

Supplementary information : Effect of sequence on the ionization of guanine in DNA

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Molecular orbitals involved in dimer and tetramer lowest ionizations

Figure 1: MOs (ω B97x-D/6-311++G(d,p)) from which ionization predominantly occurs in the stacked and H-bonded dimers.

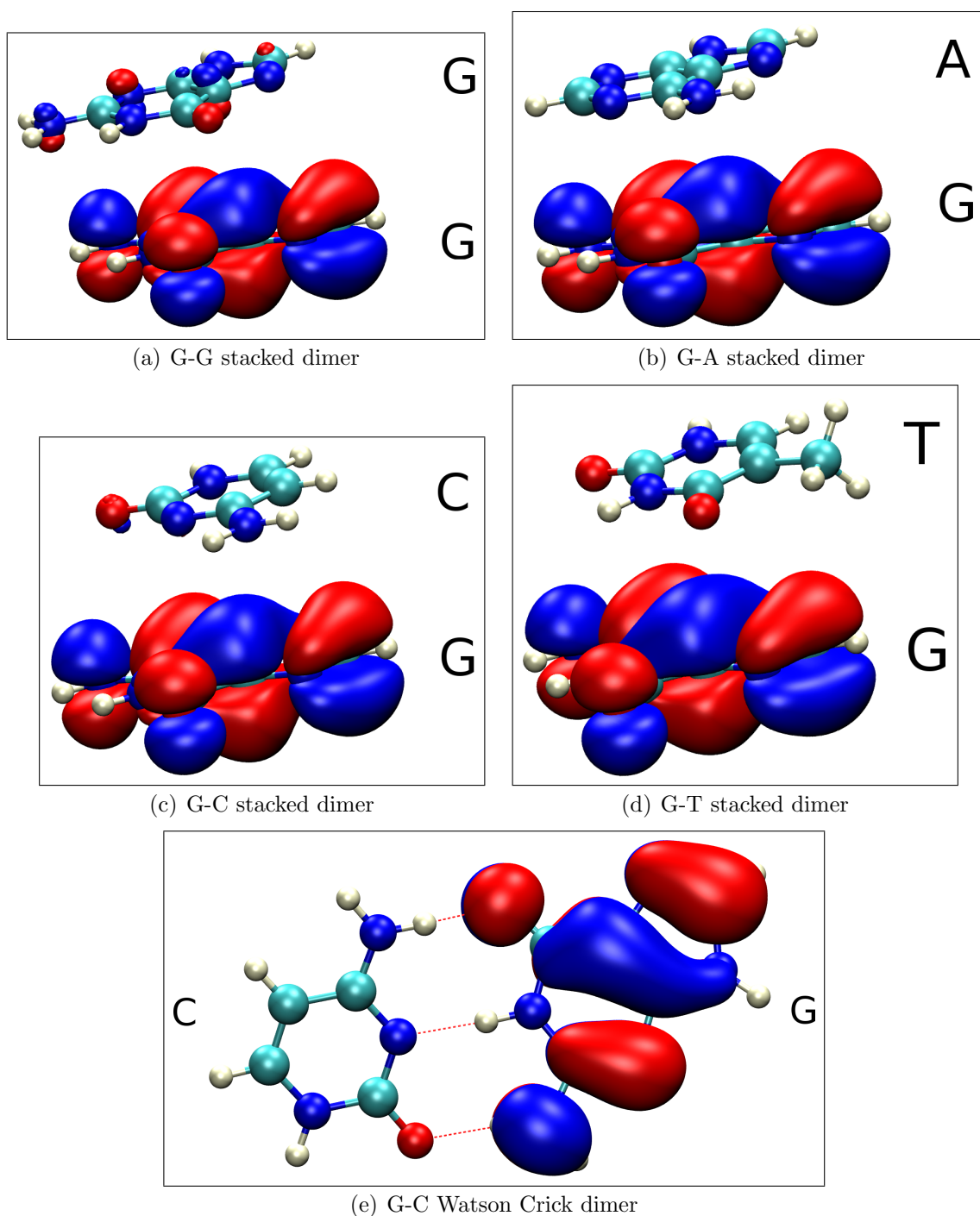
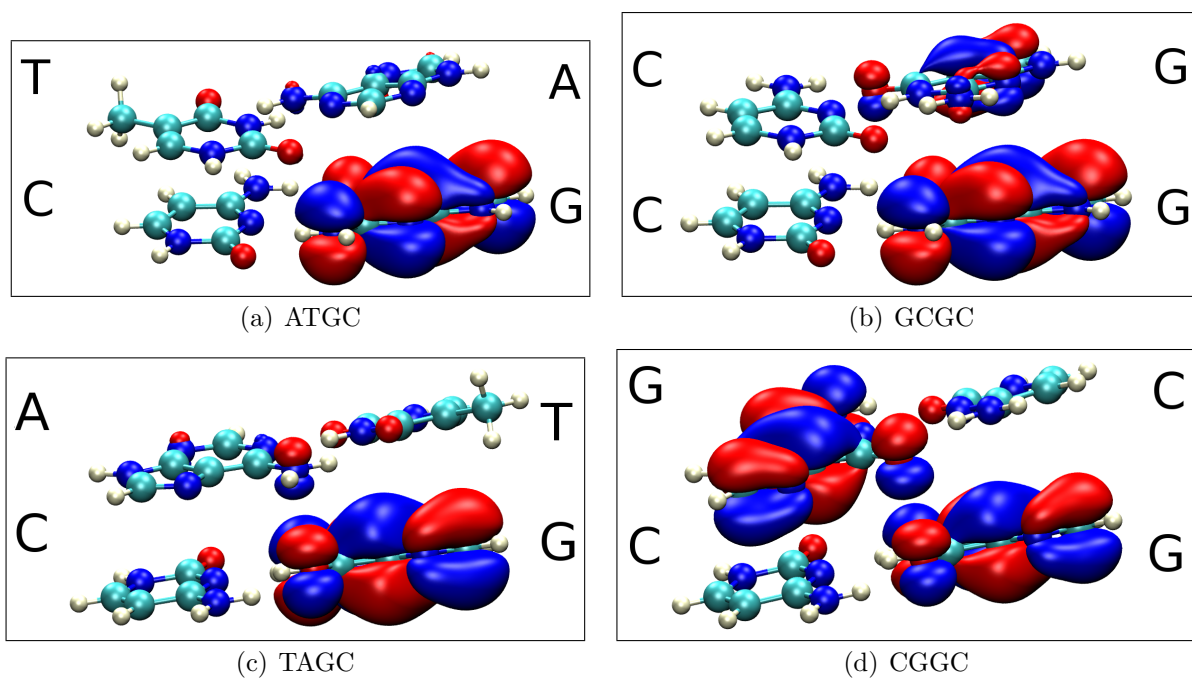


Table 1: % charge localized on the guanine in the H-bonded and stacked dimers.

Species	% charge
G-A stack	98.7
G-T stack	99.7
G-C stack	99.3
G-G stack	76.6 (23.4)
G-C WC	92.2

Figure 2: MOs most predominantly responsible for the lowest VIEs in NAB tetramers containing G-C Watson Crick dimer. The ω B97x-D/6-311++G(d,p) orbitals are shown.



Geometry of neutral monomers

Adenine

C	-0.179845	-0.514692	0.020188
C	-0.705653	0.772447	0.000091
N	-0.017797	1.919421	-0.009955
C	1.293917	1.697096	0.002642

H	1.929465	2.578287	-0.005488
N	1.943610	0.523320	0.023448
C	1.225207	-0.606937	0.033265
N	1.866434	-1.793829	0.056543
H	1.345713	-2.654037	0.055442
H	2.872380	-1.806139	0.056153
N	-2.066634	0.590296	-0.008719
H	-2.760876	1.320254	-0.022585
C	-2.282011	-0.768663	0.005865
H	-3.281351	-1.180052	0.003071
N	-1.179670	-1.469171	0.023553

Guanine (9k)

O	-0.256949	-2.678648	0.062130
H	-2.293978	-1.362391	-0.078782
C	-0.246287	-1.464038	0.025646
N	-1.485511	-0.757020	-0.019435
H	-3.665865	0.532952	0.281731
C	0.846857	-0.528263	0.008801
N	2.208274	-0.743148	0.029988
C	-1.644653	0.601590	-0.067089
N	-2.931231	1.068363	-0.154468
C	0.559273	0.827449	-0.051214
H	-3.008373	2.067757	-0.038284
N	-0.649432	1.447326	-0.077963
C	2.727585	0.451513	-0.014656
H	3.784215	0.677607	-0.014228
N	1.774398	1.447584	-0.064918

H	1.926222	2.442865	-0.106164
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Guanine (7k)

