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

Supporting Information

Enhancing the performance of a cylindrical nanopore in osmotic power generation through designing the waveform of its inner surface

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1. The frequency and amplitude of the waveform assumed for the nanopore wall

Table S1 The frequency f, wavelength λ, and width W assumed for the waveform of the nanopore wall.

f [nm^{-1}]	λ [nm]	W [nm]
0.5	4π	2π
1	2π	1π
2	1π	$(1/2)\pi$
4	$(1/2)\pi$	$(1/4)\pi$
8	$(1/4)\pi$	$(1/8)\pi$
16	$(1/8)\pi$	$(1/16)\pi$

Table S2 The amplitude a and height H of the waveform assumed for the nanopore wall.

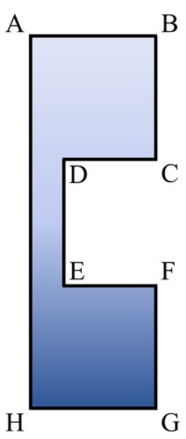
a [nm]	H [nm]
1/4	1/2
1/2	1
1	2
2	4
4	8
8	16

2. Physical parameters and schematic diagram with boundary conditions

Table S3 Values of physical parameter

Name	Symbol	Value
Radius of computational domain	R_R	1000 nm
Length of computational domain	L_R	1000 nm
Radius of nanopore	R_N	20 nm
Length of nanopore	L_N	600 nm
Gas constant	R	8.314 J/(mol·K)
Faraday constant	F	96485 C/mol
Valence of Na^+	z_1	1
Valence of Cl^-	z_2	-1
Diffusivity of Na^+	D_1	1.33×10^{-9} m^2/s
Diffusivity of Cl^+	D_2	2.03×10^{-9} m^2/s
Diffusivity of Mg^{2+}	D_3	7.10×10^{-10} m^2/s
Diffusivity of La^{3+}	D_4	6.00×10^{-10} m^2/s
Vacuumm permittivity	ε_0	8.85×10^{-12} F/m
Permittiivity of NaCl solution	ε	6.95×10^{-10} F/m
Viscosity of NaCl solution	μ	0.001 Pa·s
Density of NaCl solution	ρ	998 kg/m^3
Surface charge density of nanopore	σ	-0.01 C/m^2
Salt concentration (high)	C_H	10, 50, 100 mM
Salt Concentration (low)	C_L	1 mM

Table S4 Boundary conditions assumed in numerical modeling

Scheme	Surface	Navier -Stokes	Nernst -Planck	Poisson
	AB	$p = 0$ $n \cdot [\mu(\nabla u + (\nabla u)^T)] = 0$	$C_i = C_L$	$\phi = 0$
	BC, FG	slip	$n \cdot J_i = 0$	uncharged $-n \cdot (\varepsilon \nabla \phi) = 0$
	CD, DE, EF	no slip	$n \cdot J_i = 0$	$-n \cdot (\varepsilon \nabla \phi) = \sigma$
	HG	$p = 0$ $n \cdot [\mu(\nabla u + (\nabla u)^T)] = 0$	$C_i = C_H$	$\phi = 0$
	AH	Axial symmetry	Axial symmetry	Axial symmetry

