

The first tyrosyl radical intermediate formed in the S_2 – S_3 transition of Photosystem II

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Supplementary Information

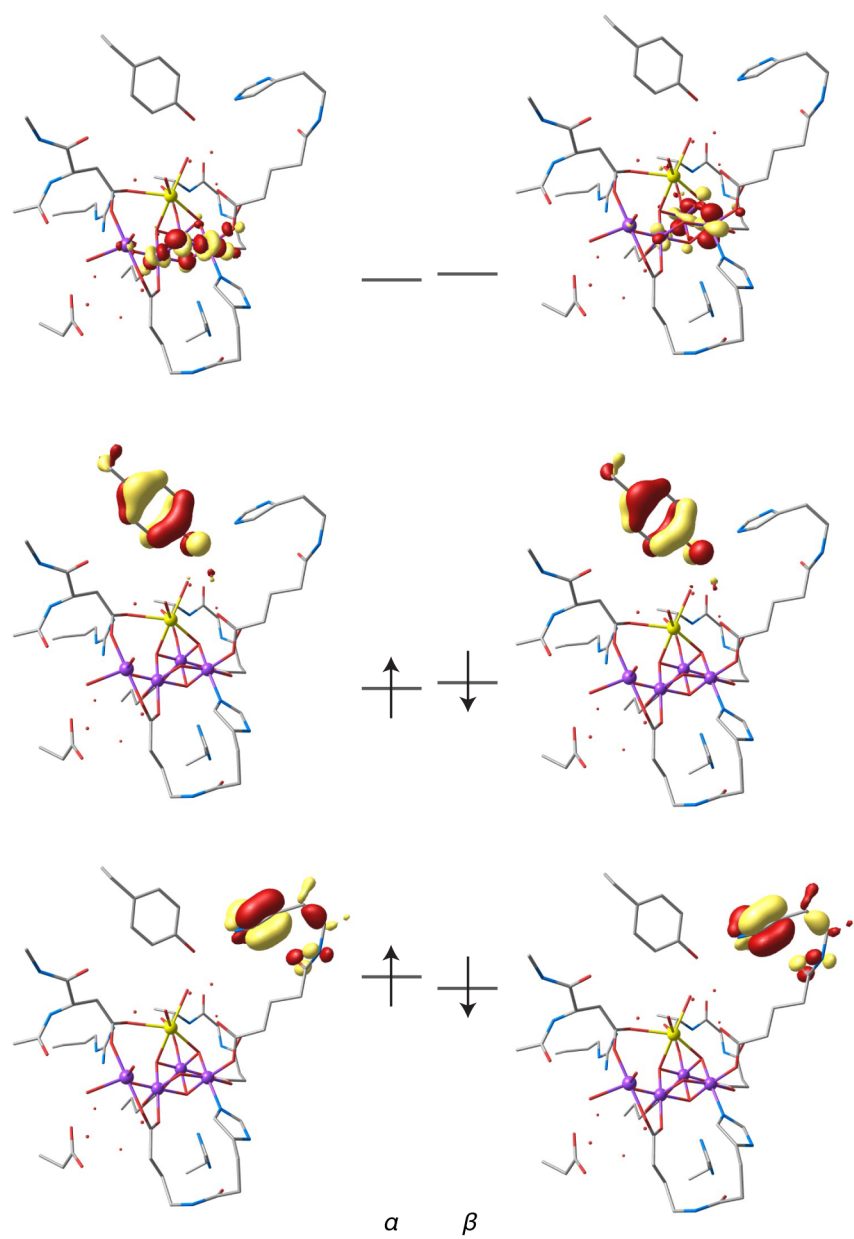


Fig. S1. Frontier orbitals of the S_2^B model of the OEC.

