Supporting Information

Mechanical properties of DNA and DNA nanostructures: comparison of atomistic, Martini and oxDNA

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I. Sequence and structure of dsDNA and DNA nanotube (DNT)

A. Sequence of dsDNA

TABLE I: Sequences of Different dsDNAs studied in our simulations

Systems	Sequence
12 bp dsDNA	d(CGCGAATTCGCG)$_2$
24 bp dsDNA	d(CGCGATTGCCTAACGGACAGGCAT)$_2$
38 bp dsDNA	d(GCCGCGAGGTGTCAGGGATTGCAGCCAGCATCTCGTCG)$_2$
56 bp dsDNA	d(CGCGATTGCCTAACGGACAGGCATAGACGTCT ATGCCTGTCCGTTAGGCAATCGCG)$_2$

B. Schematic Diagram of DNT

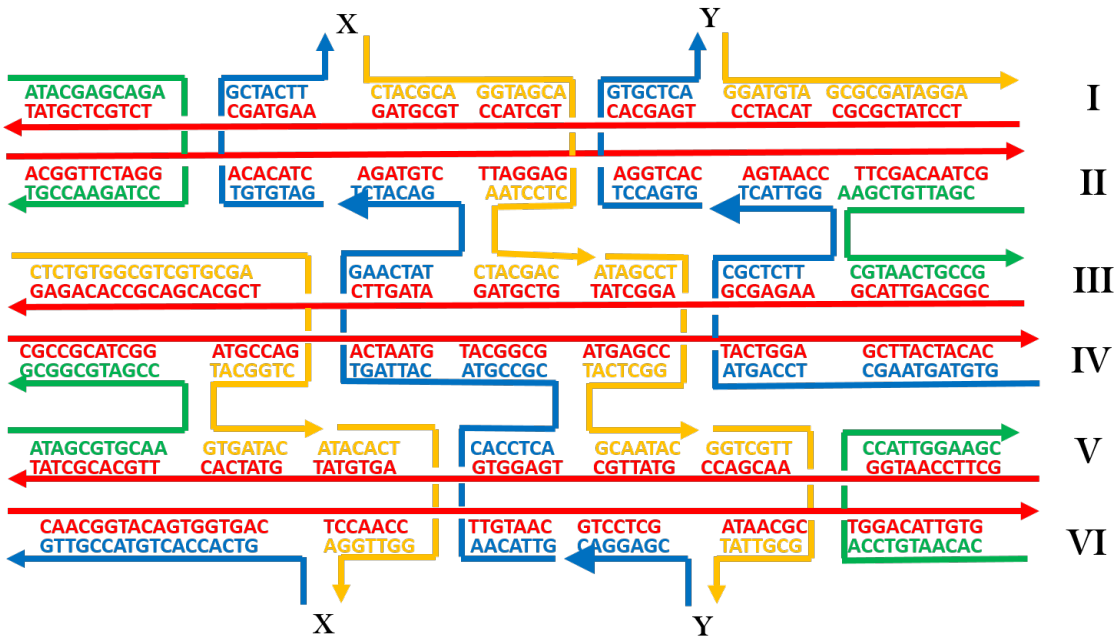

FIG. S1: Schematic Diagram representing the DNT crossovers and sequence. The roman numbers indicating six different dsDNA strands. Different Colors represent different ssDNA strands. The arrows represent the polarity of the DNA from 5' to 3'. The place X and Y are the position where the hexagonal bundle closes.