O	-0.049327	-2.634773	-0.174049
H	-2.224594	-1.461827	-0.207077
C	-0.179614	-1.419374	-0.121114
N	-1.452350	-0.817155	-0.099987
H	-3.680865	0.328243	0.393083
C	0.819531	-0.403145	-0.083119
N	2.192334	-0.473496	-0.098755
C	-1.689886	0.540870	-0.046993
N	-3.014190	0.914404	-0.087095
C	0.511642	0.949414	-0.047730
H	-3.141675	1.902694	0.078356
N	-0.760443	1.447236	-0.012459
C	2.631144	0.811505	-0.070160
H	3.684546	1.053735	-0.073748
N	1.657384	1.697623	-0.037915
H	2.745223	-1.315389	-0.127266

Thymine

N	0.722127	-1.028143	0.000022
H	1.083864	-1.973436	-0.000281
C	1.671676	-0.026264	0.000344
O	2.870662	-0.230168	-0.000197
N	1.120526	1.240484	0.000180
H	1.783978	1.999632	0.000144
C	-0.236958	1.480705	0.000146

H	-0.522993	2.526839	0.000082
C	-1.153617	0.493107	0.000104
C	-0.669798	-0.892110	0.000097
O	-1.383428	-1.879906	-0.000299
C	-2.634552	0.716453	-0.000042
H	-2.873453	1.783192	-0.000013
H	-3.093099	0.255571	0.879444
H	-3.092909	0.255669	-0.879680

Cytosine

H	1.929720	1.806414	0.036019
H	-0.388832	2.776523	-0.015800
C	1.047867	1.179978	0.025809
C	-0.198504	1.709264	-0.001543
H	3.193033	-0.321008	0.053647
N	-1.279585	0.895077	-0.011767
C	1.123284	-0.258832	0.042370
H	-2.218754	1.264692	-0.032324
N	2.340732	-0.851722	0.075448
C	-1.189080	-0.519643	0.004326
N	0.072351	-1.050521	0.031771
O	-2.223322	-1.163671	-0.007392
H	2.378604	-1.858261	0.066004

Guanine in w3DNA $VIE(\omega B97x-D) = 7.96 \text{ eV}$

O	0.1897030997	-2.6604215222	0.0005125546
N	-2.2044672524	-0.7104799974	-0.0000997671
H	-3.7198904040	0.6907167358	-0.0011873291

C	0.2409393740	-1.4330195630	-0.0000115319
C	-2.7052919693	0.5020015501	-0.0004158969
C	-0.8267391039	-0.4988880602	-0.0000700271
H	2.2906283883	-1.3563749116	-0.0007430377
N	1.4863573041	-0.7885825685	-0.0003848687
C	-0.5433841496	0.8467062090	0.0001103442
N	-1.7569066711	1.5008101922	0.0003730830
H	-1.9122581986	2.4729756977	0.0009917361
C	1.6738387973	0.5798649755	-0.0002897912
N	0.6715288639	1.4560684674	0.0001984648
H	3.6764470308	0.3425988854	-0.0003578784
N	2.9419082795	0.9981085642	0.0000079653
H	3.1423270258	1.9619924958	0.0005933473

Structures of neutral dimers

G-A stack (w3DNA) $VIE(\omega B97x-D) = 7.70$ eV

N	1.308257	2.069973	-1.368560
C	1.877013	2.707473	-0.288206
N	2.301172	1.894226	0.649694
C	1.990080	0.628685	0.155189
C	2.206337	-0.652846	0.723915
O	2.726253	-0.939859	1.799300
N	1.736042	-1.672702	-0.115777
C	1.135889	-1.477965	-1.344472
N	0.756726	-2.581570	-1.993486
N	0.933664	-0.275122	-1.877981

C	1.384003	0.725058	-1.075379
N	-2.864660	0.731136	-1.234635
C	-2.573118	1.958031	-0.711751
N	-1.920417	1.909454	0.408436
C	-1.766637	0.551339	0.647190
C	-1.152253	-0.163852	1.688068
N	-0.549198	0.421248	2.733167
N	-1.179899	-1.507725	1.617554
C	-1.779998	-2.083498	0.576727
N	-2.383622	-1.523810	-0.448086
C	-2.341957	-0.178803	-0.352769
H	0.929328	2.485298	-2.176595
H	1.962356	3.733855	-0.222647
H	1.842183	-2.600886	0.195446
H	0.910895	-3.467111	-1.590930
H	0.323054	-2.510343	-2.874677
H	-3.348650	0.539991	-2.069951
H	-2.846626	2.843588	-1.165877
H	-0.520968	1.403504	2.798591
H	-0.134773	-0.130843	3.434661
H	-1.769428	-3.115668	0.574225

G-T stack (w3DNA) VIE(ω B97x-D)=7.79 eV

N	-0.3033671104	-1.4709424996	-1.8657246801
C	-0.3181898901	-2.6636277428	-1.1770039850
N	-1.0545360982	-2.6447796239	-0.0914736952
C	-1.5622632072	-1.3470615933	-0.0591148333
C	-2.4254701863	-0.7270224062	0.8805468706

O	-2.9286577404	-1.2037054289	1.8948035350
N	-2.6902797733	0.6053271342	0.5325733304
C	-2.1864089654	1.2523433124	-0.5788592020
N	-2.5583397334	2.5251753085	-0.7353654747
N	-1.3767971586	0.6698463121	-1.4606664185
C	-1.1098638630	-0.6229606102	-1.1370418251
N	2.3525401821	1.7923708459	-0.6325983838
C	1.4402848483	2.0514455582	0.3623164364
O	0.8953863661	3.1335317371	0.4960517924
N	1.1749364091	0.9967386816	1.2138771273
C	1.7324474951	-0.2643868327	1.1534550619
O	1.4162758924	-1.1286721322	1.9729747010
C	2.6784058235	-0.4393100536	0.0756268252
C	3.3320194254	-1.7833502368	-0.0612901036
C	2.9552889470	0.5688585935	-0.7662310695
H	0.1791431483	-1.2676577029	-2.6993079943
H	0.2033328093	-3.4982097988	-1.4876949341
H	-3.2822331591	1.1200161397	1.1278358076
H	-3.1579268651	2.9474256845	-0.0779433185
H	-2.2333891003	3.0418632833	-1.5080766904
H	2.5800480871	2.5083357380	-1.2685484026
H	0.5238171782	1.1607858974	1.9344860768
H	2.9714278282	-2.4354755284	0.7062776812
H	4.3921467112	-1.6749955340	0.0314050756
H	3.0978569422	-2.1974376884	-1.0196639940
H	3.6351406915	0.4203950593	-1.5281872261

G-C stack (w3DNA) $VIE(\omega_{B97x-D}) = 7.71$ eV

N	-0.6309687431	-1.3678982774	-1.9346700097
C	-1.0429894929	-2.5143125064	-1.2919979959
N	-1.7262207773	-2.2951567411	-0.1937708962
C	-1.7684526772	-0.9048883142	-0.1027974503
C	-2.3697841741	-0.0712570785	0.8749542532
O	-3.0001048966	-0.3936760711	1.8788879064
N	-2.1729823868	1.2860902730	0.5829915437
C	-1.4851649836	1.7726654358	-0.5115174014
N	-1.4085453930	3.1018921230	-0.6125810072
N	-0.9214918071	0.9899146892	-1.4290858287
C	-1.1031014958	-0.3299080415	-1.1599726919
N	2.9712478736	0.7606148852	-0.6242787845
C	2.1892751484	1.2595714004	0.4139177542
O	2.0801020999	2.4845452529	0.5445596549
N	1.5737458072	0.3813500173	1.2473641126
C	1.7164099539	-0.9385495219	1.0729905262
N	1.0960921537	-1.7546655922	1.9116331119
C	2.5171696218	-1.4727238064	0.0111558931
C	3.1239003286	-0.5784235582	-0.8099189607
H	-0.1112866664	-1.3034319523	-2.7682026317
H	-0.8332318744	-3.4616520773	-1.6435537938
H	-2.5554749480	1.9440461998	1.2078470782
H	-1.8290472322	3.6728022275	0.0709713725
H	-0.9317785652	3.5116058114	-1.3705190558
H	3.4216526704	1.3879419452	-1.2344519393
H	1.1846759143	-2.7296560110	1.8058380244
H	0.5473114633	-1.3864979977	2.6406278829

