Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information of

Computational Investigation of Geometrical Effect in 2D Boron Nitride Nanopores for DNA Detection

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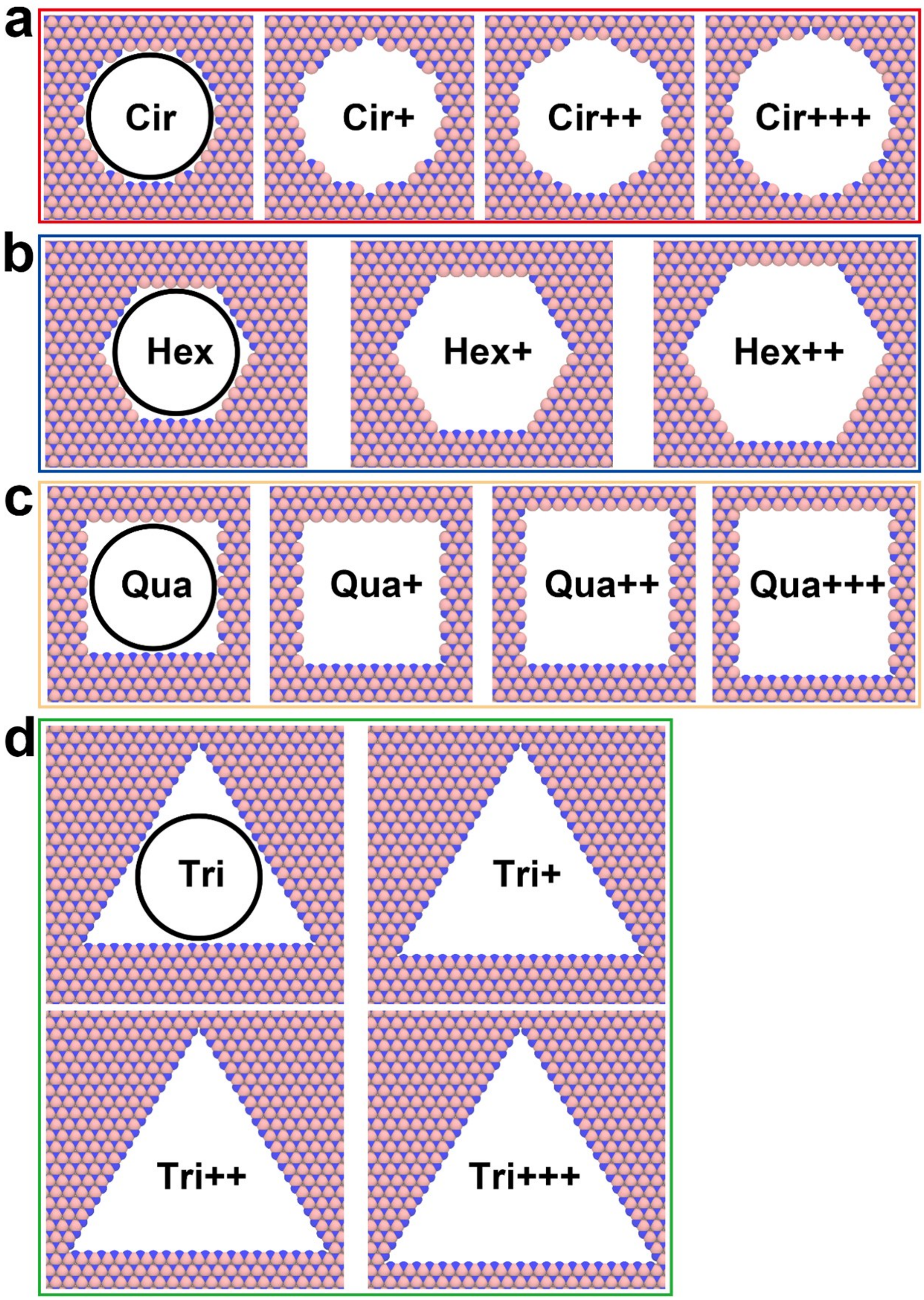

