Supplementary Material

Theoretical studies on key factors in DNA sequencing by atomically thin molybdenum disulfide nanopores

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We checked the change of pressure and temperature in all simulations. The change of pressure and temperature of system in SimV2 were displayed in Figure S1 and S2 as an example. The pressure and temperature of these systems were relatively stable during the simulation.

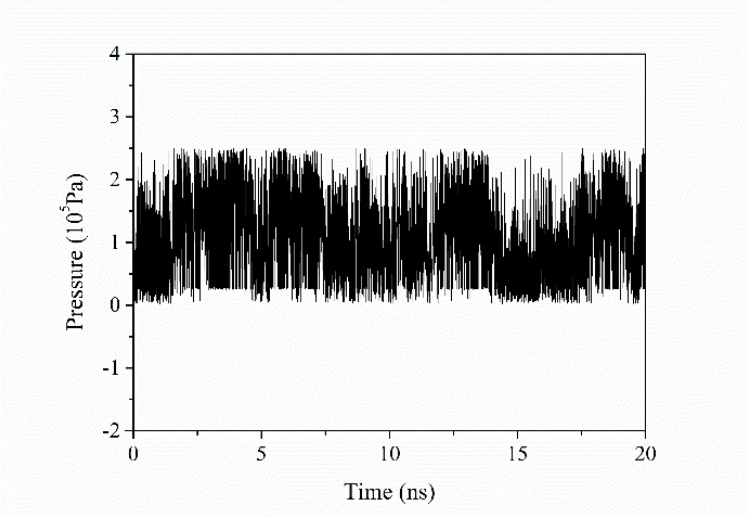

Figure S1. The change of system pressure of SimV2.

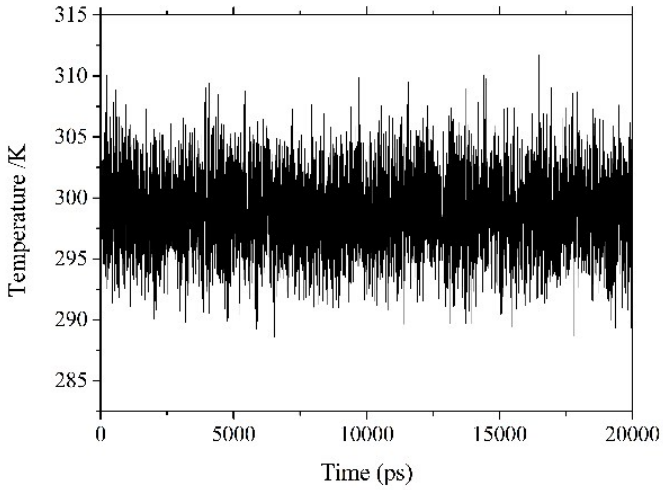

Figure S2. The change of system temperature of SimV2 (detail in manuscript)

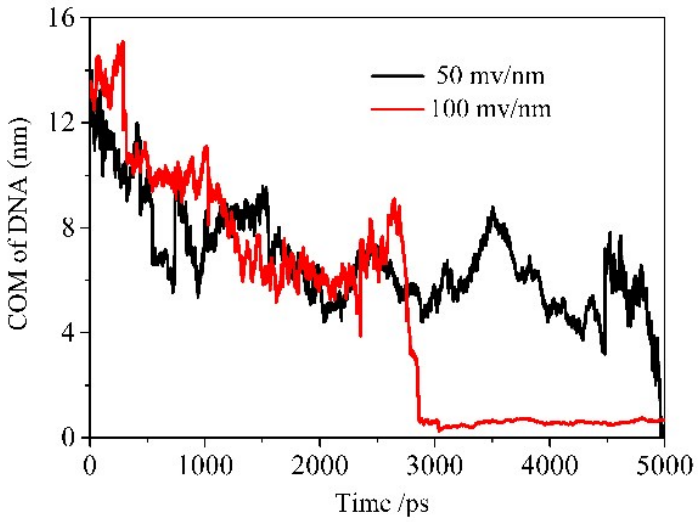

Figure S3. The axial position of center of mass of DNA translating through 2 nm MoS_2 nanopore under different applied voltage: 50 mV/nm (black line), 100 mV/nm (red line).

We have statistically counted the possibility of DNA fragments entering into and translocating through the MoS_2 nanopore and graphene nanopore from 50 independent simulations with the nanopore diameter varied from 2.0 nm, 1.8 nm to 1.6 nm under 200 mv/nm in 30 ns simulations. The possibility is defined as $P=N_{trans}/N_{total}$, where N_{trans} is counted if DNA fragment could pass through the nanopore within simulation time, and N_{total} is the total number of simulations. As seen in Table S1 and Table S2, the possibility of DNA passing through the MoS_2 nanopore is much higher than that passing through graphene nanopore under the same applied voltage and diameter of 2.0 nm and 1.0 nm.

Table S1. The possibility of DNA fragments passing through MoS_2 nanopore

Diameter	N_{total}	N_{trans}	P (%)
2.0 nm	50	31	62
1.8 nm	50	17	34
1.6 nm	50	0	0

Table S2. The possibility of DNA fragments passing through graphene nanopore

Diameter	N_{total}	N_{trans}	P (%)
2.0 nm	50	11	22
1.8 nm	50	4	8
1.6 nm	50	0	0