H	2.6267606997	-2.4903180102	-0.1230224664
H	3.7107304466	-0.9198272846	-1.5872142123

G-G stack (w3DNA) VIE (ω B97x-D) = 7.59 eV

N	-2.4526860247	1.3566972372	1.1379500083
C	-3.2049025930	1.5209695583	-0.0040827578
N	-3.1032631603	0.5303344099	-0.8580431951
C	-2.2202622255	-0.3516792253	-0.2373441566
C	-1.7226056041	-1.6057062563	-0.6758565197
O	-1.9630850733	-2.2067198195	-1.7199318626
N	-0.8470884302	-2.1674025898	0.2645327120
C	-0.4993501508	-1.5914906026	1.4708500301
N	0.3511396392	-2.2873164628	2.2294154456
N	-0.9670811402	-0.4148735338	1.8821382441
C	-1.8175273081	0.1432944999	0.9807361354
N	1.8212110029	2.3348902657	1.1624570844
C	0.9662260479	3.1866758286	0.4971781341
N	0.4945982049	2.7006173976	-0.6256483793
C	1.0792662128	1.4381432812	-0.7102558606
C	0.9490011077	0.4361306487	-1.7076242412
O	0.2808215950	0.4568239420	-2.7366577326
N	1.7183503994	-0.6949480702	-1.3998083887
C	2.5092721948	-0.8397160172	-0.2763089650
N	3.1652327612	-1.9972185883	-0.1654417784
N	2.6297778483	0.1004294368	0.6581769433
C	1.8903773549	1.2050971583	0.3752915680
H	-2.3835875033	1.9730556141	1.9023646508
H	-3.7963986261	2.3496593787	-0.1727469934

H	-0.4489130817	-3.0414499543	0.0473954364
H	0.6914895599	-3.1570718664	1.9168590997
H	0.6381214862	-1.9311481563	3.1014404205
H	2.2831360379	2.4976425278	2.0162854999
H	0.7184461673	4.1240600010	0.8512812888
H	1.6933389156	-1.4466916850	-2.0353852631
H	3.0690869637	-2.6855300607	-0.8628027342
H	3.7450799841	-2.1621385378	0.6124242823

G-C H-bond (ω 3DNA) VIE (ω B97x-D) = 7.33 eV

N	4.6435044141	-0.5253312207	0.0670598133
C	4.9470502905	0.8089031070	-0.0902063931
N	3.8962419841	1.5880709633	-0.1883713313
C	2.8209565818	0.7065971420	-0.0900290416
C	1.4256383858	0.9599302532	-0.1280877672
O	0.8414574407	2.0327549120	-0.2581680304
N	0.6855539771	-0.2233842605	0.0075840049
C	1.2248739721	-1.4857420068	0.1605051067
N	0.3495586222	-2.4876123774	0.2745524607
N	2.5343841574	-1.7228733200	0.1966964716
C	3.2662165600	-0.5850458528	0.0659066048
N	-4.2908883662	-0.9225439477	-0.1670079072
C	-2.9041607523	-1.0462271653	-0.1933705058
O	-2.4076165370	-2.1659096457	-0.3606337278
N	-2.1464520516	0.0697154062	-0.0338941697
C	-2.7230868344	1.2657382176	0.1447556606
N	-1.9423471680	2.3237706030	0.2954010873
C	-4.1481870102	1.4136670324	0.1756677114

C	-4.8863033454	0.2866065893	0.0149535759
H	5.2743454189	-1.2752045972	0.1605025540
H	5.9152870948	1.1641540496	-0.1270338096
H	-0.2961539516	-0.1480475860	-0.0074135998
H	-0.6173496290	-2.3023185394	0.2470092693
H	0.6705154573	-3.4118056333	0.3863358926
H	-4.8501568109	-1.7248749710	-0.2818718955
H	-0.9636423820	2.2207763600	0.2737648274
H	-2.3399202464	3.2141024904	0.4287081672
H	-4.5924768454	2.3348684286	0.3142300800
H	-5.9160514064	0.3483410461	0.0314698628

G-G cross (w3DNA) $VIE(\omega_{B97x-D}) = 7.63$ eV

N	4.6874213074	0.2351696469	-0.7429569834
C	4.5334603555	1.5970970904	-0.8789851565
N	3.4297007276	2.0658990359	-0.3471238779
C	2.8087202195	0.9335097112	0.1772649338
C	1.5796184240	0.8057482921	0.8740610274
O	0.7723761225	1.6806298653	1.1775129999
N	1.3267198087	-0.5273686859	1.2279062101
C	2.1546573946	-1.5961658067	0.9450810548
N	1.7354464093	-2.7909868487	1.3688649941
N	3.3082655495	-1.4756480656	0.2916120815
C	3.5678917613	-0.1884186537	-0.0590596615
N	-4.6873296987	0.2348143113	0.7428870347
C	-4.5332636175	1.5972666061	0.8787413204
N	-3.4301981941	2.0661129979	0.3472173487
C	-2.8093154032	0.9336146945	-0.1770212925

C	-1.5794147096	0.8061660385	-0.8742408590
O	-0.7724615853	1.6797606332	-1.1776105002
N	-1.3265132215	-0.5272263098	-1.2279733608
C	-2.1548122336	-1.5961873106	-0.9448600878
N	-1.7351426941	-2.7911722791	-1.3687909815
N	-3.3079251328	-1.4757368453	-0.2916707377
C	-3.5678941254	-0.1891113901	0.0590771218
H	5.4360668756	-0.3171427275	-1.0646444940
H	5.2253268665	2.1956939760	-1.3565252067
H	0.4929166248	-0.7160840695	1.7165878596
H	0.8807612777	-2.8701660337	1.8518225310
H	2.2807008856	-3.5931117766	1.1987616248
H	-5.4366699072	-0.3171664533	1.0649995732
H	-5.2252025832	2.1962593809	1.3562694593
H	-0.4930048315	-0.7160951976	-1.7164785368
H	-2.2805377705	-3.5936320200	-1.1985424135
H	-0.8806761572	-2.8697933997	-1.8516228951

G-A cross (w3DNA) $VIE(\omega_{B97x-D}) = 7.76$ eV

N	4.6000795416	0.3969134598	-0.6865769079
C	4.3852916423	1.7506324166	-0.5510588493
N	3.2527244028	2.0558612555	0.0363624680
C	2.6767284747	0.8159569220	0.3079723620
C	1.4440320964	0.4988906777	0.9344447363
O	0.5923987592	1.2599890585	1.3867620074
N	1.2476758063	-0.8876175000	1.0079585474
C	2.1286467723	-1.8417675477	0.5375482546
N	1.7586608323	-3.1140189243	0.7031225247

N	3.2855923883	-1.5436915794	-0.0498064583
C	3.4907461199	-0.2024458851	-0.1292289598
N	-4.7868461989	-0.2983577311	0.5364979521
C	-4.7158317937	1.0006592690	0.9506353542
N	-3.6430583731	1.6177990037	0.5626279626
C	-2.9501222715	0.6591752312	-0.1629545771
C	-1.7216936474	0.6913418290	-0.8439703078
N	-0.9387781866	1.7770913530	-0.9057550324
N	-1.3262048501	-0.4383844657	-1.4606031892
C	-2.1093508440	-1.5141068597	-1.3957519491
N	-3.2688408424	-1.6621905487	-0.7939113019
C	-3.6423347586	-0.5176338588	-0.1840078028
H	5.3785153675	-0.0473062541	-1.0936500103
H	5.0561033965	2.4617070275	-0.8818555968
H	0.4159140682	-1.2057916396	1.4281830445
H	0.9010528914	-3.3247249393	1.1391449954
H	2.3431426886	-3.8417933827	0.3894869122
H	-5.5095772139	-0.9424451925	0.7177249427
H	-5.4489123305	1.4505352930	1.5203488695
H	-0.0870219398	1.7421510139	-1.3976132121
H	-1.2158685849	2.6094090566	-0.4592013945
H	-1.7562408014	-2.3496968760	-1.8878501328

G1-C2 cross (w3DNA) $VIE(\omega B97x-D) = 7.86$ eV

N	4.6211432401	0.4836005692	-0.7378734404
C	4.3428433451	1.8223058800	-0.5721288808
N	3.1775071061	2.0614179263	-0.0191787208
C	2.6465765664	0.7905878808	0.1953201311

