Supporting Information for Computational approach for studying optical properties of DNA systems in solution

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Abstract

This "Supporting Information" contains additional tables and figures documenting the conclusions of the main paper.

Table S1: Averaged atomic charges and polarizabilities of the Adenine nucleotide.

Atom label	Cap. lvl. 4		Cap. lvl. 3		Cap. lvl. 2	
	q_i	α_i	q_i	α_i	q_i	α_i
O5'	-0.4726	6.0892	-0.4429	6.0330	-0.4339	5.9181
H5'	0.0537	2.5364	0.0407	2.4818	0.1061	2.4589
N9	-0.1901	7.8613	-0.2529	8.0975	-0.1589	8.1859
N7	-0.6237	8.1014	-0.6312	8.1695	-0.6721	8.2245
C5'	-0.0528	7.8193	0.0429	7.7701	-0.1570	7.5490
C5	0.0087	10.0780	-0.0025	10.1420	-0.0040	10.1670
H62	0.3541	2.1635	0.3563	2.1735	0.3759	2.1774
N1	-0.8174	8.1139	-0.8278	8.1341	-0.8466	8.1534
H2'	-0.0005	2.0883	0.0299	2.0503	0.0603	2.1572
C2'	-0.0367	7.0240	-0.1516	7.0282	-0.2427	7.1136
H5"	0.0537	2.5364	0.0407	2.4817	0.1061	2.4589
H8	0.1363	2.2571	0.1284	2.2816	0.1215	2.2668
O4'	-0.58145	5.7000	-0.5203	5.6667	-0.4292	5.8589
H2	0.0103	2.8518	0.0094	2.8728	0.0230	2.8829
C4	0.4606	9.1062	0.5057	9.1686	0.4910	9.2245
C8	0.2845	8.0294	0.3150	8.0599	0.3501	8.0433
H2"	-0.0005	2.0883	0.0299	2.0503	0.0603	2.1572
H3'	0.0802	2.1805	0.0539	2.1966	0.0264	2.2307
C4'	0.4622	7.7753	0.2704	7.6513	0.1953	7.7288
H61	0.3541	2.1635	0.3563	2.1735	0.3759	2.1774
P	1.3731	12.458	1.3750	12.346	1.3532	12.2043
C2	0.5946	8.8554	0.6057	8.9135	0.5972	8.9336
O3'	-0.5769	6.6645	-0.6052	6.5199	-0.6554	6.4098
OP2	-0.8480	7.2657	-0.8505	7.2690	-0.8489	7.3112
OP1	-0.8480	7.2657	-0.8505	7.2690	-0.8489	7.3112
H1'	0.1007	1.8709	0.0766	2.1081	0.1047	2.0937
H4'	-0.0488	2.5035	-0.0006	2.5045	0.0207	2.5613
C6	0.7280	10.115	0.7335	10.153	0.7679	10.1835
C1'	0.3632	7.4210	0.4096	7.4415	0.2263	7.7457
N3	-0.7378	8.2700	-0.7671	8.3232	-0.7676	8.3473
N6	-0.8290	8.1565	-0.8371	8.1700	-0.8832	8.1882
C3'	0.2324	8.0398	0.3531	7.8869	0.5750	7.8342

Table S2: Averaged atomic charges and polarizabilities of the Thymine nucleotide.

