Title: Photosystem II Does Not Possess a Simple Excitation Energy Funnel: Time-Resolved Fluorescence Spectroscopy Meets Theory

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Figure S1

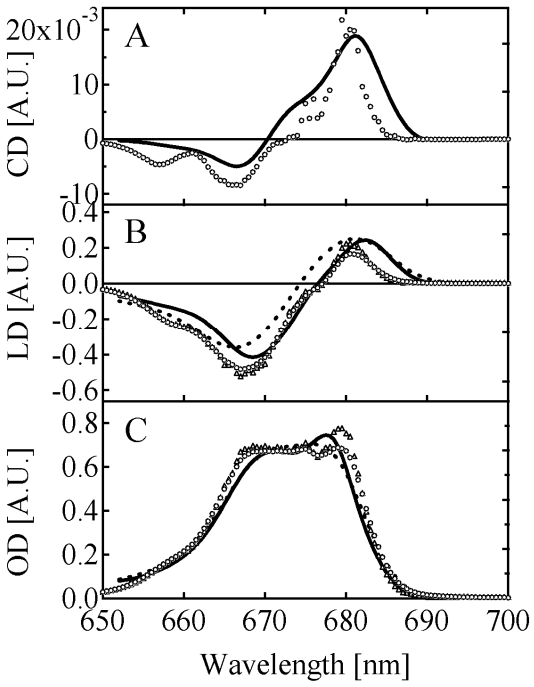

Figure S1. Comparison of the experimental circular dichroism (A), linear dichroism (B), and absorption (C) spectra of RC with the calculated curves with the site energies in Table 1. The solid and dashed lines show the experimental data at 4 K and 77 K, respectively. The circles and triangles show the calculated spectra at 4 K and 77 K, respectively.

Figure S2

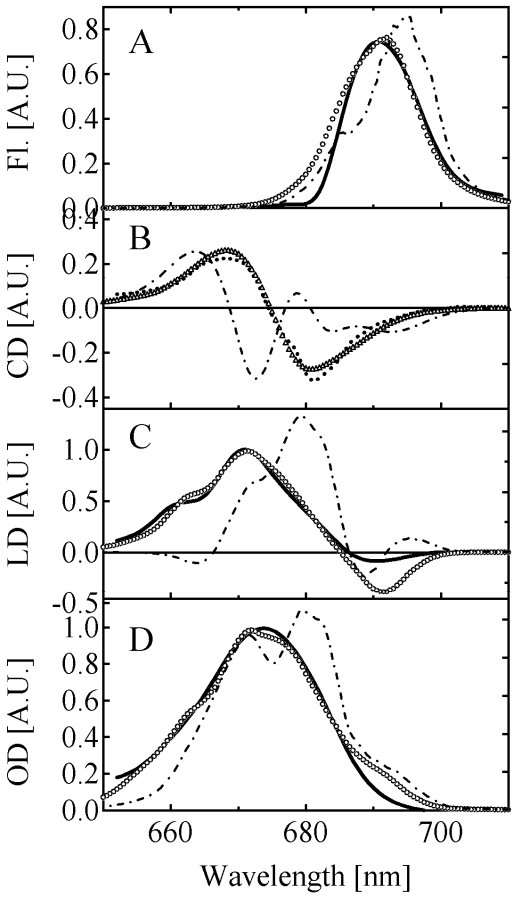

Figure S2. Comparison of the experimental fluorescence (A), circular dichroism (B), linear dichroism (C), and absorption (D) spectra of CP47 with the calculated curves with the site energies in Table 2 and those reported by Reppert et al.[11] The solid and dashed lines show the experimental data at 77 K and room temperature, respectively. The circles and triangles show the calculated spectra at 77 K and room temperature, respectively. The dashed-dotted lines show the simulated curves by using the site energies reported by Reppert et al.[11]