II. Final snapshots of the coarse-grained (CG) dsDNA

A. Soft-Martini

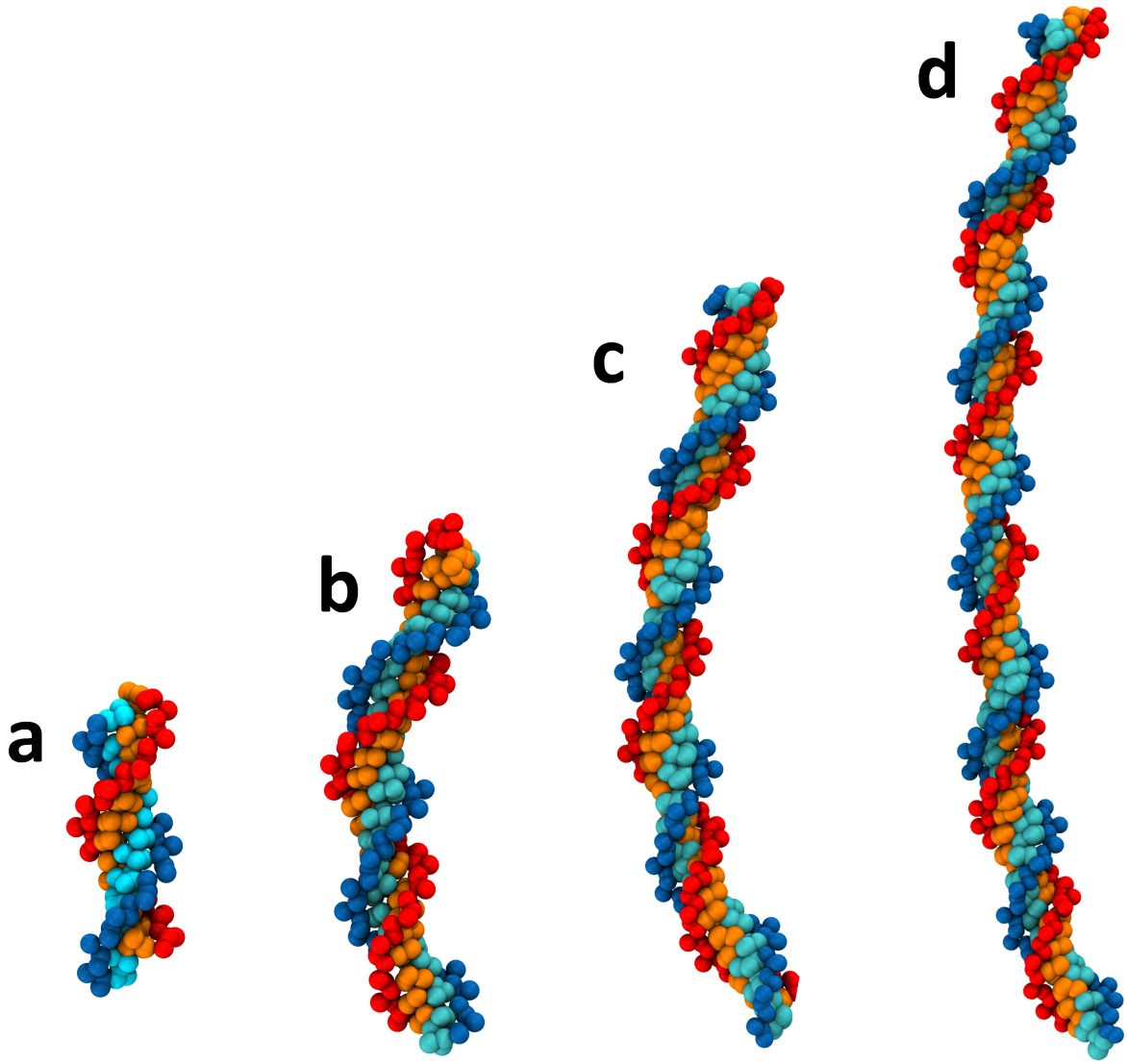

FIG. S2: Final snapshots of the coarse-grained soft-martini dsDNA model after 2 μs long MD simulation. The length of the dsDNA is (a) 12 bp (b) 24 bp (c) 38 bp (d) 56 bp.

