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

Supplementary information

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

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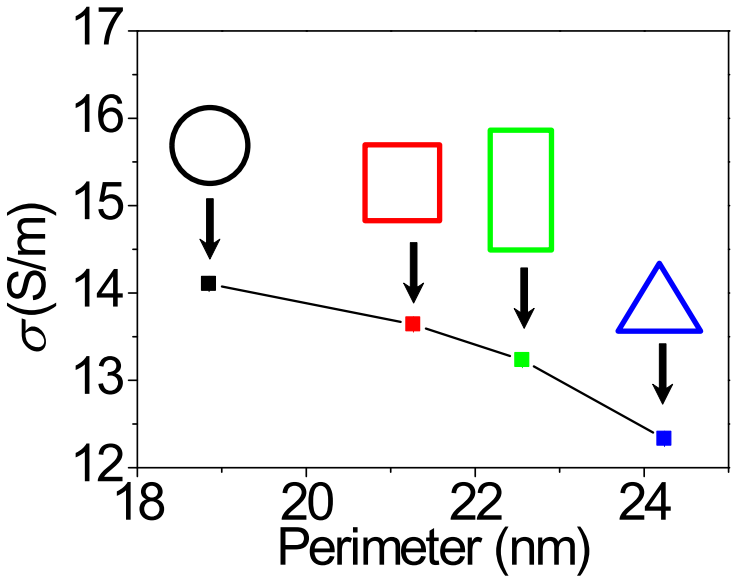

Figure S1. The relationship between the mean ionic conductivity and perimeter of the four difform nanopores. Inset images illustrate the shapes of nanochannels investigated in this work.

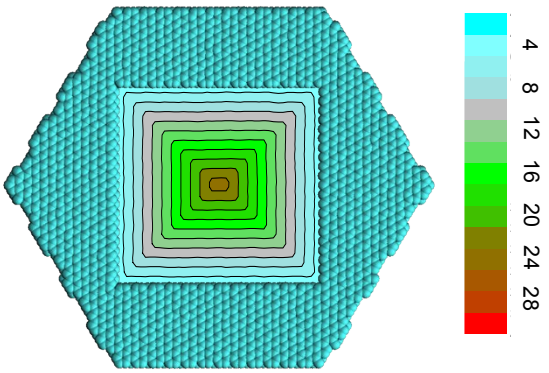

Figure S2. Cross section of a simulation system for the square nanopore. The contour plot is colored according to distance (r) to the nearest nanopore surface. Atoms of the graphene membrane are shown as cyan vdW spheres.

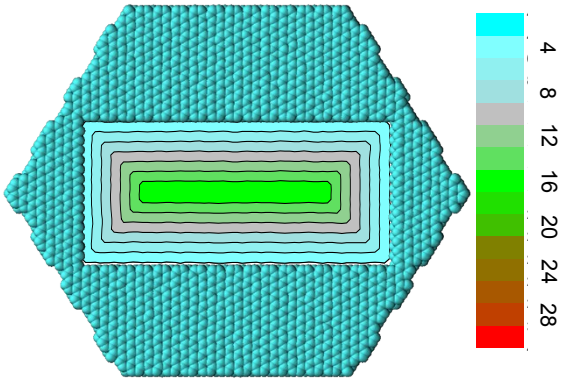

Figure S3. Cross section of a simulation system for the rectangular nanopore. The contour plot is colored according to distance (r) to the nearest nanopore surface. Atoms of the graphene membrane are shown as cyan vdW spheres.

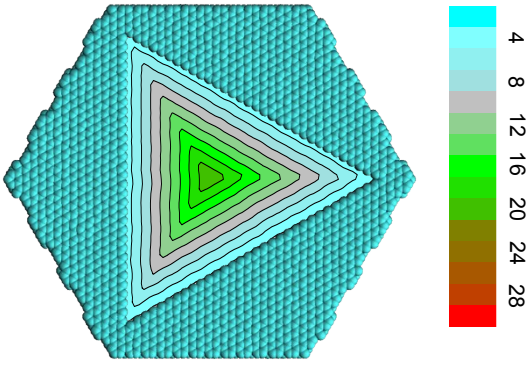

Figure S4. Cross section of a simulation system for the triangular nanopore. The contour plot is colored according to distance (r) to the nearest nanopore surface. Atoms of the graphene membrane are shown as cyan vdW spheres.

