Supporting information

Zwitterionic Polymers Functionalized Nanoporous Graphene for Water Desalination: a Molecular Dynamics Study

Membrane Fabrication. The three types of zwitterionic poly(CBMA) chains and zwitterionic poly(CBMA) functionalized graphene sheet (ZGS) were built with Accelrys Material Studio (MS) (version 7.0). The three types of poly(CBMA) chains, which have 20, 30, and 40 repeating units in fully extended conformation. The poly(CBMA) chains were then grafted to nanoporous graphene sheet to obtain zwitterionic polymers functionalized nanoporous graphene membranes.

Table S1. Size of pore of nanoporous graphene sheets, number and the type of poly(CBMA)s grafted to nanoporous graphene, and the size of box of each simulated system. The ions number of Na, Cl, are 218, 218 in each of system.

System name	Pore size / nm	Number of chains or molecules			Size box /nm
		Ploy(CBMA)20	Ploy(CBMA)30	Poly(CBMA)40	
3-ZGS20-1	3.0	1	-	-	22.00
3-ZGS20-2		2	-	-	22.09
3-ZGS20-3		3	-	-	22.19
3-ZGS20-4		4	-	-	22.29
3-ZGS30-1		-	1	-	22.04
3-ZGS30-2		-	2	-	22.09
3-ZGS30-3		-	3	-	22.37
3-ZGS30-4		-	4	-	22.53
3-ZGS40-1		-	-	1	22.09
3-ZGS40-2		-	-	2	22.31
3-ZGS40-3		-	-	3	22.60
3-ZGS40-4		-	-	4	22.82
4-ZGS20-1	4.0	1	-	-	22.00
4-ZGS20-2		2	-	-	22.09
4-ZGS20-3		3	-	-	22.19
4-ZGS20-4		4	-	-	22.29
4-ZGS30-1		-	1	-	22.04
4-ZGS30-2		-	2	-	22.09
4-ZGS30-3		-	3	-	22.37
4-ZGS30-4		-	4	-	22.53
4-ZGS40-1		-	-	1	22.09
4-ZGS40-2		-	-	2	22.31
4-ZGS40-3		-	-	3	22.60
4-ZGS40-4		-	-	4	22.82

Table S2. Atom charge (e) of an poly(CBMA) monomer.

	(e)		(e)		(e)		(e)		(e)
1 C	-0.3793	9 H	0.1370	17 H	-0.0121	25 H	0.0429	33 H	0.1135
2 C	0.2748	10 H	0.1354	18 H	0.2118	26 H	0.0419	34 C	-0.3268
3 H	0.0938	11 C	0.7513	19 H	0.2036	27 C	0.8704	35 H	0.1779
4 H	0.10297	12 O	-0.5965	20 N	0.2171	28 O	-0.7907	36 H	0.1602
5 H	0.1122	13 O	-0.5775	21 C	-0.1202	29 O	-0.7724	37 H	0.1425
6 C	-0.5004	14 C	0.5716	22 C	-0.1695	30 C	-0.2915		
7 H	-0.0014	15 C	-0.5269	23 H	0.1292	31 H	0.1678		
8 H	0.1171	16 H	-0.0037	24 H	0.1254	32 H	0.1682		

Table S3 Diffusion coefficient of Na+ and Cl- for in solution and near polymers.

position	Diffusion coefficient in solution	Diffusion coefficient near polymers
Na^+	2.017±0.443 (A^2/ps)	0.595±0.046 (A^2/ps)
Cl^-	3.833±0.343 (A^2/ps)	2.486±0.143 (A^2/ps)