B. Stiff-Martini

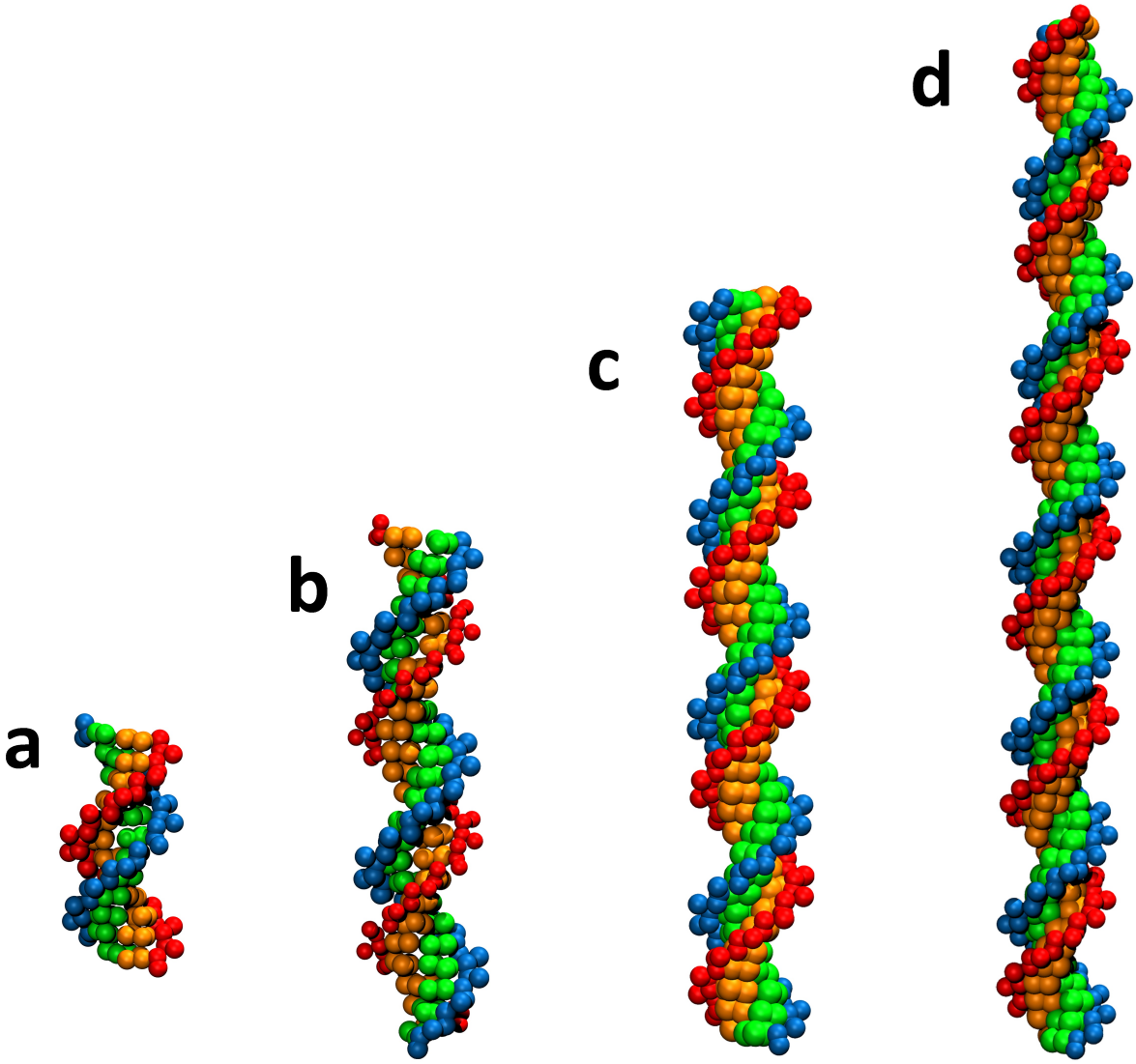

FIG. S3: Final snapshots of the coarse-grained stiff-martini dsDNA model after 2 μs long MD simulation. The length of the dsDNA is (a) 12 bp (b) 24 bp (c) 38 bp (d) 56 bp.

