Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Jianing Song,[†] Changge Ji,[*,†,‡] and John Z.H. Zhang[*,†,‡,¶]

State Key Laboratory of Precision Spectroscopy, East China Normal University, Shanghai 200062 China, Institute of Theoretical and Computational Science, East China Normal University, Shanghai 200062 China, and Department of Chemistry, New York University, New York, New York 10003 USA

E-mail: chicago.ji@gmail.com; john.zhang@nyu.edu

[*]To whom correspondence should be addressed
[†]State Key Laboratory of Precision Spectroscopy, East China Normal University, Shanghai 200062 China
[‡]Institute of Theoretical and Computational Science, East China Normal University, Shanghai 200062 China
[¶]Department of Chemistry, New York University, New York, New York 10003 USA

Figure captions

Fig. S1. (a) The total PNC and AMBER charges of individual nucleotide of G-DNA (left). the Amber result is given by the black line and red line stands for the result of PNC. (b) Some calculated PNC atomic charges of G-DNA (right).

Fig. S2. (a) The fluctuations of the backbone angle(α) as a function of time. Red line is for PNC charge, black for AMBER and yellow for XRD. (b) The fluctuations of the backbone angle(γ) as a function of time. Red line is for PNC charge, black for AMBER and yellow for XRD.

Fig. S3. (a) the structure of loop (T5-T6-T7-T8) under PNC charges aligned with the XRD structure, green color for XRD and pink for PNC. (b) the structure of loop (T17-T18-T19-T20) under PNC charges aligned with the XRD structure, green color for XRD and pink for PNC. (c) the structure of loop (T5-T6-T7-T8) under AMBER charges aligned with the XRD structure, green color for XRD and purple for PNC. (d) the structure of loop (T17-T18-T19-T20) under AMBER charges aligned with the XRD structure, green color for XRD and purple for PNC.

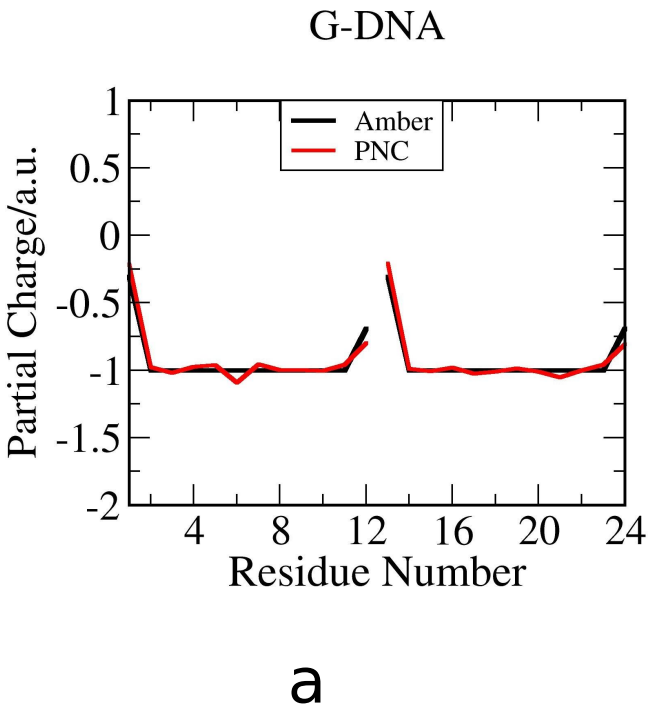
Fig. S3. (a) The fluctuations of the backbone angle(α) as a function of time. Red line is for PNC charge, black for AMBER and yellow for XRD. (b) The fluctuations of the backbone angle(γ) as a function of time. Red line is for PNC charge, black for AMBER and yellow for XRD.

Fig. S4. (a) Binding pattern for the stem-loop junction ion K26. Black dash lines indicate the distance of O4'@T8-K26 and O2'@T7-K26. (b) Binding pattern for the stem-loop junction ion K27. Black dash lines indicate the distance of O4'@T20-K27 and O2'@T19-K27.

Fig. S5. (a) Distance of K26 and the oxygen atoms in T8 and T7. Black line indicates the distance of O4'@T8-K26, with red for O2'@T7-K26. (b) Distance of K27 and the oxygen atoms in T20 and T19. Black line indicates the distance of O4'@T20-K27, with red for O2'@T19-K27.

