Electronic Supplemental Information (ESI)

for

Implication of solvent effect, metal ions and topology in the electronic structure and hydrogen bonding of human telomeric G-quadruplex DNA.

Submitted to physical chemistry chemical physics

by

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Supplemental figures:





Figure S1: The calculated total density of states (TDOS) of G4-DNA models. (a) A1 (b) B1 (c) A2, (d) B2, (e) A3 (f) B3 (g) A4, (h) B4, (i) A5 and (j) B5.







Figure S2:The calculated partial density of states (PDOS) of different functional groups in G4-DNA models. (a) A1 (b) B1 (c) A2, (d) B2, (e) A3 (f) B3 (g) A4, (h) B4, (i) A5 and (j) B5.





Figure S3: Calculated bond order (BO) distribution of: (a) A1 (b) B1 (c) A2, (d) B2, (e) A3 (f) B3 (g) A4, (h) B4, (i) A5 and (j) B5.





Figure S4: Detailed bond order (BO) distribution of hydrogen bonds and ionic bonds of G4-models: (a) A1 (b) B1 (c) A2, (d) B2, (e) A3 (f) B3 (g) A4, (h) B4, (i) A5 and (j) B5.



Figure S5: The distribution of ionic bond (Na-O or K-O) at guanine tetrad of G4-models; (a) A3, (b) B3, (c) A4, (d) B4, (e) A5, (f) B5, (g) A6, and (h) B6.

Supplemental Tables

Table S1: 0	Calculated	partial	charge	distribution	on	different	functional	groups	of	parallel
G4-DNA n	nodels									

Parallel	A1		A2		A3		A4		A5	
G4	Total	Average	Total	Average	Total	Average	Total	Average	Total	Average
Adenine	-0.904	-0.226	-0.928	-0.232	-0.926	-0.231	-0.894	-0.224	-0.951	-0.237
thymine	-1.333	-0.222	-1.196	-0.199	-1.303	-0.217	-1.119	-0.186	-1.221	-0.203
Guanine	-2.400	-0.200	-2.080	-0.173	-1.927	- 0.162	-1.796	-0.149	-2.430	-0.202
sugar	14.337	0.717	14.656	0.733	14.081	0.704	14.612	0.731	-2.431	0.701
Sugar-t	0.528	0.264	0.597	0.298	0.584	0.292	0.598	0.299	0.575	0.287
PO ₄	-27.723	-1.320	-27.116	1.291	-27.390	-1.305	-26.767	-1.275	27.406	-1.305
Na(b)	17.495	0.833	16.710	0.796	14.876	0.826	14.239	0.791	14.868	0.826
Na(c)	-	-	-	-	2.016	0.672	2.005	0.669	-	-
K(c)		-	-	-	-	-	-	-	2.529	0.843
H ₂ O	-	-	-0.643	-0.0094	-	-	-0.880	-0.012	-	-

Table S2: Calculated partial charge distribution on different functional groups of antiparallel G4-DNA models.

Anti-	B1		B2		B3		B4		B5	
parallel G4	Total	Average	Total	Average	Total	Average	Total	Average	Total	Average
Adenine	-0.972	-0.243	-0.796	-0.199	-0.975	-0.234	-0.905	-0.226	-1.023	-0.256
thymine	-1.338	-0.223	-1.420	-0.235	-1.255	-0.209	-1.283	-0.214	-1.286	-0.214
Guanine	-2.772	-0.231	-2.836	-0.236	-2.325	-0.194	-2.334	-0.194	-2.767	-0.231
sugar	14.120	0.706	14.184	0.709	13.996	0.699	14.255	0.713	13.934	0.6967
Sugar-t	0.932	0.466	0.875	0.437	0.947	0.473	0.896	0.448	0.947	0.4734
PO_4	-27.468	-1.308	-26.48	-1.261	-27.36	-1.303	-26.41	-1.261	-27.366	-1.303
Na(b)	17.514	0.834	16.706	0.795	14.954	0.831	14.151	0.7861	14.966	0.835
Na(c)	-	-			2.023	0.674	1.989	0.663	-	-
K(c)	-	-	-	-	-	-	-	-	2.595	0.865
H ₂ O	-	-	-0.267	-0.004	-	-	-0.201	-0.003	-	-