3. Code verificaiton

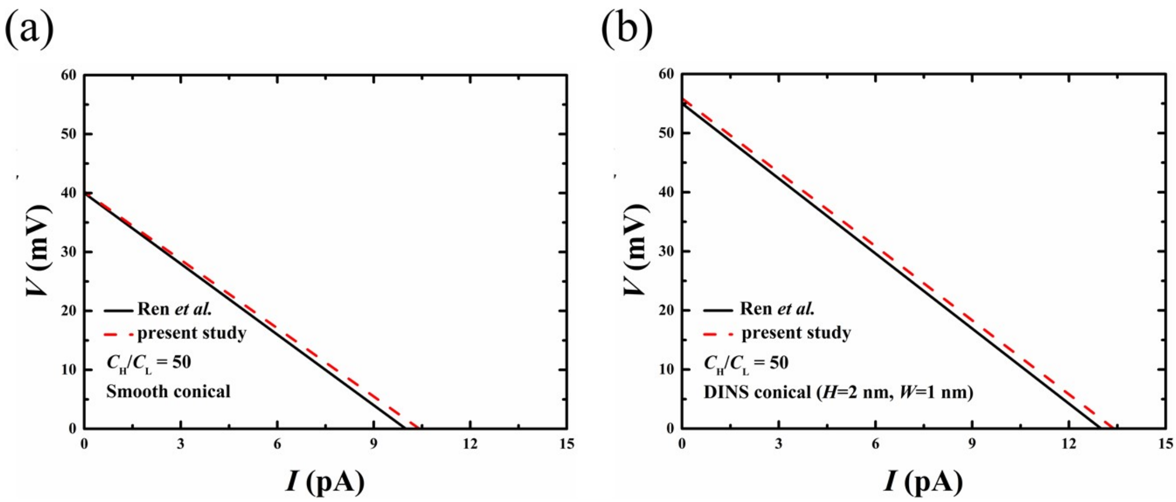


Fig. S1. Current-voltage (I-V) curve for a smooth conical nanopore, (a), and a conical nanopore with designed interfacial nanostructures (DINS), (b), at $L_N = 600$ nm, $R_{tip} = 6$ nm, $R_{base} = 40$ nm, $C_H = 50$ mM, $C_L = 1$ mM, and $T = 303$ K. Solid line: simulated results of Ren *et al*. [S1]; dotted line: present results.

4. Choice of computation domain and mesh size

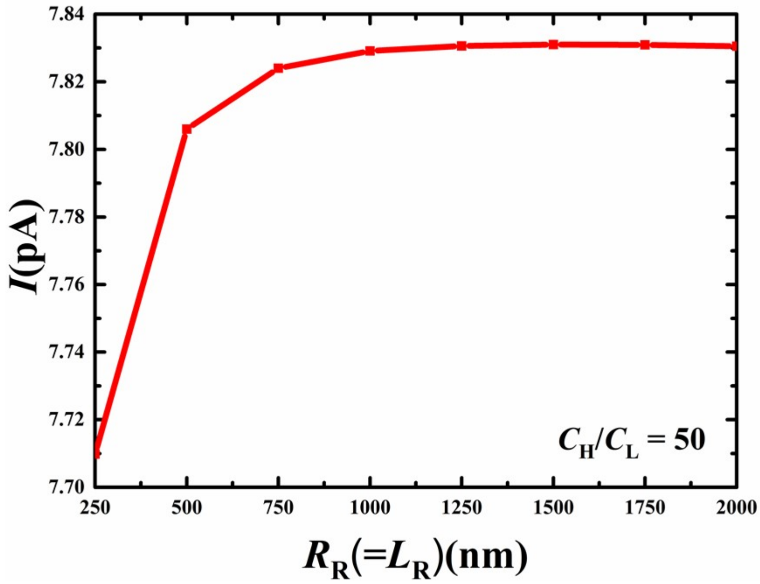


Fig. S2. Variation of ionic current with the size of computation domain (R_R=L_R) for the case of square waveform at $f = 0.5$ nm^{-1}, $a = 0.5\ nm$, and $(C_H/C_L) = 50$.

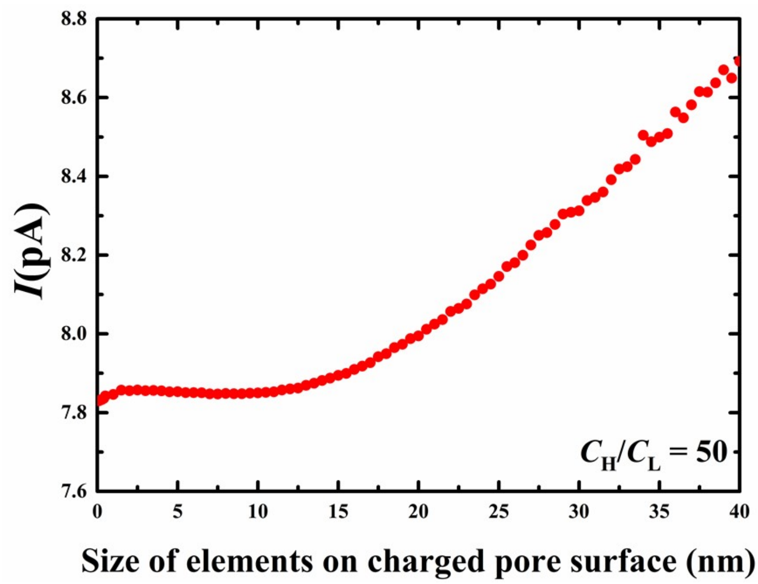


Fig. S3. Variation of ionic current with size of element on nanopore surface at $f = 0.5$ nm^{-1}, $a = 0.5\ nm$, and $(C_H/C_L) = 50$

