【Grant-in-Aid for Specially Promoted Research】

Elucidation of the mechanisms for light-induced water-splitting and light energy utilization in photosynthesis

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Purpose and Background of the Research

●Outline of the Research

Foods (energy) and oxygen are two substances indispensable for sustaining various life forms on the earth. These two substances are produced from carbon dioxide and water using the light energy from the sun via photosynthesis performed by plants and various algae (Fig. 1). The purposes of the present project is to decipher the molecular mechanism of light-induced water-splitting in photosynthesis, and to reveal the structures and functions of light-harvesting antenna protein (LHC)-photosystem supercomplexes from various organisms. The results obtained will not only be important for our understanding of photosynthesis at a molecular level, but also open a way to obtain energy from the sun with a high efficiency.

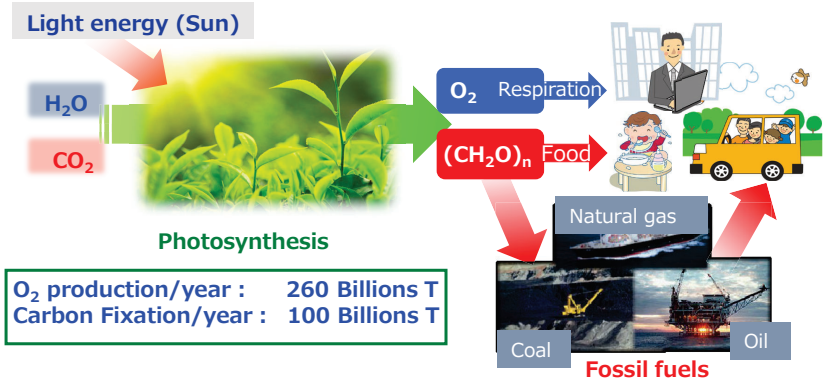

Figure 1. Photosynthesis and its effects on life activities on the earth.

●Elucdiation of the mechanism of the water-splitting reaction in photosynthesis

The water-splitting reaction in photosynthesis is catalyzed by photosystem II (PSII). The first purpose of this research is to decipher the molecular mechanism of this reaction in photosynthesis. The structure of a Mn_4CaO_5-cluster, the direct catalyst for water-splitting, has been elucidated by X-ray crystallography previously (Fig. 2), and the S_2, S_3 intermediate state structures within the S-state cycle (Fig. 2) have also been resolved by pump-probe X-ray free electron lasers (XFEL). In the present project, we will study the structural changes occurred during $S_3 \rightarrow (S_4) \rightarrow S_0$ state transitions by either pump-probe XFEL X-ray crystallography, or by cryo-electron microscopy (cryo-EM) of room-temperature excited S_0 state. We will also study the structures and functions of various amino acid residue-substituted mutants that are important for proton egress and water inlet. The results obtained will lead us to understand the molecular mechanism of O-O bond formation, proton egress and water inlet pathways within PSII.

●Structural analysis of PS-LHC supercomplexes from various organisms

The second purpose of this research is to decipher the highly efficient light energy transfer and utilization mechanisms in photosynthesis. Light energy is harvested by light-harvesting antenna proteins (LHC, FCP), and the structures of these LHC and FCP in complex with photosystems (PS) from higher plants and diatoms (Fig. 3) have been solved. However, there are still a large number organisms whose PS-LHC (FCP) supercomplex structures have not been solved. We will analyze the structures of these supercomplexes by cryo-EM. From the results obtained, we will decipher the roles of proteins and pigments in light-harvesting and energy transfer in different organisms, and to obtain insights into the changes occurred during evolution in response to the changes in the light environment.

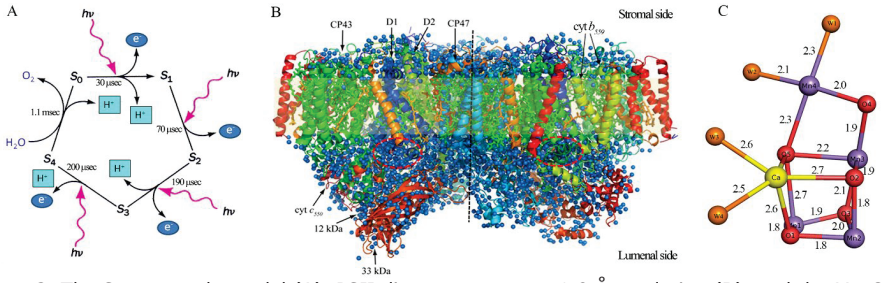

Figure 2. The S-state cycle model (A), PSII dimer structure at 1.9 Å resolution (B), and the Mn_4CaO_5 cluster (C).

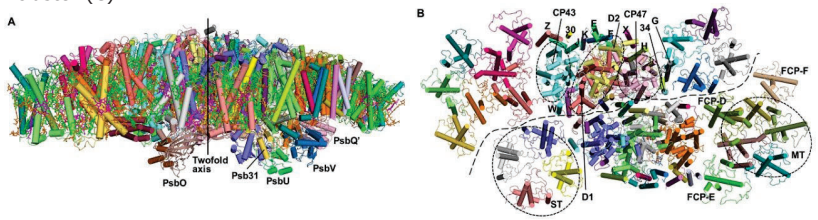

Figure 3. Cryo-EM structure of the PSII-FCPII supercomplex from a diatom viewed from the side of the membrane (A) and top of the stromal side (B).

Expected Research Achievements

●Elucdiation of the mechanism of the water-splitting reaction in photosynthesis

We will analyze the unsolved structural changes occurred during the $S_3 \rightarrow (S_4) \rightarrow S_0$ state transition by pump-probe XFELs using microcrystals of PSII from a thermophilic cyanobacterium *Thermosynechococcus vulcanus*. In case that these transitions did not occur or have a low efficiency in the PSII crystals, we will use cryo-EM to analyze the S_0 state structure. We will also analyze the structures and functions of various amino acid residue-substituted PSII mutants to reveal the participation of these amino acid residues in the proton egress and water inlet pathways. The results obtained will be important not only for elucidating the mechanism of water-splitting, but also for developing artificial catalysts for water-splitting in artificial photosynthesis.

● Structural analysis of PS-LHC (FCP) supercomplexes from various organisms

We will analyze the structures of PSII-LHCII and PSI-LHCI supercomplexes from various algae such as Charophyceae, Dinoflagellate, Phaeophyceae, Euglena, Chlorolla, as well as cyt c_6-PSI-Fd、Fd-FNR-PSI supercomplexes from cyanobacteria and higher plants. From the results obtained, we will elucidate the mechanisms of energy transfer from antenna to the reaction center in various organisms, as well as the changes occurred during evolution in response to the changes in the light environment that each organism lives. These results will aid in designing and synthesizing highly efficient light-energy harvesting devices in artificial photosynthesis.

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