Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

"Influence of temperature on bend, twist and twist-bend coupling of dsDNA"

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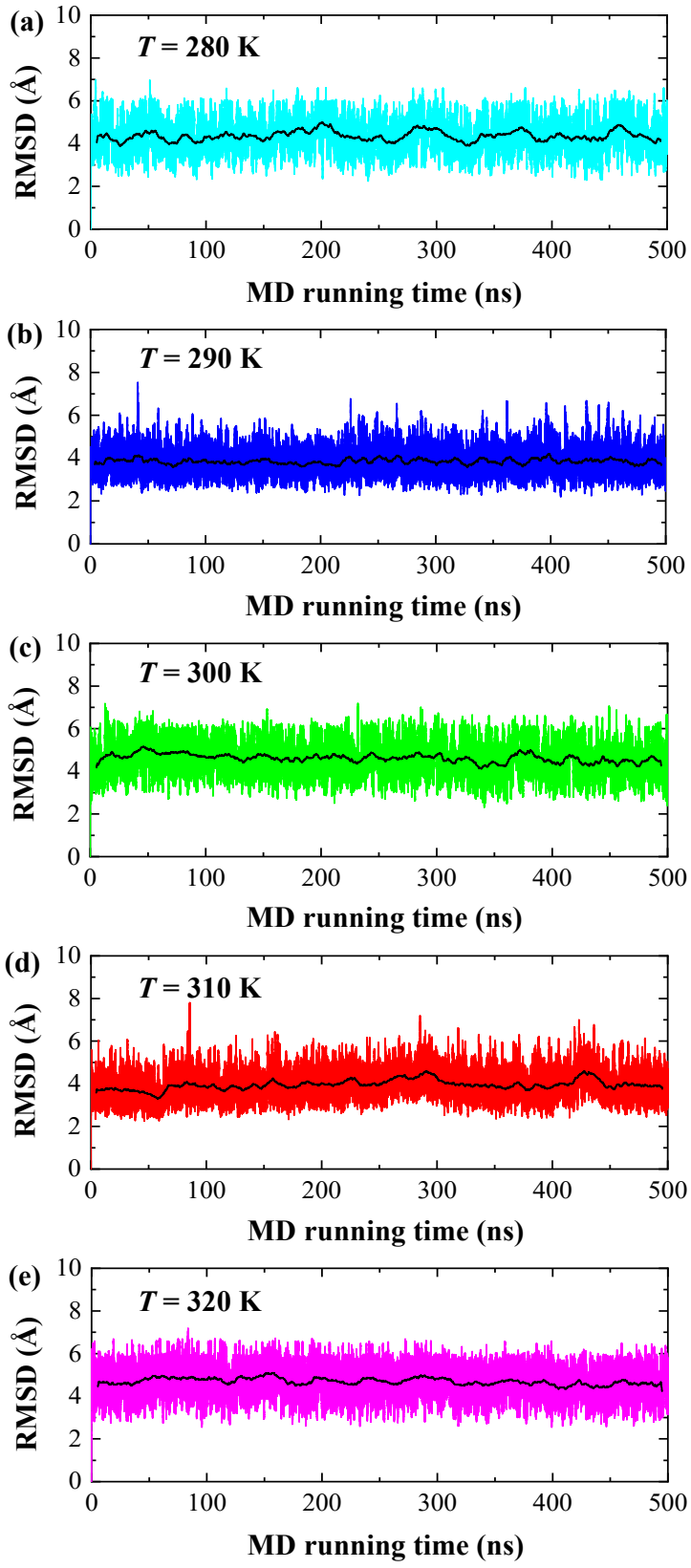
Figure S1


(a)
T = 280 K
RMSD (Å)
MD running time (ns)
(b)
T = 290 K
RMSD (Å)
MD running time (ns)
(c)
T = 300 K
RMSD (Å)
MD running time (ns)
(d)
T = 310 K
RMSD (Å)
MD running time (ns)
(e)
T = 320 K
RMSD (Å)
MD running time (ns)

Caption of Fig. S1

(a) The root mean square deviation (RMSD) curve of 29 base fragments in the center of dsDNA sequence at $T = 280\ K$, where the black line represents the average of the relevant parameters every 2 ns.