Figure S3

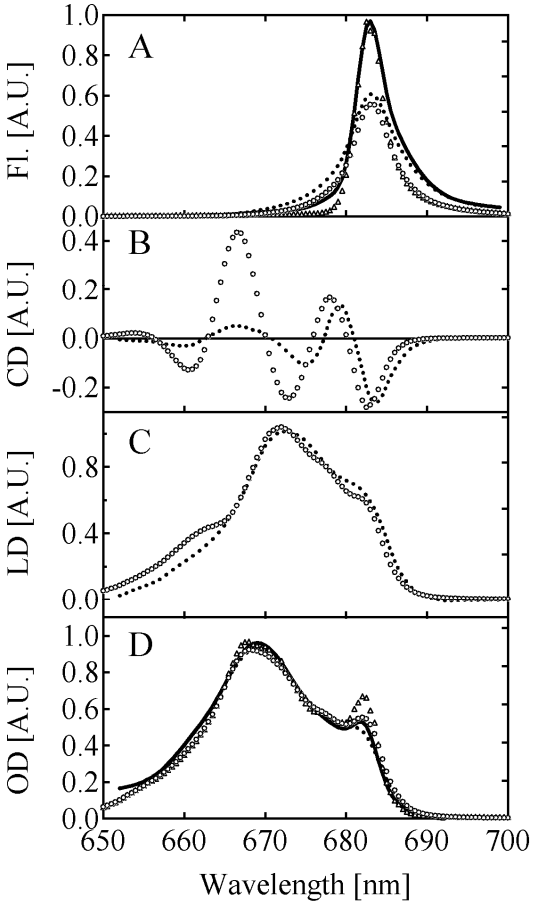

Figure S3. Comparison of the experimental fluorescence (A), circular dichroism (B), linear dichroism (C), and absorption (D) spectra of CP43 with the calculated spectra with the site energies listed in Table 3. The solid and dashed lines show the experimental data at 4 K and 77 K, respectively. The triangles and circles show the calculated spectra at 4 K and 77 K, respectively.

Figure S4

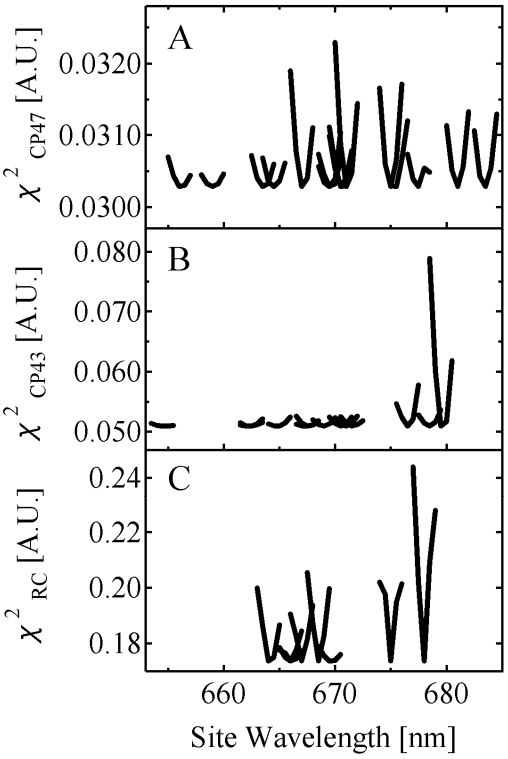

Figure S4. The dependencies of χ^2 values on perturbations on the site energies. (A) CP47, (B) CP43, and (C) RC.

Figure S5

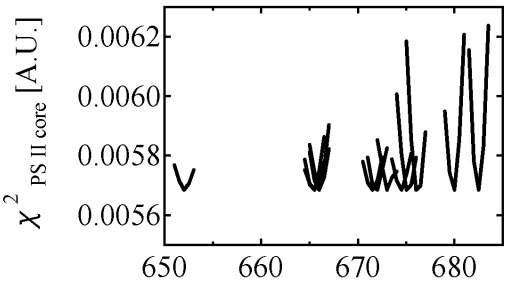

Figure S5. The dependencies of χ^2 values for PS II core complex on perturbations on the site energies in CP43.

