Supporting Information for

Na^+ and K^+ ion selectivity by size-controlled biomimetic graphene nanopores

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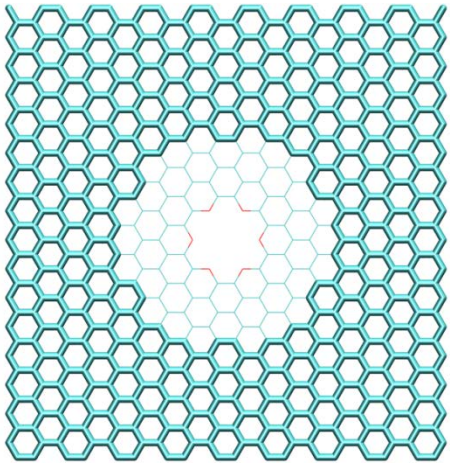

Figure S1. The structure of a partially flexible grapheme used in the MD simulation, where atoms around the nanopore (line model) are allowed to relax in the simulation.

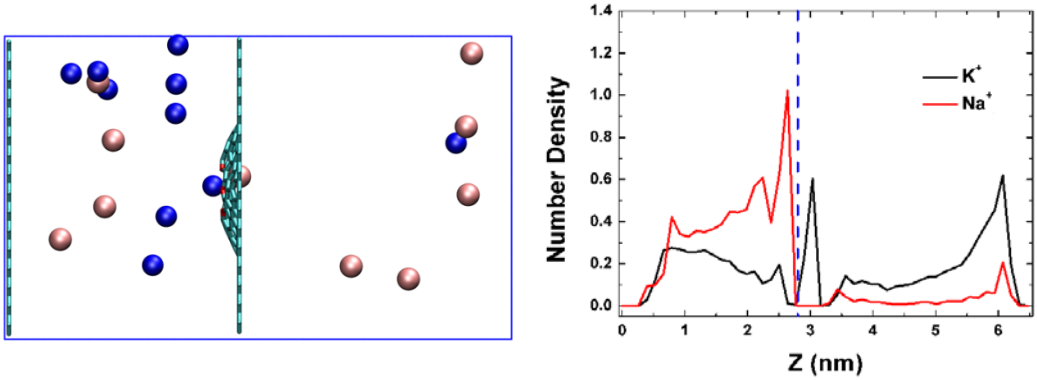

Figure S2. A snapshot from the MD simulation (400 mV/nm) in which a partially flexible graphene was employed (left figure). The nanopore tends to select K^+ over Na^+, which could also be proved by the position distribution of the ions in the last 6 ns MD simulation (right figure, in which vertical dash blue line is the position of the nanopore). It turns out that under an electric field of 400 mV/nm, the K^+ selectivity of the graphene over Na^+ is about 6: 1, which is fundamentally not so different from that using the rigid graphene, proving that the flexibility of the graphene has no significant effect on the results.

Table S1. Number of ions passing through the nanopores under different electric fields. (errors in parenthesis)

Nanopore	mV/nm	Na^+	K^+	K^+/Na^+
I	200	1.0(0.0)	0.0(0.0)	0.0(0.0)
	400	2.7(0.6)	1.3(0.6)	0.5(0.2)
	600	2.7(0.6)	4.7(0.6)	1.8(0.6)
	800	3.7(0.6)	4.0(1.0)	0.9(0.3)
	1000	3.7(0.6)	8.3(1.5)	1.8(0.5)
II	200	2.0(0.0)	1.0(1.0)	0.5(0.5)
	400	1.0(0.0)	6.7(0.6)	6.7(0.6)
	600	3.3(0.6)	6.0(1.0)	1.9(0.5)
	800	3.1(0.0)	5.8(1.2)	1.9(0.2)
	1000	3.4(1.0)	8.7(0.6)	2.9(0.3)
III	200	1.0(0.0)	2.7(0.6)	2.7(0.6)
	400	1.7(0.6)	4.0(1.0)	2.7(1.3)
	600	2.7(0.6)	7.0(0.0)	2.7(0.7)
	800	3.3(0.6)	8.7(0.6)	2.7(0.4)
	1000	4.3(0.6)	9.7(0.6)	2.2(0.4)