C	1.4069521052	0.4028234872	0.7658540653
O	0.5071474866	1.1131687717	1.2073313865
N	1.2686171247	-0.9923522959	0.7925555144
C	2.2067740873	-1.8937000429	0.3286247517
N	1.8867755815	-3.1849064581	0.4440151747
N	3.3701780592	-1.5292896755	-0.2062156751
C	3.5194813969	-0.1787644698	-0.2397743153
N	-4.7647738989	-0.6460071018	0.1119706458
C	-3.6273765598	-0.9839898106	-0.6160966463
O	-3.5290117393	-2.1301562605	-1.0712546749
N	-2.6660529700	-0.0427785373	-0.8000621179
C	-2.8103101942	1.1874250389	-0.2908980830
N	-1.8459997453	2.0705182772	-0.4972102027
C	-3.9727475035	1.5558537756	0.4619490249
C	-4.9214811171	0.6001219364	0.6347500142
H	5.4324300019	0.0852408941	-1.1279059512
H	4.9936096094	2.5708217955	-0.8572064025
H	0.4368093983	-1.3580145117	1.1720789660
H	1.0239110138	-3.4448169883	0.8414006980
H	2.5133787106	-3.8774748501	0.1319902703
H	-5.4682793338	-1.3212681371	0.2511670432
H	-1.0480820191	1.8161544915	-1.0147199771
H	-1.9268589065	2.9816223153	-0.1335355845
H	-4.0831593201	2.5040781848	0.8549957150
H	-5.7748793718	0.8221557345	1.1715129147

G2-C1 cross (w3DNA) $VIE(\omega B97x-D) = 7.42$ eV

H	3.8924568418	-3.2056497521	0.4906945921
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H	5.5493899723	-1.6772636365	-0.3907857364
N	3.2711491785	-2.4726283637	0.7049297004
H	2.3984421504	-2.6710836039	1.1150982155
C	4.8788858589	-0.9288708960	-0.1555060307
C	3.6091174769	-1.2203993795	0.4415269662
O	-2.1859945374	-2.4966513912	-0.8742676775
H	6.0624120441	0.6310677103	-0.8256811231
C	5.1587548821	0.3765814939	-0.3971201601
N	2.7390344002	-0.2486906510	0.7475197546
H	-0.4778819417	-0.7886467665	-1.3967764923
C	-2.3100912854	-1.3002486242	-0.6313223829
N	-1.2797195035	-0.4109688789	-0.9682252260
N	4.2678552806	1.3552405937	-0.0837541338
C	3.0389744209	1.0520862951	0.4967243789
N	-4.6102043772	-1.1220012379	0.4562260685
C	-3.4002950506	-0.6234389550	-0.0237646309
H	0.5348063311	1.1490958284	-1.5618368123
H	4.4958028000	2.2945823598	-0.2706156469
C	-1.2992285177	0.9526686822	-0.7471415311
O	2.2614496173	1.9749529231	0.7650420391
N	-0.2161950187	1.6267043699	-1.1409718650
C	-5.2283013430	-0.0568004804	0.9064798715
C	-3.3307079381	0.7379671201	0.1561134735
H	-6.1673333966	-0.0905498206	1.3332160714
N	-2.3218617243	1.5855744895	-0.1767815012
H	-0.1685463877	2.6013599459	-1.0105250710
N	-4.5127776475	1.1117460460	0.7593103873

H	-4.7868041937	2.0185693705	1.0273050886
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G-T cross (w3DNA) VIE (ω B97x-D) = 7.74

N	4.8356703603	0.6727606447	-0.7347261377
C	4.4430303934	1.9916447115	-0.6761371056
N	3.2487315567	2.1714393285	-0.1640226807
C	2.8202854778	0.8795870443	0.1367390742
C	1.6036934206	0.4314991035	0.7126383394
O	0.6374431216	1.0937750648	1.0826274080
N	1.5812794884	-0.9645486676	0.8426892383
C	2.6021718548	-1.8150253388	0.4655073087
N	2.3879712139	-3.1165903915	0.6728102254
N	3.7439040646	-1.3939581677	-0.0744074980
C	3.7811260040	-0.0418554599	-0.2077071402
N	-4.4416539850	-1.1823378221	0.0291793992
C	-3.2827732103	-1.4886007645	-0.6429391619
O	-3.0185978485	-2.6134004974	-1.0303794013
N	-2.4229300780	-0.4286707560	-0.8553683613
C	-2.6212833741	0.8785520423	-0.4617409667
O	-1.7776651085	1.7430221722	-0.7091871556
C	-3.8654751201	1.1015216792	0.2365551310
C	-4.1606084458	2.4976173030	0.7007817234
C	-4.7202039334	0.0896334373	0.4574597298
H	5.6865328712	0.3167954794	-1.0787083884
H	5.0360250631	2.7694321403	-1.0054485650
H	0.7737801779	-1.3702636822	1.2338301216
H	1.5403007770	-3.4185350552	1.0731703763
H	3.0774186093	-3.7747657501	0.4256068955

H	-5.0923227275	-1.8989301879	0.2091226371
H	-1.5865525430	-0.6254713638	-1.3350923858
H	-5.1079022835	2.5149049128	1.1981312218
H	-4.1886212797	3.1550270793	-0.1422299415
H	-3.3957639672	2.8177362432	1.3777128777
H	-5.6029227619	0.2727945422	0.9593974544

VIEs of NAB dimers (structures taken from earlier work)

We have compared the VIEs of alternative structures that have been used in earlier work and we find similar trends in the Δ VIEs.

Table 2: Δ VIE (defined by eq 1) of G-NAB stacking and H-bonding interaction. Structures taken from Ref. 1.

Species	
G-G	-0.25
G-A	-0.24
G-C	-0.31
G-T	-0.14
G-C (hb)	-0.55

$$\Delta\text{VIE} = \text{VIE}(\text{dimer}) - \text{VIE}(\text{guanine}), \quad (1)$$

Dipoles of GT and GC stacked dimers

Table 3: The dipoles $\vec{\mu}$ on each of the NABs for GT and GC stacked dimers in their ground (g.s.) and ionized states (i.s.).

	GT				GC			
	g.s.		i.s.		g.s.		i.s.	
	G	T	G	T	G	C	G	C
μ_x	1.61	0.64	0.73	0.36	1.73	-0.70	0.84	-0.30
μ_y	-0.147	1.03	0.156	0.546	-0.21	1.760	0.077	0.897
μ_z	0.22	-0.077	0.089	-0.049	0.239	-0.262	0.107	-0.129

Geometry of tetramers

GCGC VIE(ω B97x-D) = 6.79 eV

N	4.4475083877	-0.5364003878	2.0006329827
C	4.3323202761	0.6289416727	2.7257285494
N	3.0970321778	1.0430448801	2.8790871092
C	2.3411968128	0.0840288641	2.2068466893
C	0.9374460837	-0.0094822942	2.0244225846
O	0.0570524024	0.7474488924	2.4257991467
N	0.5918022937	-1.1443047099	1.2767104373
C	1.4868862249	-2.0674728746	0.7723461882
N	0.9576767369	-3.0825325221	0.0849458466
N	2.8041039730	-1.9795408409	0.9442861824
C	3.1556848960	-0.8836866655	1.6673563594
N	4.3784342007	-0.4607589452	-2.3826494778
C	5.0840018514	0.5264800641	-1.7294516297
N	4.3289229892	1.4136657430	-1.1276356420
C	3.0317360475	0.9840074997	-1.4024734712

C	1.7840107834	1.5410792241	-1.0169935638
O	1.5636706827	2.5429684353	-0.3435915676
N	0.7117022159	0.7857436787	-1.5125846755
C	0.8287472464	-0.3575789353	-2.2793179154
N	-0.3162784868	-0.9334129032	-2.6531083807
N	1.9993270809	-0.8789430999	-2.6392918851
C	3.0506129194	-0.1584154112	-2.1674169700
N	-4.2320429790	1.6401372595	-1.1650835148
C	-2.9515668190	1.2218203928	-1.5163367034
O	-2.8226387738	0.3987121832	-2.4308925707
N	-1.8895820310	1.7324113894	-0.8415403310
C	-2.0712784839	2.6220334342	0.1428467964
N	-1.0048355799	3.0913377459	0.7711508592
C	-3.3806437725	3.0655033798	0.5205714956
C	-4.4286068756	2.5424205361	-0.1661137839
N	-3.9220342614	-2.6552237604	-0.3439956364
C	-2.5640962983	-2.4261972834	-0.1377012804
O	-1.7429536585	-3.0520176419	-0.8176245438
N	-2.1907054786	-1.5221771658	0.8047476162
C	-3.1118162006	-0.8638569105	1.5210321122
N	-2.6984710653	0.0073244658	2.4276024673
C	-4.5138400053	-1.0859917440	1.3242216277
C	-4.8651437284	-1.9932618338	0.3785172984
H	5.2744674150	-1.0180555434	1.7700921444
H	5.1456553196	1.1314544333	3.1143273561
H	-0.3646734337	-1.2946002008	1.0972210269
H	-0.0180238525	-3.1392978939	-0.0366685131