Figure S6

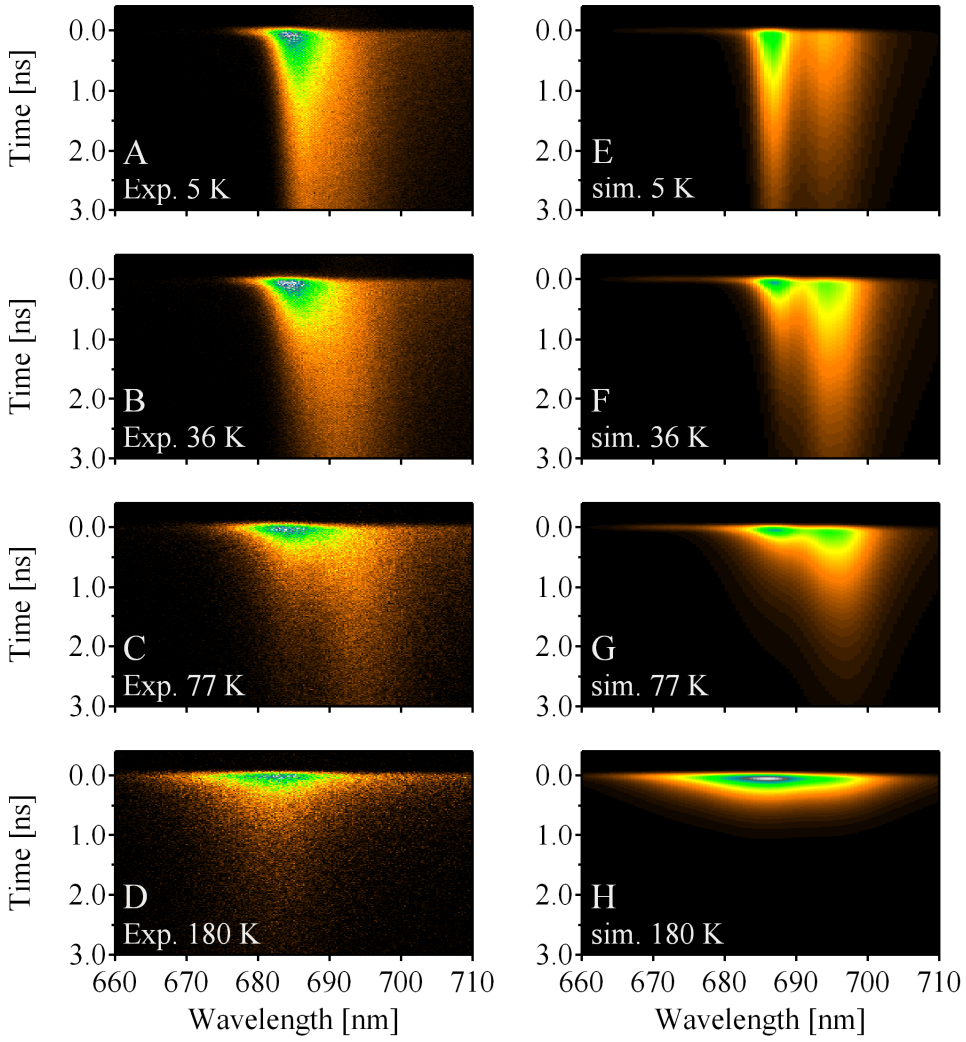

Figure S6. The temperature dependence of the experimental (left, A, B, C, and D) time-resolved fluorescence spectrum of the PS II core complex dimer from *T. vulcanus*, compared with that of the calculated (right, E, F, G, and H) ones using the site energies reported by Reppert et al.[11] The calculated time-resolved fluorescence spectra were convolved with the instrumental response functions approximated by a Gaussian function with FWHM of 89 ps.

The MS Excel file “Coupling_SI.xls” contains excitonic couplings between pigments in unit of cm^{-1}.

The MS Excel file “InterdomainRate_SI.xls” contains the disorder-averaged interdomain transfer rate constants in unit of ns^{-1} from a donor domain (arranged in the left column) to an acceptor domain (arranged in the top row).