

# Dna Translocation Through Hybrid Bilayer Nanopores

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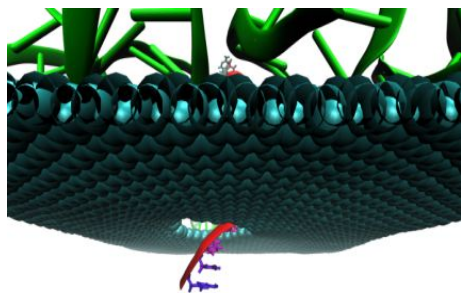
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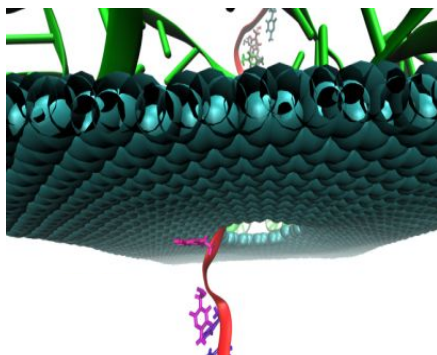
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## Supporting Information S.I.

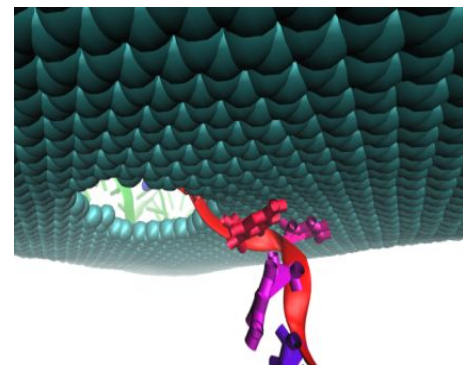
a)  $t = 0$  ns



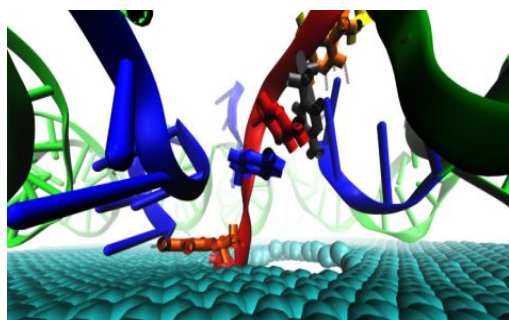
b)  $t = 4.7$  ns



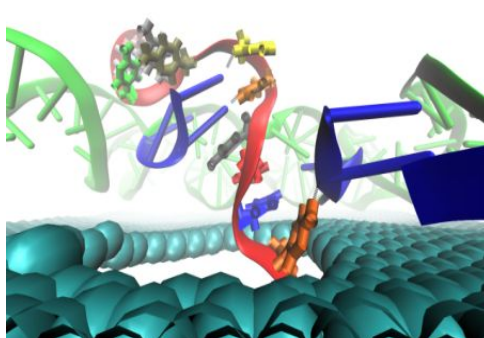
c)  $t = 18$  ns



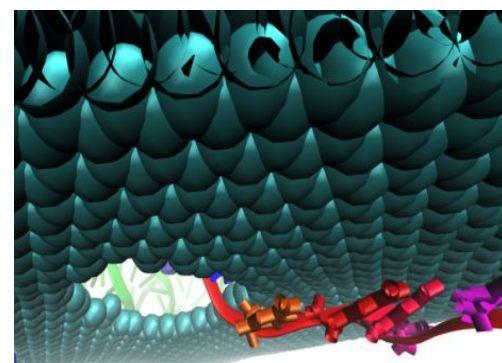
d)  $t = 55$  ns



e)  $t = 93$  ns



f)  $t = 105$  ns



**Figure S1:** Translocating DNA, graphene, Origami interaction. Origami sheet is shown in green; Overhangs are highlighted in blue; the translocating strand's backbone is shown in red; it's each base shown in different colours.