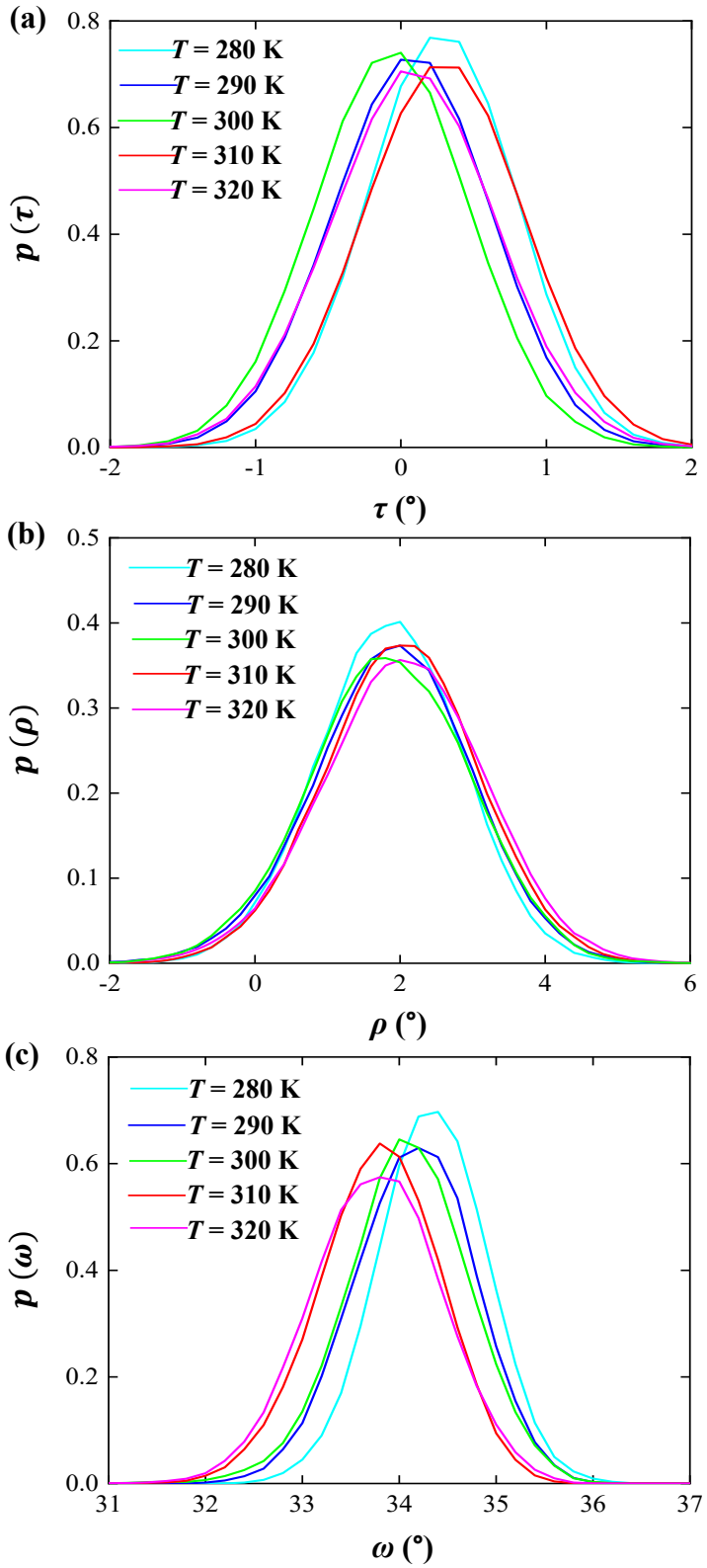
(b) The root mean square deviation (RMSD) curve of 29 base fragments in the center of dsDNA sequence at $T = 290\ K$, where the black line represents the average of the relevant parameters every 2 ns.

