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Supplementary Information for

Ionic Flow Through Partially Blocked Nanopores

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In this supplementary information, we provide (i) the concentration profiles of ions, and (iii) the potential of mean force.

S1: The concentration profiles of ions

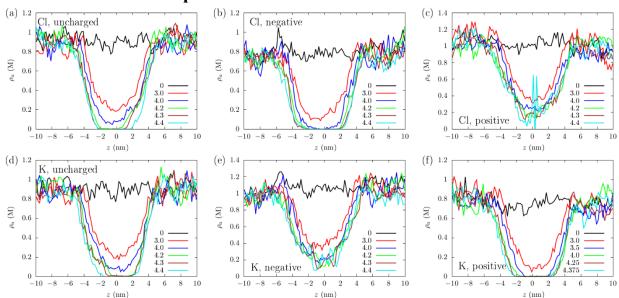


Fig. S1: The concentration profiles of ions in the axial direction of pore with radius 5 nm. The sampling bin width is 0.1 nm. The blockage radius is indicated on the plots.

S2: The potential of mean force (a)6 (b) 9 0.6 $\frac{0.7}{0.8}$ 0.75 7.5 0.80.9 0.9PMF (kcal/mol) PMF (kcal/mol) 1.0 6K, uncharged Cl, uncharged 4.53 1 1.5 0 0 0.6 0.8 1.4 0.6 0.8 1 1.2 0.20.4 1.2 0.20.41.4 z (nm)z (nm)(d) 12 (c) 3 $0.6 \\ 0.7$ $0.6 \\ 0.7$ 2.5 10 0.8 0.80.90.9PMF (kcal/mol) PMF (kcal/mol) 1.0 1.0 2 K, negative Cl, negative 1.5 6 1 0.52 0 0 0.8 0 0.20.40.6 0.8 1 1.2 1.4 0 0.2 0.40.61 1.2 1.4 z (nm) $z \, (\text{nm})$ (e)12 (f) 5 $0.6 \\ 0.7$ 0.60.70.8 10 0.8 4 0.9PMF (kcal/mol) PMF (kcal/mol) 1.0 1.0 3 K, positive Cl, positive

Fig S2: The potential of mean force of ions around the blockage inside pores with radius 1.49 nm. Pore gaps of 0.6 to 1.0 nm are created by placing the spherical blockages of radius 0.89 to 0.49 nm at the pore center.

2

0

0.2

0.4

0.6

0.8

 $z \, (\text{nm})$

1

1.2

1.4

1

0

0

0.2

0.4

0.8

 $z \, (\text{nm})$

1

1.2

1.4

0.6