

Supplementary Material for:

A facile construction of quaternized polymer brush-grafted graphene modified polysulfone based composite anion exchange membranes with enhanced performance

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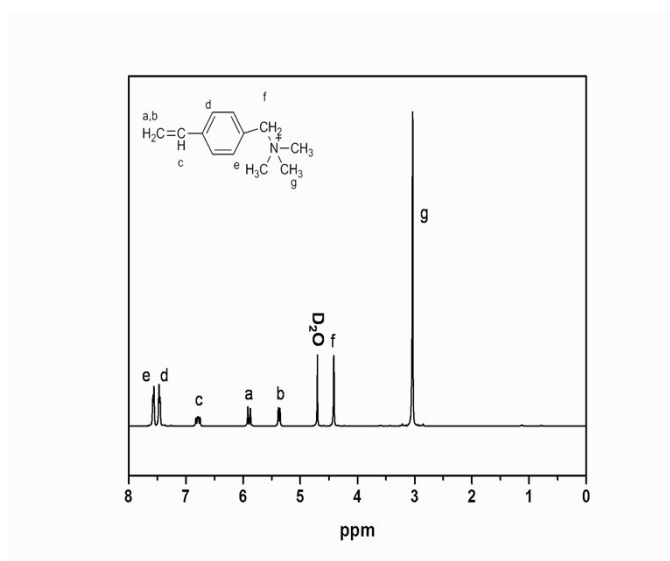