C. OxDNA

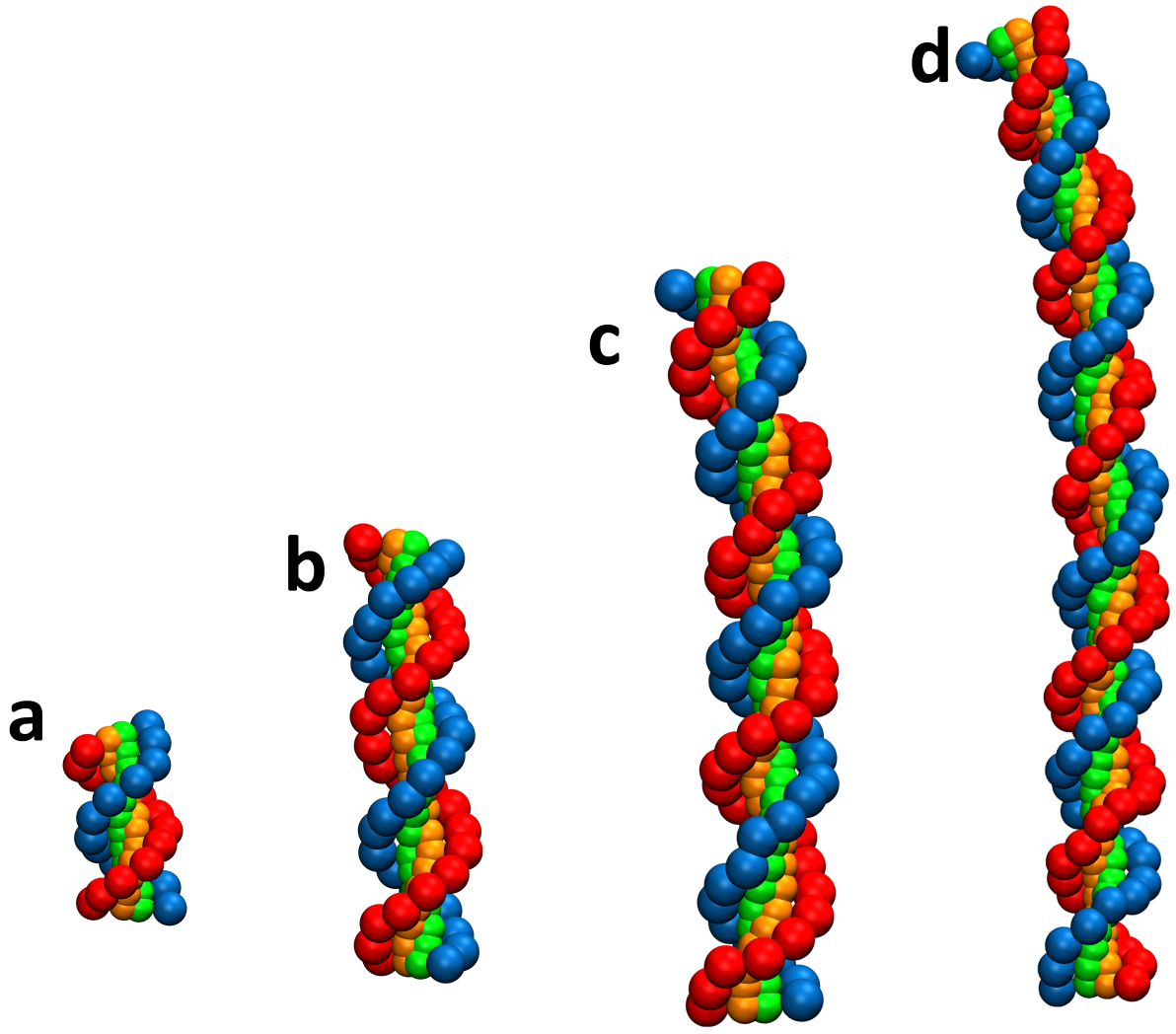

FIG. S4: Final snapshots of the coarse-grained oxDNA dsDNA model after 2×10^9 long MD simulation steps. The length of the dsDNA is (a) 12 bp (b) 24 bp (c) 38 bp (d) 56 bp.