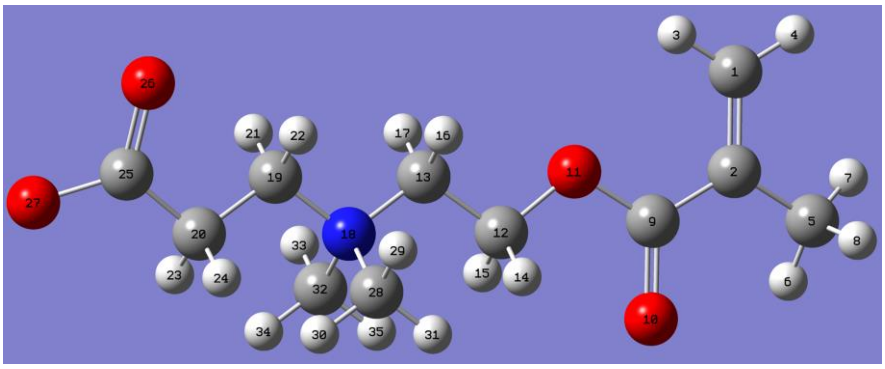

Figure S1. Definition of atom names in an poly(CBMA) monomer.

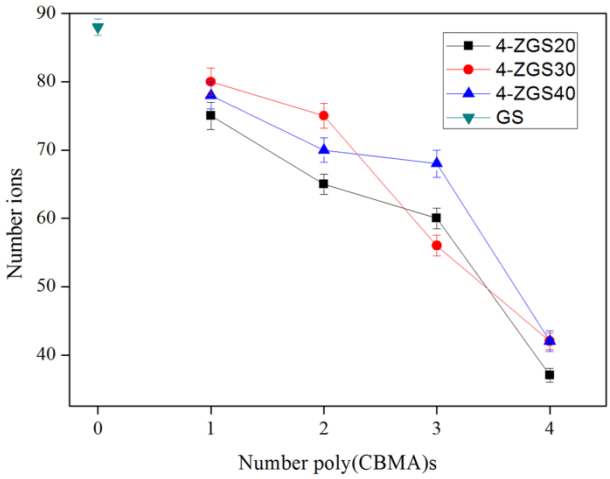

Figure S2. Number of ions through ZGS membranes considered and unfunctionalized nanoporous graphene at 5 ns. Each of membrane pore size is 4.0 nm.

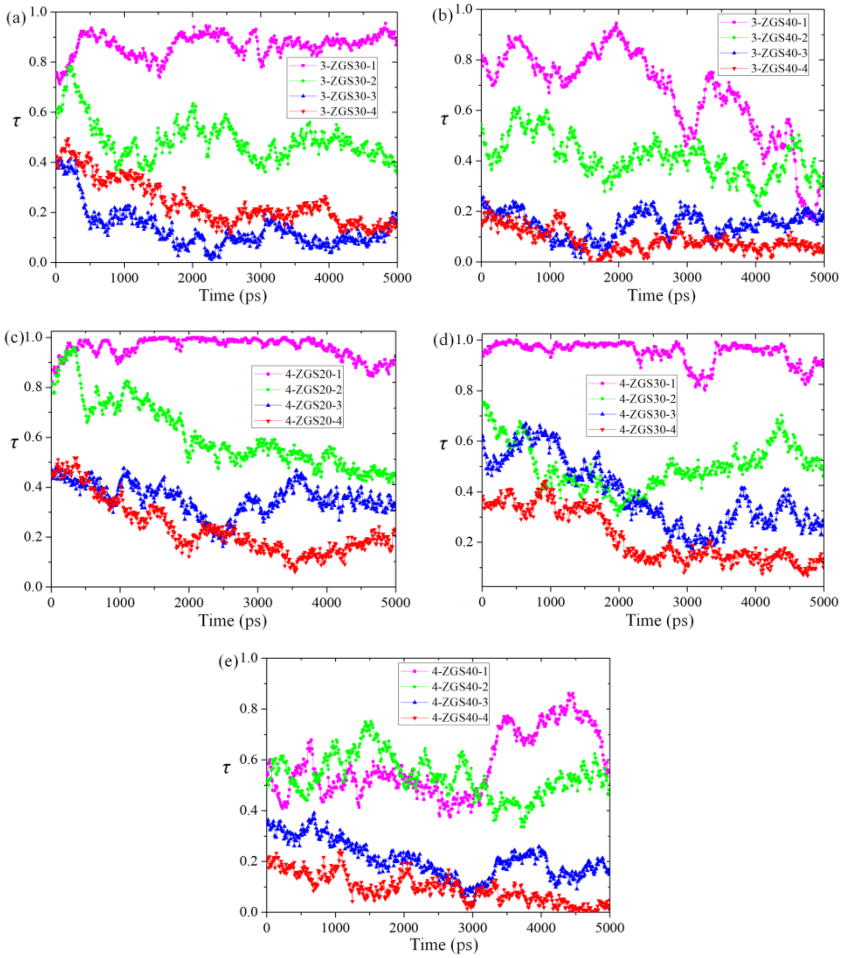

Figure S3. Effective parameter τ representing the pore size area with time evolution.