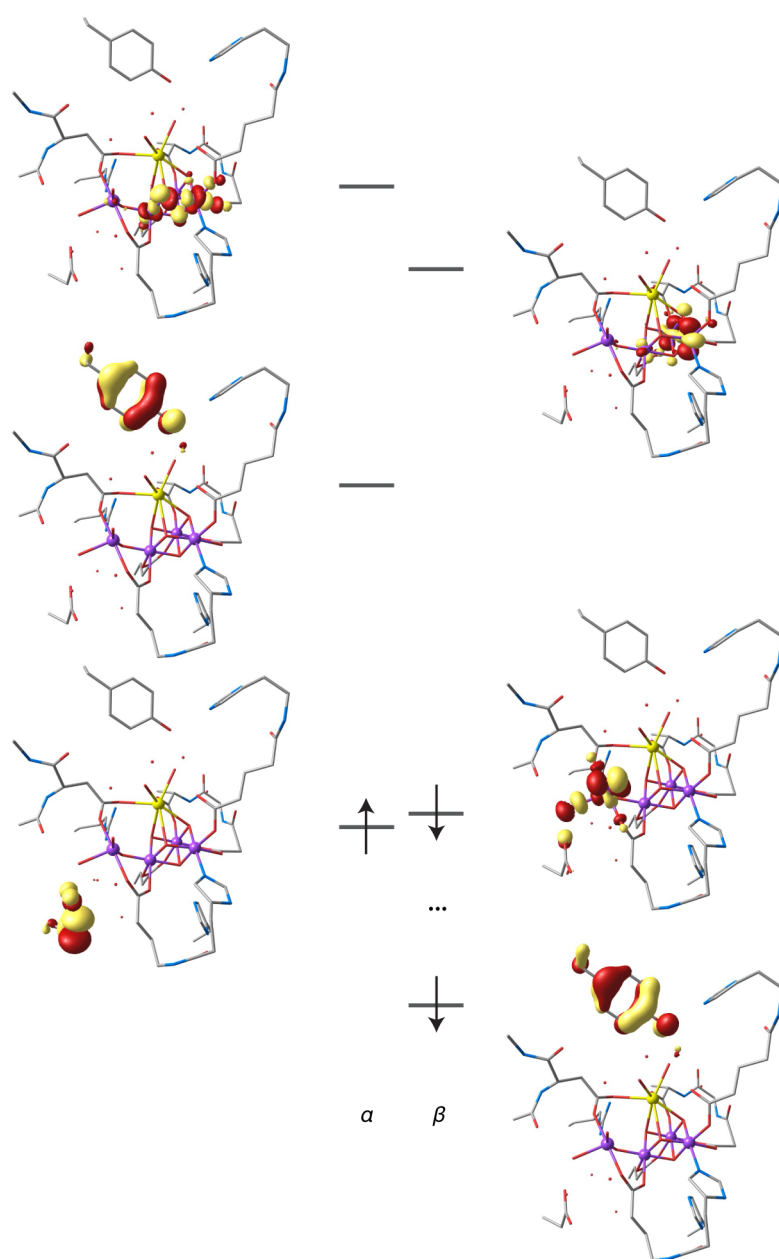


Fig. S2. Frontier orbitals of the $S_2^B Y_Z$ model of the OEC.

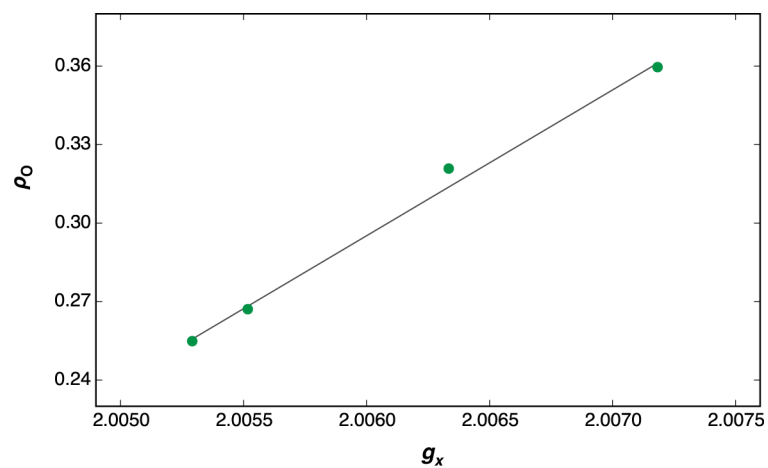


Fig. S3. Correlation between the g_x value of the Y_Z radical and the spin population of the tyrosyl O atom. The models used are those described in Table 1 of the main text.