H	1.5427006513	-3.7745594307	-0.3003952717
H	4.7436275074	-1.2190990315	-2.8929828613
H	6.1154210741	0.5642640615	-1.7146274443
H	-0.1981186414	1.0948418590	-1.2972098333
H	-1.1765067605	-0.5389994867	-2.3814939960
H	-0.3005833179	-1.7511744953	-3.2003895151
H	-5.0093463921	1.2760827028	-1.6483398483
H	-0.1059306764	2.7859870189	0.5105344593
H	-1.1105216553	3.7458904301	1.4986804031
H	-3.5203046673	3.7506928540	1.2800556751
H	-5.3896007485	2.8334372759	0.0736820326
H	-4.2042758622	-3.3082524679	-1.0248797572
H	-1.7351709331	0.1590807914	2.5616243788
H	-3.3540298727	0.5041612074	2.9679004429
H	-5.2234763606	-0.5795744455	1.8766370175
H	-5.8641809779	-2.1839970712	0.2052843823

GCAT VIE(ω B97x-D) = 6.95 eV

N	-4.5267161521	-2.1597697418	0.7223781357
C	-4.4245666368	-2.8625012138	-0.4431157316
N	-3.2126492056	-2.9574020187	-0.8951931335
C	-2.4528863746	-2.2667596406	0.0391320486
C	-1.0763364508	-2.0016749739	0.1318597519
N	-0.1793568123	-2.4228477793	-0.7710721371
N	-0.6535710355	-1.2848003956	1.1897511653
C	-1.5498552042	-0.8694430137	2.0839826421
N	-2.8512208281	-1.0543376945	2.1026231893
C	-3.2489149723	-1.7739096673	1.0333671191

N	-4.6717164157	2.2222426958	0.6978848644
C	-5.3685551303	1.5462499854	-0.2801660859
N	-4.6069509503	0.9915802206	-1.1921559570
C	-3.3145572322	1.3245414808	-0.7900474187
C	-2.0635010110	1.0063275804	-1.3810975393
O	-1.8351662117	0.3553811049	-2.3959541328
N	-0.9984496020	1.5452811482	-0.6454464344
C	-1.1247311483	2.2929325793	0.5094718781
N	0.0144768071	2.7157280152	1.0624974234
N	-2.2983856969	2.5898153511	1.0626939135
C	-3.3427496864	2.0751932390	0.3616261997
N	3.9341676903	1.4481247673	-1.6207460217
C	2.6487033662	1.7320691055	-1.1680385178
O	2.4956439118	2.6302624031	-0.3311612247
N	1.6085633041	1.0119747506	-1.6614326516
C	1.8160820174	0.0473286200	-2.5668898988
N	0.7702405342	-0.6269971582	-3.0183468035
C	3.1310648854	-0.2613747124	-3.0457440616
C	4.1569310675	0.4697754706	-2.5393874815
N	3.7684185870	0.5662681560	2.6705560129
C	2.4311640686	0.3120081246	2.4853475096
O	1.5532756682	0.8976919042	3.0952560820
N	2.1358633256	-0.6631868187	1.5519203331
C	3.0463271058	-1.3851133317	0.8081059646
O	2.6623686000	-2.2348806969	0.0004115354
C	4.4247519269	-1.0476025646	1.0725629453
C	5.4807685490	-1.7874569956	0.3051274009

C	4.7400398428	-0.1040379692	1.9750541554
H	-5.2378378789	-3.2808183978	-0.9214739868
H	-0.4741433239	-2.9477219626	-1.5496156518
H	0.7743227280	-2.2067601109	-0.6549151144
H	-1.1679607338	-0.3256940987	2.8742286361
H	-5.0427005895	2.7059211622	1.4707444143
H	-6.3986605324	1.4816536265	-0.2937001538
H	-0.0870273814	1.3778179795	-0.9785644660
H	0.8770340079	2.4906091043	0.6445912721
H	-0.0078700399	3.2526730295	1.8869291489
H	4.6957634989	1.9646545945	-1.2694032233
H	-0.1325621098	-0.4137766812	-2.6886887773
H	0.8951241538	-1.3413607340	-3.6839268236
H	3.2906777986	-1.0056664306	-3.7431388968
H	5.1210712865	0.2802158271	-2.8559357079
H	4.0370929084	1.2514621980	3.3238769400
H	1.1832968065	-0.8617679267	1.4030023347
H	6.4478070088	-1.4371744099	0.6003438087
H	5.3451076090	-1.6180117744	-0.7422648019
H	5.4025145849	-2.8350805640	0.5100546464
H	5.7324914037	0.1199825411	2.1482006546
H	-5.3465856974	-1.9698217978	1.2329490977

GCCG VIE(ω B97x-D) = 7.00 eV

N	-4.2712254031	-2.0688742689	-0.7296875771
C	-4.2225649564	-1.8694047972	-2.0916340118
N	-3.0128274001	-1.6752048264	-2.5604179876
C	-2.2036033078	-1.7505821423	-1.4279955272

C	-0.7967736504	-1.6200505783	-1.3002034076
O	0.0391195391	-1.4078867264	-2.1750805851
N	-0.3870763501	-1.7657832590	0.0329414112
C	-1.2281724601	-2.0066804897	1.1017369285
N	-0.6420213125	-2.1147869267	2.2965874758
N	-2.5482900059	-2.1296284716	0.9811904266
C	-2.9616963585	-1.9903397065	-0.3060662795
N	-4.2057536870	1.3341602234	2.0341372543
C	-2.8372503732	1.3940220913	1.7853276141
O	-2.0522863160	1.3068929372	2.7370560099
N	-2.4130652044	1.5465143494	0.5040801541
C	-3.2945713951	1.6370423399	-0.4997353263
N	-2.8319371773	1.7847376720	-1.7319352571
C	-4.7072176738	1.5783313986	-0.2651409601
C	-5.1100794783	1.4261869104	1.0219539941
N	4.2712302043	2.0687749618	-0.7294897635
C	4.2224695608	1.8691079979	-2.0919230658
N	3.0135238578	1.6749314963	-2.5607874101
C	2.2043947378	1.7504742873	-1.4283222434
C	0.7966594749	1.6198599736	-1.3009043063
O	-0.0388945188	1.4076140236	-2.1745032877
N	0.3869405791	1.7657727099	0.0324601974
C	1.2284308885	2.0068598289	1.1014228068
N	0.6417445045	2.1150705512	2.2963782564
N	2.5479897744	2.1297295040	0.9810010914
C	2.9618016469	1.9903095068	-0.3055970582
N	4.2056093529	-1.3338978360	2.0341905247

C	2.8368148522	-1.3938259609	1.7855618161
O	2.0526792786	-1.3064748952	2.7372567217
N	2.4124923916	-1.5465087378	0.5043430919
C	3.2945814209	-1.6371096299	-0.4999499045
N	2.8322414960	-1.7849409508	-1.7312373180
C	4.7069972636	-1.5783920349	-0.2646145453
C	5.1094535481	-1.4261163145	1.0221453562
H	-5.0694413207	-2.2326223718	-0.1773833967
H	-5.0632077100	-1.8729254388	-2.6902569030
H	0.5764263959	-1.6903413324	0.2216792563
H	0.3353507375	-2.0227262026	2.3757878480
H	-1.1867122798	-2.2866833886	3.0987130000
H	-4.5243427358	1.2235116217	2.9587847032
H	-3.4588195866	1.8541593954	-2.4881396403
H	-1.8618655367	1.8256690337	-1.8913925735
H	-5.3864434505	1.6479963620	-1.0392928426
H	-6.1186044833	1.3799980563	1.2360985809
H	5.0702244200	2.2326847456	-0.1775007907
H	5.0632025267	1.8725566819	-2.6908898316
H	-0.5762312436	1.6903932368	0.2213066297
H	1.1865835033	2.2870931812	3.0988374019
H	-0.3353813195	2.0230478707	2.3749781945
H	4.5246217720	-1.2230758294	2.9592092052
H	1.8618507389	-1.8249233962	-1.8914939326
H	3.4584145146	-1.8545446420	-2.4872721564
H	5.3866139378	-1.6491257394	-1.0381279060
H	6.1177454757	-1.3799239768	1.2358710134