(c) The root mean square deviation (RMSD) curve of 29 base fragments in the center of dsDNA sequence at $T = 300\ K$, where the black line represents the average of the relevant parameters every 2 ns.

(d) The root mean square deviation (RMSD) curve of 29 base fragments in the center of dsDNA sequence at $T = 310\ K$, where the black line represents the average of the relevant parameters every 2 ns.

(e) The root mean square deviation (RMSD) curve of 29 base fragments in the center of dsDNA sequence at $T = 320\ K$, where the black line represents the average of the relevant parameters every 2 ns.

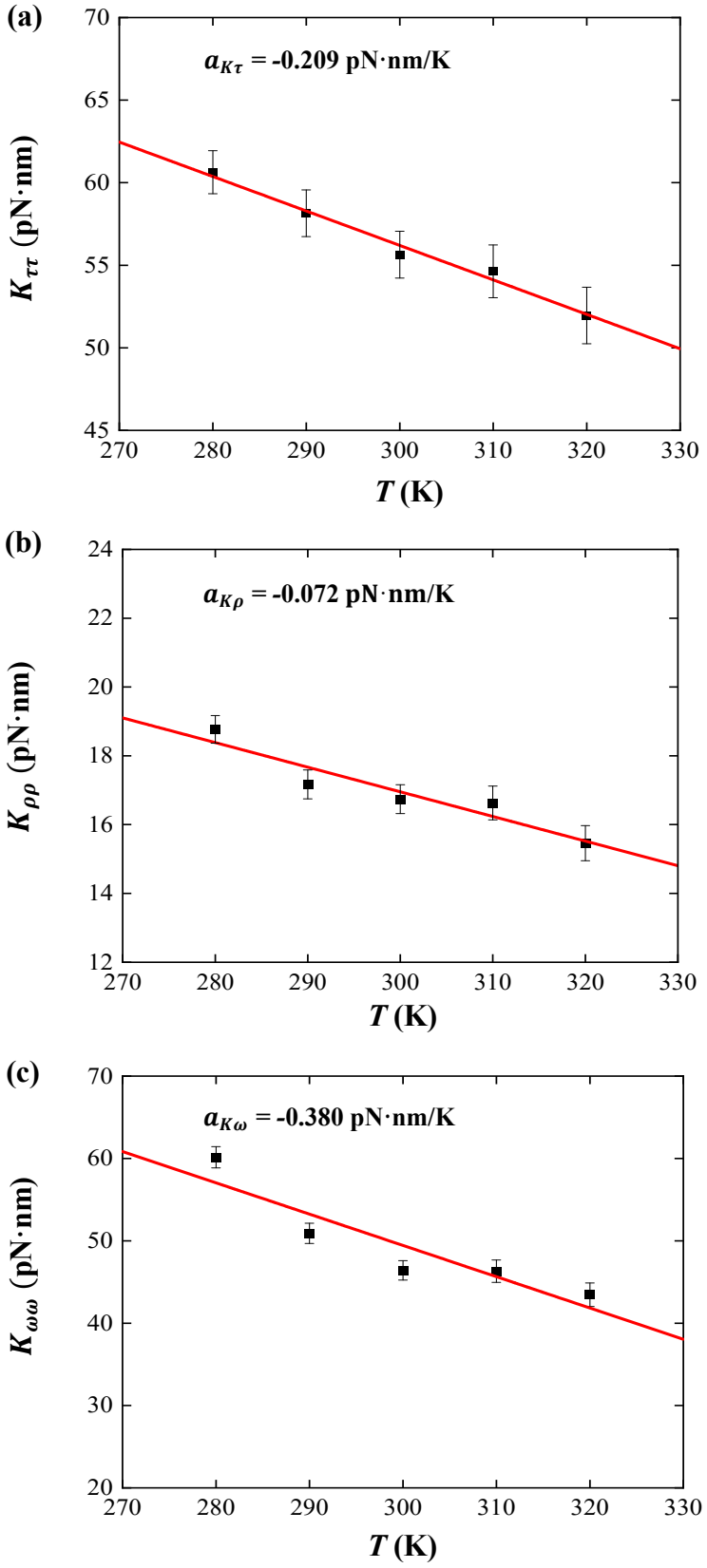
Figure S2



Caption of Fig. S2