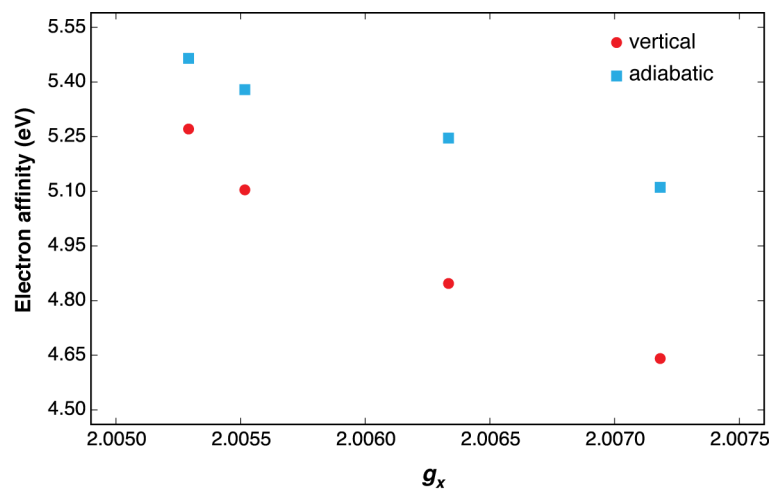


Fig. S4. Correlation between the g_x value of the Y_Z radical and the vertical/adiabatic electron affinity for the models described in Table 1 of the main text.

Cartesian coordinates of optimized structures

$S_2^A Y_Z^*$

25	-24.840238894	-35.510264666	203.970335556
25	-27.326655458	-35.211090075	205.234696641
25	-27.320418575	-33.343045701	203.153420824
25	-27.578210976	-33.181624944	200.415450329
20	-27.864431308	-36.722647315	202.225624937
8	-26.407290423	-36.495138140	204.230172698
8	-28.347518806	-34.729811833	203.800170145
8	-25.993958540	-34.045792559	204.486645331
8	-28.496655243	-32.616153015	201.978872761
8	-26.769799593	-34.313952071	201.675061519
8	-28.443759743	-31.703651409	199.327824392
8	-26.639416140	-33.801360825	198.946372264
8	-27.610604032	-37.363371424	199.914757633
8	-27.942415101	-39.132552786	202.550973164
1	-30.444125946	-26.807342602	200.178392151
6	-30.241436243	-27.113397027	201.222178400
1	-30.724379276	-26.361922999	201.871660392
6	-28.736972624	-27.347441011	201.419475787
6	-28.200792243	-28.505859752	200.557917545
8	-28.977601690	-29.546494750	200.469853984
8	-27.070437359	-28.412274226	200.008481274
6	-32.924383416	-41.850906151	196.489849980
6	-31.569540960	-41.351969795	195.930862060
6	-30.590703811	-41.216135816	197.064906897
6	-30.096536928	-42.402006685	197.705298153
6	-30.211466818	-39.940971578	197.591092707
6	-29.296936347	-42.333131091	198.828405425
6	-29.410435341	-39.845456143	198.717828547
6	-28.928028365	-41.043301764	199.379542472
8	-28.157986566	-40.960477057	200.417948046
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6	-32.844741711	-31.791424452	197.688635420
6	-31.628843209	-32.691777736	197.684660241
8	-30.474636719	-32.230039364	197.570262174
1	-32.689405434	-30.979290836	198.418610035
7	-31.869450579	-34.039058249	197.749638444
6	-30.825023497	-35.049753456	197.612836071
6	-30.938807189	-35.899983072	196.337953355
8	-30.149791210	-36.850080076	196.159800543
6	-30.639583384	-35.885041223	198.894386949
6	-29.817096415	-35.246497324	200.024825972
8	-29.862458018	-35.764651811	201.175531954
8	-29.053618531	-34.268961951	199.684090858
7	-31.863918030	-35.487389392	195.445854707
6	-31.935593501	-35.967613512	194.072831837
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8	-25.224851798	-38.040757461	201.929368229
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1	-25.622563955	-45.846540993	202.133284565
1	-22.819921121	-30.461834863	207.603910499

$S_2^B Y_Z$

25	-25.066182762	-35.474742055	203.966288409
25	-27.410467609	-35.261860927	205.394948445
25	-27.081154786	-33.531881015	203.264638536
25	-27.492704929	-33.221964126	200.166063380
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8	-26.489277442	-36.559617329	204.434761619
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6	-30.181470406	-39.921890505	197.585460144
6	-29.307439986	-42.302481674	198.855500359
6	-29.374792079	-39.827341347	198.713586133
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6	-29.749752789	-35.303187025	199.976215221
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8	-28.968169105	-34.367477821	199.568075625
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