Supporting Information

Computational Investigation of DNA Detection using Graphene Nanopores

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Supporting Tables

Pore Diameter (nm)	KCl Concentration (M)	Temperature (K)	Average RMSD fluctuation of pore mouth (Å)	Maximum RMSD fluctuation of pore mouth (Å)
3	1	295	0.72	3.3
3	2	295	0.93	4.4
3	1	305	1.7	4.4

Table S1: Breathing fluctuations of graphene around the pore from simulations SimA2, SimA7 and SimA8.

Applied bias Voltage (V)	Open pore current (nA)	Average blockade current (nA)	Reduction in current (%)	Translocation time (ns)
0.8	7.2	3.20	56	27.0
2.5	16.0	10.56	34	3.7
4.3	25.4	22.30	12	1.6

Table S2: Details of voltage-dependent DNA translocation. This table complements Figure 3. The reduction in current is determined as $100-$(Average blockade current/Open pore current)$\times100$.
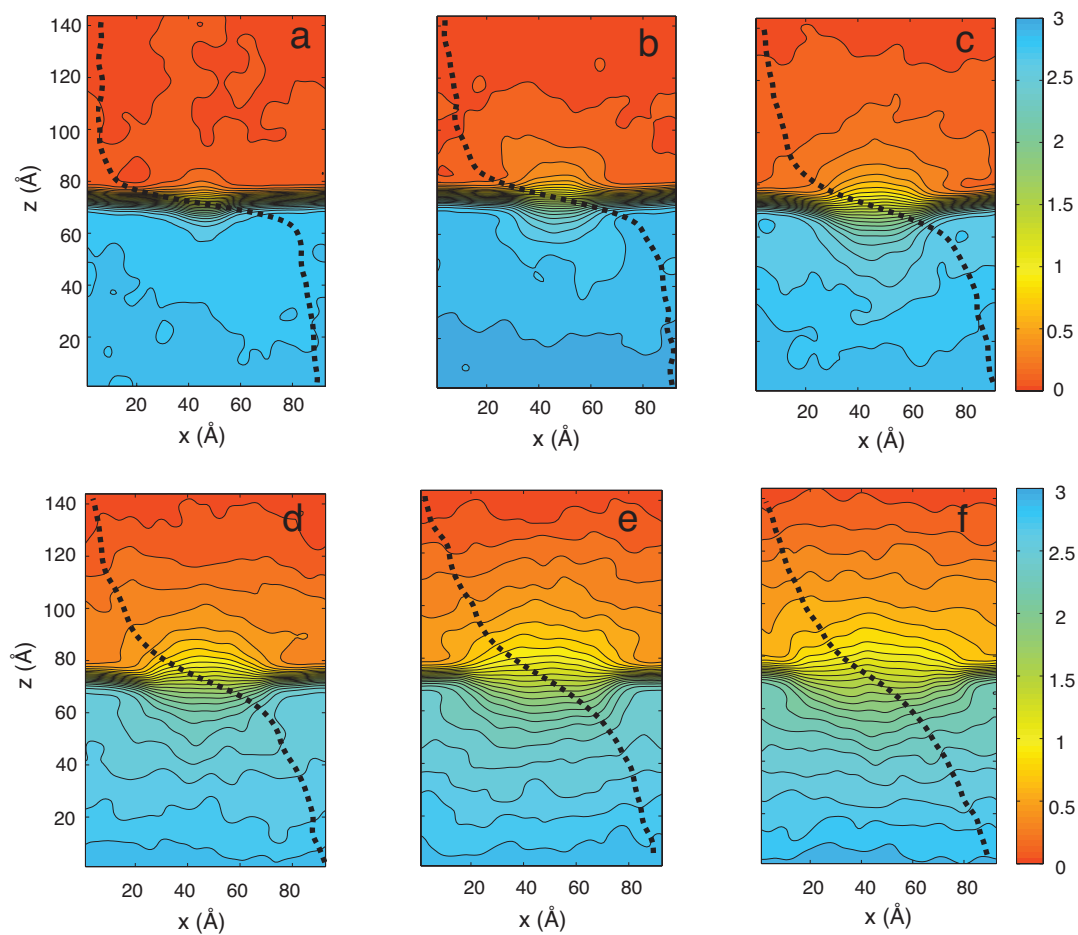
Supporting Figures