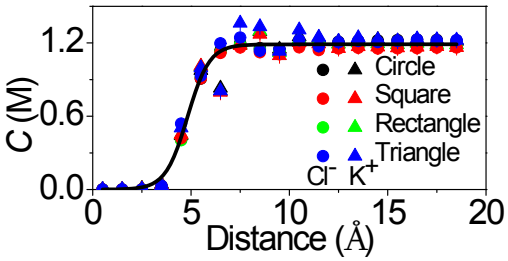

Figure S5. The ion concentration distributions depending on the distance r from the nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function $y=\frac{1}{2}(1+\tanh(\frac{x-a}{b}))$.

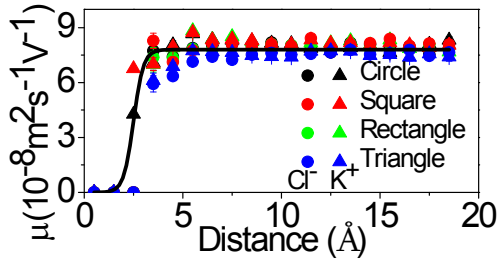

Figure S6. The ion mobility distributions depending on the distance *r* from the nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function $y=\frac{1}{2}(1+\tanh(\frac{x-a}{b}))$.

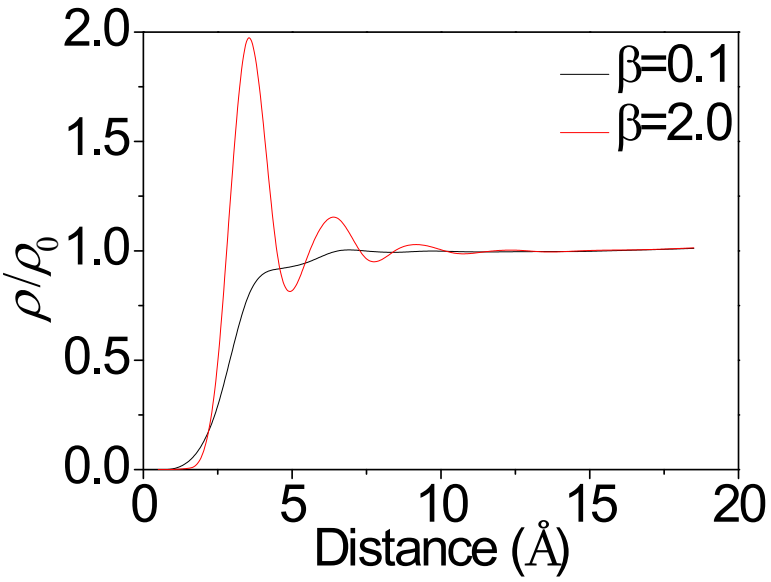

Figure S7. The relative water density distributions $\rho(r)/\rho_0$ depending on the distance r from the hydrophobic and hydrophilic square nanopore surfaces. ρ_0 is the averaged water density in the bulk area of the simulated systems.

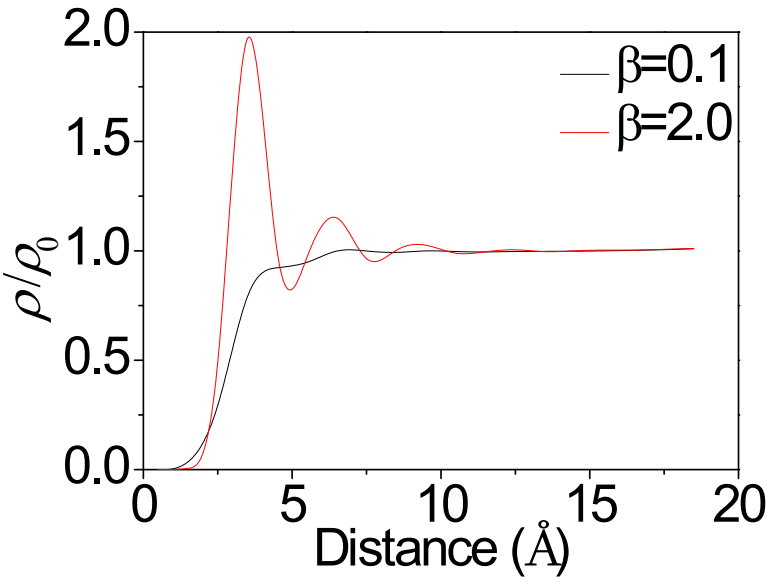

Figure S8. The relative water density distributions $\rho(r)/\rho_0$ depending on the distance r from the hydrophobic and hydrophilic rectangular nanopore surfaces. ρ_0 is the averaged water density in the bulk area of the simulated systems.

