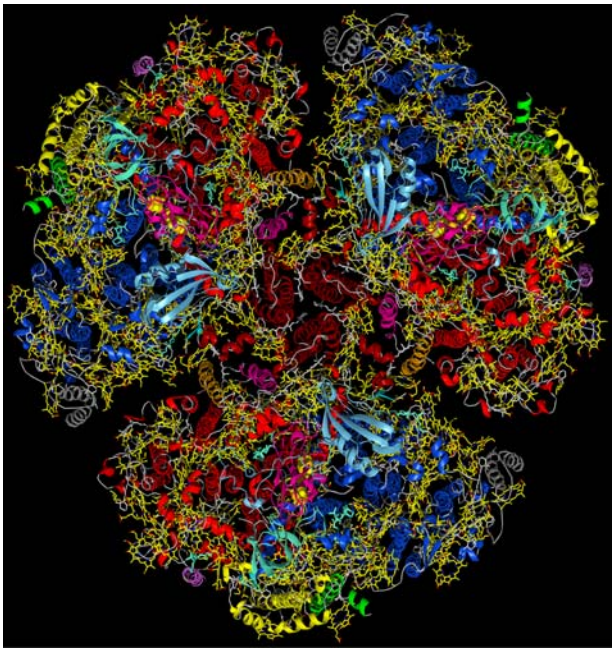
Structure and function of Photosystem I

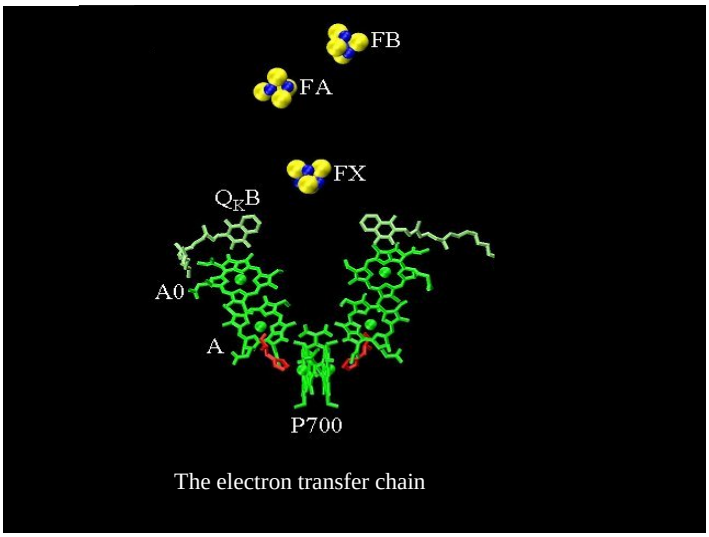
(Yana Bukman, Devendra Chauhan, Raimund Fromme, Ingo Grotjohann, Craig Jolley, Daqun Ni, Rajagopal Subramanyam, HongQi Yu)

Photosynthesis is the main life process on earth; it converts the light energy from the sun into chemical energy. Two photosystems, acting in series, catalyze the first step of this energy conversion, the light-induced charge separation. Photosystem I (PS I) captures the light energy from the sun by an internal large antenna system of more than 110 cofactors. This antenna system of high complexity is a unique feature of Photosystem I, not present in any other protein in nature, representing the key invention for the high efficiency of energy transduction. Light energy is transferred from the antenna system to the core of the complex (the reaction centre) with an efficiency of more than 99.99% , driving the electron transfer from the soluble electron carriers cytochrome c_6 or plastocyanin at the inner (lumenal) side of the thylakoid membrane to ferredoxin or flavodoxin at the cytoplasmic (stromal) side. In the thermophilic cyanobacterium *Synechococcus elongatus*, PS I consists of 12 protein subunits. A large number of cofactors (~ 100 chlorophyll *a*, ~ 20 carotenoid, 2 phylloquinone molecules and 3 Fe_4S_4 clusters) are coordinated with the protein subunits. *In vivo* , cyanobacterial PS I exists as a trimer with a molecular mass of ~1 020 000 Da. My group and coworkers have determined the structure of the native trimeric Photosystem I from Synechococcus elongatus at 2.5 Å which was a breakthrough in understanding of the organization and function of this large complex biosolar energy converter.