Figure S1. Atomic models of BN nanopore. Atomic models of BN nanopore with circular (a), hexagonal (b), quadrangular (c) and triangular (d) shapes investigated in this study. The solid circles in the Cir, Hex, Qua and Tri systems indicate the minimum inscribed circles with same 2.46 nm effective diameter, which is defined as the distance between the pore atoms at the diameter minus the van der Waals radius of boron and nitrogen (~0.3 nm). More geometrical information of the nanopore is list in table S1.

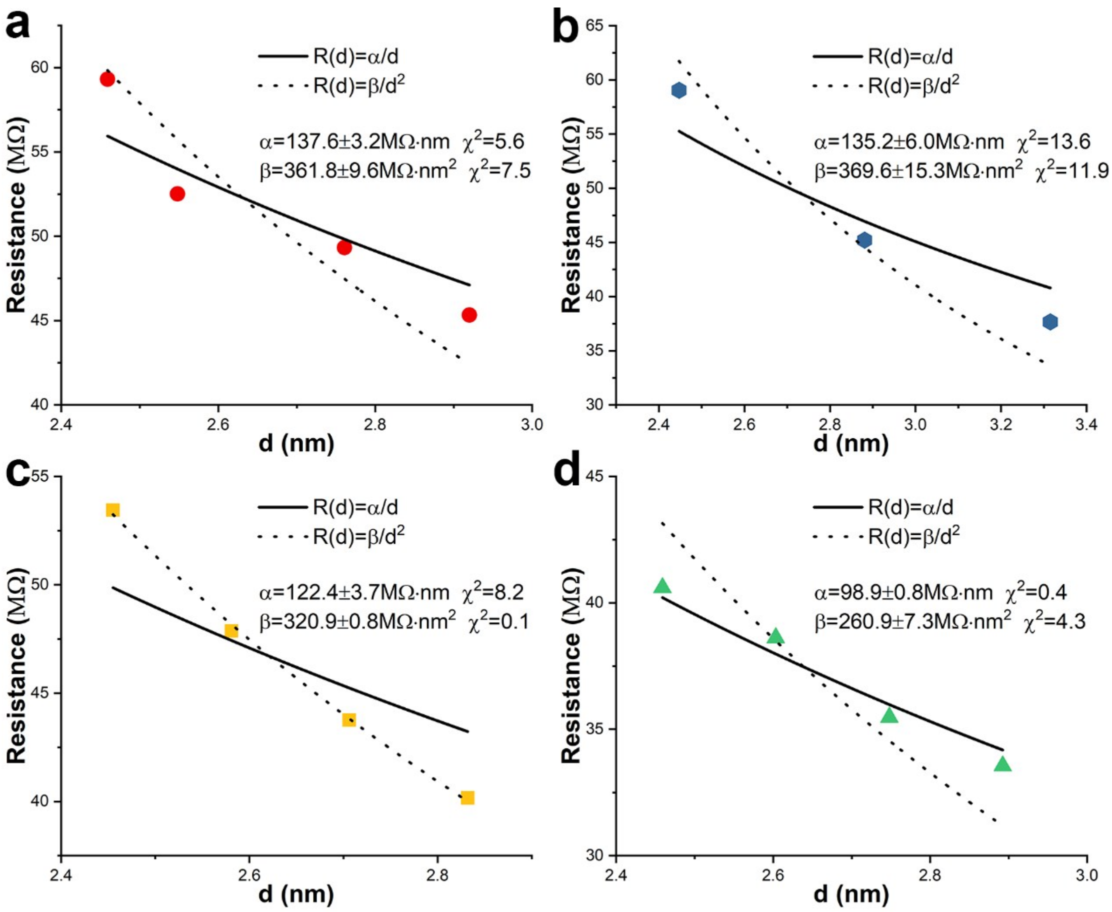

Figure S2. Ionic resistance for circular (a), hexagonal (b), quadrangular (c) and triangular (d) shape nanopores of various size, fitted according to two functional dependences *R(d)=α/d* and *R(d)=β/d²*. The effective diameter (*d*) of the minimum inscribed circle is used for the hexagonal, quadrangular and triangular shape nanopores.