The pore diameter of the nanoporous graphene was 3.0 nm, the polymer chains grafting to the membrane were from one to four, and the polymerization degree of

poly(CBMA) is 30 (a) and 40 (b). The pore diameter is 4.0 nm, and the polymerization degree of poly(CBMA) is 20 (c), 30 (b) and 40 (e).

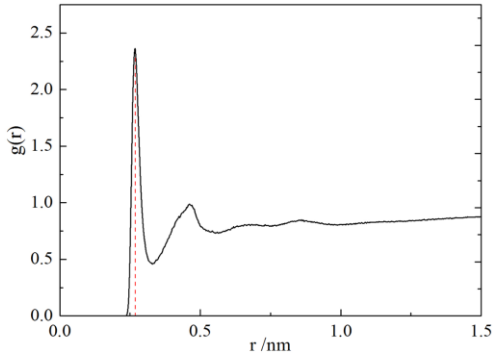

Figure S4. Radial distribution function between $-COO^-$ of poly(CBMA) and oxygen atoms of water.

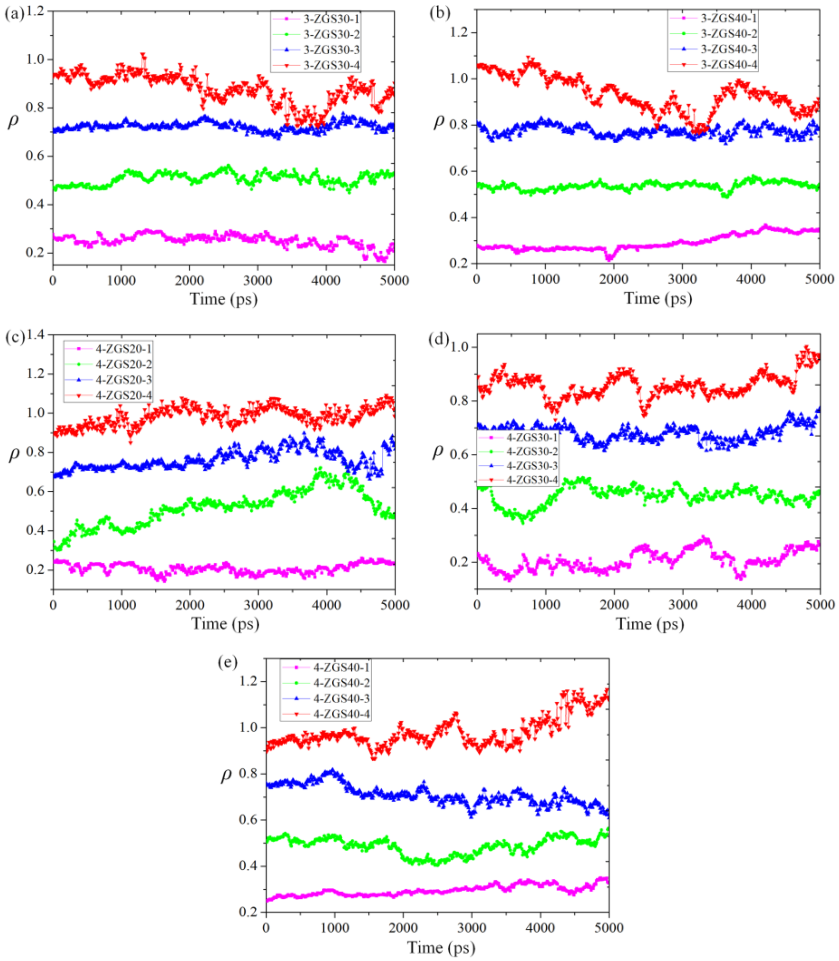

Figure S5. Volume charge density of defined polymer channels with time evolution. The pore diameter of the nanoporous graphene was 3.0 nm, the polymer chains grafting to the membrane were from one to four, and the polymerization degree of poly(CBMA) is 30 (a) and 40 (b). The pore diameter is 4.0 nm, and the polymerization degree of polymer is 20 (c), 30 (b) and 40 (e).

