Explicit calculation of the excited electronic states of the photosystem II reaction centre: Supplementary Information

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Table S1: Excitation energies of a chlorophyll dimer (AB) with various modifications (eV). CAM-B3LYP/6-31G(d,p)

Excitation	Character[a]	Full chlorophyll	Truncated tail[b]	With diffuse[c]	With His[d]
1	A^*	2.1291	2.1296	2.0888	2.1301
2	B^*	2.1771	2.1779	2.1409	2.1802
3	A^*	2.5588	2.5595	2.5299	2.4762
4	B^*	2.5682	2.5689	2.5391	2.5010
5	A^+B^-	2.7152	2.7161	2.6743	2.7744
6	A^-B^+	2.7158	2.7166	2.6773	2.7805
7	A^+B^-	3.2444	3.2456	3.2060	3.2317
8	A^-B^+	3.2453	3.2465	3.2075	3.2419
9	A^*	3.4027	3.4047	3.3466	3.3832
10	B^*	3.4152	3.4185	3.3542	3.4047

[a] Principle nature of excited state
[b] Truncated at ether, converted to carboxylic acid
[c] Truncated tail configuration, CAM-B3LYP/6-31+G(d,p)
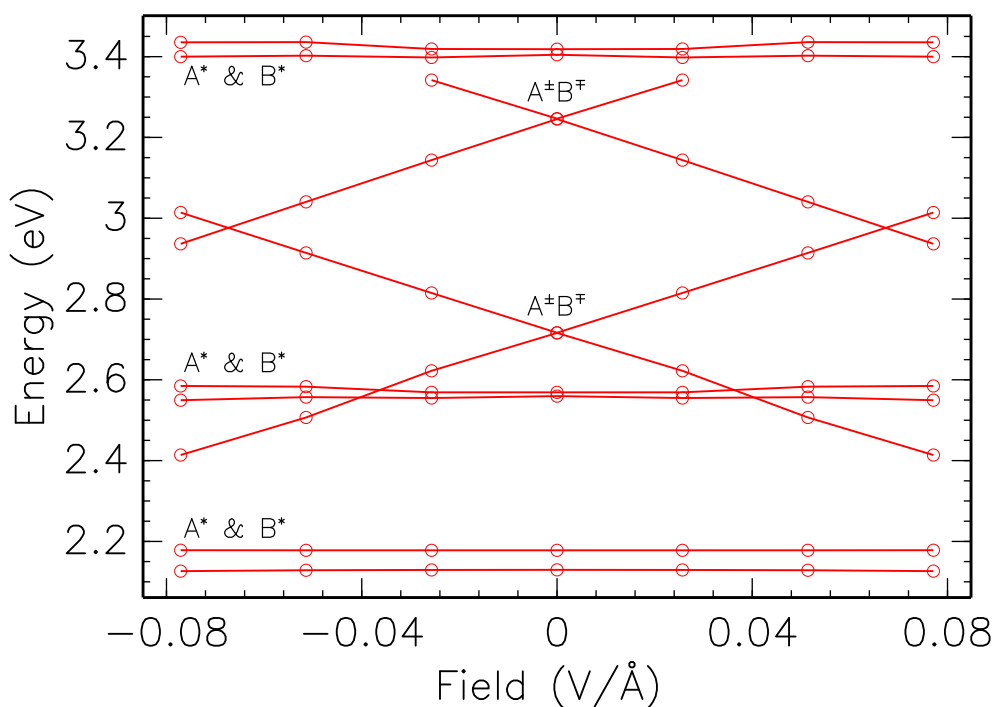[d] Truncated Chl and protonated His, Chl–His monomer optimised in gas phase

Figure S1: Excitation energies of a dimer of truncated chlorophyll molecules (3.8 Å separation between the planes of the rings) under a uniform external electric field. The field is oriented approximately along the vector between the centres of the chlorophylls.