III. Contour length and bending angle distribution of a 12bp dsDNA

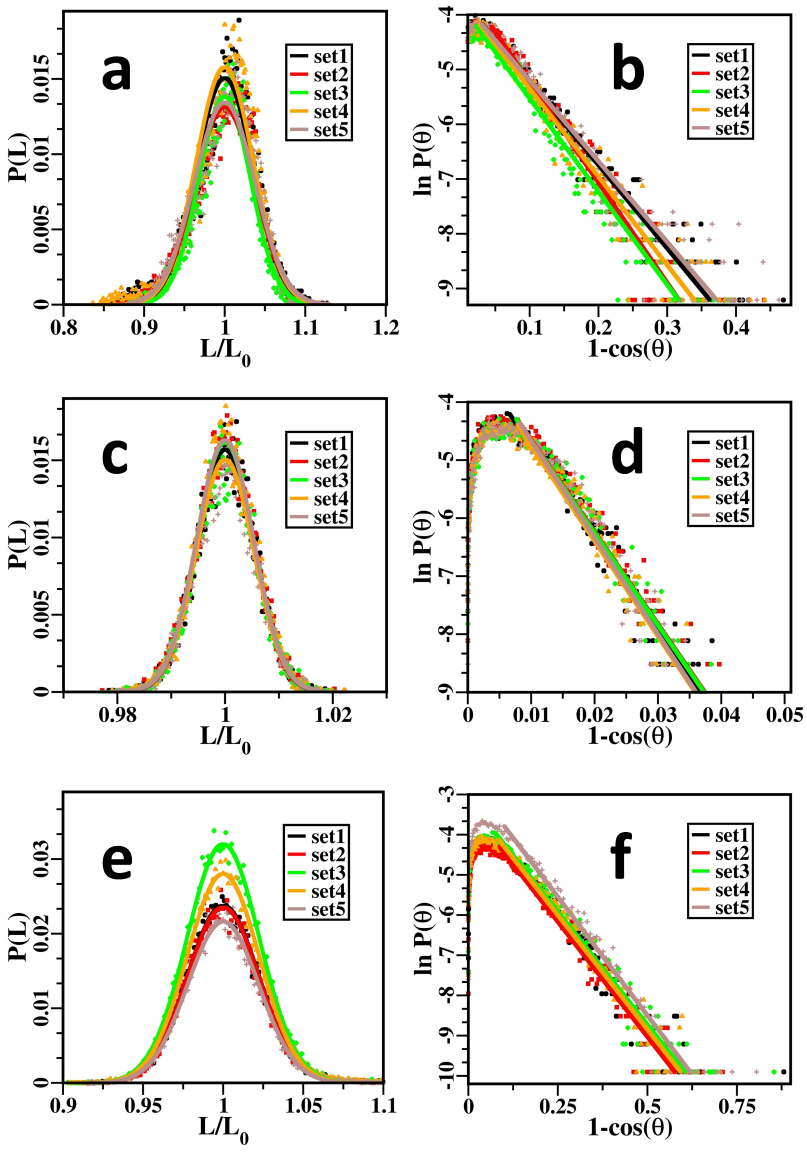

FIG. S5: Contour length distribution and logarithm of bending angle distribution of a 12 bp dsDNA for various CG models. The trajectory is divided into five intervals of equal length and Different sets represent different time interval of the same trajectory. (a) Contour length distribution and (b) logarithm of bending angle distribution of a 12 bp soft martini dsDNA. (c) Contour length distribution and (d) logarithm of bending angle distribution of a 12 bp stiff martini dsDNA. (c) Contour length distribution and (d) logarithm of bending angle distribution of a 12 bp oxDNA.

IV. Elastic properties of CG dsDNA

TABLE II: Mechanical properties of soft-martini dsDNA at different salt concentration

