Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

DNA Translocation through Single-layer Boron Nitride Nanopores

Zonglin Gu[1,‡], Yuanzhao Zhang[2,‡], Binquan Luan[2], Ruhong Zhou[*,1,2,3]

1. School for Radiological and Interdisciplinary Sciences (RAD-X) and Collaborative Innovation Center of Radiation Medicine of Jiangsu Higher Education Institutions, Soochow University, Suzhou, China, 215123

2. Computational Biological Center, IBM Thomas J. Watson Research Center, Yorktown Heights, NY 10598, USA

3. Department of Chemistry, Columbia University, New York, NY 10027, USA

‡These authors contribute equally

*Corresponding author, E-mail: ruhongz@us.ibm.com

Table S1. List of Performed Simulations

	DNA	Nanopore diameter (nm)	Voltage (V)
A1	N/A	2.5	1.0
A2	N/A	3.5	1.0
A3	N/A	4.5	1.0
A4	N/A	5.5	1.0
A5	N/A	6.5	1.0
B1	poly(G-C, A-T)$_{20}$	2.5	1.0
B2	poly(G-C, A-T)$_{20}$	3.5	1.0
B3	poly(G-C, A-T)$_{20}$	4.5	1.0
B4	poly(G-C, A-T)$_{20}$	5.5	1.0
B5	poly(G-C, A-T)$_{20}$	6.5	1.0
C1	poly(A-T)$_{40}$	2.5	0.5
C2	poly(A-T)$_{40}$	2.5	0.7
C3	poly(A-T)$_{40}$	2.5	1.0
C4	poly(A-T)$_{40}$	2.5	1.2
C5	poly(A-T)$_{40}$	2.5	1.5
D1	poly(G-C)$_{40}$	2.5	0.5
D2	poly(G-C)$_{40}$	2.5	0.7
D3	poly(G-C)$_{40}$	2.5	1.0

D4	poly(G-C)$_{40}$	2.5	1.2
D5	poly(G-C)$_{40}$	2.5	1.5
E1	poly(G-C, A-T)$_{20}$	4.5	1.0
E2	poly(G-C, A-T)$_{20}$	4.5	1.0
E3	poly(G-C, A-T)$_{20}$	4.5	1.0
E4	poly(G-C, A-T)$_{20}$	4.5	1.0
E5	poly(G-C, A-T)$_{20}$	4.5	1.0

Movie S1-S3: Movies for the translocation of three different dsDNA sequences, poly(G-C, A-T)$_{20}$, poly(A-T)$_{40}$ and poly(G-C)$_{40}$, through the 2.5 nm BN nanopore, respectively, which demonstrates that dsDNA moves smoothly and unobstructedly through the BN nanopore

