

Supplementary Information for:

The energetics of phosphoric acid interactions reveal a new acid loss mechanism

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Table S1. ΔE_{Base} of PA-BI and biposphate-TMA.

Number of PA	1	2	3	4	5	6	7	8	9	10	11	12
PA-BI	17.1	42.9	65.9	89.8	123.2	152.4	189.1	212.7	232.3	262.4	286.9	324.2
Biphosphate-TMA	105.1	128.5	147.8	185.0	218.7	246.4	277.8	299.7	318.9	357.7	387.9	419.3

Table S2. Weight of dry membrane, $Weight_{dry}$, weight at equilibrated hydrated state, $Weight_{wet}$, and weight of total dope, $Uptake_{total}$

RH (%)	5%		20%		40%		60%		80%		95%	
	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP
$Weight_{dry}$ (g)	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
$Weight_{wet}$ (g)	0.1898	0.13	0.1898	0.1299	0.19	0.129	0.194	0.131	0.188	0.131	0.190	0.13
$Uptake_{total}$ (g)	0.0898 ± 0.002	0.03 ± 0.002	0.09 ± 0.002	0.0299 ± 0.002	0.09 ± 0.002	0.029 ± 0.002	0.094 ± 0.002	0.031 ± 0.002	0.088 ± 0.002	0.031 ± 0.002	0.09 ± 0.002	0.03 ± 0.002

Table S3. Weight and λ values for phosphoric acid (PA) and water (H_2O).

RH (%)	5%		20%		40%		60%		80%		95%	
	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP
$Weight_{PA}$ (mg)	80	25	44	24	29	22	18	18	11	17	9.7	12
$Weight_{H_2O}$ (mg)	10	4	45	6	67	9	80	13	83	16	85	18
λ_{PA}	12.6	13.8	7.7	13.0	4.6	11.7	2.8	9.6	1.8	8.9	1.5	6.6
λ_{H_2O}	12.0	11.5	38.5	17.3	56.4	26.6	68.4	39.1	71.2	47.4	72.6	52.9

Table S4. Volume uptake and λ values for phosphoric acid (PA) and water (H_2O).

RH (%)	5%		20%		40%		60%		80%		95%	
	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP	PA-PBI	BPA-QAP
Volume Uptake _{PA} (10^{-3} cm ³)	40	13	24	12.1	15	10.9	8.8	8.9	5.9	8.2	4.8	6.2
Volume Uptake _{H₂O} (10^{-3} cm ³)	10	4	45	6	67	9	80	13	83	16	85	18
λ_{PA} (Vol _{uptake} %)	52.2	16.7	31.9	15.7	19.1	14.2	11.5	11.6	7.6	10.7	6.4	8.0
λ_{H_2O} (Vol _{uptake} %)	16.5	4.7	53.1	7	77.9	10.7	94.4	15.8	98.4	19.1	100.3	23.3

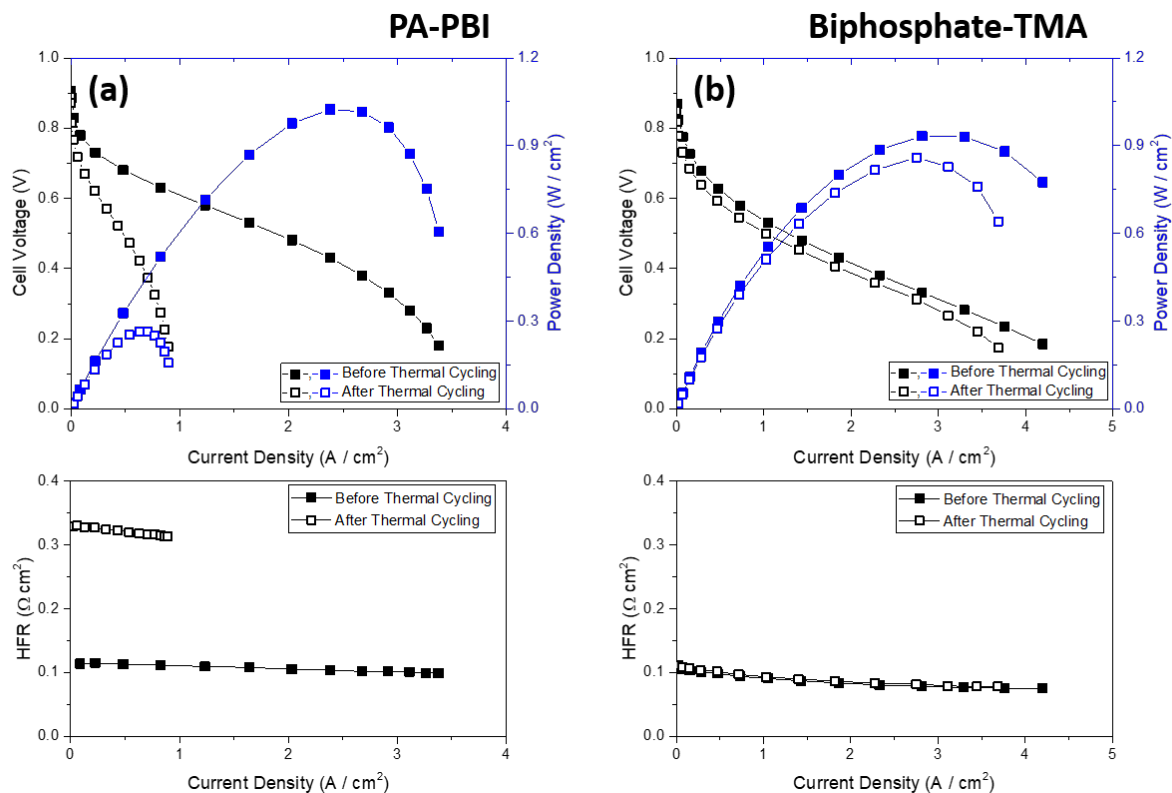


Fig. S5. Polarization curves for membrane electrode assemblies with (a) PA-PBI and (b) biphosphate-TMA membranes before and after thermal cycling. The polarization curves were measured at 160 °C under dry H₂/O₂ conditions. The anode and cathode flows are 500 sccm with 10 psi backpressure.