(a) Probability distribution $p(\tau)$ of tilt τ at T = 280K, 290K, 300K, 300K and 310K, respectively. (b) Probability distribution $p(\rho)$ of roll ρ at T = 280K, 290K, 300K, 300K and 310K, respectively. (c) Probability distribution $p(\omega)$ of twist ω at T = 280K, 290K, 300K, 300K and 310K, respectively.

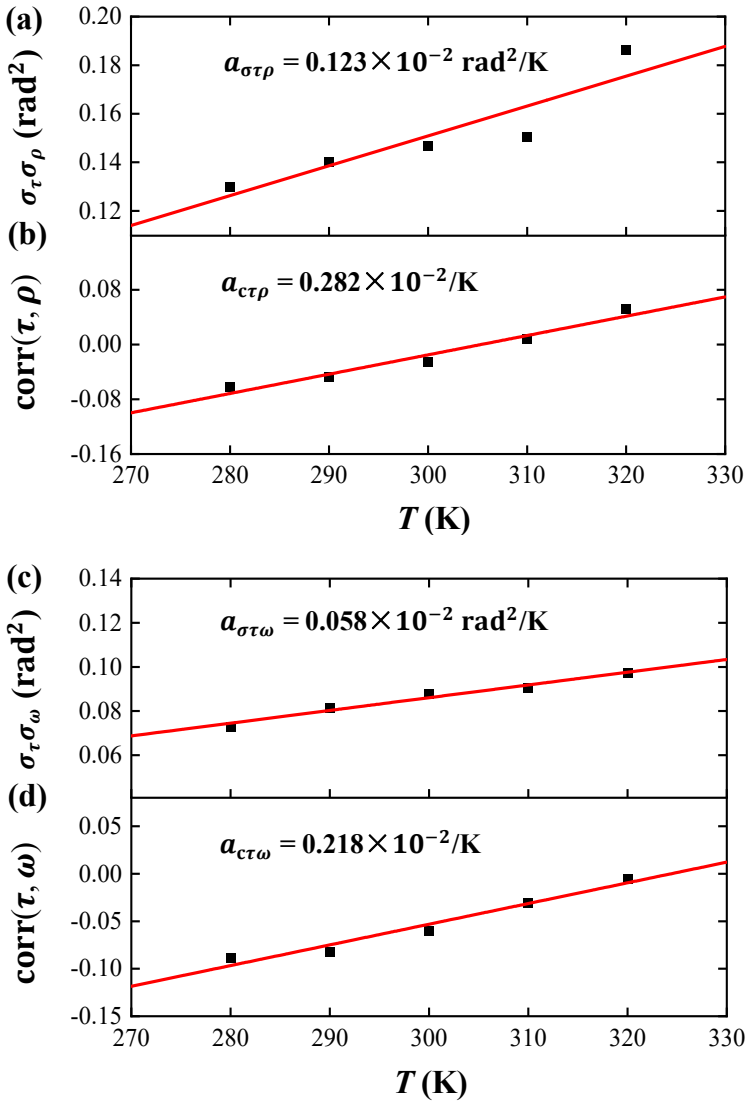
Figure S3



Caption of Fig. S3

(a) The temperature dependence of tilt modulus $K_{\tau\tau}$. The line is a fitting result with a slope of -0.209 pN·nm/K. (b) The temperature dependence of roll modulus $K_{\rho\rho}$. The line is a fitting result with a slope of -0.072 pN·nm/K. (c) The temperature dependence of twist modulus $K_{\omega\omega}$. The line is a fitting result with a slope of -0.380 pN·nm/K.