Fig. S6. (a) Projected force along the direction of the channel (vector Vc) on stem-loop junction ion K27 as a function of simulation time. Red lines stands for the changes under PNC. Black line

is the changes under AMBER charges. Green color describes the average force of AMBER charges, while blue one for PNC. (b) The same as in (a) but for K26. (c) F_{27} and F_{26} is, respectively, the total force on K27 and K26. The vector Vc denotes the direction of the channel.



a

G-DNA				
Residue	Atom	Charge	Atom	Charge
DG^{1}			O6	-0.631
DG^{2}	P	0.925	O6	-0.722
DG^{3}	P	1.134	O6	-0.693
DG^{4}	P	0.891	O6	-0.696
DT^{5}	P	1.061		
DT^{6}	P	0.871		
DT^{7}	P	0.980		
DT^{8}	P	0.791		
DG^{9}	P	0.918	O6	-0.693
DG^{10}	P	0.896	O6	-0.707
DG^{11}	P	1.062	O6	-0.692
DG^{12}	P	0.918	O6	-0.626
DG^{13}			O6	-0.720
DG^{14}	P	0.921	O6	-0.758
DG^{15}	P	1.079	O6	-0.709
DG^{16}	P	0.856	O6	-0.659
DT^{17}	P	0.944		
DT^{18}	P	0.944		
DT^{19}	P	0.922		
DT^{20}	P	0.813		
DG^{21}	P	0.918	O6	-0.617
DG^{22}	P	0.879	O6	-0.722
DG^{23}	P	1.059	O6	-0.660
DG^{24}	P	0.918	O6	-0.673

b

Figure S1

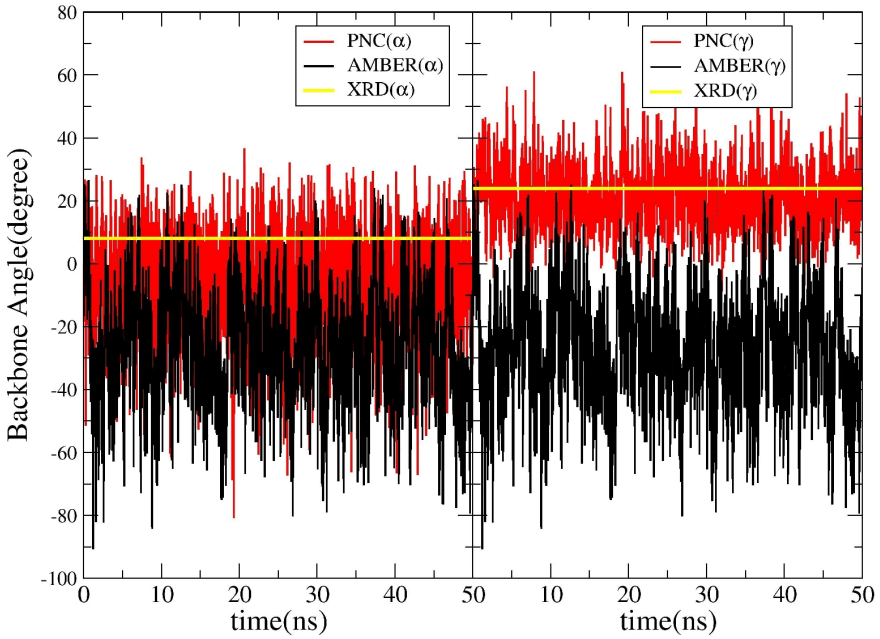

PNC(α)
AMBER(α)
XRD(α)
PNC(γ)
AMBER(γ)
XRD(γ)
Backbone Angle(degree)
time(ns)
time(ns)
80
60
40
20
0
-20
-40
-60
-80
-100
0
10
20
30
40
50
10
20
30
40
50