System	NaCl Salt Concentration	Stretch Modulus (pN)		Persistence length (nm)	
		γ_G	γ_{WLC}	L_P	L_P^{WLC}
12 bp dsDNA	0mM	767.16 ± 85.29	1160. ± 91.69	70.03 ± 5.53	25.14 ± 1.19
	150mM	758.10 ± 63.43	1083.18 ± 178.42	65.38 ± 10.77	23.75 ± 2.00
	250mM	750.46 ± 77.14	1117.00 ± 192.69	67.42 ± 11.63	24.73 ± 2.04
24 bp dsDNA	0mM	916.04 ± 159.80	1729.78 ± 130.23	104.40 ±7.86	29.39 ± 2.23
	150mM	848.18 ± 409.60	973.97 ± 140.79	58.79 ± 8.50	16.94 ± 6.15
	250mM	1028.84 ± 208.48	1563.22 ± 269.75	94.35 ± 16.28	38.09 ± 30.89
38 bp dsDNA	0mM	854.68 ± 75.21	1150.11 ± 105.08	69.42 ± 6.34	29.98 ± 2.54
	150mM	1020.37 ± 117.91	1094.74 ± 241.57	66.07 ± 14.58	29.27 ± 1.91
	250mM	1225.32 ± 122.33	1083.33 ± 305.68	65.39 ± 18.45	29.59 ± 1.67
56 bp dsDNA	0mM	1023.36 ± 241.80	1946.10 ± 308.86	117.46 ± 18.64	51.52 ± 7.44
	150mM	789.30 ± 183.54	1317.08 ± 635.32	116.00 ± 16.29	45.81 ± 9.73
	250mM	1178.63 ± 244.82	1881.61 ± 124.13	113.57 ± 7.49	55.70 ± 42.07

TABLE III: Mechanical properties of stiff-martini dsDNA at 0mM NaCl

System	Stretch Modulus (pN)		Persistence length (nm)	
	γ_G	γ_{WLC}	L_P	L_P^{WLC}
12 bp dsDNA	38983.44 ± 789.02	9964.32 ± 204.59	601.42 ± 12.35	102.32 ± 0.82
24 bp dsDNA	47375.90 ± 2535.07	13920.78 ± 536.98	840.22 ± 32.41	200.77 ± 5.24
38 bp dsDNA	50697.57 ± 1162.17	9478.05 ± 248.87	572.07 ± 15.02	280.85 ± 1.41
56 bp dsDNA	51901.02 ± 416.46	18054.48 ± 2585.72	1089.72 ± 156.07	400.25 ± 7.69

TABLE IV: Mechanical properties of oxDNA at different salt concentration

System	NaCl Salt Concentration	Stretch Modulus (pN)		Persistence length (nm)	
		γ_G	γ_{WLC}	L_P	L_P^{WLC}
12 bp dsDNA	0mM	2151.60 ± 25.77	728.42 ± 11.91	43.96 ± 0.72	23.00 ± 0.14
	150mM	2149.84 ± 26.43	704.18 ± 13.07	42.50 ± 0.79	22.61 ± 0.21
	250mM	2180.13 ± 22.67	662.07 ± 6.15	39.96 ± 0.37	22.81 ± 1.74
24 bp dsDNA	0mM	1470.48 ± 74.31	825.73 ± 65.87	49.83 ± 3.98	31.16 ± 0.56
	150mM	1520.40 ± 48.68	657.87 ± 37.86	39.71 ± 2.28	25.78 ± 0.30
	250mM	1528.58 ± 56.27	649.91 ± 28.96	39.22 ± 1.75	25.42 ± 0.27
38 bp dsDNA	0mM	2209.62 ± 15.99	1268.88 ± 26.88	76.59 ± 1.62	52.45 ± 0.12
	150mM	2288.43 ± 19.05	941.91 ± 21.16	56.85 ± 1.27	34.50 ± 0.14
	250mM	2313.52 ± 23.13	909.22 ± 16.79	54.88 ± 1.01	33.73 ± 0.12
56 bp dsDNA	0mM	1398.29 ± 245.41	1502.17 ± 43.65	90.67 ± 2.63	73.45 ± 1.11
	150mM	2309.68 ± 62.19	867.50 ± 28.31	52.36 ± 1.71	37.21 ± 0.67
	250mM	2228.92 ± 58.90	884.10 ± 30.63	53.36 ± 1.85	36.78 ± 0.85