Figure S1. ¹H NMR spectrum of VBTAC

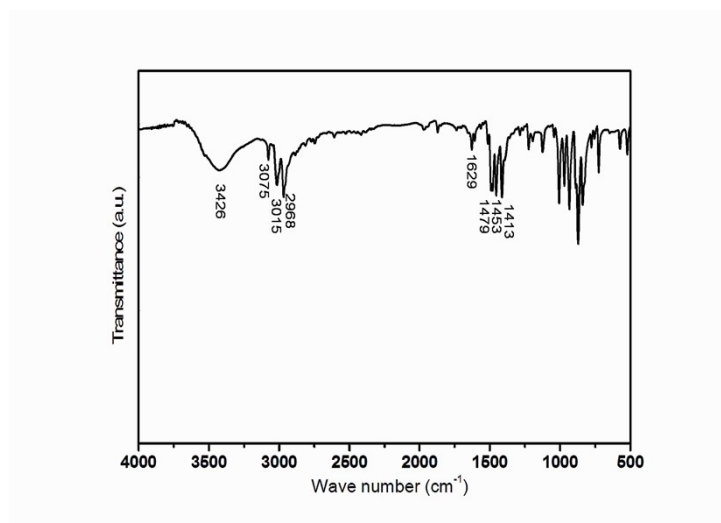


Figure S2. FTIR spectra of VBTAC

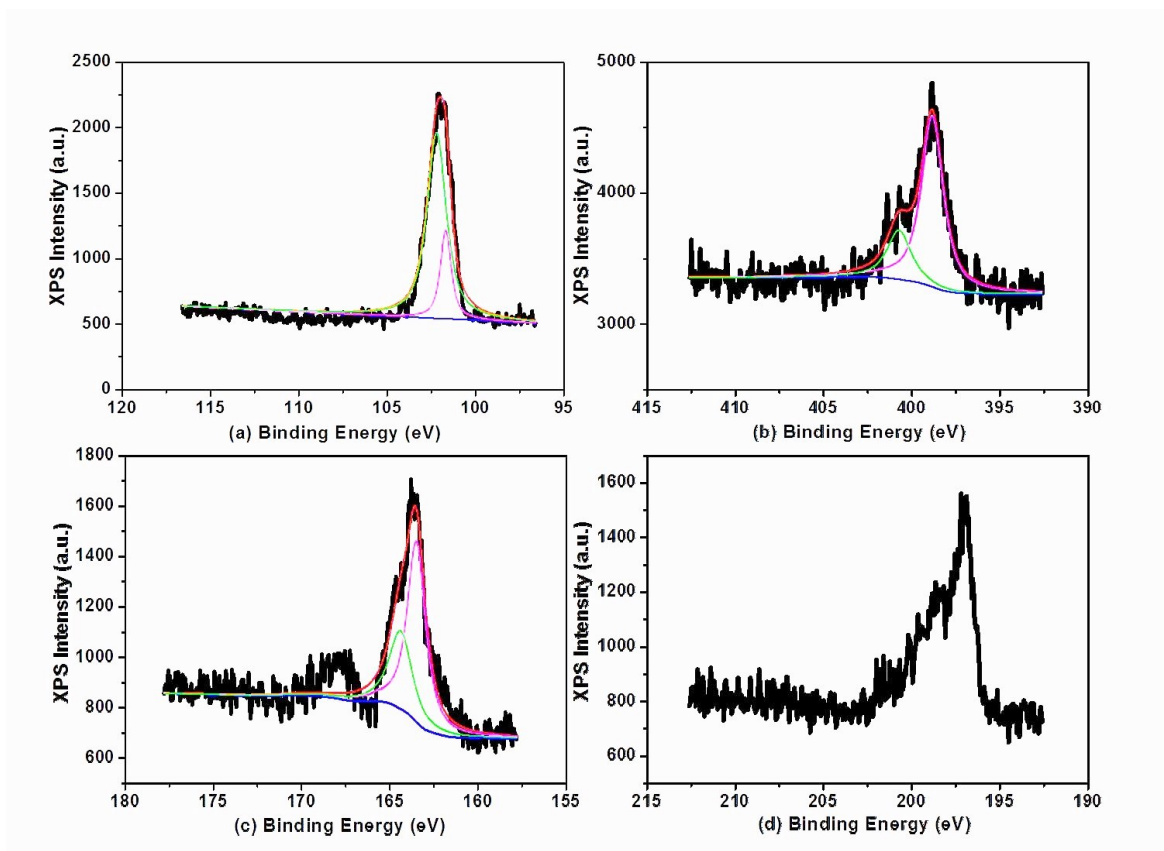


Figure S3. Deconvoluted XPS spectra (a), in the Si_{2p} region of A-FGs (b), in the N_{1s} region of A-FGs (c), in the S_{2p} region of R-FGs (d), and in the Cl_{2p} region of QPbGs.

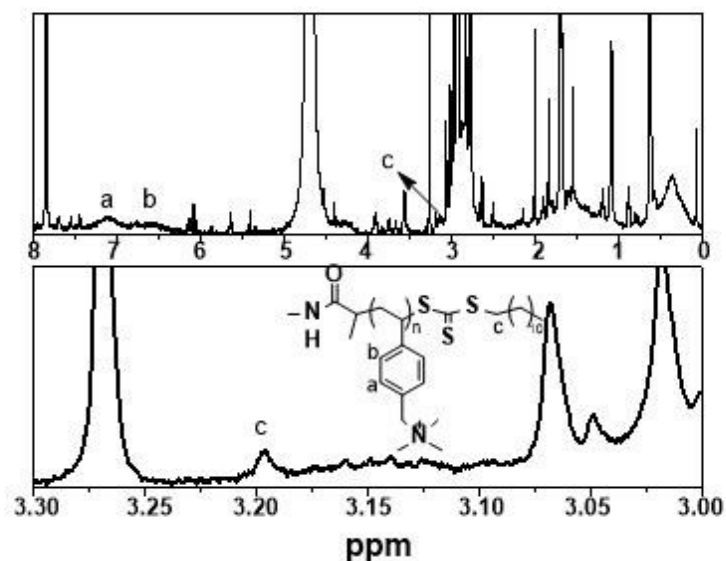


Figure S4. ^1H NMR spectra of QPbGs.

There are two broad peaks (a and b) at 6.56 and 7.11 ppm, which belongs to the hydrogen of benzene ring of PVBTAC brushes. Peak c at 3.19 is attributed to the hydrogen on $-\text{CH}_2-$ nearby the sulfur atom. The area integral ratio of c and (a + b) of hydrogen is 1 : 14, and the degree of polymerization (n) can be calculated as 7. The theoretical molecular weight of PVBTAC calculated by ^1H NMR is 1500 g mol^{-1} , which is close to the result of GPC.