Figure S2

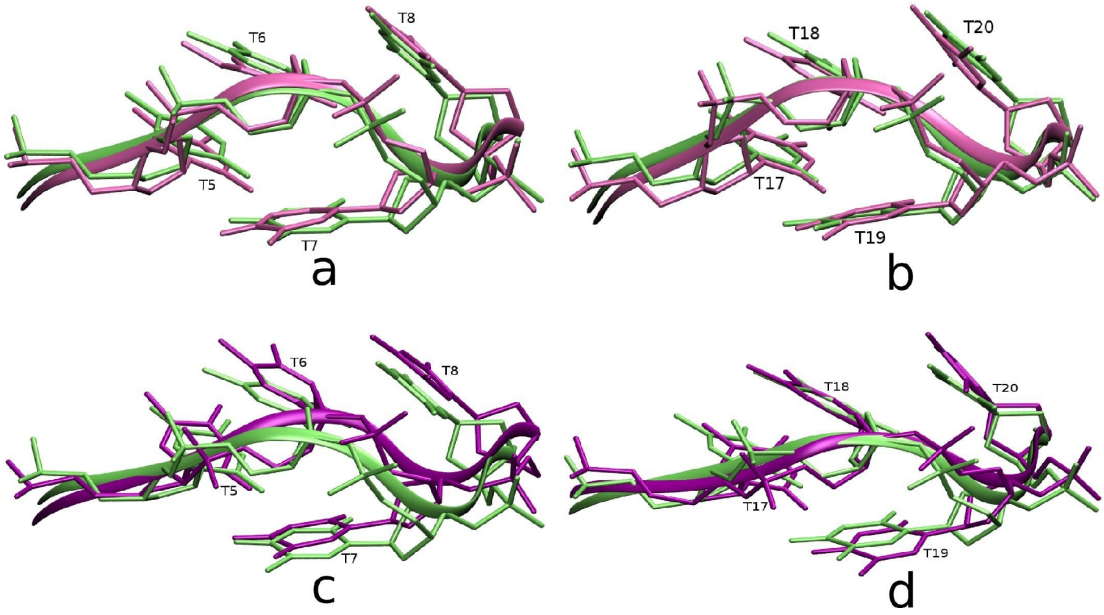


Figure S3

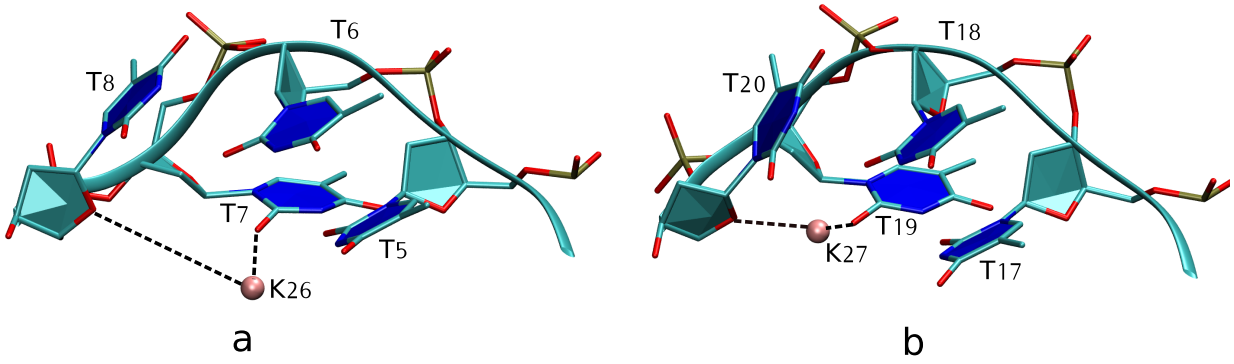


Figure S4

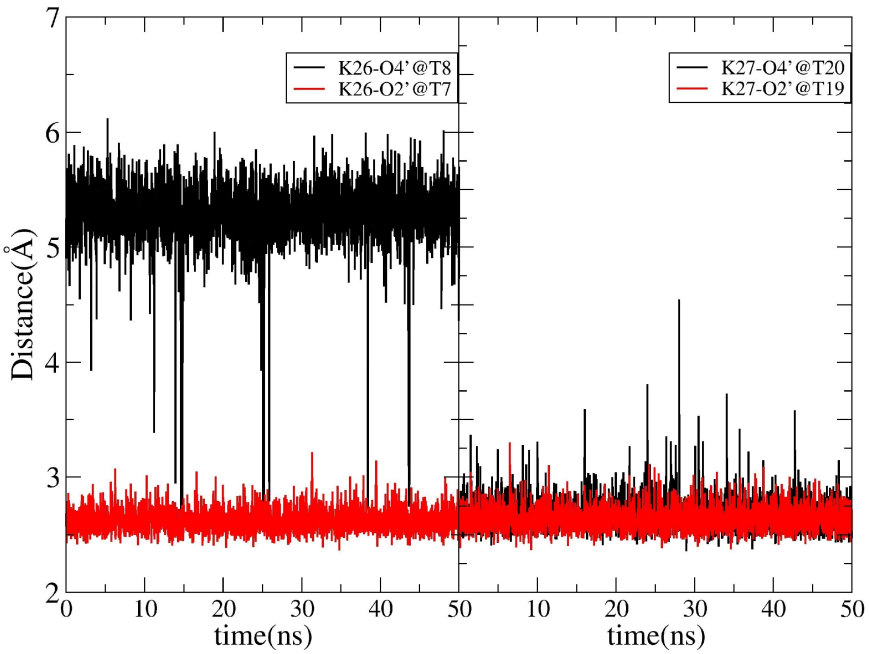

K26-O4'@T8
K26-O2'@T7
K27-O4'@T20
K27-O2'@T19
Distance(Å)
time(ns)
time(ns)