Atom label	Cap. lvl. 4		Cap. lvl. 3		Cap. lvl. 2	
	q_i	α_i	q_i	α_i	q_i	α_i
C5	-0.0934	9.9783	-0.1013	10.0497	0.0770	10.0669
H72	0.0945	2.4266	0.0819	2.4434	0.1308	2.4331
N1	-0.1785	7.9109	-0.2594	8.1879	-0.1948	8.2600
H6	0.2595	1.9389	0.2264	1.9629	0.2301	1.9414
H2'	0.0298	2.0438	0.0733	2.0012	0.0716	2.1832
H5'	0.0312	2.5369	0.0416	2.4841	0.0752	2.4551
O2	-0.6267	6.2489	-0.6395	6.2846	-0.6282	6.2945
O5'	-0.5085	6.0389	-0.4473	5.9978	-0.4902	5.8939
H3	0.3422	2.1701	0.3466	2.1887	0.3559	2.1912
C5'	0.0555	7.6591	0.0729	7.6407	-0.0263	7.4503
C7	-0.3063	7.3155	-0.2647	7.3625	-0.4423	7.3097
H73	0.0945	2.4266	0.0819	2.4434	0.1308	2.4331
P	1.3850	12.302	1.3690	12.2237	1.3792	12.1097
H2"	0.0298	2.0438	0.0733	2.0012	0.0716	2.1832
H3'	0.0827	2.0346	0.0508	2.0477	0.0238	2.0700
C2	0.7342	8.6302	0.7614	8.7018	0.7555	8.7496
O4	-0.6324	7.1515	-0.6315	7.1970	-0.6275	7.1812
H5"	0.0312	2.5369	0.0416	2.4841	0.0752	2.4551
C2'	-0.0532	6.9189	-0.2660	6.8864	-0.2471	7.0284
O4'	-0.5208	5.5579	-0.4611	5.5607	-0.3737	5.7423
C4	0.7154	8.7715	0.7077	8.8386	0.6976	8.8195
OP1	-0.8477	7.2197	-0.8475	7.2245	-0.8508	7.2603
H4'	-0.0432	2.5110	0.0056	2.5297	0.0263	2.5886
H1'	0.1343	1.8770	0.1155	2.0988	0.1366	2.0975
O3'	-0.5485	6.5353	-0.5922	6.4639	-0.6621	6.3189
C4'	0.3929	7.5938	0.2102	7.5389	0.1296	7.6725
OP2	-0.8477	7.2197	-0.8475	7.2245	-0.8508	7.2603
C3'	0.2233	7.9129	0.3918	7.8094	0.6240	7.7560
H71	0.0945	2.4266	0.0819	2.4434	0.1308	2.4331
N3	-0.6165	7.5998	-0.6238	7.6348	-0.6471	7.6764
C6	-0.1370	8.8325	-0.0580	8.8596	-0.0518	8.8334
C1'	0.2358	7.3895	0.3098	7.4372	0.1271	7.7515

Table S3: Averaged atomic charges and polarizabilities of the Guanine nucleotide.