5. Effective bulk concentration range

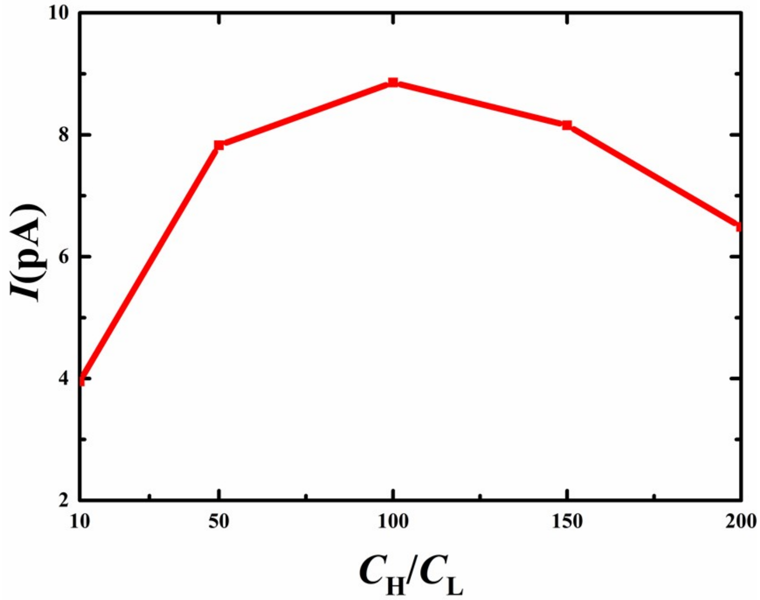


Fig. S4. Variation of ionic current with bulk concentration ratio (C_H/C_L) at $f = 0.5$ nm^{-1} and $a = 0.5\ nm$

