Supplementary information

Computational Modeling of Ionic Currents Through Difform Graphene Nanopores with Consistent Cross-sectional Area

Wei Si¹,², Chenhan Liu¹,², Jingjie Sha¹,², Yin Zhang¹,², Yunfei Chen¹,²*

¹School of Mechanical Engineering, Southeast University, Nanjing 211189, China
²Jiangsu Key Laboratory for Design and Manufacture of Micro-Nano Biomedical Instruments, Southeast University, Nanjing 211189, China

*The correspondence should be addressed to yunfeichen@seu.edu.cn, major212@seu.edu.cn and wei.si@seu.edu.cn.
Figure S1. The relationship between the mean ionic conductivity \( \sigma \) (S/m) and perimeter \( P \) (nm) of the four different nanopores. Inset images illustrate the shapes of nanochannels investigated in this work.
Figure S2. Cross section of a simulation system for the square nanopore. The contour plot is colored according to distance ($r$) to the nearest nanopore surface. Atoms of the graphene membrane are shown as cyan vdW spheres.
Figure S3. Cross section of a simulation system for the rectangular nanopore. The contour plot is colored according to distance ($r$) to the nearest nanopore surface. Atoms of the graphene membrane are shown as cyan vdW spheres.
Figure S4. Cross section of a simulation system for the triangular nanopore. The contour plot is colored according to distance ($r$) to the nearest nanopore surface. Atoms of the graphene membrane are shown as cyan vdW spheres.
Figure S5. The ion concentration distributions depending on the distance \( r \) from the nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function

\[
y = \frac{1}{2} \left( 1 + \tanh \left( \frac{x-a}{b} \right) \right).
\]
Figure S6. The ion mobility distributions depending on the distance $r$ from the nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function $y = \frac{1}{2} \left(1 + \tanh \left(\frac{x-a}{b}\right)\right)$. 
Figure S7. The relative water density distributions $\rho(r)/\rho_0$ depending on the distance $r$ from the hydrophobic and hydrophilic square nanopore surfaces. $\rho_0$ is the averaged water density in the bulk area of the simulated systems.
Figure S8. The relative water density distributions $\rho(r)/\rho_0$ depending on the distance $r$ from the hydrophobic and hydrophilic rectangular nanopore surfaces. $\rho_0$ is the averaged water density in the bulk area of the simulated systems.
Figure S9. The relative water density distributions $\rho(r)/\rho_0$ depending on the distance $r$ from the hydrophobic and hydrophilic triangular nanopore surfaces. $\rho_0$ is the averaged water density in the bulk area of the simulated systems.
Figure S10. The ion concentration distributions depending on the distance \( r \) from the hydrophobic and hydrophilic square nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function \( y = \frac{1}{2} (1 + \tanh(\frac{x-a}{b})) \).
Figure S11. The ion concentration distributions depending on the distance $r$ from the hydrophobic and hydrophilic rectangular nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function $y = \frac{1}{2} \left( 1 + \tanh \left( \frac{x-a}{b} \right) \right)$. 
Figure S12. The ion concentration distributions depending on the distance $r$ from the hydrophobic and hydrophilic triangular nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function $y=\frac{1}{2}(1+\tanh\left(\frac{x-a}{b}\right))$. 

$\beta = 0.1$  
$\beta = 2.0$  
Cl$^-$  K$^+$
Figure S13. The ion mobility distributions depending on the distance $r$ from the hydrophobic and hydrophilic square nanopore surfaces.
Figure S14. The ion mobility distributions depending on the distance $r$ from the hydrophobic and hydrophilic rectangular nanopore surfaces.
Figure S15. The ion mobility distributions depending on the distance $r$ from the hydrophobic and hydrophilic triangular nanopore surfaces.
Table S1. Parameters of $a$ and $b$ used for predicting ionic currents through difform nanopores with different hydrophobicity.

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$a$</th>
<th>$b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>2.8</td>
<td>1.3</td>
</tr>
<tr>
<td>1.0</td>
<td>3.3</td>
<td>1.0</td>
</tr>
<tr>
<td>2.0</td>
<td>4.2</td>
<td>1.6</td>
</tr>
</tbody>
</table>