0.454
C1	0.472	C1	0.470	C2	–0.294
C2	–0.309	C2	–0.307	C3	0.128
C3	0.144	C3	0.143	C4	0.113
C4	0.148	C4	0.149	C5	–0.245
C5	–0.320	C5	–0.320	C6	0.184

C6	0.193	C6	0.192	C7	0.583
C7	0.090	C7	0.093	C8	–0.247
C8	–0.192	C8	–0.214	C9	–0.268
C9	–0.048	C9	0.144	N1	–0.301
C10	–0.303	N1	–0.307	N2	–0.455
N1	–0.307	O1	–0.511	O1	–0.495
O1	–0.515	O2	–0.248	O2	–0.493
O2	–0.246	O3	–0.531		

Table S3 Atomic charges by the EQeq method.

TpPa-OC3OH		TpPa-AM2	
Atom	Charges (*e*)	Atom	Charges (*e*)
H1	0.066	H1	0.090
H2	0.053	H2	0.031
H3	0.020	H3	0.095
H4	0.112	H4	0.116
H5	0.087	H5	0.063
H6	0.009	H6	0.045
H7	0.135	C1	0.208
C1	0.212	C2	–0.124
C2	–0.128	C3	0.081
C3	0.086	C4	0.053
C4	0.054	C5	–0.086
C5	–0.100	C6	0.075
C6	0.108	C7	0.231
C7	0.070	C8	–0.139
C8	–0.143	C9	–0.100
C9	0.092	N1	–0.156
N1	–0.152	N2	–0.187
O1	–0.223	O1	–0.222
O2	–0.205	O2	–0.226
O3	–0.271		

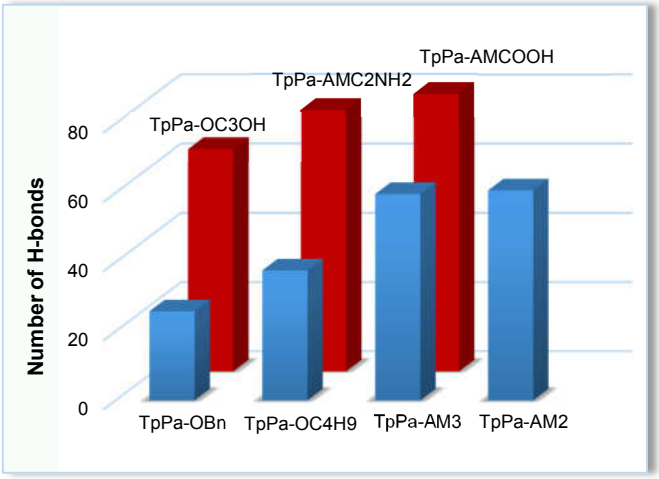

Fig. S3 Numbers of hydrogen bonds formed between TpPa-X membranes and water.

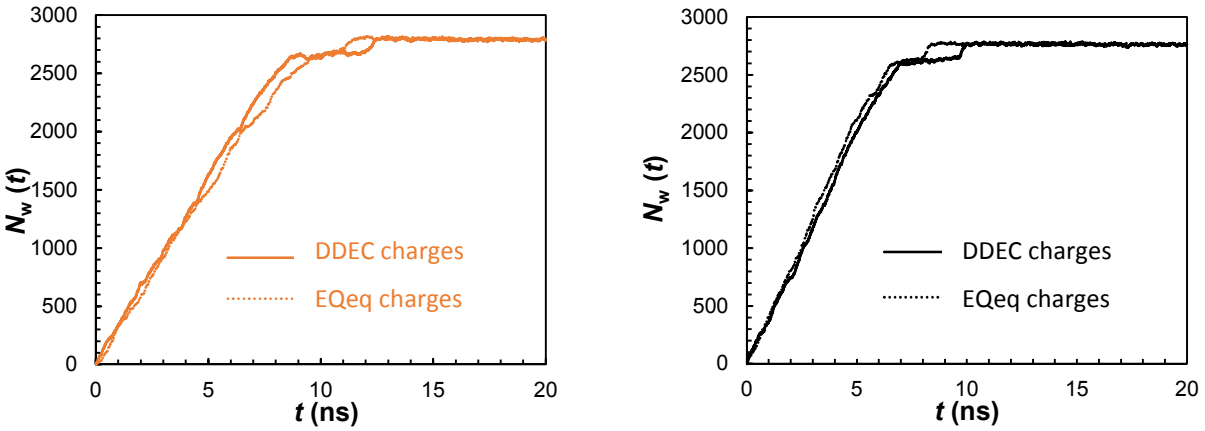

Fig. S4 Net water flow through TpPa-OC3OH and -AM2 membranes with different atomic charges.

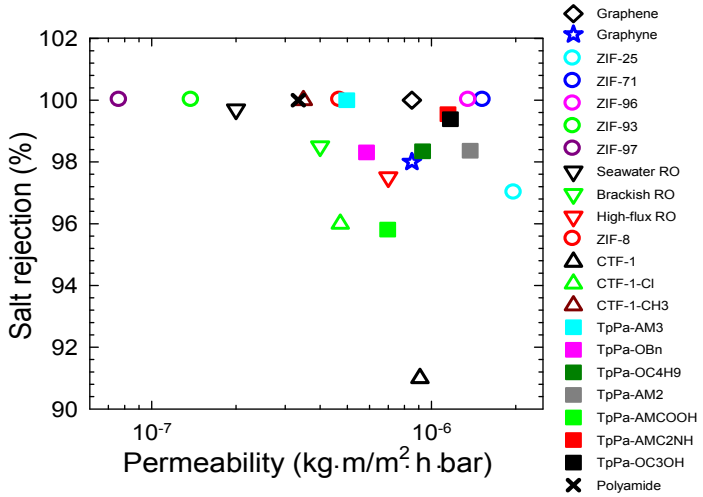

Fig. S5 Performance (salt rejection versus permeability) of TpPa-X and other membranes.