Figure S1: Averaged potential maps along the (x, z)-plane for pore diameter (a) 2 nm, (b) 3 nm, (c) 4 nm, (d) 5 nm, (e) 6 nm and (f) 7 nm. The dashed line shows the potential change normal to the graphene membrane. This figure complements Figure 2.
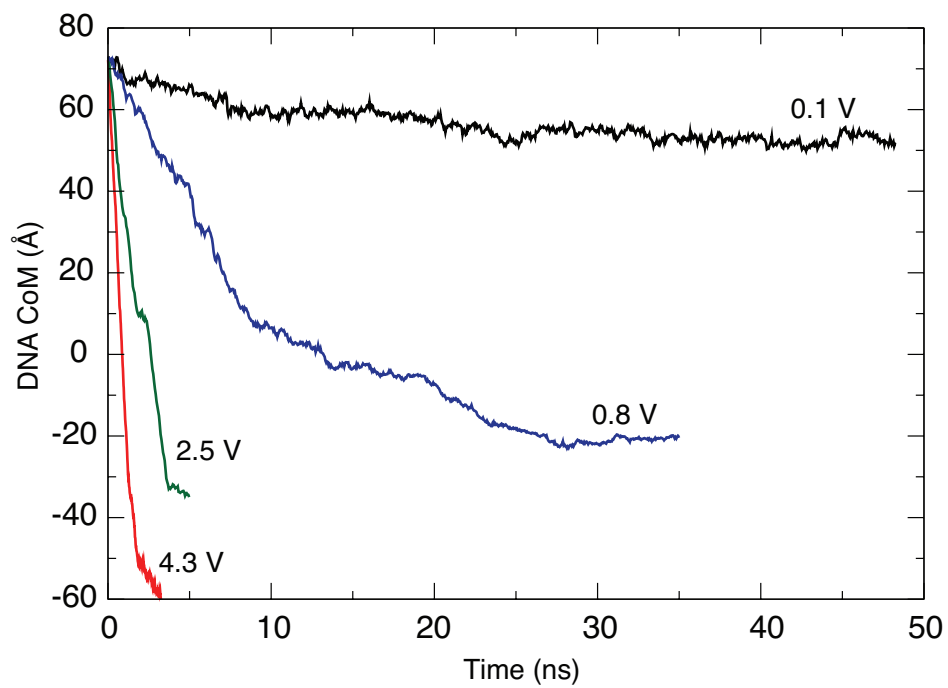
Figure S2: Comparison of DNA center of mass (CoM) motions for various applied bias voltages. This figure complements Figure 2.
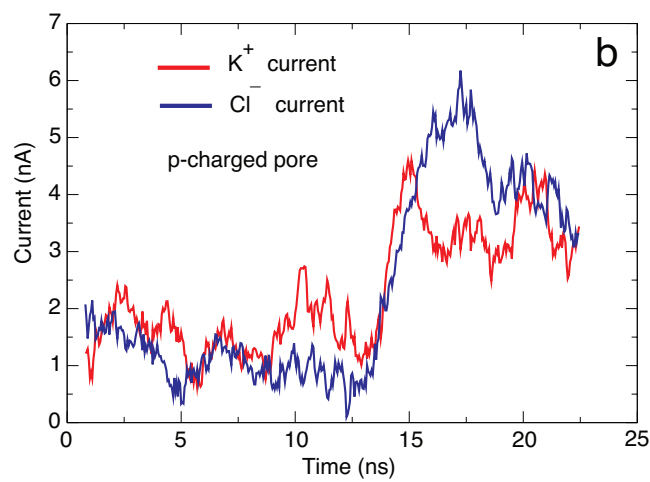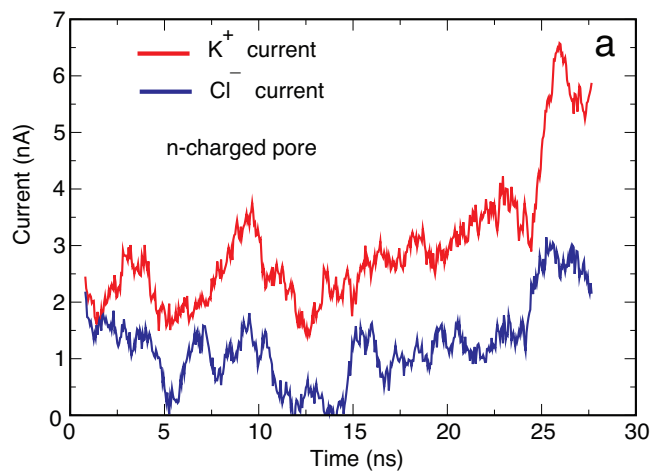
Figure S3: Profiles of K^+ (red line) and Cl^- (blue line) ion currents for (a) an n-charged pore and (b) a p-charged pore. This figure complements Figure 5a.