GCTA VIE(ω B97x-D) = 7.02 eV

N	-4.3789684129	0.6175565651	-1.5752553861
C	-3.1004492775	0.1711395175	-1.8061246995
O	-2.8564647511	-0.8823785957	-2.3685063635
N	-2.0913899736	1.0005555925	-1.3551676108
C	-2.2538541318	2.2088496293	-0.7094022369
O	-1.2724779322	2.8651419038	-0.3515192877
C	-3.6314891018	2.5925968638	-0.5125115328
C	-3.8972455606	3.8950943708	0.1834674531
C	-4.6319086283	1.8050266183	-0.9404190921
N	-3.7752597805	-3.0996929456	0.6700174175
C	-4.6213159592	-2.1516497238	1.2034375073
N	-4.0081389583	-1.0915017424	1.6719726960
C	-2.6608272694	-1.3566776499	1.4326633753
C	-1.5108385377	-0.5756284431	1.7211595688
O	-1.4436863559	0.5272642584	2.2549388054
N	-0.3368555937	-1.2224710704	1.3096420569
C	-0.2806385785	-2.4606583213	0.6993159319
N	0.9381430862	-2.9042369610	0.3827764486
N	-1.3598167703	-3.1913572040	0.4289225646
C	-2.5077007480	-2.5790717845	0.8219835508
N	4.4568843543	0.1924956902	1.8657790700
C	3.2608377795	-0.4954097933	1.6807233033
O	3.3017938750	-1.7044576976	1.4217488580
N	2.0915829214	0.1862056189	1.7907619625
C	2.0897478651	1.4954161742	2.0725834563
N	0.9246124802	2.1161377380	2.1699347530

C	3.3094258481	2.2225114366	2.2662251289
C	4.4671118632	1.5225589952	2.1512961498
N	4.3401076901	-1.2621545034	-2.2683197465
C	4.9951323502	-0.0898120336	-2.0250137083
N	4.2091391912	0.9032237814	-1.7453377814
C	2.9374306763	0.3499318500	-1.8071074482
C	1.6571149433	0.8926082318	-1.6069775691
N	1.4392800812	2.1765148116	-1.2885802274
N	0.6048471595	0.0650437726	-1.7471331153
C	0.8278673082	-1.2100418155	-2.0632276523
N	1.9701585030	-1.8257649863	-2.2733271599
C	3.0072402344	-0.9758047607	-2.1274433107
H	-5.1373714497	0.0667098749	-1.8750849340
H	-1.1668421338	0.7002176420	-1.5100947142
H	-2.9678183726	4.3597005645	0.4376645951
H	-4.4618206962	3.7150665113	1.0743411176
H	-4.4524990193	4.5399742481	-0.4658849477
H	-5.6092269497	2.0994833836	-0.7878769274
H	-4.0224515102	-3.9629417730	0.2668007131
H	-5.6468617136	-2.2654317652	1.2314116525
H	0.5163870885	-0.7572152727	1.4684374217
H	1.7295648925	-2.3556308154	0.5877443033
H	1.0455579818	-3.7793134468	-0.0544879840
H	5.3107336274	-0.2924944950	1.7883262521
H	0.0875011281	1.6154119871	2.0368621917
H	0.8951401864	3.0782619275	2.3757415262
H	3.3075719789	3.2319513508	2.4826359023

H	5.3692338216	2.0070791632	2.2821326089
H	4.7410277181	-2.1315753912	-2.4970542017
H	6.0228285312	-0.0012883148	-2.0600866427
H	2.1990904890	2.7930159633	-1.1830507336
H	0.5188707343	2.5022730284	-1.1604427291
H	-0.0160633150	-1.7975685932	-2.1559012126

Geometry of hexamers

TAGCTA VIE(ω B97x-D) = 6.82 eV

N	1.3547975307	5.1081044569	-1.0849742535
C	0.5205656585	4.4962778720	-0.1811349905
O	0.6737069740	4.5789152622	1.0252732319
N	-0.5187996001	3.7695694772	-0.7298687769
C	-0.7842309008	3.6101728572	-2.0743095313
O	-1.7466582812	2.9345368359	-2.4473356753
C	0.1461238796	4.2893050364	-2.9444390997
C	-0.0704973483	4.1670100827	-4.4241796810
C	1.1656027586	5.0021601514	-2.4377721476
N	3.6673489470	2.1260588307	1.1473267634
C	4.0205456110	2.3712783498	-0.1619682774
N	3.1711472329	1.8984458903	-1.0419551299
C	2.1863931945	1.2969000955	-0.2601379258
C	1.0036179549	0.6135292867	-0.6471638552
O	0.5752688925	0.3954687981	-1.7762204101
N	0.2869478790	0.1591966805	0.4690591894

C	0.6627172283	0.3411696442	1.7860440931
N	-0.1590467292	-0.1682902835	2.7066648512
N	1.7716112407	0.9826989673	2.1472271446
C	2.4794128876	1.4298815110	1.0766793402
N	4.5406932185	-1.7441889088	3.0139984588
C	3.4512521562	-2.2288453170	2.3316823021
O	2.5025389682	-2.7564166292	2.8851602125
N	3.4968393222	-2.0801143839	0.9584157876
C	4.5164250120	-1.5008019787	0.2308058933
O	4.4448112998	-1.4243625890	-0.9970925129
C	5.6161439901	-1.0225080346	1.0355878963
C	6.7681842613	-0.3784190555	0.3218984677
C	5.5983929962	-1.1543271439	2.3718931102
N	-1.8142144640	-4.6805353088	-2.5555641063
C	-1.5763512066	-4.0666386124	-3.7509409996
N	-0.5318691018	-3.2976373056	-3.7477593441
C	-0.0394510099	-3.4091903175	-2.4545562091
C	1.0663935752	-2.8314641066	-1.8086946304
N	1.9150858017	-1.9859669485	-2.4097221343
N	1.2686092620	-3.1548452733	-0.5182112183
C	0.4214819643	-3.9963834982	0.0737125586
N	-0.6380617411	-4.5940208265	-0.4246675774
C	-0.8188736601	-4.2536676477	-1.7168331100
N	-3.9234993985	-2.5839219922	0.6660253563
C	-2.7154690607	-1.9378626671	0.9135269753
O	-2.2123727354	-2.0245680295	2.0404334788
N	-2.1328259770	-1.2349098377	-0.0915846387

C	-2.7097111255	-1.1653298292	-1.2981587755
N	-2.1031754993	-0.4681528030	-2.2459835105
C	-3.9531328777	-1.8223443601	-1.5738637855
C	-4.5191485654	-2.5191876135	-0.5553282085
N	-4.6140279539	0.4876191656	3.7171271622
C	-5.6379546644	0.1991272934	2.8621484892
N	-5.4488134023	0.6265732955	1.6523387941
C	-4.2070596154	1.2448245733	1.7071374254
C	-3.4331283196	1.9042088130	0.7376010548
N	-3.8174141479	2.0563376586	-0.5377131090
N	-2.2458447888	2.4040388222	1.1278596604
C	-1.8692844795	2.2492182349	2.3966109832
N	-2.5028764285	1.6566328056	3.3842798301
C	-3.6880595823	1.1655250648	2.9678580740
H	2.1126848528	5.6391320220	-0.7501287188
H	-1.1293223456	3.3225129045	-0.1002685879
H	-0.9316274259	3.5600471749	-4.6095469325
H	0.7884577259	3.7151247981	-4.8745205186
H	-0.2226668115	5.1397532497	-4.8442394215
H	1.8188069762	5.4785894750	-3.0792270173
H	4.1574272722	2.3911093458	1.9587806805
H	4.8774261192	2.8822375963	-0.4268256789
H	-0.5515726920	-0.3290705842	0.3011892094
H	-0.9764265700	-0.6412642041	2.4282499340
H	0.0523731250	-0.0718129961	3.6629549632
H	4.5626530599	-1.8231677019	3.9946620686
H	2.7265486296	-2.4202818429	0.4492671366

H	6.5791063018	-0.3763189909	-0.7311405226
H	7.6640882513	-0.9275280732	0.5223812031
H	6.8830230885	0.6288919644	0.6655589877
H	6.3962074926	-0.8053997224	2.9255018925
H	-2.5477094997	-5.3006636981	-2.3405877977
H	-2.1729900081	-4.2020034053	-4.5818751205
H	1.7792891491	-1.7404011085	-3.3536578776
H	2.6739982650	-1.6107483281	-1.9074982203
H	0.6261730264	-4.2082732122	1.0629194723
H	-4.3545530203	-3.0967115821	1.3881836572
H	-1.2489474690	-0.0174651701	-2.0552870766
H	-2.5060218224	-0.4006324976	-3.1415636846
H	-4.3979197763	-1.7677449096	-2.5039119105
H	-5.4156464825	-3.0071875858	-0.7097610796
H	-4.5531755618	0.2570034614	4.6721467344
H	-6.4859473882	-0.3129865478	3.1517581472
H	-4.6829891983	1.6962161637	-0.8370696542
H	-3.2333082228	2.5285085353	-1.1745536946
H	-0.9494826717	2.6513889253	2.6378958149

ATGCAT VIE(ω B97x-D) = 6.63 eV

N	-1.8513428582	4.5862103714	2.8064515225
C	-1.5712013333	3.9256430011	3.9674052147
N	-0.5234098433	3.1643153976	3.8993076848
C	-0.0736095333	3.3313474227	2.5966296802
C	1.0136982770	2.7876087186	1.8924507630
N	1.8862401381	1.9237971444	2.4307306761
N	1.1719540003	3.1646754023	0.6100507310