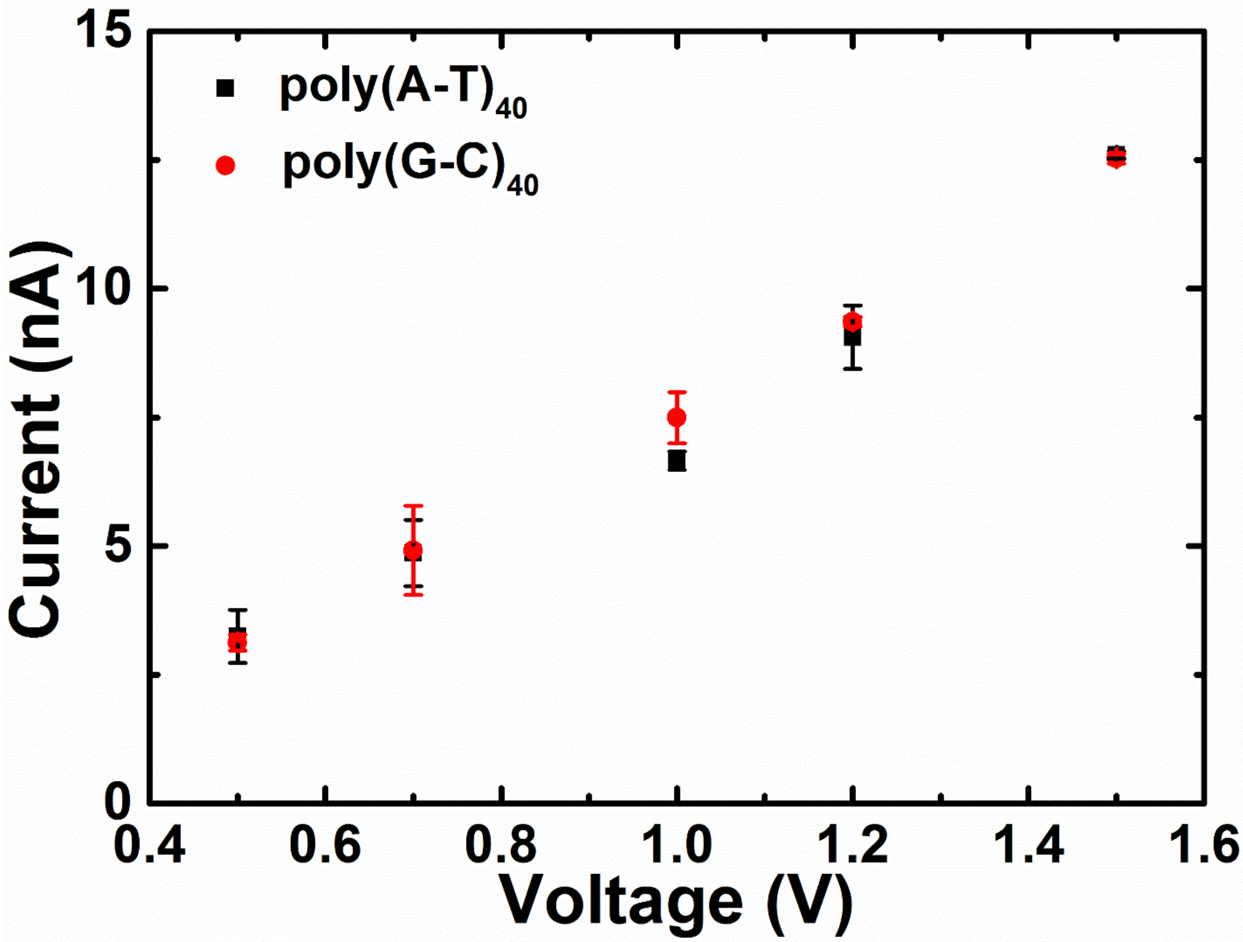

Fig. S1 The blockage currents of poly(A-T)$_{40}$ and poly(G-C)$_{40}$ transporting through a 2.5 nm graphene nanopore under different voltages. The current signals are not well separated for all the voltages studied,.