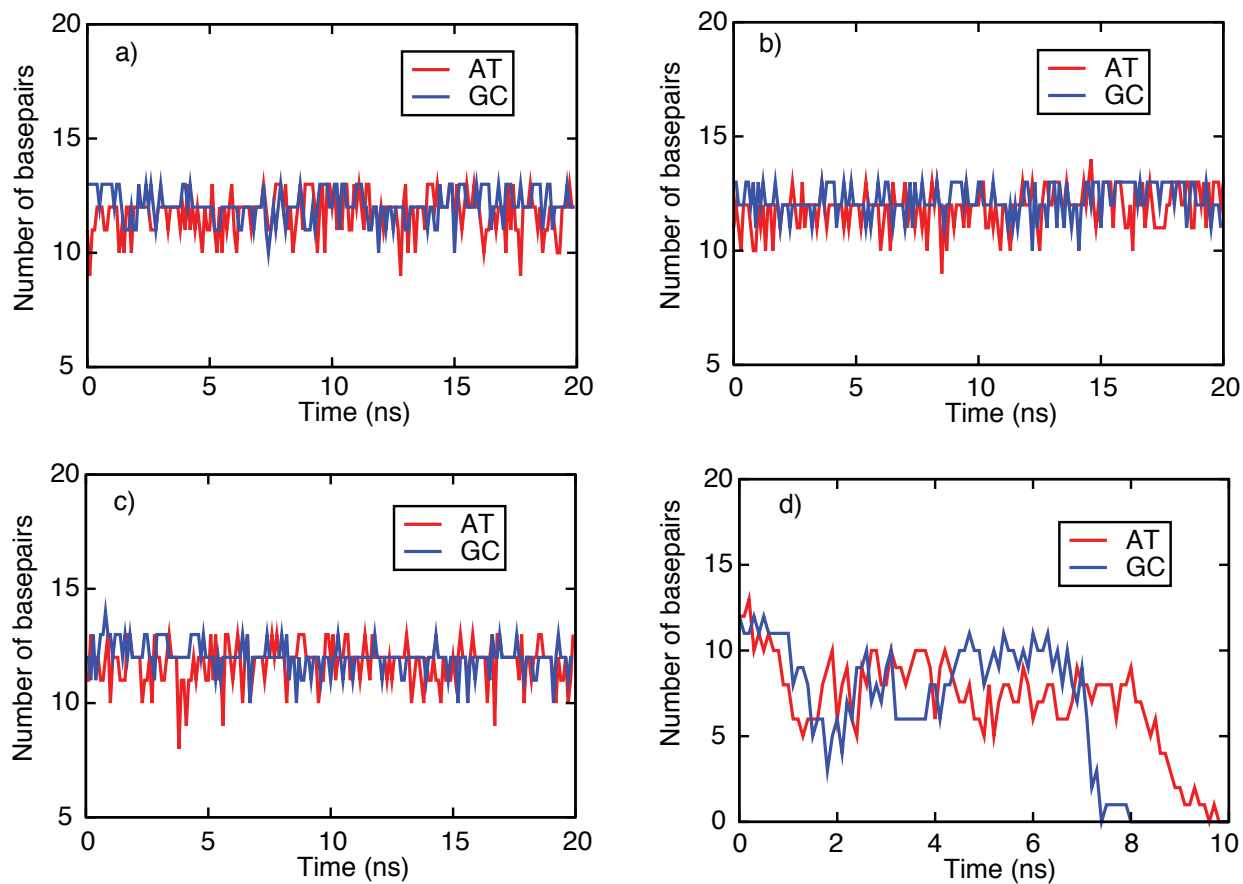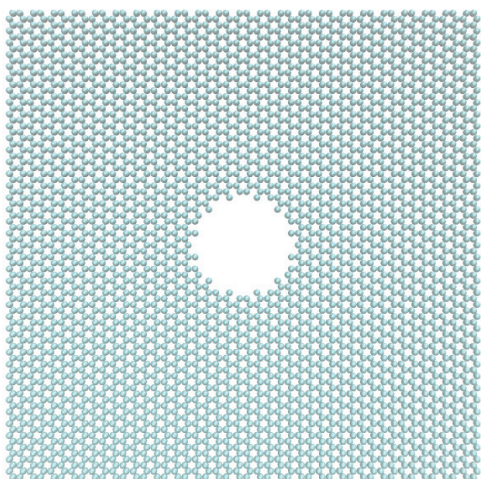
Figure S4: Number of base pairs near the pore mouth (± 2 nm) for (a) 0.1 V, (b) 0.3 V, (c) 0.5 V and (d) 1.2 V. This figure complements Figure 6.
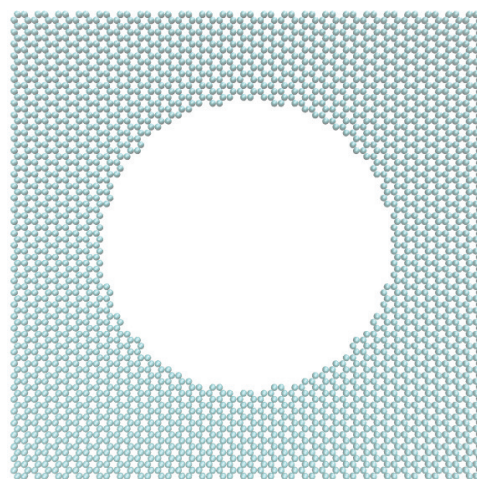
Figure S5: Graphene nanopores with diameters of (a) 2 nm and (b) 6 nm. This figure complements Figure 1.

Supporting Movies

- **Movie S1** shows the DNA translocation trajectory of simulation SimB1 (see Table 1) at an applied bias voltage of 4.3 V.

- **Movie S2** shows the DNA translocation trajectory of simulation SimB2 (see Table 1) at an applied bias voltage of 2.5 V.

- **Movie S3** shows the DNA translocation trajectory of simulation SimB3 (see Table 1) at an applied bias voltage of 0.8 V.

- **Movie S4** shows the DNA translocation trajectory of simulation SimC (see Table 1).

- **Movie S5** shows the DNA translocation trajectories of simulation SimD1-D2 (see Table 1) through an n-charged (red colored DNA) and a p-charged pore (blue colored DNA).

- **Movie S6** shows the DNA translocation of simulation SimE4 (see Table 1).

- **Movie S7** shows the DNA translocation of simulation SimF4 (see Table 1).