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Divergence of protein structure in solvent from that in X-ray quality crystals: probing the local environment of Chl a in the cytochrome b_6f complexes by ultrafast spectroscopy SERGEI SAVIKHIN, NARANBAATAR DASHDORJ, HANYOUP KIM, JOHN SCHAIBLEY, Department of Physics, Purdue University, HUAMIN ZHANG, JIUSHENG YAN, EIKI YAMASHITA, WILLIAM CRAMER, Department of Biological Sciences, Purdue University — The cytochrome b_6f complex in oxygenic photosynthesis mediates electron transfer between the reaction centers of photosystems I and II, and coupled proton translocation across the membrane. High-resolution X-ray crystallographic structures of the b_6f complex show a single chlorophyll a(Chl a) molecule as an intrinsic component of the complex. Using ultrafast optical spectroscopy, we have shown that the excited state lifetime of the Chl a in dissolved complex is unusually short (∼200 ps) and attributed the observed quenching to the electron transfer exchange with a nearby amino acid. Similar optical time resolved experiments performed on single crystals of theb_6f complex reveal significant changes in the lifetime of the excited state and suggest structural dissimilarities between the complexes within crystals and in solvents. The extent of the structural variations is discussed and modeled using molecular dynamic simulation methods (NSF MCB-0516939, NIH GM-38323).

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