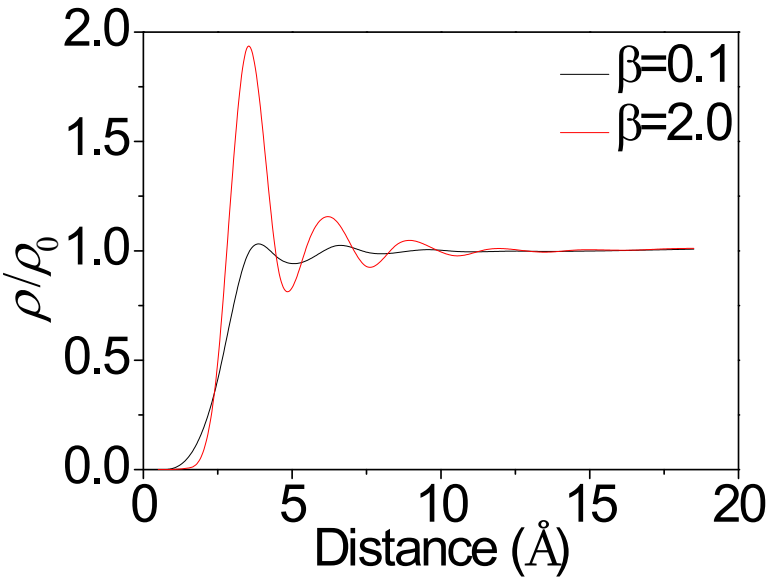

Figure S9. The relative water density distributions $\rho(r)/\rho_0$ depending on the distance r from the hydrophobic and hydrophilic triangular nanopore surfaces. ρ_0 is the averaged water density in the bulk area of the simulated systems.

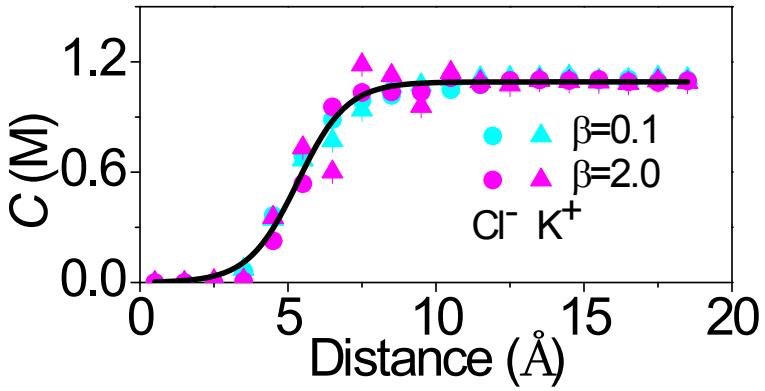

Figure S10. The ion concentration distributions depending on the distance *r* from the hydrophobic and hydrophilic square nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function $y=\frac{1}{2}(1+\tanh(\frac{x-a}{b}))$.

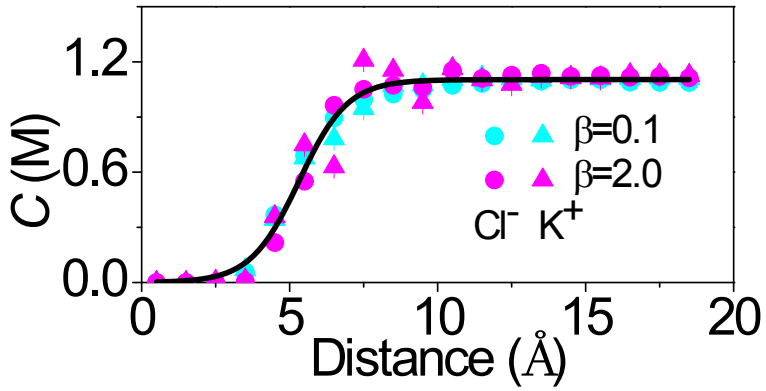

Figure S11. The ion concentration distributions depending on the distance *r* from the hydrophobic and hydrophilic rectangular nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function $y=\frac{1}{2}(1+\tanh(\frac{x-a}{b}))$.