6. Influence of frequency and amplitude of the waveform on the I_+ and I_-

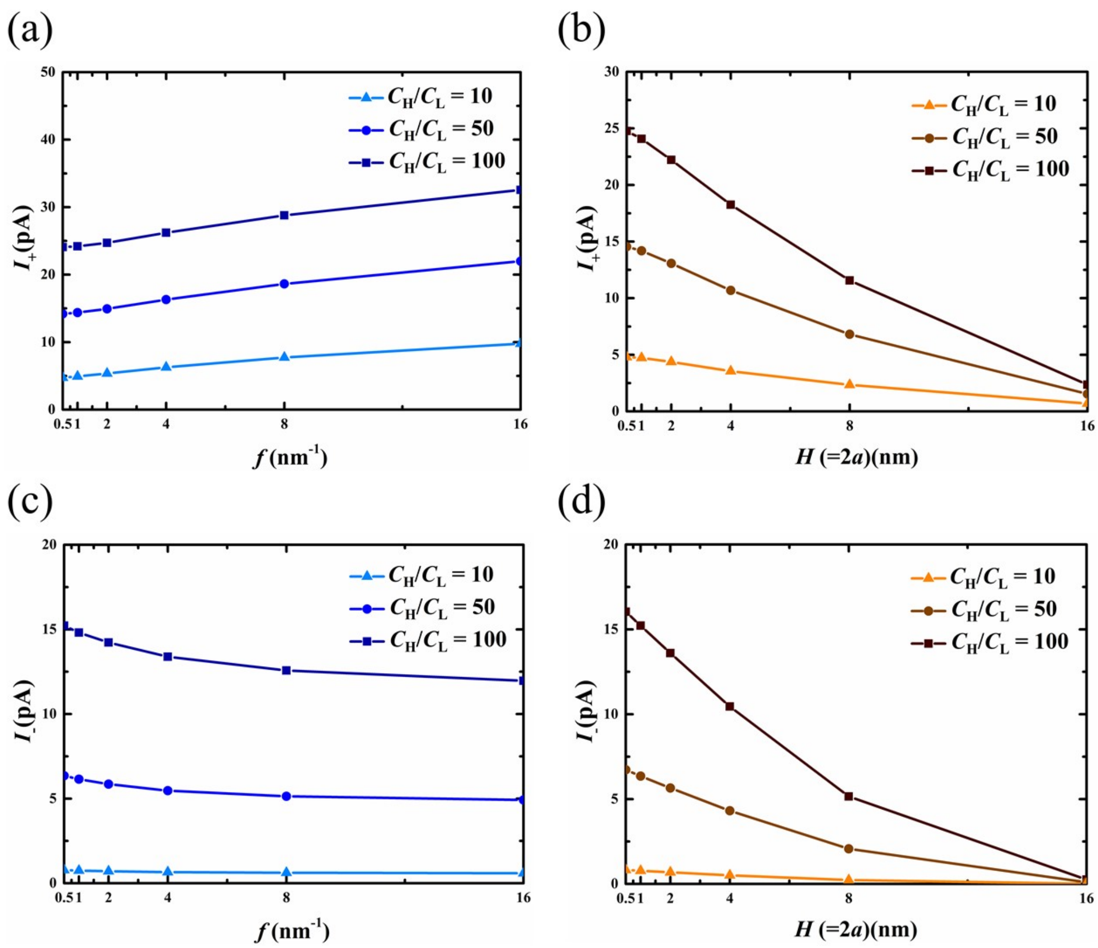


Fig. S5. Variation of I_+ with f, (a), and $H(=2a)$, (b), for various levels of bulk concentration ratio (C_H/C_L), (c) and (d) are the corresponding variation of I_-. (a) and (c): $a = 0.5\ nm$; (b) and (d): $f = 0.5\ \mathrm{nm}^{-1}$.