Atom label	Cap. lvl. 4		Cap. lvl. 3		Cap. lvl. 2	
	q_i	α_i	q_i	α_i	q_i	α_i
H5'	0.0313	2.5468	0.0352	2.4910	0.1119	2.4632
N9	-0.021	8.0741	-0.0401	8.2922	0.0631	8.3625
O5'	-0.501	6.2148	-0.4693	6.1470	-0.4447	5.9872
C5'	0.0238	7.9298	0.0480	7.8841	-0.1892	7.6352
N7	-0.593	8.3328	-0.5986	8.3917	-0.6282	8.4280
H2'	0.0136	2.0734	0.0370	2.0449	0.0786	2.1435
C5	0.1029	10.2921	0.1006	10.3451	0.1221	10.3567
N1	-0.687	7.2861	-0.6931	7.3073	-0.6849	7.3173
H8	0.1263	2.3570	0.1316	2.3711	0.1384	2.3549
C2'	-0.077	7.0578	-0.1952	7.0536	-0.3164	7.1413
H5"	0.0313	2.54685	0.0352	2.4910	0.1119	2.4632
C8	0.2201	8.3981	0.2280	8.4193	0.2322	8.4072
C4	0.1738	9.3766	0.1796	9.4273	0.1418	9.4553
O4'	-0.578	5.8086	-0.5381	5.7672	-0.4290	5.9473
P	1.4117	12.4803	1.4198	12.4008	1.4072	12.2392
H3'	0.0707	2.1405	0.0434	2.1599	0.0200	2.1947
H2"	0.0136	2.0734	0.0370	2.0449	0.0786	2.1435
C2	0.8530	9.1508	0.8573	9.1952	0.8523	9.2032
O3'	-0.603	6.6080	-0.6331	6.4992	-0.6827	6.3749
N2	-0.903	7.5690	-0.8984	7.5890	-0.9493	7.5897
H22	0.3819	2.0249	0.3780	2.0258	0.4022	2.0213
OP2	-0.853	7.2350	-0.8546	7.2432	-0.8575	7.2881
H1	0.3502	2.3048	0.3503	2.3158	0.3496	2.3105
OP1	-0.853	7.2350	-0.8546	7.2432	-0.8575	7.2881
C4'	0.4481	7.8251	0.3297	7.7506	0.2386	7.7852
H4'	-0.053	2.5470	-0.0242	2.5354	0.0081	2.5899
O6	-0.634	7.2598	-0.6385	7.2781	-0.6376	7.2813
H1'	0.0905	1.9272	0.0693	2.1260	0.0983	2.1220
C1'	0.3047	7.5147	0.3540	7.5291	0.1477	7.7962
N3	-0.644	8.4565	-0.6533	8.4837	-0.6337	8.4818
H21	0.3819	2.0249	0.3780	2.0258	0.4022	2.0213
C6	0.6666	9.8142	0.6710	9.8610	0.6656	9.8634
C3'	0.2897	8.0420	0.4070	7.9380	0.6362	7.8929

Table S4: Averaged atomic charges and polarizabilities of the Cytosine nucleotide.

Atom label	Cap. lvl. 4		Cap. lvl. 3		Cap. lvl. 2	
	q_i	α_i	q_i	α_i	q_i	α_i
H42	0.3696	2.1590	0.3896	2.1766	0.3888	2.1805
O5'	-0.5023	6.0467	-0.4147	5.9801	-0.4712	5.8900
O2	-0.6836	6.5448	-0.6935	6.5632	-0.6807	6.5810
H5'	0.0334	2.5538	0.0843	2.4931	0.1109	2.4613
H2'	0.0154	2.0537	0.0447	2.0112	0.0683	2.1777
C5'	0.0303	7.7658	-0.1003	7.7274	-0.1524	7.5205
C5	-0.7032	9.7979	-0.8024	9.8748	-0.7740	9.9096
H6	0.1723	2.0093	0.1219	2.0314	0.1321	2.0155
N1	-0.2738	8.0350	-0.3853	8.2666	-0.2546	8.3418
C2'	-0.0063	6.9629	-0.1697	6.9179	-0.2276	7.0418
H5"	0.0334	2.5538	0.0843	2.4931	0.1109	2.4613
C4	0.9351	8.9981	0.9843	9.0429	0.9533	9.0502
O4'	-0.5367	5.6450	-0.4759	5.6276	-0.3745	5.7808
H3'	0.0768	2.0632	0.0555	2.0824	0.0255	2.1039
H2"	0.0154	2.0537	0.0447	2.0112	0.0683	2.1777
C4'	0.4325	7.7257	0.2909	7.6653	0.1897	7.7353
H5	0.2088	2.5920	0.2291	2.6248	0.2178	2.6634
H41	0.3696	2.1590	0.3896	2.1766	0.3888	2.1805
C2	0.9216	9.1116	0.9637	9.1690	0.9299	9.2222
O3'	-0.5750	6.6285	-0.6134	6.5398	-0.6780	6.3996
P	1.4190	12.2855	1.4018	12.1844	1.4258	12.0668
OP2	-0.8576	7.1538	-0.8608	7.1616	-0.8663	7.2057
OP1	-0.8576	7.1538	-0.8608	7.1616	-0.8663	7.2057
H1'	0.1343	1.8716	0.1159	2.0761	0.1570	2.0753
H4'	-0.0524	2.5532	-0.0032	2.5608	0.0196	2.6035
C1'	0.1937	7.5330	0.2679	7.5536	0.0234	7.8279
C6	0.2056	8.5244	0.3557	8.5588	0.3229	8.5443
N3	-0.8235	8.5331	-0.8533	8.5665	-0.8449	8.6043
N4	-0.9095	8.0029	-0.9618	8.0439	-0.9506	8.0530
C3'	0.2327	7.9597	0.3664	7.8499	0.6057	7.7805