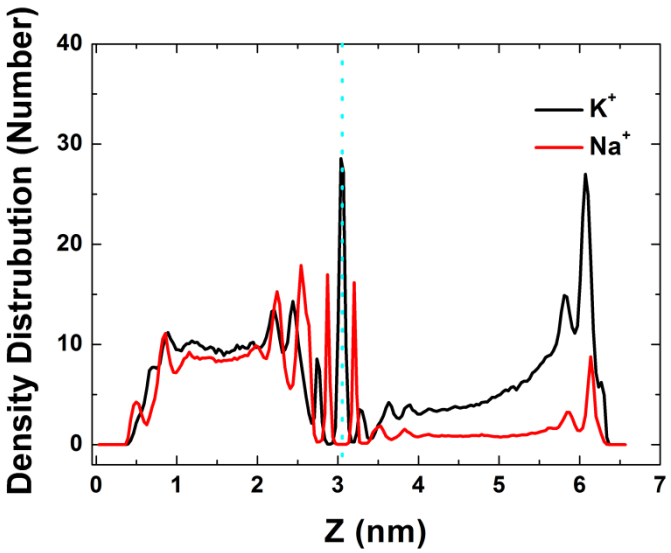

Figure S3. Average density distribution of K^+/Na^+ extracted from 10 parallel trajectories along z-axis (atomic charge of O is -0.43e). The cyan vertical dash line represents the position of graphene nanopore.

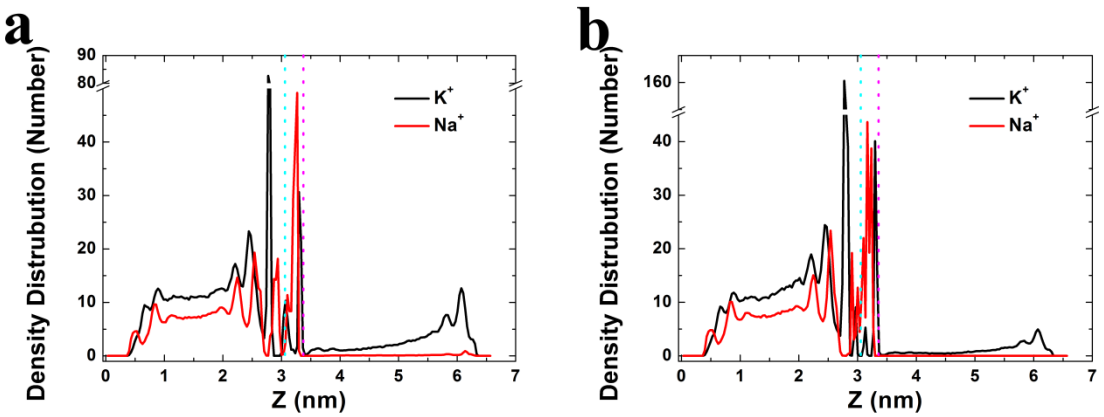

Figure S4. Average density distribution of K^+/Na^+ extracted from 10 parallel trajectories along *z*-axis: a) atomic charge of O is -0.76e; b) atomic charge of O is -1.00e. The cyan vertical dash line represents the position of graphene nanopore. The purple vertical dash line is the edge of Na^+ distribution peak, beyond which the distribution of Na^+ is nearly 0.