Structural model of Photosystem I at 2.5 Å resolution

The structural model opens the way for detailed investigations on the function-structure relationship in this large membrane protein complex by spectroscopy,



The electron transfer chain

mutagenesis computational studies with the aim to

The electron transfer chain in Photosystemm I

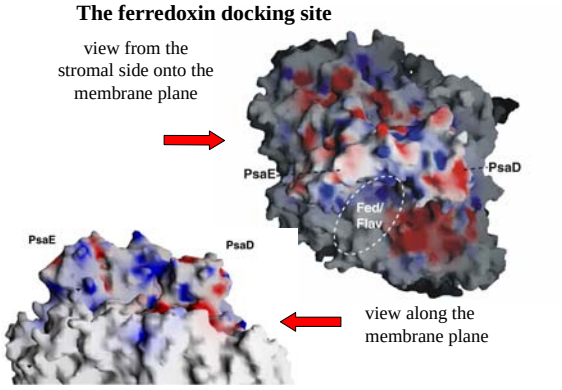
achieve a detailed insight into the complex function of light capturing, energy transfer and electron transfer.

The present projects regarding Photosystem I include the study of:

- **Interaction of Photosystem I with its natural electron acceptor ferredoxin** (**HongQi Yu, Daqun Ni** and **Raimund Fromme** in cooperation with **Robert Blankenship** and **Dmitry Matyushov** (ASU) and **Pierre Setif,** CEA France
- **Interaction of Photosystem I with its electron donors: plastocyanin/ cytochrome c6** (**Yana Bukman**)
- **Structure and function of supercomplexes of Photosystem I with its external antenna systems in cyanobacteria, algae and plants.** (**Rajagopal Subramanyam**, **Devendra Chauhan** and **Craig Jolley** in cooperation with **Alexander Melkozernov** (Chemistry ASU) and **Andrew Webber** SOLS ASU and **Nathan Nelson** Tel Aviv University)
- **Pathways of energy transfer from the antenna system to the electron transfer chain**. (**Craig Jolley** in cooperation with **Klaus Schulten and Melih Sener at Urbana**)
- **Assembly of Photosystem I** (**Craig** Jolley in Cooperation with **Michael Thorpe** Physics and Astronomy ASU)

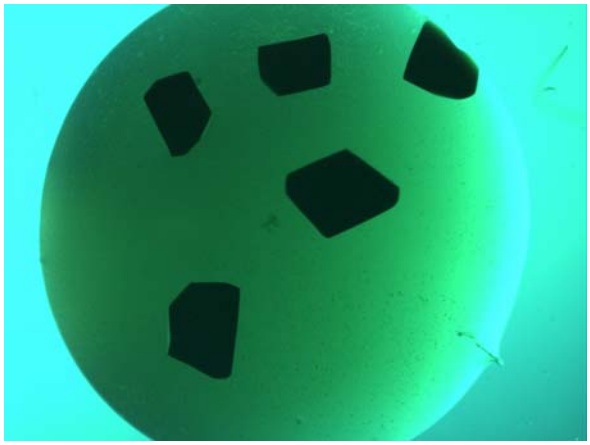
Interaction of Photosystem I with its natural electron acceptor ferredoxin: a model system for protein recognition and inter-protein electron transfer

Photosystem I can be described as a large biosolar energy converter, capturing the light energy from the sun ands converting it into electrical energy by performing a light driven charge separation across the membrane. The charge separation process is coupled to the inter-protein electron transfer between Photosystem I and smaller soluble electron transfer proteins.
The interaction between Photosystem I and its natural electron acceptor ferredoxin is used to study protein-protein interaction and the mechanism of inter-protein electron transfer. Reduced ferredoxin is an essential redox intermediate involved in many assimilatory processes, in redox regulation of the cell and it is necessary for the reduction of $NADP^+$ to NADPH. We are investigating the structure and function of the intact complex between Photosystem and ferredoxin.



Surface of Photosystem I with proposed docking site of ferredoxin

Three different approaches will be made 1) determination of the structure of the Photosystem I/ferredoxin complex by X-ray structure analysis, based on co-crystals of Photosystem I with ferredoxin.