7. Influence of *f* and *a* on ionic flux

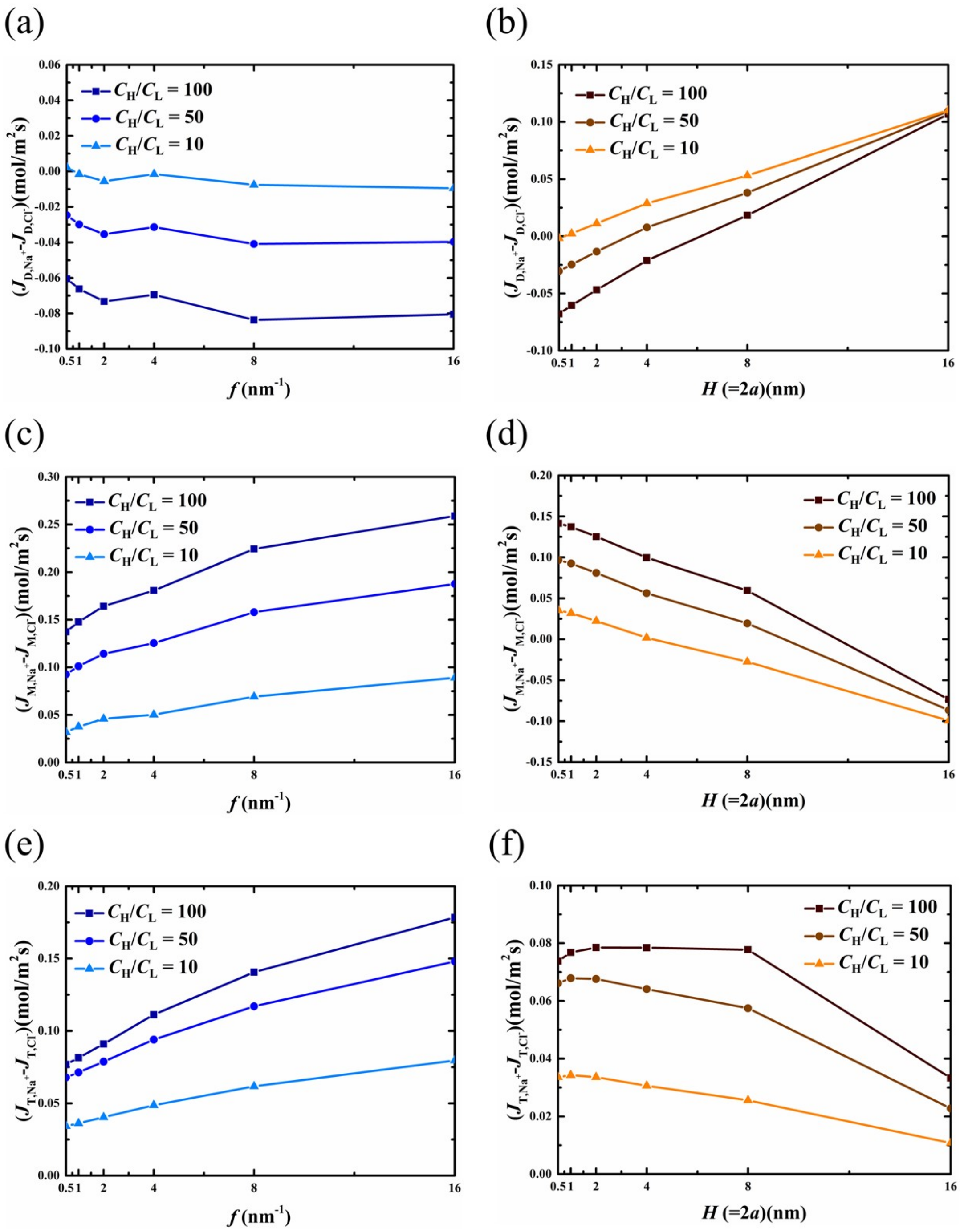


Fig. S6. Variation of $(J_{D,Na^+} - J_{D,Cl^-})$ with f, (a), and $H(=2a)$, (b), for various levels of bulk concentration ratio (C_H/C_L), (c) and (d) are the corresponding variation of $(J_{D,Na^+} - J_{D,Cl^-})$, (e) and (f) are the corresponding variation of $(J_{T,Na^+} - J_{T,Cl^-})$. (a), (c), and (e): $a = 0.5\ nm$; (b), (d), and (f): $f = 0.5\ \mathrm{nm}^{-1}$.

8. Influence of various electrolytes

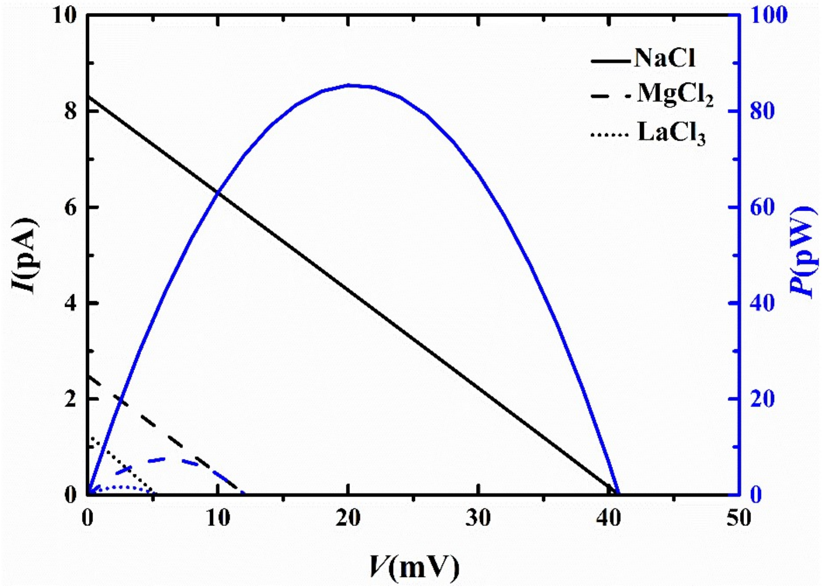


Fig. S7 Current-voltage (I-V) curve and power-voltage (P-V) curve for various electrolytes in the case of a square waveform at $f = 2\ \mathrm{nm}^{-1}$, $a = 0.5\ nm$, and $(C_{H,\ \mathrm{Cl}^-}/C_{L,\mathrm{Cl}^-}) = 10$

References

1 Q. Ren, Q. Cui, K. Chen, J. Xie and P. Wang, *Desalination*, 2022, **535**, 115802.