Supporting Information for "Non-Empirically Tuned Range-Separated DFT Accurately Predicts Both Fundamental Excitation Gaps in DNA and RNA Nucleobases"

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Nucleobase	Optimal μ (Bohr^{-1})
Guanine	0.2692
Adenine	0.2699
Cytosine	0.2800
Thymine	0.2735
Uracil	0.2923

Table S1. LC-BLYP/aug-cc-pVTZ optimal μ values for the different DNA/RNA nucleobases

	LDA-KS[†]	B3LYP / aug-cc-pVTZ	LC-BLYP / aug-cc-pVTZ	GW[†]	CASPT2[†,‡]	Experiment[†]
Guanine						
HOMO-1	6.34	7.27	9.40	9.82	9.56	9.9
HOMO	5.69	5.91	7.91	7.81	8.09	8.0 - 8.3
LUMO	1.8	0.93	-0.09	-1.58	-1.14	
Fundamental gap	3.89	4.98	8.00	9.39	9.23	
Adenine						
HOMO-1	6.28	7.13	9.24	9.47	9.05	9.45
HOMO	6.02	6.25	8.28	8.22	8.37	8.3 - 8.5, 8.47
LUMO	2.22	1.02	-0.37	-1.14	-0.91	-0.56 to -0.45
Fundamental gap	3.80	5.23	8.65	9.36	9.28	
Cytosine						
HOMO-1	6.172	7.11	9.33	9.52	9.42	9.45, 9.55
HOMO	6.167	6.60	8.74	8.73	8.73	8.8 - 9.0, 8.89
LUMO	2.57	1.40	-0.20	-0.91	-0.69	-0.55 to -0.32
Fundamental gap	3.60	5.20	8.94	9.64	9.42	
Thymine						
HOMO-1	6.68	7.62	9.76	10.41	9.81	9.95 - 10.05, 10.14
HOMO	6.54	6.91	8.95	9.05	9.07	9.0 - 9.2, 9.19
LUMO	2.83	1.65	-0.21	-0.67	-0.6	-0.53 to -0.29
Fundamental gap	3.71	5.26	9.16	9.72	9.67	
Uracil						
HOMO-1	6.88	7.68	9.99	10.54	9.83	10.02 - 10.13
HOMO	6.72	7.27	9.47	9.47	9.42	9.4 - 9.6
LUMO	3.01	1.81	-0.16	-0.64	-0.61	-0.30 to -0.22
Fundamental gap	3.71	5.46	9.63	10.11	10.03	
MAE HOMO-1	3.06 (3.48)	2.17 (2.59)	0.01 (0.41)	0.42		
MAE HOMO	2.51 (2.43)	2.15 (2.07)	0.07 (0.01)	0.08		
MAE LUMO	3.28 (3.47)	2.15 (2.35)	0.58 (0.78)	0.20		
MAE Fundamental gap	5.78 (5.90)	4.30 (4.42)	0.65 (0.77)	0.12		

Table S2. HOMO-1, HOMO, and LUMO energy levels (in eV) for the DNA/RNA nucleobases calculated at different levels of theory (note: the negative of the orbital energies are reported). The fundamental gap is determined by the difference between the HOMO and LUMO orbital energies. The MAE (mean absolute error) values are with respect to the CASPT2 values; the values in parentheses are with respect to the GW values. [†]Values were obtained from Ref. 1. [‡]The reported CASPT2 HOMO/LUMO energies are actually the vertical ionization energies and electron affinities, respectively (see main text).

Reference Cartesian coordinates (in Å) for **guanine**

N	0.95103344	0.74588413	0.00000144
C	-1.49642563	-0.09935178	0.00002235
C	-1.33220817	1.30207573	0.00005918
C	0.66682489	-0.59425707	-0.00001277
C	0.01635877	1.82442902	0.00002553
N	-0.56066108	-1.07640186	-0.00000210
N	1.71481265	-1.46581979	-0.00006470
H	1.48440682	-2.46212880	-0.00002519
H	2.68872896	-1.16135180	0.00005104
O	0.44367551	2.97649997	0.00000553
N	-2.54986302	1.94040224	0.00006419
C	-3.43506077	0.96689703	0.00002738
H	-4.53758831	1.09743659	0.00002927
N	-2.85224920	-0.28793673	-0.00000073
H	-3.31793982	-1.20257220	-0.00003749
H	1.92439341	1.08388113	-0.00002583

Reference Cartesian coordinates (in Å) for **adenine**

N	1.00978880	0.74572335	-0.00001530
C	-1.51369985	-0.16385117	0.00000078
C	-1.32432583	1.23295247	0.00003944
C	0.66277242	-0.55578813	-0.00003259
C	0.02778638	1.66502787	0.00001047
N	-0.56155283	-1.10622262	-0.00003458
H	1.51767039	-1.27471790	-0.00004805
N	0.34848568	2.97812545	-0.00001164
H	1.33873147	3.23936680	-0.00000435
H	-0.39663209	3.68061172	0.00003808
N	-2.52110889	1.91313209	0.00005519
C	-3.42770742	0.95225575	0.00002734
H	-4.52692639	1.11164669	0.00002556
N	-2.88257926	-0.31447295	-0.00000432
H	-3.38561856	-1.20919409	-0.00005145

Reference Cartesian coordinates (in Å) for **cytosine**

N	1.14904057	0.63518420	-0.00001193
C	-1.34371073	-0.61250622	0.00001462
C	-1.29668275	0.76105602	0.00004891
C	1.10204936	-0.73362929	-0.00001209
C	0.02516335	1.33831302	0.00001304
N	-0.19399492	-1.32366089	-0.00002833
H	-2.29935893	-1.18252596	0.00002318
H	-2.22055810	1.37511297	0.00008373
O	2.07616821	-1.48560443	0.00000314
N	0.15733385	2.68981983	0.00000293
H	-0.64893280	3.31620742	0.00000038
H	1.11285301	3.06166983	-0.00003074
H	-0.18520792	-2.35219256	-0.00003407

Reference Cartesian coordinates (in Å) for **thymine**

N	1.14690489	0.58634304	-0.00071387
C	-1.26069863	-0.63223611	0.02350754
C	-1.26694288	0.73620614	0.04078617
C	1.17720310	-0.79915753	-0.00059683
C	0.02554195	1.42878862	0.01299201
N	-0.09540930	-1.35981377	-0.00151990
H	2.06801258	1.05028816	-0.01001415
H	-2.20509683	-1.22254263	0.03068533
C	-2.49142777	1.58328610	0.09410188
H	-3.42395829	0.96780564	0.05051049
H	-2.50067321	2.19422848	1.03437753
H	-2.49235540	2.32136907	-0.74816232
O	2.20568578	-1.47198873	-0.00180910
O	0.15320249	2.65511204	0.00150994
H	-0.10220997	-2.38662822	-0.01132262

Reference Cartesian coordinates (in Å) for **uracil**

N	1.14697849	0.58666204	-0.00319763
C	-1.24841389	-0.65900001	0.01722627
C	-1.25016037	0.70766060	0.01500134
C	1.18738494	-0.79659357	0.00039035
C	0.01719519	1.42946040	0.00310714
N	-0.08115913	-1.37461681	0.00593386
H	2.06175024	1.06249266	-0.00986687
H	-2.18662482	-1.25766722	0.02955514
H	-2.18805773	1.29756107	0.02544546
O	2.21427357	-1.46996815	-0.00050242
O	0.15220447	2.65263034	-0.00007986
H	-0.06964598	-2.40144502	0.01504209