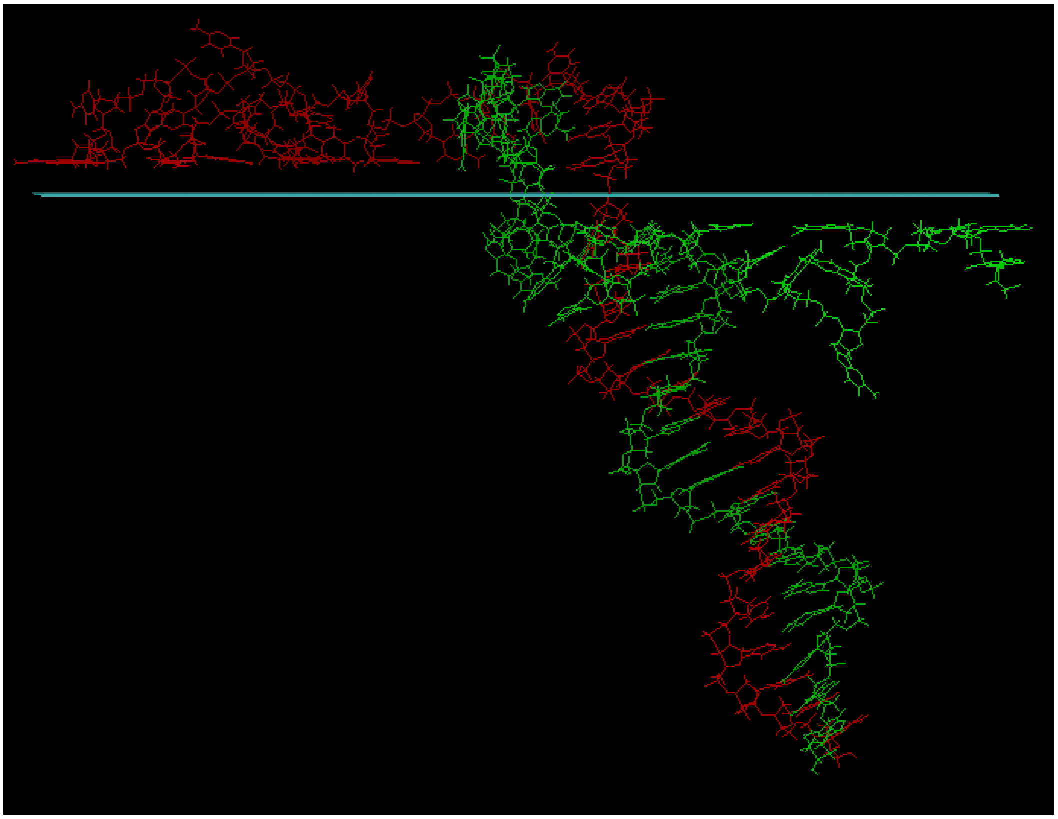

Fig. S2 The snap-shot, from an independent simulation, for a failed transport of dsDNA through the 2.5-nm graphene pore.

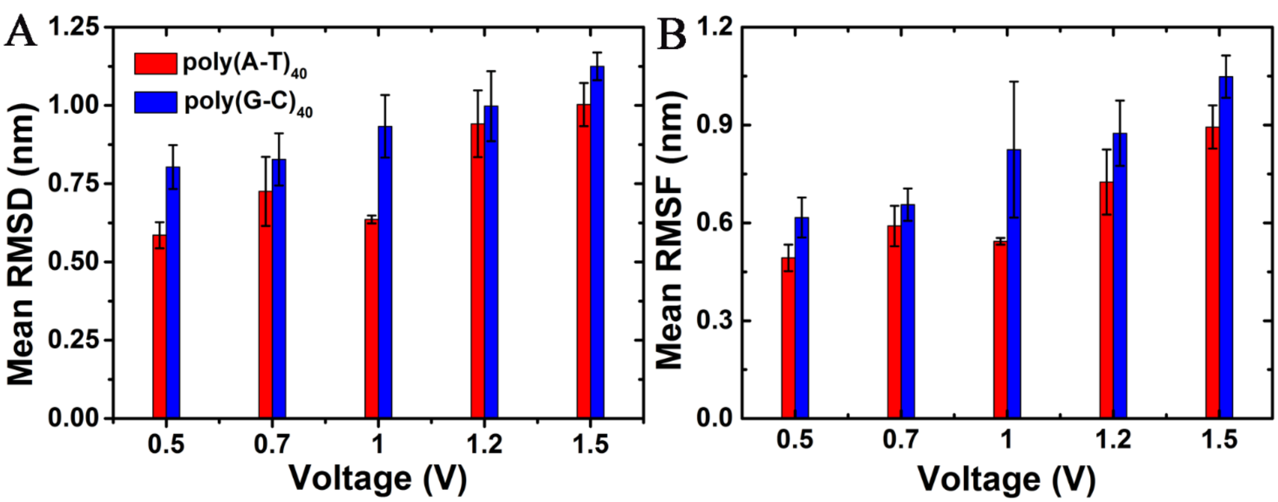

Fig. S3 Root mean square deviations (RMSD) and root mean square fluctuations (RMSF) for poly(A-T)$_{40}$ and poly(G-C)$_{40}$ at different biasing voltages. Results suggest that poly(A-T)$_{40}$ is more flexible and is easier to be stretched.