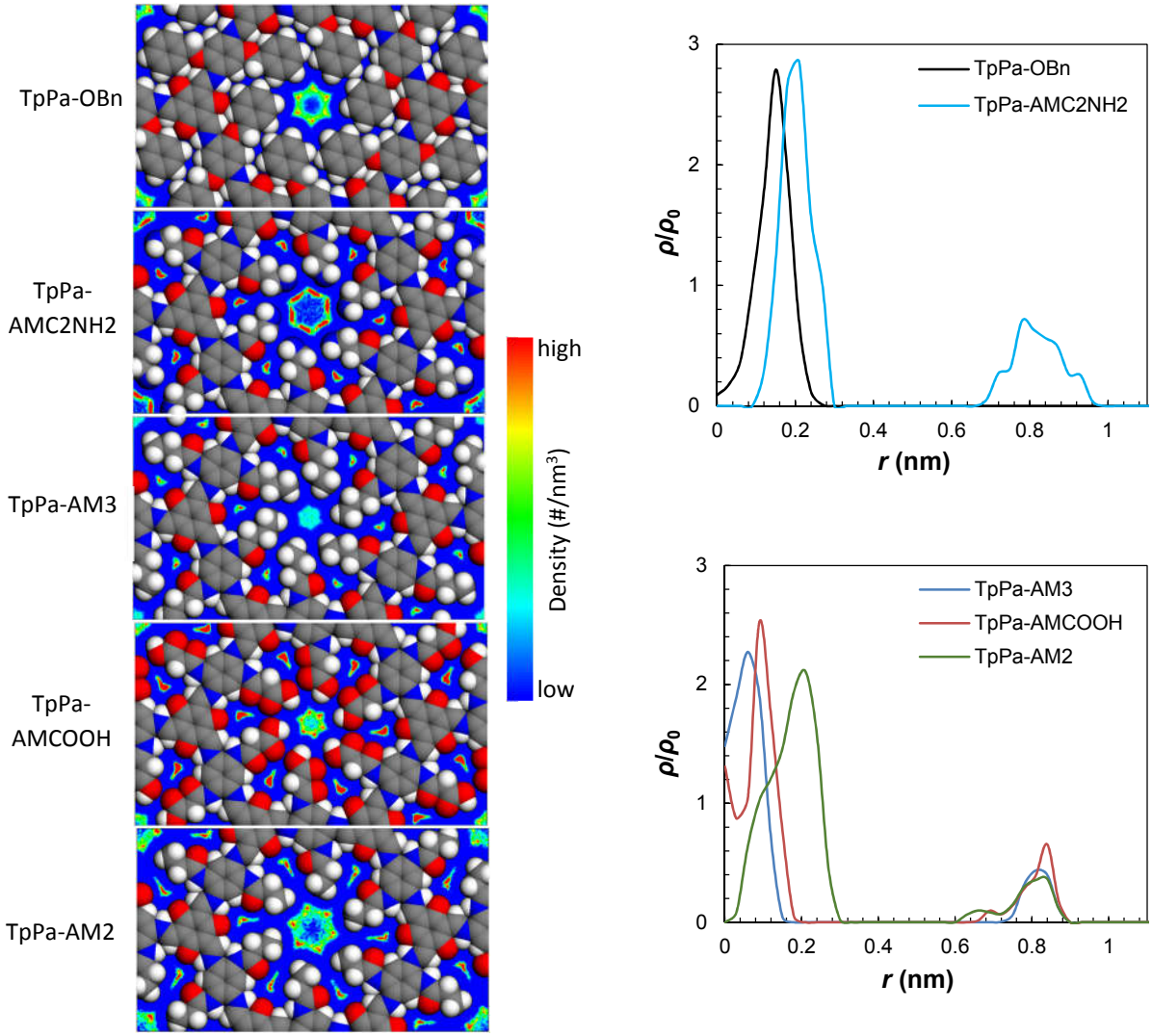

Fig. S6 (Left) Density contours of water molecules at membrane apertures. (Right) Density profiles along radial direction.

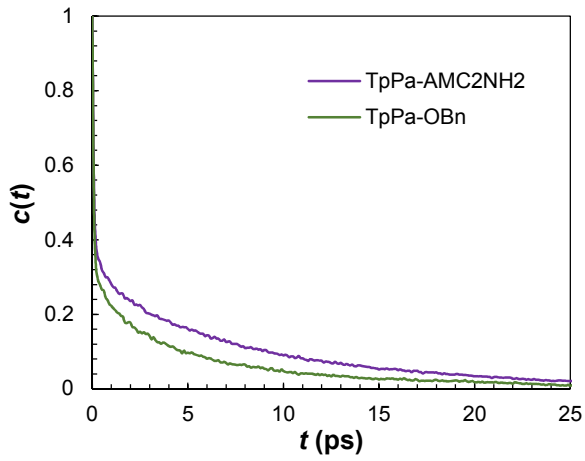

Fig. S7 Autocorrelation functions $c(t)$ in TpPa-AMC2NH2 and -OBn membranes.