Supporting Information

Proton Release Process during the S_2-to-S_3 Transition of Photosynthetic Water Oxidation As Revealed by the pH Dependence of Kinetics Monitored by Time-Resolved Infrared Spectroscopy

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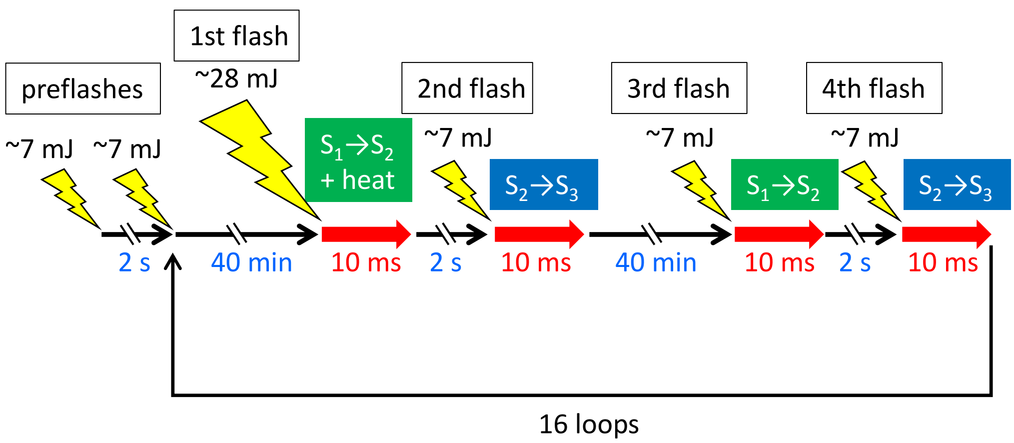

Figure S1: Scheme of the TRIR measurement.

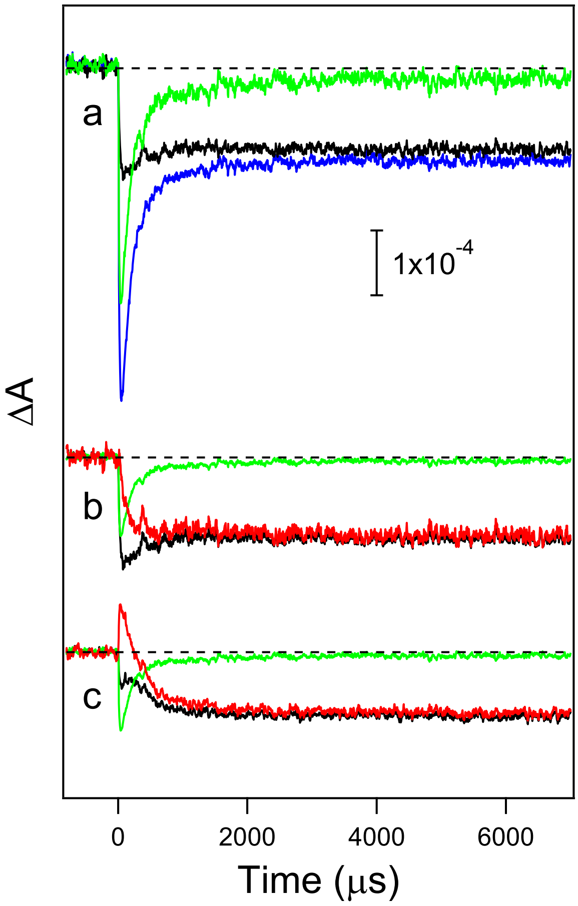

Figure S2: Example of heat-signal correction of the TRIR traces. (a) A heat signal corresponding to a laser power of 21 mJ cm^{-2} pulse^{-1} (green lines) was calculated by subtraction of a TRIR trace upon a flash with 7 mJ cm^{-2} pulse^{-1} (black lines) from that upon a flash with 28 mJ cm^{-2} pulse^{-1} (blue lines). (b, c) Heat-corrected TRIR traces (red lines) obtained by subtraction of a heat signal corresponding to a laser power of 7 mJ cm^{-2} pulse^{-1} (green line; the 1/3 intensity of the heat signal obtained in a) from raw TRIR traces (black lines) by (b) the 1st flash (the 3rd flash in the scheme of Figure S1) and (c) the 2nd flash (the 2nd and 4th flashes in the scheme of Figure S1) with 7 mJ cm^{-2} pulse^{-1}. The TRIR traces were measured at 1400 cm^{-1} for the Y_D-less PSII core complexes at pH 6.0.

Table S1. Relative amplitudes of the components obtained in the global fit analysis of the time courses of ΔA in the $S_2 \rightarrow S_3$ transition

pH	Wavenumber (cm^{-1})	I_A[a]	I_B[a]	I_C[a]	I_D[a]
5.0	1514	−0.27	1.00	0.39	0.68
	1400	0.44	1.00	0.54	−1.00
	1256	1.00	0.08	−0.15	0.44
6.0	1514	0.10	1.00	0.23	0.96
	1400	0.02	1.00	0.50	−0.83
	1256	1.00	−0.18	−0.51	0.64
7.0	1514	0.55	0.93	0.02	1.00
	1400	0.50	1.00	0.45	−0.87
	1256	1.00	−0.50	−0.59	0.17
8.0	1514	0.67	0.73	0.53	1.00
	1400	0.71	1.00	0.14	−0.83
	1256	−0.33	1.00	0.79	0.04

[a] I_A, I_B, I_C, and I_D are the amplitudes of component A, B, C, and D, respectively, in the fitting function (Equation 1 in the main text).