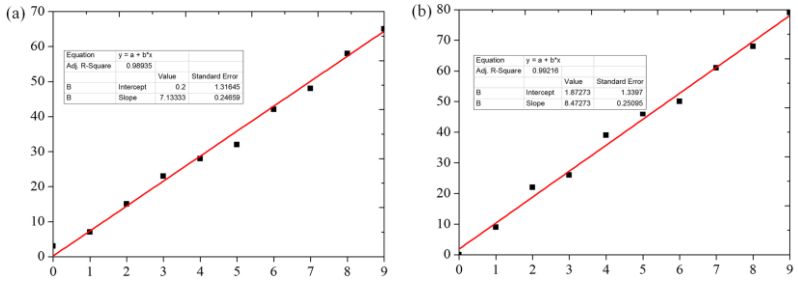

Figure S6. Number of ions through pristine nanoprous graphene. (a) The pore size is 3.0 nm. (b) The pore size is 3.0 nm.

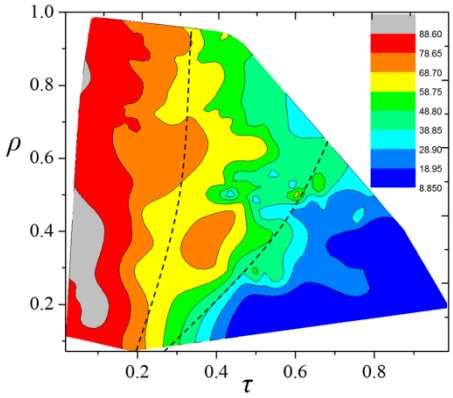

Figure S7. Contours of rejection distribution of ZGS membranes as a function of effective parameter of pore size τ and volume charge density of polymer channel ρ.

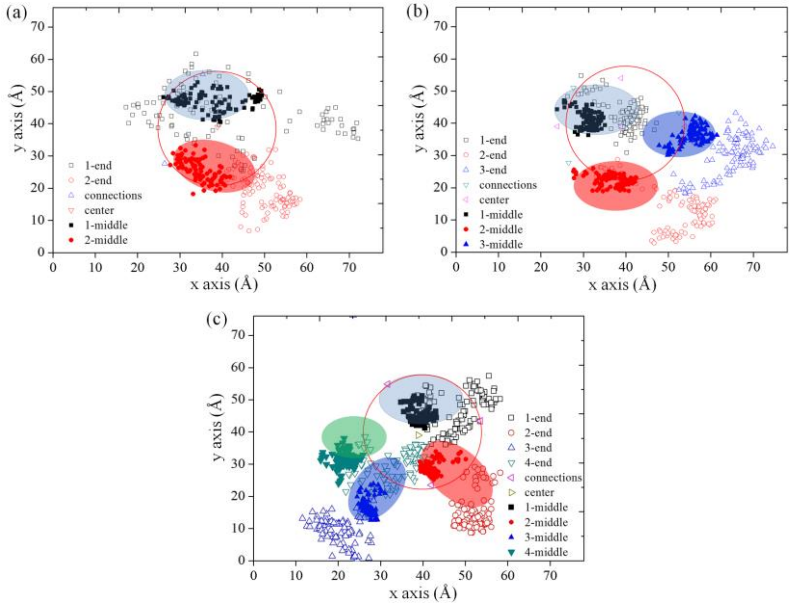

Figure S8. The projection distribution of trajectories of chains grafted to graphene, with pore diameter 3.0 nm, for middle atom (solid shape) and end atom (empty shape) of polymer main chain during 5.0 ns NMD run. (a) Graphene with two zwitterionic

poly(CBMA) chain. (b) Graphene with three poly(CBMA) chains. (c) Grapehene with four poly(CBMA) chains.