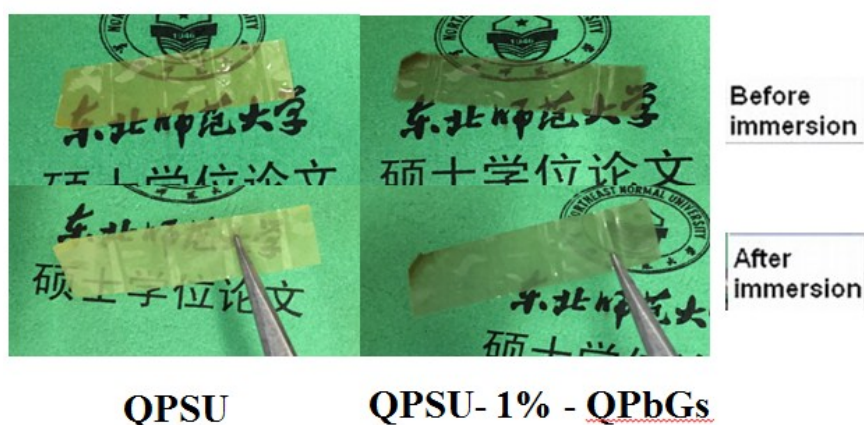


Figure S5. Digital photos of QPSU and QPSU-1%- QPbGs before and after alkaline resistance test.

Table S1.

Elementary Composition of GO, A-FGs, R-FGs and QPbGs.

sample	atomic composition (wt %)					
	C	N	Si	S	Cl	O
GO	68.65	0	0	0	0	31.35
A-FGs	73.56	2.85	4.92	0	0	18.67
R-FGs	67.24	4.53	8.02	2.40	0	17.80
QPbGs	70.42	3.97	5.59	1.64	1.84	16.54

Table S2.

Ionic conductivity values reported in the literature for different AEMs.

Membrane material	IEC (meq g ⁻¹)	Conductivity (mS cm ⁻¹) 80 °C	Reference
QPSU-1%-QPbGs	1.84	56.0 ^a	This study
QPSU-2%-QPbGs	1.87	49.7 ^a	This study
QPSU-0.5%-QGs	1.20	18.7 ^a	35
PVA-20wt%FGO	--	21.0 ^b	36
fGO-PEI-5	2.83	72.0 ^b	37
CLQCPAES/10%ZrO2	1.18	49.4 ^b	14

^a bicarbonate conductivities.^b hydroxide conductivities.

The calculation of grafting density

The grafting density can be determined from the data of TGA analysis combined with the molar mass of the PVBTAC brushes.¹ The weight fractions of A-FGs, R-FGs and QPbGs can be obtained from Figure 6 and the molar mass of the PVBTAC brushes was determined to be 1200 g mol⁻¹ by GPC according to the method reported in literature.²

The grafting density is calculated by the following formula:

$$\text{Functional groups per carbon: } A_{\text{mg}} = M_{\text{c}} \times W_{\text{R}} / M_{\text{R}} \times W_{\text{c}}$$

$$\text{Chain per carbon: } A_{\text{pg}} = M_{\text{c}} \times W_{\text{p}} / M_{\text{p}} \times W_{\text{c}}$$

where M_{c} is the relative molar mass of carbon ($M_{\text{c}}=12 \text{ g mol}^{-1}$), M_{R} is the molar mass of RAFT agent ($M_{\text{R}}=350 \text{ g mol}^{-1}$), M_{p} is the average-number molar mass (M_{n}) of grafted polymer ($M_{\text{n}}=1200 \text{ g mol}^{-1}$), The values of W_{c} , W_{R} and W_{p} were obtained from the TGA curves in Figure 6. When calculating the functional groups per carbon, $W_{\text{c}} = 73.8\%$ and $W_{\text{R}} = 26.2\%$, and so the grafting density of RAFT agent on A-FGs was calculated to be 1.22 functional groups per 100 carbons. When calculating the Chain per carbon, $W_{\text{c}} = 52.9\%$ and $W_{\text{p}} = 47.1\%$, so the grafting density of PVBTAC chains on QPbGs was calculated to be 0.9 chains per 100 carbons.

References

- 1 P. Ding, J. Zhang, N. Song, S. Tang, Y. Liu and L. Shi, *COMPOS. PART A-APPL. S.*, 2015, **69**, 186-94.
- 2 Y. Yang, X. Song, L. Yuan, M. Li, J. Liu, R. Ji and H. Zhao, *J. Polym. Sci. Part A: Polym. Chem.*, 2012, **50**, 329-337.