C	0.3017141521	4.0238413890	0.0808877940
N	-0.7443912250	4.5940240086	0.6364427601
C	-0.8808678191	4.1999108132	1.9191359926
N	-4.0528591405	2.6081768196	-0.4284159132
C	-4.4599690573	2.3761929377	0.8675698098
N	-3.6435538830	1.6151941173	1.5558808285
C	-2.6242838744	1.3218585975	0.6515142423
C	-1.4535892056	0.5360386748	0.8179565489
O	-1.0695416057	-0.0716036790	1.8124816672
N	-0.6897029977	0.5010865819	-0.3573069163
C	-1.0134282635	1.1411787917	-1.5380905185
N	-0.1520357356	0.9844819948	-2.5459779263
N	-2.1110688166	1.8781117577	-1.6922787789
C	-2.8642120976	1.9224981183	-0.5618660006
N	-4.8252675653	-0.3417053577	-3.5792239628
C	-5.8227222815	-0.0947970733	-2.6801114069
N	-5.5922679506	-0.5695970377	-1.4958627864
C	-4.3495278700	-1.1770732410	-1.6157366972
C	-3.5412452381	-1.8700385874	-0.6994140380
N	-3.8829585608	-2.0764712937	0.5804650746
N	-2.3651591818	-2.3455705963	-1.1472040519
C	-2.0302982299	-2.1372685063	-2.4199033024
N	-2.6987243701	-1.5090548371	-3.3626339536
C	-3.8720295653	-1.0434630502	-2.8875958427
N	1.3197068049	-5.1135443095	0.8361867778
C	0.4534762558	-4.4711886105	-0.0141836072
O	0.5685953751	-4.5041943671	-1.2277808255

N	-0.5712218828	-3.7741563759	0.5963250239
C	-0.7937388308	-3.6713730322	1.9548594519
O	-1.7467127536	-3.0178009720	2.3848248746
C	0.1681521661	-4.3791523918	2.7655080121
C	-0.0014743696	-4.3182236610	4.2557534711
C	1.1739295289	-5.0638402225	2.1976563844
N	3.5430350257	-2.0283177402	-1.3459446660
C	2.3417429686	-1.3266406583	-1.3962802022
O	1.8849086253	-1.0041122173	-2.4998289268
N	1.7146179647	-1.0209283389	-0.2313256076
C	2.2420903832	-1.3883140678	0.9435188817
N	1.5934321047	-1.0674987700	2.0519560619
C	3.4776826318	-2.1105215455	1.0177290845
C	4.0886936175	-2.4056267385	-0.1582630500
N	4.3355826086	1.9196247331	-3.0797369133
C	3.2662409058	2.3691276212	-2.3437644436
O	2.2970508171	2.9127003899	-2.8446648501
N	3.3564654788	2.1655596031	-0.9799779543
C	4.4022742257	1.5640296980	-0.3107785533
O	4.3710562411	1.4370106402	0.9159205118
C	5.4777909204	1.1257835151	-1.1681641857
C	6.6562470895	0.4607127366	-0.5197546568
C	5.4162163135	1.3115300798	-2.4970425779
H	-2.5948183698	5.2097530967	2.6409594280
H	-2.1411922211	4.0231261869	4.8222931701
H	1.7827597680	1.6391542905	3.3671025353
H	2.6304880955	1.5743521698	1.8888135351

H	0.4737135380	4.2778491674	-0.9049576603
H	-4.5116524994	3.1476678872	-1.1120415723
H	-5.3301095327	2.7670494122	1.2619804709
H	0.1445575203	-0.0218065155	-0.3401547524
H	0.6565601552	0.4368722952	-2.4209767175
H	-0.3254839796	1.4154248520	-3.4135613289
H	-4.7964697777	-0.0721159853	-4.5261269450
H	-6.6818292595	0.4227127280	-2.9211110045
H	-4.7404022588	-1.7344190916	0.9221222065
H	-3.2759567082	-2.5702812164	1.1783208358
H	-1.1174647120	-2.5228212688	-2.7065634425
H	2.0690241927	-5.6255000089	0.4557675168
H	-1.2038419276	-3.3048682178	0.0050564693
H	-0.8597765983	-3.7245292690	4.4927708822
H	0.8689806055	-3.8790848437	4.6958400939
H	-0.1352189244	-5.3078752778	4.6402415352
H	1.8501024018	-5.5615204692	2.7973534896
H	4.0060882988	-2.2552950018	-2.1851919413
H	0.7446390955	-0.5715230494	1.9995298066
H	1.9595194237	-1.3251411557	2.9286022139
H	3.8843749611	-2.3928065113	1.9236664705
H	4.9814216056	-2.9239795648	-0.1512568647
H	4.3252866653	2.0384963029	-4.0566036102
H	2.6009395313	2.4799765496	-0.4328796757
H	6.5021453113	0.4141853043	0.5377886473
H	7.5423497098	1.0234540098	-0.7270115163
H	6.7649492212	-0.5307793743	-0.9082932526

H	6.1974610729	0.9906969120	-3.0902100960
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GCGCGC VIE(ω B97x-D) = 6.44 eV

N	-1.4618015974	4.8795519903	2.4312027963
C	-1.1714224810	4.3398041642	3.6646557759
N	-0.1462686252	3.5212756779	3.6618828758
C	0.2707198466	3.5184858186	2.3318382033
C	1.3377007873	2.8199220052	1.7104693347
O	2.1485766762	2.0469892315	2.2146480929
N	1.4074429510	3.1044948527	0.3391490493
C	0.5568163196	3.9538060710	-0.3412205477
N	0.7893958662	4.0931869603	-1.6486637481
N	-0.4440073591	4.6095501343	0.2424828767
C	-0.5253848572	4.3438346743	1.5729373093
N	-3.8134867656	2.6228888740	-0.5014933095
C	-4.2045292334	2.5716344888	0.8189584224
N	-3.4092214601	1.8639864176	1.5845593323
C	-2.4223175282	1.4141891295	0.7090371860
C	-1.2846940043	0.6010903915	0.9548524827
O	-0.9082838671	0.1033770640	2.0114502549
N	-0.5467769923	0.3859606804	-0.2178306334
C	-0.8652158415	0.8900726630	-1.4641186452
N	-0.0319847896	0.5703345931	-2.4570343420
N	-1.9318049364	1.6528110246	-1.6927600553
C	-2.6594684590	1.8712643451	-0.5659007275
N	-4.7793771653	-0.6534929627	-3.2507457163
C	-5.7465044788	-0.2555924961	-2.3528270240
N	-5.4971293474	-0.6014278573	-1.1122586273

C	-4.2804757117	-1.2759149480	-1.1944601788
C	-3.5021086648	-1.8844732066	-0.1759418499
O	-3.7305422798	-1.9537830128	1.0290960061
N	-2.3349621564	-2.4588497651	-0.6965814537
C	-1.9669670621	-2.4469713138	-2.0284941809
N	-0.8135800264	-3.0500680363	-2.3238476797
N	-2.6977127249	-1.8751341406	-2.9837213914
C	-3.8339605207	-1.3135087143	-2.4940604608
N	1.2340069327	-5.1264241005	1.6338328455
C	0.3602759863	-4.5381783893	0.7230462532
O	0.5080193199	-4.7717514147	-0.4822539373
N	-0.6232483029	-3.7282061720	1.1925725887
C	-0.7499388514	-3.5005208674	2.5066437081
N	-1.7256103023	-2.7029049150	2.9146179872
C	0.1388984424	-4.0954097154	3.4599587262
C	1.1150456510	-4.9010285820	2.9702426156
N	3.5484749004	-2.4407795288	-0.9457136768
C	2.3788642049	-1.6953538877	-1.0654568798
O	1.9148740843	-1.4903059406	-2.1938231800
N	1.7893997336	-1.2194786974	0.0614590178
C	2.3233712508	-1.4635039920	1.2651138996
N	1.7119417727	-0.9786171208	2.3343901574
C	3.5268041443	-2.2279398746	1.4105994730
C	4.1004255819	-2.6939084743	0.2716478891
N	4.4812623044	1.2220884296	-3.1669122224
C	3.4415869965	1.8123675545	-2.4530132037
O	2.5045287490	2.3241065538	-3.0761239785