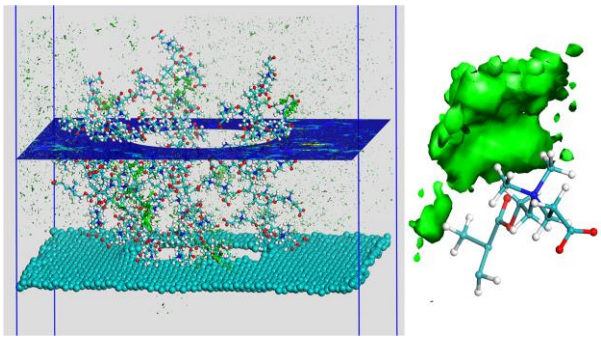

Figure S9. The spatial distribution functions (SDFs) of Cl^- ions in the solution box (left). A local SDFs of the Cl^- ions around amido group of polymer (right).

We calculate the water flux of all systems and supplemented in the supporting information. Here, the number of net transferred water molecules defined N_w and we calculated water flux J_w through $J_w = N_w/(At)$, where A is the membrane area and t is time duration. As shown in Figure S10,

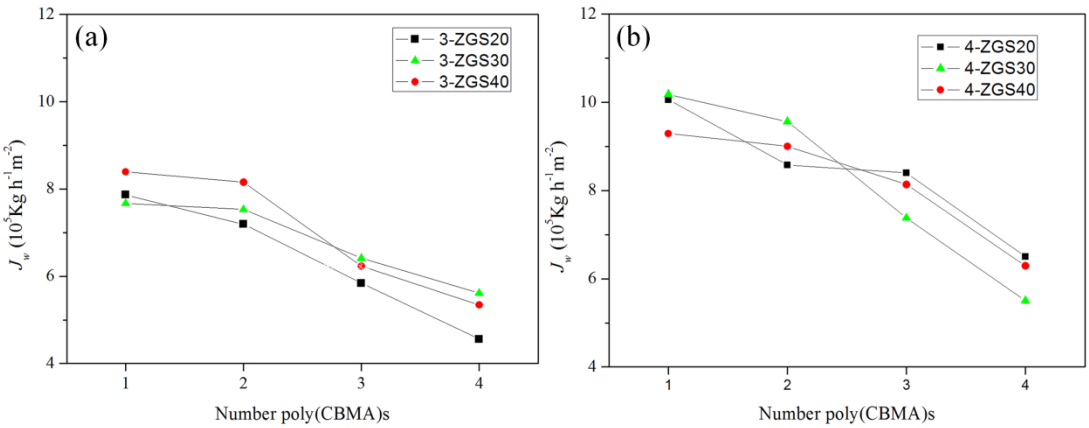

Figure S10. Water flux for all considered systems. The pore size in the graphene sheet is 3.0 nm (a) and 4.0 nm (b).

As shown in the Figure S10, the water flux is decrease with the increase number polymers with the same degree of polymerization. We can also find that the water flow will increase, When the size of the graphene hole increased from 3 nm to 4 nm. We note that the water flow does not decrease as the increase degree of polymerization of the polymer and have not regular change, may be because of the

exclusion between the polymer functional groups and is not conducive to folding, covering the graphene pores, which is similar to the change effective pore ratio τ for the different degree of polymerization."

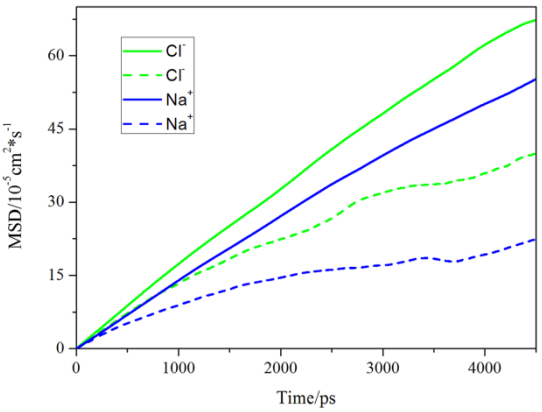

Figure S11 Mean square displacements of Na^+ and Cl^- for in solution is represented by straight lines, for near polymers dash lines.