## **Supporting Information**

## Multi-physics Simulation of Ion Concentration Polarization Induced by A Surface-patterned Nanoporous Membrane in Single Channel Devices

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## **Governing Equations**

Ionic concentration of species *i* ( $c_i$ ), fluid velocity ( $\bar{u}$ ), and electric potential ( $\phi$ ) are the main variables in the governing equations, respectively. The generation and development of ICP phenomena depend on the complex effect of those variables on each other.

First, the Nernst-Planck equation is in charge of the concentration distribution of different species of ions and trace molecules. The equation is shown as below:

$$\frac{\partial c_i}{\partial t} + \nabla c_i \cdot \overline{\mathbf{u}} = \nabla \left( D_i \nabla c_i + z_i c_i D_i \frac{F}{RT} \nabla \phi \right)$$
(1)

where  $c_i$ ,  $D_i$ , and  $z_i$  are the concentration of an ion species *i*, its corresponding diffusion coefficient, and ionic valence in an electrolyte solution, respectively. *T* represents the temperature of 25°C and *F* and *R* are the Faraday and ideal gas constant, respectively.

Second, the Navier-Stokes equation describes the motion of incompressible fluid flow with the continuity equation:

$$\rho \frac{\partial \overline{\mathbf{u}}}{\partial t} + \rho(\overline{\mathbf{u}} \cdot \nabla)\overline{\mathbf{u}} = -\nabla p + \eta \nabla^2 \overline{\mathbf{u}} - \rho_E \nabla \phi$$
<sup>(2)</sup>

$$\nabla \cdot \overline{\mathbf{u}} = 0 \tag{3}$$

where  $\rho$  is the density of the solution,  $\eta$  is the dynamic viscosity, and  $\rho_E$  represents the net charge density in the solution.

$$\rho_E = F \sum_i z_i c_i \tag{4}$$

Third, the Poisson equation relates the ionic concentration of a buffer solution to the electric potential:

$$\nabla^2 \phi = -\frac{\rho_E}{\varepsilon} \tag{5}$$

where  $\varepsilon$  is the permittivity of the medium. When it comes to the domain of the membrane, the fixed volumetric charge of the membrane ( $\rho_{fix}$ ) is added to the right hand side of the Poisson equation as follows:

$$\nabla^2 f = -\frac{\Gamma_E + \Gamma_{fix}}{\varrho} \tag{6}$$

Since the governing equations are coupled with each other, we performed numerical multiphysics simulations to find out CEFs, ionic concentration distributions, ionic currents, electric fields, flow fields including vortex flows, and so on.

Table S1 Properties used in simulations unless otherw
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Diffusion coefficient of H <sup>+</sup>	$9.36 \times 10^{-9} \text{ m}^2/\text{s}$
Diffusion coefficient of $C1^{-}$	$2.032 \times 10^{-9} \text{ m}^{2/s}$
Diffusion coefficient of Ci	$2.032 \times 10^{-111/8}$
	0 4 7 4 0 9 2 4
Diffusion coefficient of trace molecule	$0.45 \times 10^{5} \text{ m}^{2}/\text{s}$
Valence of trace molecule	-2
Diffusion apofficient of U <sup>+</sup> in membrane	$0.26 \times 10^{-10} \text{ m}^2/c$
Diffusion coefficient of H In memorane	$9.30 \times 10^{-111}$ III /S
	10 2
Diffusion coefficient of Cl <sup>-</sup> in membrane	$2 \times 10^{-10} \text{ m}^2/\text{s}$
Ion concentration in electrolyte solution $c_{0}$	1 mM
Ton concentration in creetionyte solution, e0	1 11111
Assumed charge density of the membrane, $\rho_{fix}$	-0.5 mM
Zeta-notential at the channel walls $\zeta$	-60 mV
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Note that these properties are found in literature[1-4].



Fig. S1. (a) The distribution of normalized electric fields along the *x*-axis near the top surface of the channel (at  $z = 20 \ \mu\text{m}$ ) when the electric potentials range from 1.5 to 5 V. (b) The distribution of normalized concentrations of the trace molecules along the same line in (a) ( $z = 20 \ \mu\text{m}$ ) for the different electric potentials.

## References

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