Figure S5

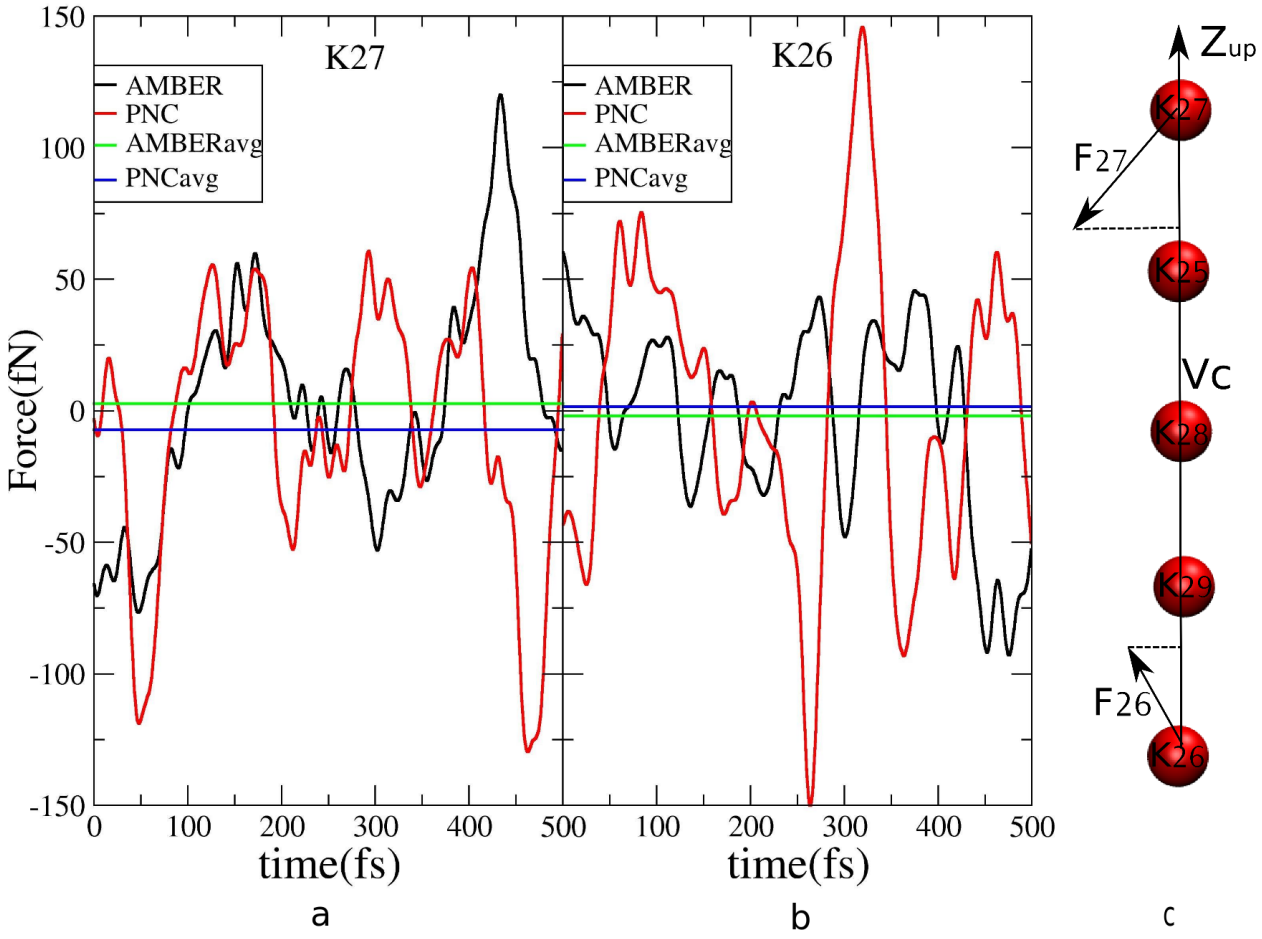

K27
K26
AMBER
PNC
AMBERavg
PNCavg
Force(fN)
time(fs)
a
b
c
Zup
F27
F26
Vc
K27
K25
K28
K29
K26

Figure S6