V. Contour length distribution of DNT

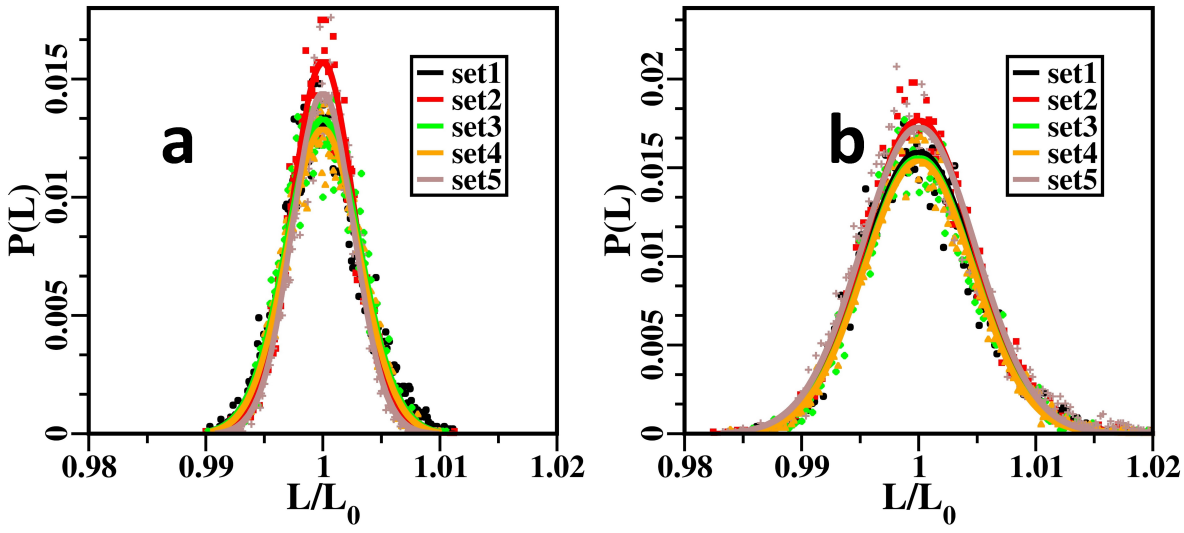

FIG. S6: Contour length distribution of DNT for (a) soft martini (b) oxDNA.

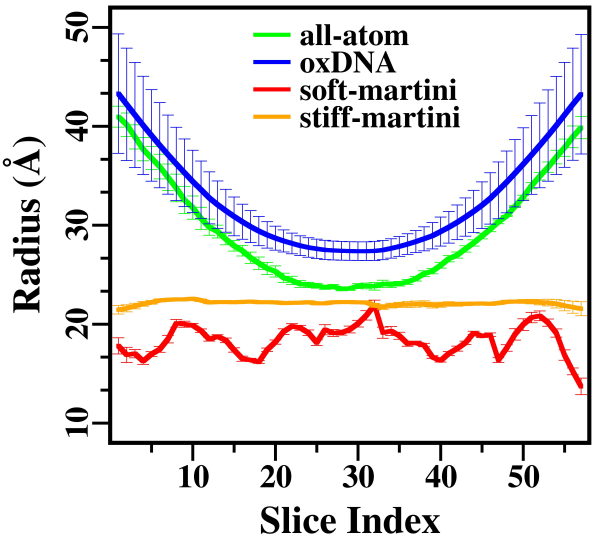

FIG. S7: Radius of the pore of DNTs. The average value of the pore radius is used to estimate area moment of inertia, I (equation 10 of the main airticle).

TABLE V: Mechanical properties of DNT.

Quantity	Salt concentration	all-atom	soft martini	stiff martini	oxDNA
Stretch modulus (pN)	0 mM	8294.87 ± 48.19	16799.39 ± 2684.95	113205.86 ± 3468.73	9504.72 ± 340.30
	500 mM	10540.9 ± 148.13	16790.09 ± 4365.83	–	8856.86 ± 121.76
	1000 mM	13066.8 ± 155.91	14562.56 ± 4226.89	–	9736.46 ± 386.64
Persistence length (μm)	0 mM	6.35 ± 0.11	12.97 ± 1.8	88.55 ± 2.71	7.34 ± 0.26
	500 mM	8.28 ± 0.12	12.38 ± 1.99	–	6.84 ± 0.09
	1000 mM	10.42 ± 0.12	11.69 ± 2.43	–	7.52 ± 0.29