Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for Control the ion transport in a C_2N-based nanochannel with tunable interlayer spacing

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1 The details of simulation systems

Table S1: The number of atom in the simulation systems.

d/nm	Concentration	Water molecules	Cation (K^+, Na^+ or Li^+)	Anion (Cl^-)
0.6	0.5	3485	53	53
0.7	0.5	3625	54	54
0.8	0.5	3738	55	55
1.0	0.5	3917	57	57
1.2	0.5	4117	59	59
1.4	0.5	4322	61	61
1.6	0.5	4575	63	63
0.7	0.1	3711	11	11
0.7	0.3	3669	32	32
0.7	0.7	3581	76	76
0.7	1.0	3517	108	108
1.0	0.1	4009	11	11
1.0	0.3	3963	34	34
1.0	0.7	3871	80	80
1.0	1.0	3803	114	114
1.4	0.1	4420	12	12
1.4	0.3	4370	37	37
1.4	0.7	4272	86	86
1.4	1.0	4200	122	122

2 The force field parameters

Table S2: The Lennard Jones and force field parameters adopted in this work.

Atom	σ/nm	ε/kJ mol^{-1}	q/e	Ref.
Li^+	0.202590	7.65672×10^{-2}	1.0	[1]
Na^+	0.332840	1.15897×10^{-2}	1.0	[1]
K^+	0.472302	1.37235×10^{-3}	1.0	[1]
Cl^-	0440104	4.18400×10^{-1}	-1.0	[1]
O_w	0.315061	6.36386×10^{-1}	-0.834	[2]
H_w	0	0	0.417	[2]
C_{gra}	0.339967	3.59824×10^{-1}	0	[3]
C_{c_2n}	0.339967	3.59824×10^{-1}	0.24	[4]
N_{c_2n}	0.325000	7.11280×10^{-1}	-0.48	[4]

Bond type	length/nm
C_{c_2n}-C_{c_2n}(involved in pyrazine)	0.143
C_{c_2n}-C_{c_2n}(presented in benzene rings)	0.147
C_{c_2n}-N_{c_2n}	0.134
C_{gra}-C_{gra}	0.142

Angle type	angle/degree
C_{c_2n}-C_{c_2n}-C_{c_2n}	120
C_{c_2n}-N_{c_2n}-C_{c_2n}	120
N_{c_2n}-C_{c_2n}-C_{c_2n}	120
C_{gra}-C_{gra}-C_{gra}	120

3 The dehydration free energy

Table S3: The dehydration free energy of alkali ion in the bulk solution, the water model is TIP3P.

	Li^+/kCal mol^{-1}	Na^+/kCal mol^{-1}	K^+/kCal mol^{-1}
This work	109.1	83.9	66.5
Joung's work[5]	113.7	88.7	70.7
Åqvist's work[6]	109.5	84.2	67.0

4 The number of water molecules, anion and nitrogen atom in the first coordination shell of cation

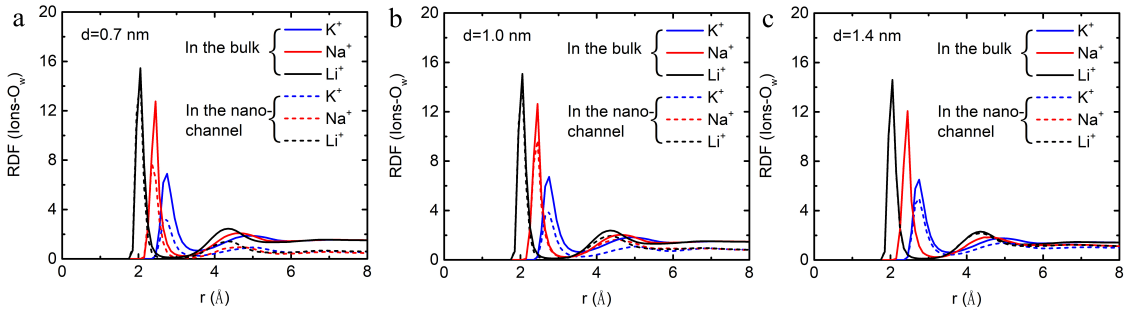

Figure S1: The radial distribution function of water molecules around K^+,Na^+ and Li^+ ions at d=0.7 nm (a),1.0 nm (b) and 1.4 nm (c). The solid and dashed lines represent the case of the alkali ion in the bulk and the nanochannel, respectively. The first peak position from the center of K^+,Na^+ and Li^+ ions are in good agreement with the previous work.[7, 8]

The hydration diameter could be defined as [9]

$$D_{hd}^3 = \frac{6}{\pi} \upsilon_w h + D_{eff}^3 \tag{1}$$

where D_{hd} is the hydration diameter, υ_w (υ_w=2.991×10^{-29} m^3) is the volume of a water molecule , h is the hydration factor and D_{eff} is the effective ionic diameter defined as the double difference between the peak position of radial distribution function and the effective radius of a water molecule (0.138 nm). The results is shown in the Table S4, which is good agreement with that of the previous work.

Table S4: The hydration diameter of cations

	Li^+/nm	Na^+/nm	K^+/nm
This work	0.79	0.72	0.63
Previous work[10]	0.76	0.72	0.66

Table S5: The number of oxygen in water, Cl^- and nitrogen in the C_2N membrane within the first coordination shell of alkali ions in the bulk and in the nanochannel, respectively. The radius of the first coordination shell was defined at first minima in the radial distribution function.

d/nm	Ion	In the bulk		In the nanochannel		
		Ion-O_w	Ion-Cl^-	Ion-O_w	Ion-Cl^-	Ion-N
0.7	Li^+	4.3	0.2	3.8	0.2	0.6
	Na^+	5.5	0.2	3.5	0.2	1.2
	K^+	6.5	0.3	2.8	0.1	4.7
1.0	Li^+	4.3	0.2	3.9	0.2	0.2
	Na^+	5.5	0.2	4.4	0.6	0.6
	K^+	6.5	0.3	3.5	0.1	3.8
1.4	Li^+	4.3	0.2	4.3	0.2	0.2
	Na^+	5.5	0.2	5.4	0.2	0.2
	K^+	6.5	0.3	4.9	0.1	3.3

5 The concentration of ions outside the nanochannel

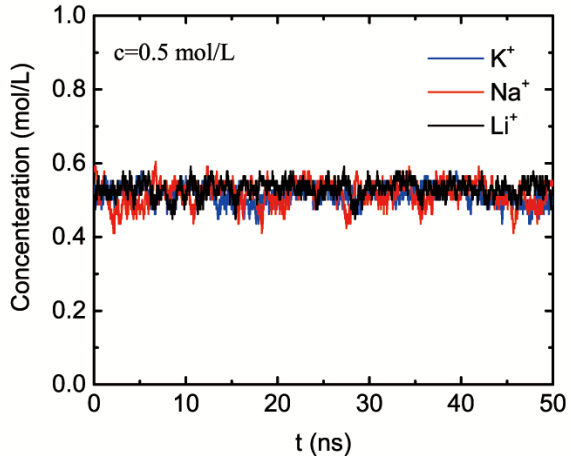

Figure S2: The concentration of ions outside the nanochannel as a function of simulated time at d=1.4 nm.

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