Cocrystals of Photosystem I with ferredoxin

2) Biophysical investigations of the complex in solution and in single crystals. This part of the project will include optical spectroscopy and EPR-spectroscopy experiments.
3) dynamic simulation of the protein-protein interaction.

The main goal of the project to get a deeper knowledge of the structure of the PS I /ferredoxin complex and to understand the dynamics of these docking and electron transfer processes, also in respect to the outstanding regulatory function of ferredoxin in cells of plants, green algae and cyanobacteria. This knowledge is a prerequisite for understanding the complex processes of redox regulation in plant cells, which could directly lead to implications for the growth development and crop production of plants.

Group members working on this project:
HongQi Yu, Raimund Fromme Daqun Ni
cooperation with R. Blankenship (ASU), P. Setif (CEA, France), D. Matyushov (ASU)
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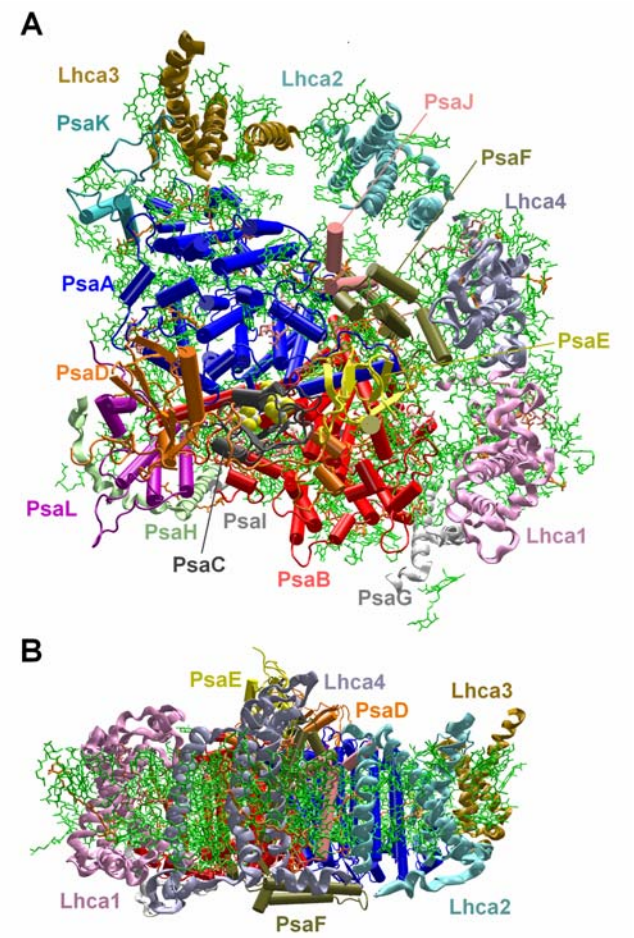
Structure and function of photosystem I with its peripheral antenna systems in green algae and cyanobacteria



In this project, we will apply the experimental experience of structure determination to the larger challenge of determination of the atomic structure and function of both the eukaryotic PSI in a supercomplex with LHCI and the cyanobacterial PS I in its supercomplex with the IsiA protein. As cyanobacterial model organism

Structural model of plant Photosystem I as revealed from computational modeling

We use the thermophilic cyanobacterium *Thermosynechococcus elongatus* that had already served as a basis for the determination of the structure of the trimeric PS I core. The green alga *Chlamydomonas reinhardtii,* which is easily transformable and can be grown in the laboratory under reproducible experimental conditions, will be used as a model system for the eukaryotic LHCI-PS I supercomplex. The overall goal of the project is to determine the structure of both PS I-antenna supercomplexes and to understand the general principles and the differences of the peripheral and core antenna system in plant-type and cyanobacterial PS I.

Specific proposed experiments include crystallization of the complex and determination of the structure of the PS I supercomplex by X-ray structure analysis, design of structurally and functionally improved complexes by mutagenesis and functional investigations on the wild type and mutant supercomplexes by time-resolved spectroscopy. The obtained experimental results will lead to detailed insights into the structural organization of the photosynthetic system in pro- and eukaryotes and will provide a better knowledge of the protein assembly during formation of large supercomplexes of membrane proteins. Furthermore, it will provide detailed information on the functional external antenna complexes to the core units of Photosynthesis.

Group Members working on this project:
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