N	3.4951835465	1.8044709138	-1.0958293353
C	4.5284663228	1.2390729029	-0.4574362014
N	4.5353512340	1.2564204907	0.8659430561
C	5.6082752307	0.6272716174	-1.1739980687
C	5.5353543324	0.6465443944	-2.5287013951
H	-2.1828323454	5.5121372545	2.2099505784
H	-1.7120868481	4.5601901139	4.5156282051
H	2.1191730449	2.6638404188	-0.1794210454
H	1.5324364438	3.6042480044	-2.0715507275
H	0.2182311813	4.6848696157	-2.1902581887
H	-4.2613722874	3.0948461990	-1.2401006766
H	-5.0483349414	3.0482996913	1.1742825166
H	0.2635400250	-0.1691980472	-0.1479227038
H	0.7537538574	0.0051629632	-2.2766879883
H	-0.2033791608	0.8987026424	-3.3687883624
H	-4.7657439260	-0.4996447283	-4.2230110379
H	-6.5913205077	0.2680442226	-2.6315894033
H	-1.7285769020	-2.9070117737	-0.0631102727
H	-0.2809926097	-3.4702592963	-1.6106738239
H	-0.4958204894	-3.0754830384	-3.2552487503
H	1.9508091806	-5.7158059310	1.3047210173
H	-2.3350199181	-2.2954182379	2.2578794333
H	-1.8408742173	-2.5183554794	3.8745454510
H	0.0415374429	-3.9190497796	4.4727484421
H	1.7773962363	-5.3490638844	3.6218760018
H	3.9840834849	-2.7908111926	-1.7568832001
H	0.8852052441	-0.4538095825	2.2330305989

H	2.0836460819	-1.1430705036	3.2308827627
H	3.9385530926	-2.4151066156	2.3386282520
H	4.9691396897	-3.2485457768	0.3300881279
H	4.4527548946	1.2217169775	-4.1512379762
H	3.7929300729	1.6768087340	1.3568845441
H	5.2825538913	0.8486438011	1.3598381465
H	6.4047783114	0.1925191774	-0.6822886441
H	6.2923392665	0.2177454476	-3.0832915797

CGGCCG VIE(ω B97x-D) = 6.74 eV

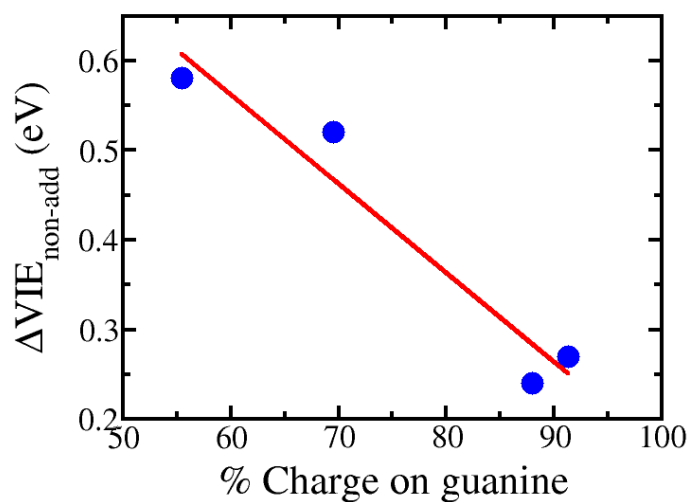
N	1.2365492262	5.0912083644	-1.8888485703
C	0.4033942030	4.5373044500	-0.9203191898
O	0.5983518043	4.8196211403	0.2673300935
N	-0.5946214959	3.7055128557	-1.3165141019
C	-0.7733607881	3.4245022460	-2.6141963830
N	-1.7596999092	2.6086398791	-2.9506257762
C	0.0737166603	3.9837884005	-3.6258325793
C	1.0645393224	4.8115165293	-3.2086436569
N	3.6663108429	2.5191663501	0.7004595154
C	4.0213582917	2.6210956133	-0.6272022391
N	3.2053621271	2.0038607887	-1.4473220051
C	2.2424535626	1.4536399919	-0.6029878465
C	1.0983440895	0.6709537384	-0.9098391822
O	0.6932541282	0.2968883442	-2.0060960883
N	0.3924629490	0.3204033693	0.2498307080
C	0.7447528914	0.6788630373	1.5367512428
N	-0.0613160256	0.2447849837	2.5084596067
N	1.8173735367	1.4132948870	1.8226774734

C	2.5142495494	1.7618520759	0.7091696337
N	4.7055164888	-1.0486829312	3.0278000860
C	3.6406730048	-1.6707414587	2.3798451932
O	2.7324840374	-2.1598115165	3.0604223586
N	3.6406981238	-1.7163762471	1.0223506387
C	4.6440101686	-1.1741289710	0.3211631943
N	4.5977932514	-1.2445182692	-1.0002358156
C	5.7489063873	-0.5302712039	0.9678644557
C	5.7310278444	-0.4950978784	2.3244573184
N	-1.4395026972	-4.9477120272	-2.1744417685
C	-1.2020364224	-4.4572382270	-3.4394631990
N	-0.1822829156	-3.6362766603	-3.5110515468
C	0.2883157683	-3.5783469876	-2.1999905140
C	1.3766766586	-2.8512620140	-1.6514004905
O	2.1622923528	-2.0968876563	-2.2178793598
N	1.5027609729	-3.0804305119	-0.2735450753
C	0.6845160140	-3.9045350469	0.4748404555
N	0.9704126687	-3.9903415089	1.7762018019
N	-0.3363159723	-4.5869522470	-0.0414906601
C	-0.4721772806	-4.3749822282	-1.3766773197
N	-3.6823386926	-2.5828489866	0.7582393421
C	-2.5096948042	-1.8528094254	0.9312582717
O	-2.0151935074	-1.7774683701	2.0627768057
N	-1.9508944623	-1.2489218208	-0.1489856540
C	-2.5174058661	-1.3545286454	-1.3578574537
N	-1.9350817145	-0.7482503240	-2.3804219648
C	-3.7245635901	-2.1005901913	-1.5577108975

C	-4.2671972456	-2.6959750130	-0.4648043919
N	-4.5534475094	0.7978543311	3.4101125493
C	-5.5531457319	0.3615248476	2.5691166838
N	-5.3563392714	0.6575592628	1.3063546943
C	-4.1404352928	1.3390629806	1.3123711194
C	-3.4070888907	1.9085248279	0.2397783453
O	-3.6840994579	1.9286566040	-0.9568840370
N	-2.2219223466	2.5078591974	0.6898267606
C	-1.8015143189	2.5500651243	2.0048452966
N	-0.6397322794	3.1686742142	2.2295969074
N	-2.4898379745	2.0150264465	3.0109775734
C	-3.6425245260	1.4300367189	2.5909338466
H	1.9632377040	5.6958544739	-1.6131006087
H	-1.9128070959	2.3851133281	-3.8967336297
H	-2.3398176072	2.2248463876	-2.2540146851
H	-0.0633252196	3.7666127155	-4.6254621332
H	1.6977761565	5.2351539537	-3.9043500926
H	4.1342123940	2.9043899228	1.4760605324
H	4.8553469198	3.1378237152	-0.9480262359
H	-0.4196124210	-0.2253388298	0.1384707263
H	-0.8518221877	-0.2981433981	2.2856193501
H	0.1348540405	0.4666908220	3.4469542013
H	4.7165484912	-1.0089302237	4.0116943980
H	5.3230015553	-0.8540946730	-1.5390598421
H	3.8388047663	-1.6876538266	-1.4434145124
H	6.5223403790	-0.1132912041	0.4270303406
H	6.5071829218	-0.0409210258	2.8308609937

H	-2.1481518706	-5.5734864591	-1.8990371401
H	-1.7753587131	-4.7134098352	-4.2582621109
H	2.2323619714	-2.6170690092	0.1974416558
H	0.4245579826	-4.5615932152	2.3634352732
H	1.7272080253	-3.4824546434	2.1481382480
H	-4.0958728052	-3.0250081314	1.5352578929
H	-1.1057480300	-0.2362257687	-2.2417623296
H	-2.3310266194	-0.8096493982	-3.2795136098
H	-4.1614007840	-2.1810416790	-2.4896480328
H	-5.1373368179	-3.2426825208	-0.5631406799
H	-4.5005099115	0.6828274074	4.3863135622
H	-6.3831381315	-0.1530920588	2.9027692820
H	-1.6439978416	2.9320604781	0.0147656225
H	-0.2848640493	3.2325423505	3.1459109368
H	-0.1374444618	3.5611084619	1.4787931318

Figure 3: Correlation between the charge on guanine in the cationic state and the non-additivity in the ΔVIE s of the hexamers.



References

- (1) Petr Jurečka and Jiří Šponer and Jiří Černýa and Pavel Hobza, Benchmark database of accurate (MP2 and CCSD(T) complete basis set limit) interaction energies of small model complexes, DNA base pairs, and amino acid pairs, *Phys. Chem. Chem. Phys.*, 2006, 8, 1985-1993,