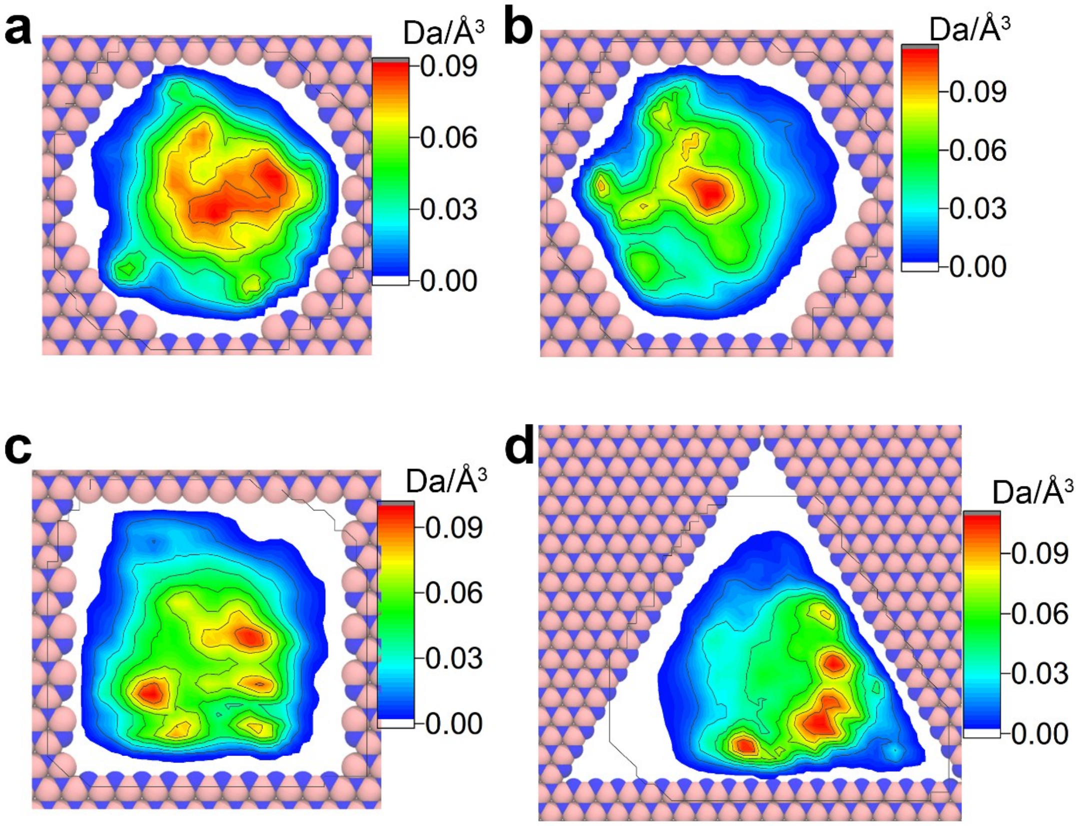

Figure S3. Mass density of DNA for the Cir (a), Hex (b), Qua (c) and Tri (d) systems. Heavy atoms of DNA molecule within 6 Å of the BN membrane are counted.