Trial	No Overhangs (ns)	A as unpaired bases (ns)			G as unpaired bases (ns)		
		2 (A2)	4 (A4)	Strip (AS)	2 (G2)	4 (G4)	Strip (GS)
1	4.29	5.8	7.05	5.33	8.89	27.74	27.99
2	7.05	7.13	10.84	6.94	9.42	32.52	47.37
3	7.32	7.83	20.37	7.81	9.85	32.83	79.72
4	7.33	10.86	21.38	9.91	10.07	38.71	112.35
5	7.51	11.89	37.01	10.72	10.5	65.74	117.48
6	8.04	12.08	39.52	15.82	10.57	135.07	184.66
7	8.91	12.19	46.33	53.14	18.45	313	187.95
8	8.93	14.98	46.39	177	19.04	336	476

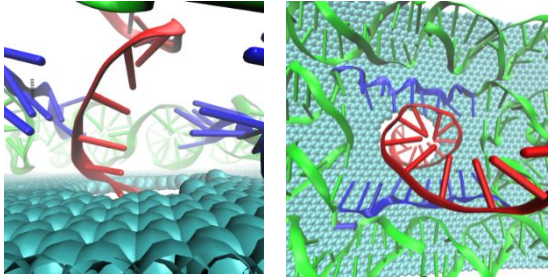
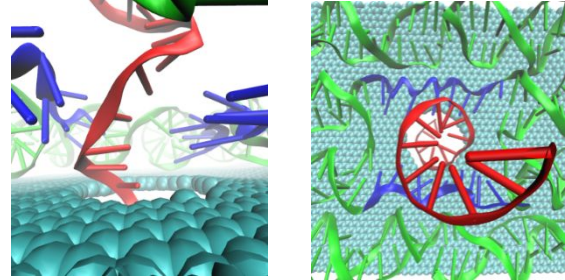
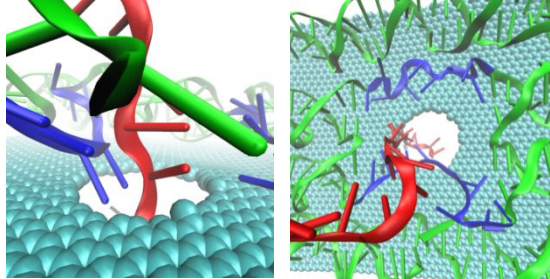
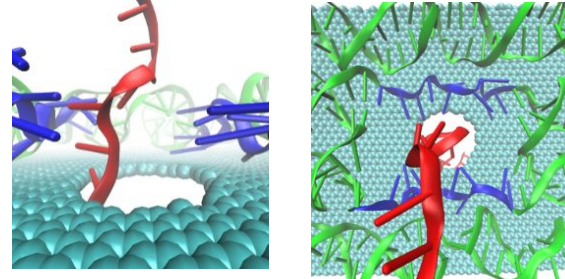
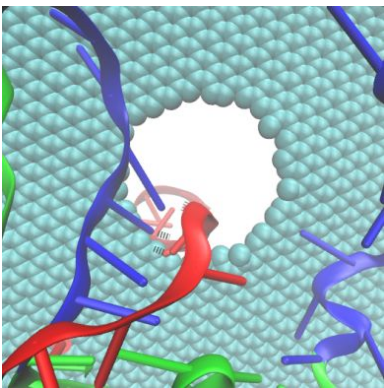
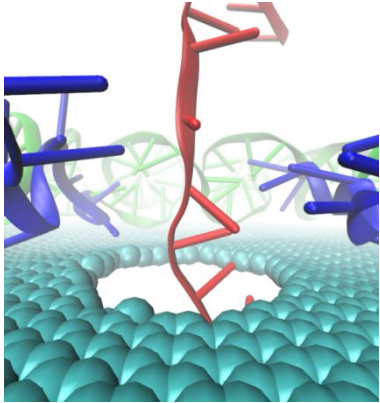
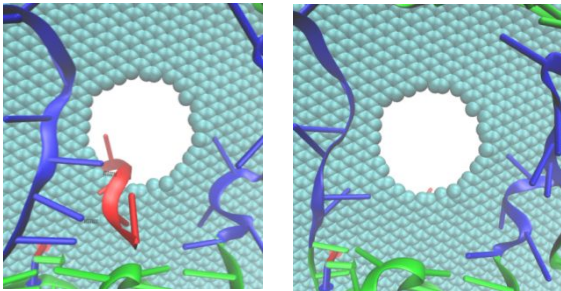
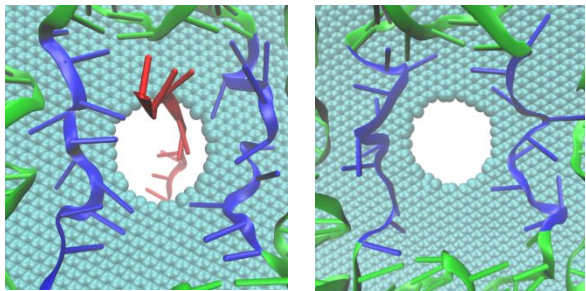
**Table S1:** Translocation times for poly(C)<sub>18</sub> in different systems. The trials are arranged in the ascending order of their translocation times. The red values indicate the instances where the translocation is not complete, and the simulation was stopped owing to the poly(C)<sub>18</sub> getting stuck

