Directly Observing the Motion of DNA Molecules near Solid-State Nanopores

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Supporting Information

We have used COMSOL Multiphysics Software (Version 4.2) with the Electrostatic (Poisson equation) and Transport of Diluted Species (Nernst-Planck equation) modules. Since the simulation geometry has cylindrical symmetry, simulation domains are defined with axial symmetry in 2 dimensions as shown in Figure S1. The thickness of the freestanding membrane is set as 200 nm, the pore's inner diameter is around 100 nm. Electrical setup is also shown in Figure S1. The voltage is applied along the blue line and ground is set along the black line in the Figure S1. To obtain electric field around a nanopore we used Poisson-Nernst-Planck equations (PNP).

The Nernst-Planck equation describes the motion of chemical ions in fluid. It accounts the flux of ions under the influence of both an ionic concentration gradient (∇c_i) and an electric field(- $\nabla \Phi$).

$$J_{i} = -D_{i}\nabla c_{i} - \frac{z_{i}F}{RT}D_{i}c_{i}\nabla\Phi + c_{i}\mathcal{U}$$
(S1)

S1

Here J_i , D_i , c_i , and z_i are the flux, diffusion constant, concentration, and charge species i, respectively. Φ and u are the local electric potential and fluid velocity, and *F*, *R*, *T* are, respectively, the Faraday constant, the gas constant, and the absolute temperature. The ionic concentration is increased by 5 mM to compensate the effect from TE buffer in solution.

The electric potential generated by chemical ions is described by the Poisson equation (S2), where ε is the dielectric constant of the fluid.

$$\nabla^2 \Phi = -F/\epsilon \sum_{i} z_i c_i \tag{S2}$$

The Figure S2 and S3 are generated by the COMSOL simulation for the purpose to compare with experimental results in the main text.

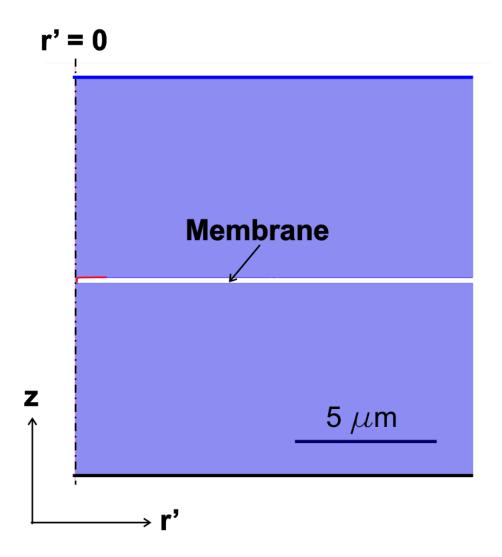


Figure S1. Electrostatic conditions used for the simulation. Electric potential is applied to the blue line and electrical ground is set at the black line. The red line, indicating an area of $1.1 \mu m$ radius, around a nanopore can be electrically charged. Other boundaries are set as insulators.

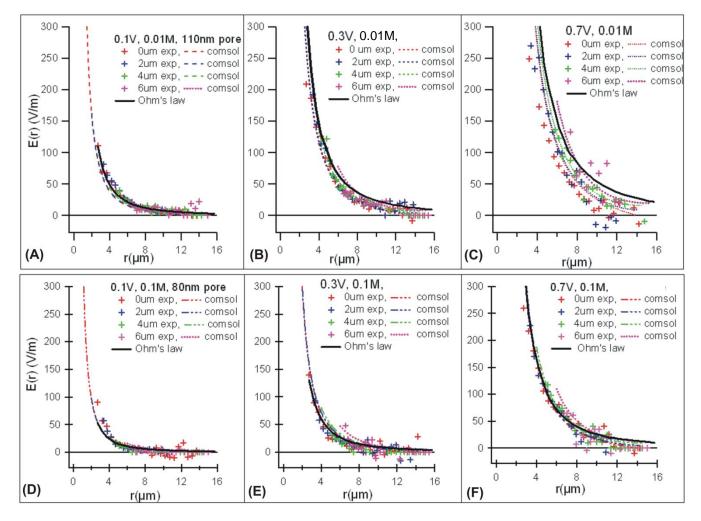


Figure S2. The dashed curves in Fig.S2 are the result of simulation using the PNP equations. The solid curve is from Ohm's law using equation (3).

(a) 0.01 M KCl

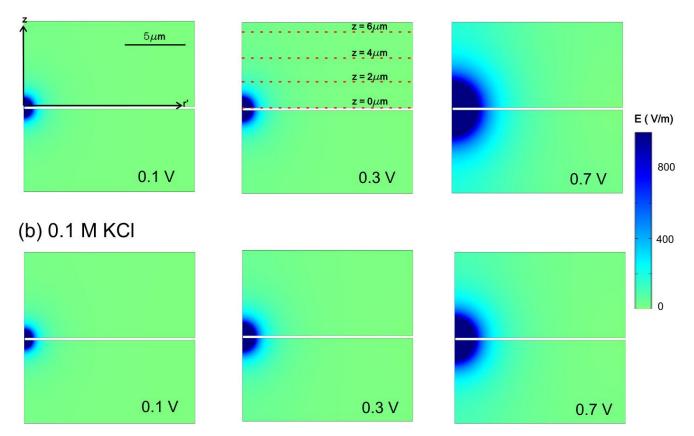


Figure S3. The strength of the electric field in two dimensions near a nanopore for bias voltages, 0.1, 0.3 and 0.7 V. The salt concentrations are 0.01M for (a) and 0.1 M KCl for (b). Electric field magnitude only less than 1000 V/m is shown in this figure.

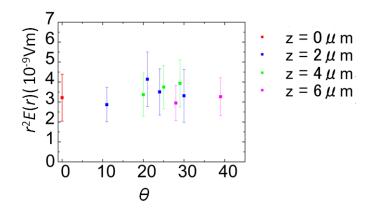


Figure S4. The theta angle dependence of $r^{2}*E(r)$. This plot demonstrates that $r^{2}*E(r)$ vs theta is approximately a constant.