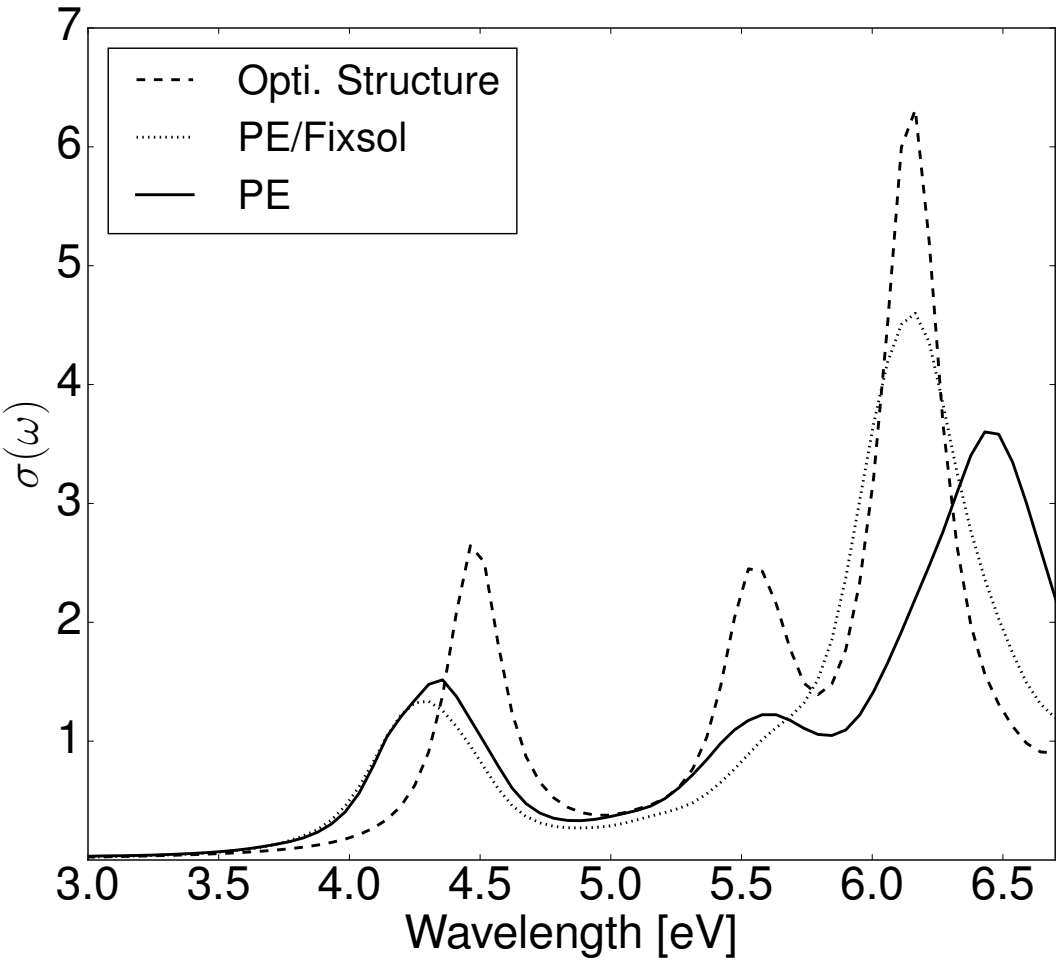

Figure S1: Near UV absorption spectra of the 2AP unit embedded in a DNA helical structure. The full curve is the PE-QM/MM calculation including 12 Åof water molecules. The dotted curve represents the PE-QM/MM/FixSol calculation with no explicitly included water molecules. Finally, the dashed line represents a PE-QM/MM/FixSol calculation using a single QM/MM geometry-optimized structure. DNA atoms have all been represented using averaged parameters developed using capping level 4.