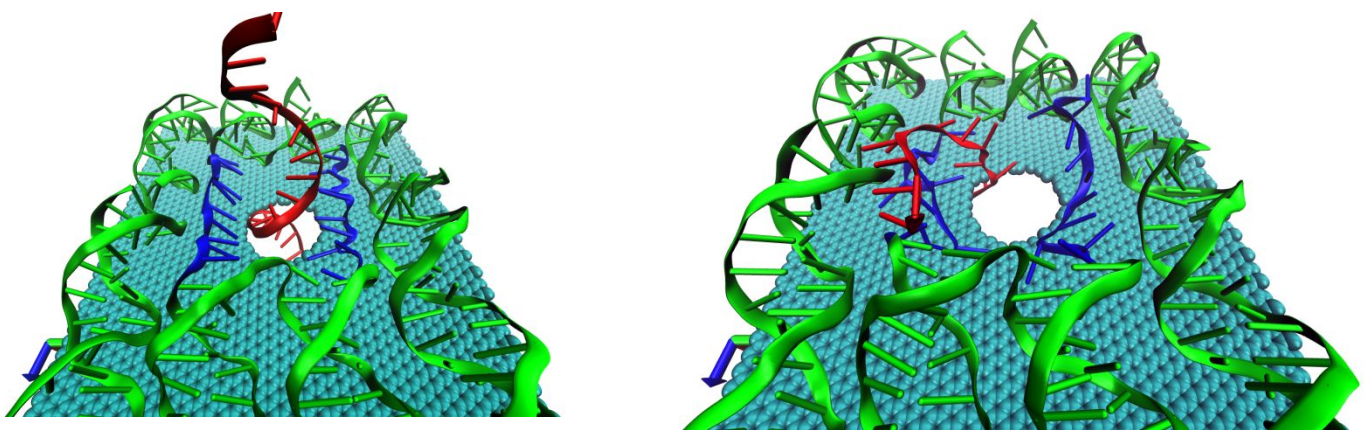
Trial	A as unpaired bases			G as unpaired bases		
	2 (A2)	4 (A4)	Strip (AS)	2 (G2)	4 (G4)	Strip (GS)
1	0	0.23963	0	0	1.25052	7.0476
2	0	1.39869	0.46935	0.44952	0.42991	57.4579
3	0	0.50966	0.09989	0.60794	2.01937	15.3278
4	0	0.01999	0.47954	0.45949	1.44969	50.9957
5	0	2.35939	1.19892	0.34965	26.1658	9.63923
6	0	1.58949	1.58896	0.06997	196.925	75.0957
7	0	13.7971	6.83859	2.86842	--	71.5263
8	0	5.08898	--	0.2399	--	--
<b>MEAN</b>	<b>0</b>	<b>3.125</b>	<b>1.525</b>	<b>0.63</b>	<b>38.04</b>	<b>41.02</b>

Trial	A as unpaired bases			G as unpaired bases		
	2 (A2)	4 (A4)	Strip (AS)	2 (G2)	4 (G4)	Strip (GS)
1	0	0.03399	0	0	0.04508	0.25179
2	0	0.12903	0.06763	0.04772	0.01322	1.21296
3	0	0.02502	0.01279	0.06172	0.06151	0.19227
4	0	9.35E-04	0.04839	0.04563	0.03745	0.4539
5	0	0.06375	0.11184	0.0333	0.39802	0.08205
6	0	0.04022	0.10044	0.00662	1.45795	0.40667
7	0	0.2978	0.12869	0.15547	--	0.38056
8	0	0.1097	--	0.0126	--	--
<b>MEAN</b>	<b>0</b>	<b>0.08756</b>	<b>0.06711</b>	<b>0.04538</b>	<b>0.33554</b>	<b>0.42574</b>