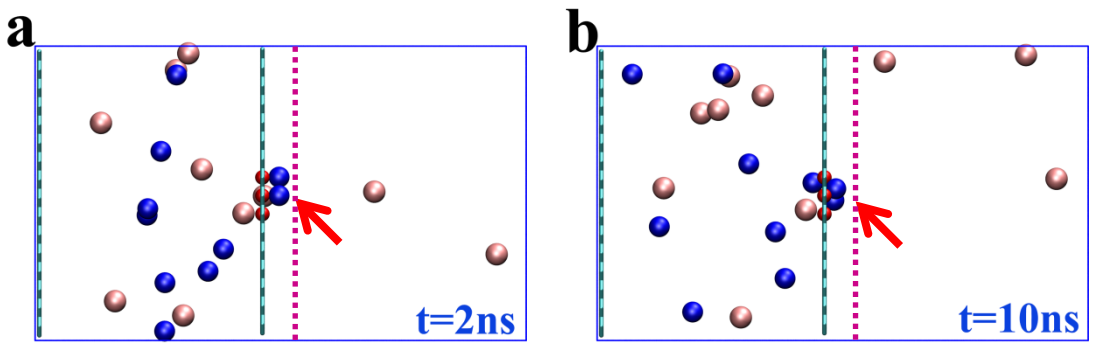

Figure S5. Snapshot of MD simulation for the system of O atoms charged -0.76e. The two Na^+ ions were not able to escape the attraction of O atoms in 10 ns (red arrow).

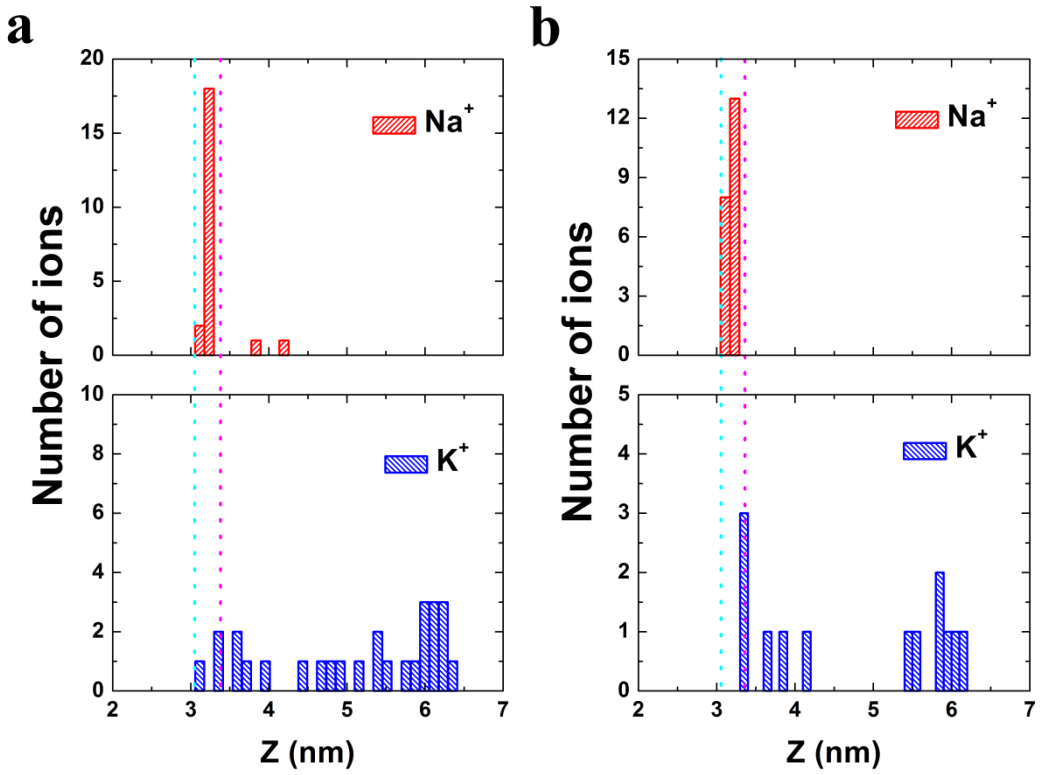

Figure S6. Position distribution of K^+/Na^+ passed through graphene nanopore in all of 10 trajectories at t=10 ns: a) atomic charge of O is -0.76e; b) atomic charge of O is -1.00e.