Figure S4



Caption of Fig. S4

(a) The standard deviations for cumulative tilt angle and cumulative roll angle, $\sigma_\tau\sigma_\rho$, as function of temperature T. The line is a fitting result with a slope of 0.123×10^{-2} rad^2/K. (b) The correlation coefficient corr (τ, ρ) as function of temperature T, and the line is a fitting result with a slope of 0.282×10^{-2} /K. Here, corr (τ, ρ) denote Pearson correlation coefficient between roll and tilt. (c) The standard deviations for cumulative tilt angle and cumulative twist angle, $\sigma_\tau\sigma_\omega$, as function of temperature T. The line is a fitting result with a slope of 0.058×10^{-2} rad^2/K. (d) The correlation coefficient corr (τ, ω) as function of temperature T, and the line is a fitting result with a slope of 0.218×10^{-2} /K. Here, corr (τ, ω) denote Pearson correlation coefficient between tilt and twist.

Table S1

Table S1 Summary of dsDNA elasticity parameters in the literatures.

Subject		Elastic parameters					
Length	Temperature	K_{SS}	l_B	k_T	l_T	K_{ST}	References
48bp	298 K	1401±313 pN	52.5±12.4 nm				Baumann et al.[1]
16400 nm			49 nm		120 nm		Moroz et al.[2]
16.5 μm	298 K	1010 pN	45 nm				Williams et al.[3]
69 bp	298 K	1256±217 pN	47±2 nm				Wenner et al.[4]
1.4 kbp	296 K			410±30 pN·nm^2			Bryant et al.[5]
14.8 kb	296 K	1045±92 pN		436±17 pN·nm^2		-90±10 pN·nm, 0.5±0.1 nm/turn	Gore et al.[6]
7.4 kbp						0.42±0.2 nm/turn	Lionnet.[7]
15 bp			11±2 nm				Yuan et al.[8]
2.2kbp/2.4kbp				90±0.3nm k_BT/ 88±4nm k_BT			Forth et al.[9]
4.2 kbp	296 K	1200 pN	43 nm		100 nm		Sheinin et al.[10]
11 bp	298 K	2399.09±30.27 pN	56.93±5.45 nm		87.93±5.20 nm		Faustino et al.[11]
7.9 kb					103±5 nm		Lipfert et al.[12]
8.4 kb	293 K	1450±50 pN	38±2 nm				Gross et al.[13]
160 bp	298 K		47.7nm/48.5 nm				Geggier et al.[14]
56 bp	298 K	1518 pN	43 nm				Noy et al.[15]
4.0 kb	296 K	935±121 pN	49±2 nm				Herrero-Galán et al.[16]
38 bp	298 K	955 pN	43 nm				Mogurampelly et al.[17]
3 kbp	298 K		54.7±0.6 nm		100 nm		Chou et al.[18]
4.2 kbp	300 K	1000±200 pN	45±2 nm		109±4 nm	0.44±0.1 nm/turn	Lipfert et al.[19]
2 kbp			42±1.2 nm				Zhang et al.[20]
1201bp/ 2060 bp	298 K		46.2±0.8 nm/ 47.8±0.7 nm				Brunet et al.[21]
24 bp	300 K	966.4±30.7 pN	45.84±0.88 nm				Garai et al.[22]
2060 bp	298 K	1448±5 pN		399±1 pN·nm^2		-120±1 pN·nm	Snodin et al.[23]
16.5 um	300 K	1760±50 pN	42.5±0.2 nm				Broekmans et al.[24]
25 bp	300 K		50.9 nm				Drozdetski et al.[25]
20.6 kbp	~ 298 K		43(56) nm		110(110) nm		Nomidis et al.[26]
150 bp	295 K				118nm/105 nm		Skoruppa et al.[27]
40 bp	298 K	1441 pN				0.61 nm/turn	Bao et al.[28]
16 bp	300 K	1280±70 pN		303±23 pN·nm^2			Marin-Gonzalez et al.[29]
7.9 kb					103±4 nm		Kriegel et al.[30]
12 bp	298 K	1096±32 pN	49.87±0.77 nm				Garai et al.[31]
30 bp	298 K	1860±41 pN	46.3±0.2 nm		105±2 nm	0.47±0.02 nm/turn	Xiong et al.[32]
17 bp	298 K			420-495 pN·nm^2	102-120 nm		Reymer et al.[33]
2686 bp	298 K		49.3 nm				Schurr et al.[34]
100 bp	300 K		39 nm		105 nm		Nomidis et al.[35]
16 bp	298 K	834±34 pN				0.59±0.02 nm/turn	Liu et al.[36]
104 bp	300 K				118 nm		Caraglio et al.[37]
16 bp	310 K	1435±61 pN	39.17±0.82 nm	448±16 pN·nm^2			Chen et al.[38]
20 bp	295 K	1336 pN	48 nm			0.69±0.17 nm/turn	Fu et al.[39]
38 bp	300 K	1150.11±105.08 pN	29.98±2.54 nm				Naskar et al.[40]