**Table S2: a)** Total number of hydrogen bonds formed during the translocation time /100. ( $N_h$ ) **b)** Rate of hydrogen bonds formed per frame. ( $N_h / T_h = R_h$ )

**Table S3:** Dynamics of translocation poly(C)<sub>18</sub> in LS (strip) designs

Translocation stages	LS with G (GS)	LS with A (AS)
Initial Configuration (t = 0 s)	 <p style="text-align: center;">Side view                      Top view</p>	 <p style="text-align: center;">Side view                      Top view</p>
Translocation of initial bases	 <p style="text-align: center;">Side view                      Top view</p>	 <p style="text-align: center;">Side view                      Top view</p>
Translocation of middle bases		
Final translocation stages		



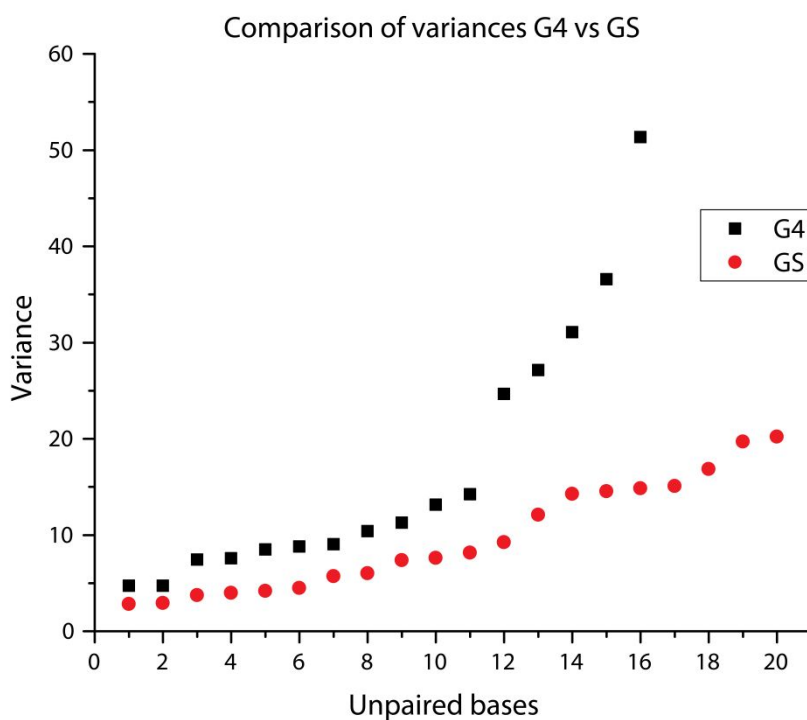
**Figure S2:** a) Initial Configuration b) Final snapshot when the simulation was stopped due to entanglement of the bases with the origami sheet. One can clearly see that the translocating DNA is totally bent over and entangled too much that there isn't much of translocation happening after this. The simulations were stopped after this phenomenon is observed.

Parameter	Origami with G Overhangs			Origami with A overhangs		
	G2	G4	GS (G-Strip)	A2	A4	AS (A-Strip)
Mean Translocation time (ns)	39.78	147.67	91.9	41.14	233.37	390.5
Mean Residence time for a single base (ns)	3.51	11.31	12.58	3.07	16.93	48.04
Mean number of Hydrogen bonds per ns	2.971	5.581	31.141	4.854	25.49	53.3

**Table S4:** Comparison of Mean per base residence time, total translocation time and mean number of hydrogen bonds formed between the bases of translocating DNA and the traps per ns for translocating poly T

### Section S1: Calculation of mean variances of center of mass:

A comparison of mean variances of the center of masses of unpaired bases in the G4 and GS was computed for a potential difference of 2V. In the case of G4, as there are 16 unpaired bases, 16 values of variances were computed. Similarly, 20 values were computed for GS. The total variance of each unpaired base was calculated ( $\sigma^2_{\text{COM}} = \sigma^2_{\text{COMx}} + \sigma^2_{\text{COMy}} + \sigma^2_{\text{COMz}}$ ). From this the mean  $\sigma^2_{\text{COM}}$  was found to be  $16.91 \text{ \AA}^2$  and  $9.69 \text{ \AA}^2$  for G4 and GS.



**Figure S3:** Comparison of  $\sigma^2_{\text{COM}}$  of G4 and GS arranged in ascending order of values. It can be clearly concluded that the GS motion is more restrained when compared to G4 owing to lower value of variance in GS.