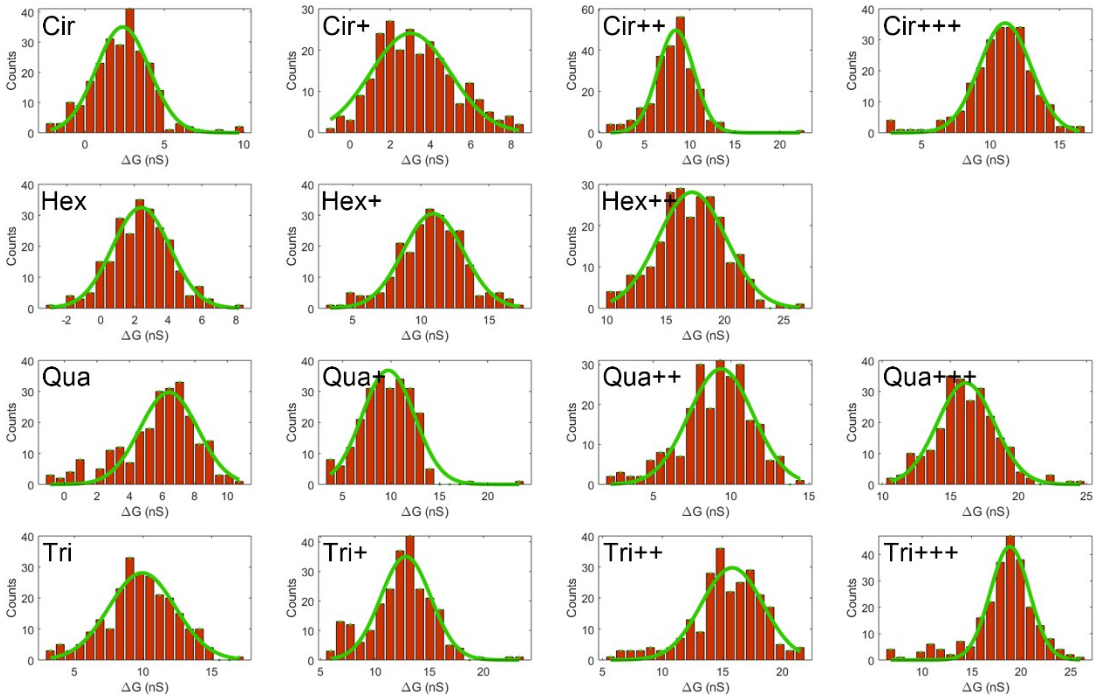

Figure S4. Histograms of conductance blockades for all the systems with dsDNA translocating through the nanopores. Gaussian fit (Green solid line) was performed to obtain the expectation of every distribution.

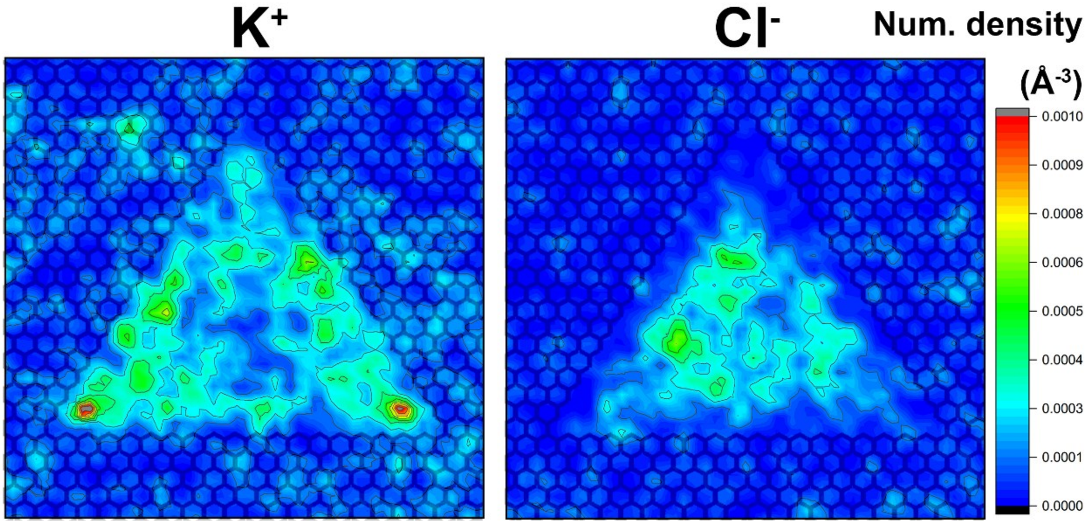

Figure S5. Number density of K^+ and Cl^- of the open-pore Tri system. Atoms within 6 Å of the BN membrane are counted.