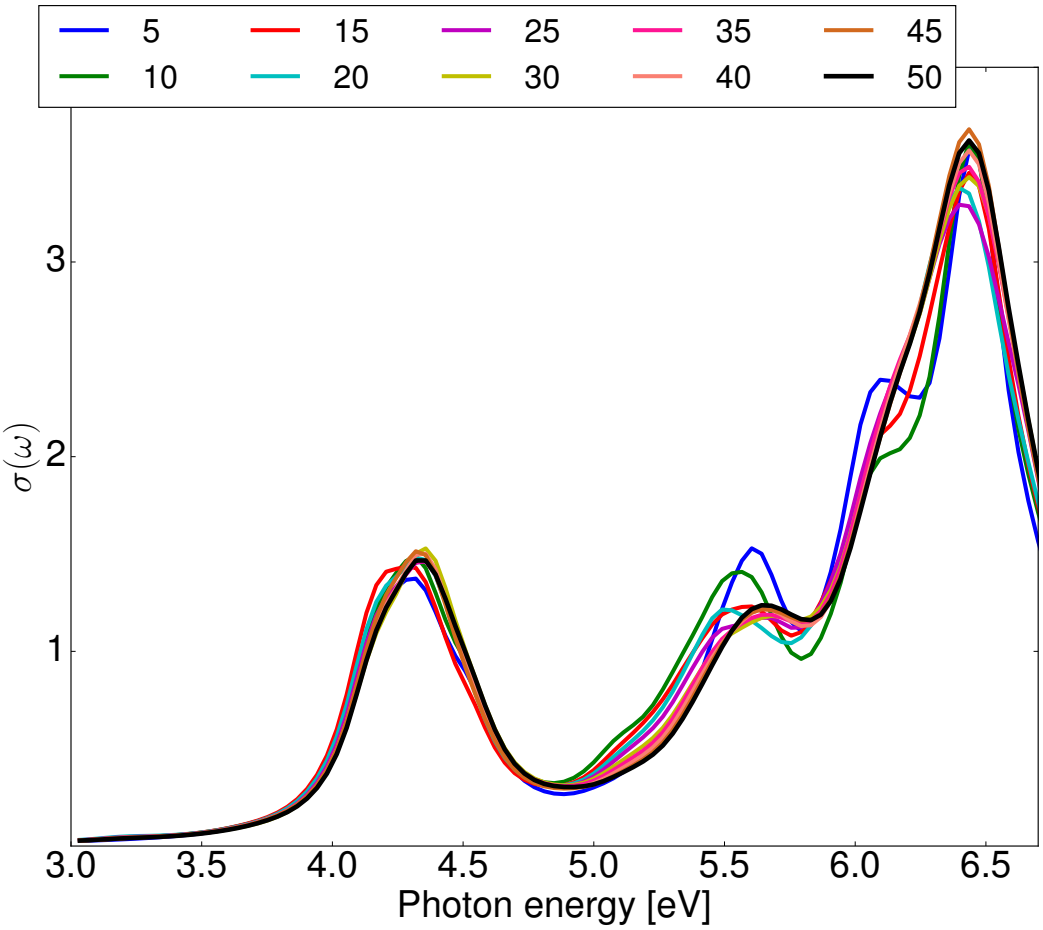

Figure S2: Averaged spectra of the near UV absorption of the 2AP unit embedded in a DNA helical structure. The numbers in the legend indicate the number of snapshots included in the averaged spectrum.