20 bp	298 K		49 nm				Qiang et al.[41]
N = 200			51.14 nm		219.82 nm		Segers et al.[42]
32 bp	300 K		42 nm		86 nm		Skoruppa et al.[43]
100 bp	300 K	1038±21 pN		386±3 pN·nm^2		-125±6 pN·nm	Assenza et al.[44]
~20-30 bp	300 K		58±1 nm				Segers et al.[45]
16 bp	300 K	1368.6±49.1 pN	57.78±1.39 nm	464.02±10.93 pN·nm^2			Chhetri et al.[46]
13.7 kbp	293 K					0.3 nm/turn	Qiang et al.[47]
25 bp	295 K					2.8K_BT (deg.nm)	Zhang et al.[48]
35 bp	300 K	1398.5±25.2 pN	55.14±0.19 nm	402.2±7.2 pN·nm^2	95.6±1.7 nm	-116.7±1.8 pN·nm	Zhang et al.[49]

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Table S2

Table S2 The Pearson correlation coefficients for dsDNA at different temperatures.

Structure Parameters	280K	290K	300K	310K	320K
corr (ρ,ω)	-0.4391	-0.4082	-0.3624	-0.3473	-0.2914
corr (τ,ω)	-0.0882	-0.0819	-0.0599	-0.0306	-0.0049
corr (τ,ρ)	-0.0622	-0.0473	-0.025	0.0077	0.0514

Table S3

Table S3 Comparison of dsDNA elasticity parameters in the present works.

	280K	290K	300K	310K	320K
[a]$K_{\tau\tau}$ (pN·nm)	60.63	58.15	55.64	54.63	51.96
[a]$K_{\rho\rho}$ (pN·nm)	18.77	17.17	16.74	16.63	15.46
[b]$K_{\rho\rho}$ (pN·nm)	18.55	17.09	16.55	16.83	15.37
[a]$K_{\omega\omega}$ (pN·nm)	60.15	50.91	46.31	46.42	43.45
[b]$K_{\omega\omega}$ (pN·nm)	59.08	50.03	45.82	46.78	43.48
[a]$K_{\tau\rho}$ (pN·nm)	3.80	2.80	1.53	0.09	-1.48
[a]$K_{\tau\omega}$ (pN·nm)	7.76	6.04	3.76	1.50	-0.50
[a]$K_{\rho\omega}$ (pN·nm)	15.03	12.23	10.12	9.47	7.54
[b]$K_{\rho\omega}$ (pN·nm)	14.54	11.99	9.96	9.74	7.49

a) Obtained from the third-order covariance matrix in Eqs.(2), Eq.(3) and Eq.(4).

b) Obtained from the second-order covariance matrix in Eqs.(10), Eq.(12) and Eq.(13).