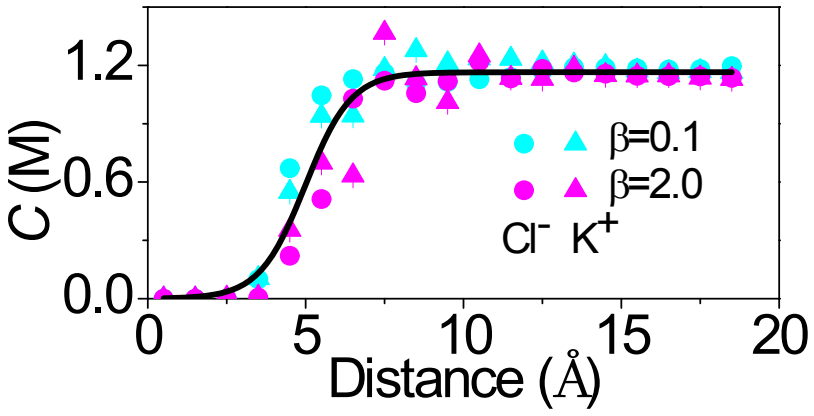

Figure S12. The ion concentration distributions depending on the distance *r* from the hydrophobic and hydrophilic triangular nanopore surfaces. The black solid line is plotted by fitting the results using a smooth-step function $y=\frac{1}{2}(1+\tanh(\frac{x-a}{b}))$.

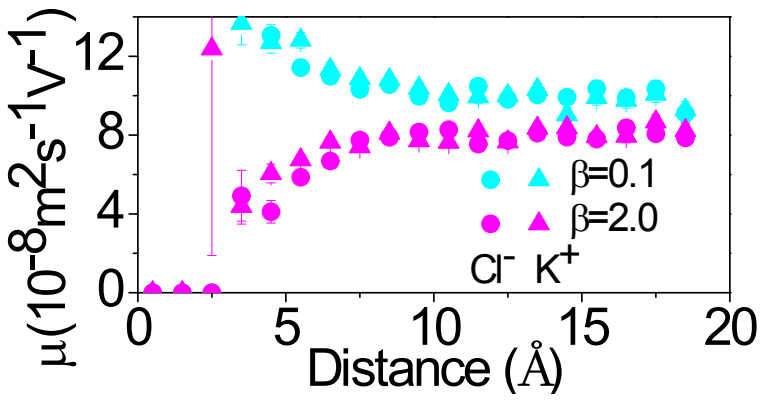

Figure S13. The ion mobility distributions depending on the distance *r* from the hydrophobic and hydrophilic square nanopore surfaces.

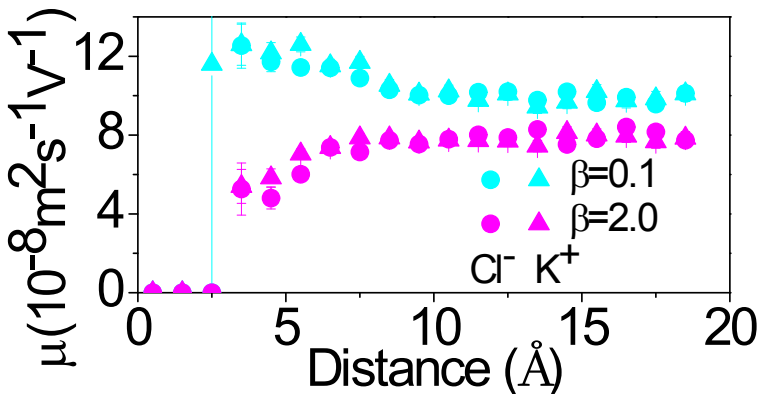

Figure S14. The ion mobility distributions depending on the distance *r* from the hydrophobic and hydrophilic rectangular nanopore surfaces.

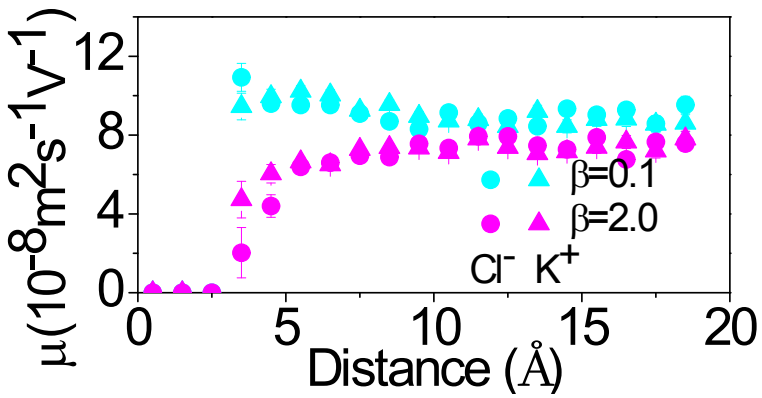

Figure S15. The ion mobility distributions depending on the distance *r* from the hydrophobic and hydrophilic triangular nanopore surfaces.

Table S1. Parameters of *a* and *b* used for predicting ionic currents through difform nanopores with different hydrophobicity.

β	*a*	*b*
0.1	2.8	1.3
1.0	3.3	1.0
2.0	4.2	1.6