Table S1. Geometrical information of BN nanopores

Nanopore geometry	Diameter d (nm)	*Area A* (nm^2)
Cir	2.46	4.75
Cir+	2.55	5.10
Cir++	2.76	5.99
Cir+++	2.92	6.70
Hex	2.46*	5.19
Hex+	2.88*	7.19
Hex++	3.32*	9.52
Qua	2.46*	6.36
Qua+	2.58*	7.06
Qua++	2.71*	7.80
Qua+++	2.83*	8.98
Tri	2.46*	7.85
Tri+	2.60*	8.80
Tri++	2.75*	9.81
Tri+++	2.89*	10.87

* List is the effective diameter of the minimum inscribed circle.

Table S2. Information of systems simulated

Nanopore geometry	*DNA (bp)*	*No. of atoms*	*Simulation duration (ns)*
Cir	n/a	193815	27
Cir	$[\text{A-T}]^{45}$	208847	60[*]
Cir	$[\text{C-G}]^{45}$	208994	75[*]
Cir+	n/a	205491	27
Cir+	$[\text{A-T}]^{45}$	204680	90[*]
Cir+	$[\text{C-G}]^{45}$	204992	65[*]
Cir++	n/a	205482	27
Cir++	$[\text{A-T}]^{45}$	204635	70[*]
Cir++	$[\text{C-G}]^{45}$	204935	60[*]
Cir+++	n/a	205482	27
Cir+++	$[\text{A-T}]^{45}$	204647	70[*]
Cir+++	$[\text{C-G}]^{45}$	204761	65[*]
Hex	n/a	193809	27
Hex	$[\text{A-T}]^{45}$	208787	70[*]
Hex	$[\text{C-G}]^{45}$	209012	70[*]
Hex+	n/a	205473	27
Hex+	$[\text{A-T}]^{45}$	204677	70[*]
Hex+	$[\text{C-G}]^{45}$	208790	75[*]
Hex++	n/a	205479	27
Hex++	$[\text{A-T}]^{45}$	208787	60[*]
Hex++	$[\text{C-G}]^{45}$	208796	70[*]
Qua	n/a	193815	27
Qua	$[\text{A-T}]^{45}$	208718	75[*]
Qua	$[\text{C-G}]^{45}$	208904	65[*]
Qua+	n/a	209501	27
Qua+	$[\text{A-T}]^{45}$	208663	75[*]
Qua+	$[\text{C-G}]^{45}$	208828	75[*]

Qua++	n/a	209510	27
Qua++	[A-T]^{45}	208732	60*
Qua++	[C-G]^{45}	208744	60*
Qua+++	n/a	209508	27
Qua+++	[A-T]^{45}	208721	60*
Qua+++	[C-G]^{45}	208739	75*
Tri	n/a	205488	27
Tri	[A-T]^{45}	208718	90*
Tri	[C-G]^{45}	208748	60*
Tri+	n/a	205499	27
Tri+	[A-T]^{45}	208777	65*
Tri+	[C-G]^{45}	208795	70*
Tri++	n/a	205472	27
Tri++	[A-T]^{45}	208834	80*
Tri++	[C-G]^{45}	208816	75*
Tri+++	n/a	205500	27
Tri+++	[A-T]^{45}	208871	80*
Tri+++	[C-G]^{45}	208757	60*

*Simulations with three replicas (refer to simulation S1, S2 and S3).