

motors. Our findings suggest that structural features unique to each myosin confer selective advantages to cellular functions. Beyond the biological relevance, our study uncovers a simple engineering principle for designing efficient molecular transporters.

Light Energy Harvesting, Trapping, and Transfer

915-Pos Board B670

Dynamic Mechanical Responses of Arabidopsis Thylakoid Membranes during PSII-Specific Illumination

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Remodeling of thylakoid membranes in response to illumination is an important process for the regulation of photosynthesis. We investigated the thylakoid network from individual chloroplasts of *Arabidopsis thaliana* using atomic force microscopy to capture dynamic changes in height, elasticity, and viscosity of thylakoid membranes caused by changes in illumination. We also correlated the mechanical response of the chloroplast with membrane ultrastructure using electron microscopy. We find that the elasticity of the thylakoid membranes increases immediately upon PSII-specific illumination, followed by a delayed height change. While the change in stiffness depends primarily on the transmembrane pH gradient, the height change requires both a pH gradient, and the STN7-kinase-dependent phosphorylation of LHClI. Direct visualization by electron microscopy and image analysis further indicate that there is a significant change in the packing repeat distance of the membrane stacks. We propose that the stiffness change is due to a pH-dependent lumen expansion, while the height change may additionally require the disruption of stromal interactions between membranes by phosphorylation. Our studies indicate that lumen expansion in response to illumination is not simply a result of the influx of water, and we propose a model in which protein interactions within the lumen drive these changes.

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Light-Harvesting Lipid Vesicles Incorporated with Proteorhodopsins and Photosystem II; Generation of Photo-Induced Proton Gradients and Extended Absorbing Light Spectrum

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The most common uses of electrochemical potentials in living cells are to use for energy storages, which are transferable to various essential cellular activities, i.e. the generation of ATP or NADPH, and ions or molecular transport across a membranes. Often, the electrochemical potentials (i.e. proton gradient) are produced by activation of light-harvesting membrane proteins. Depending on the cells from various species, different membrane protein complexes are acting similar roles, in terms of generating an electrochemical potential, by absorbing different light-spectrum. For example, proteorhodopsin and photosystemII are well-known photoactive transmembrane proteins, functioning as a light-driven proton pump in marine bacteria or eukaryotes, and a light-driven proton production in plants, respectively. In their natural habitats, not only their biological roles, but also their activating absorption wavelengths are very different; PR functions as a light-driven H⁺ pump activated by green light, while as PS II captures photons of light to energize electrons, which replaced by oxidizing water to form hydrogen ions by absorbing blue and red light. Although their light-driven mechanisms and their utilizing wavelength bands are very much different, both systems can result a similar proton gradient across the membrane. Consequently, we hypothesized that we can build an artificial light-harvesting system, which allows utilizing multiple maximum absorption bands. By reconstitution of two different purified proteins into a single giant vesicle, we could successfully build the hybrid light-harvesting liposomes incorporated both with PR and PSII, activated by the wide wavelength bands, from blue up to NIR. This new system, generating a improved gradient of electrochemical potential across a membrane, can be used as numerous energy storages in vitro, providing photo-induced energies for flagella rotation, NADPH synthesis or ATP synthesis with highly improved light efficiencies.

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Simulation of Photosystem II Dynamics in the Thylakoid Membrane

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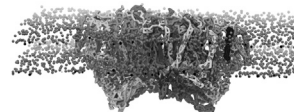
Virtually all life on earth is dependent on the process of photosynthesis, which transforms solar energy into biochemical energy usable by most organisms. Photosystem II (PSII), a protein complex localized in the thylakoid membrane of plants and green algae, is a key player in this process.

Using the MARTINI coarse-grain force field [1,2], we performed molecular dynamics simulations of PSII embedded in the thylakoid membrane resulting in a detailed view on the mobility of the various co-factors and protein subunits on a microsecond time scale. We furthermore provide evidence for the existence of binding sites for specific glycolipids at the membrane-exposed surface of the complex.

Side view of the PSII dimer embedded in the thylakoid membrane. For clarity only the glycerol region of the lipids is shown.

[1] S.J. Marrink, D.P. Tieleman. Perspective on the Martini model. *Chem. Soc. Rev.*, 42, 6801-6822, 2013.

[2] C.A. Lopez, Z. Sovova, F.J. van Eerden, A.H. de Vries, S.J. Marrink. Martini force field parameters for glycolipids. *J. Chem. Theo. Comput.*, 9, 1694-1708, 2013.



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The Dependence of the Photocurrent on the Concentration of Electron Mediator (*Para*-Benzoquinone) in Thylakoids

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The photocurrent harvested from the isolated thylakoids has been investigated as a function of concentration of electron mediator. This photocurrent measured has been verified indeed from the photosynthesis on the thylakoid membranes. The photocurrent has a linear dependence on light intensity; the photocurrent shares similar frequency dependence as that of absorption spectrum of chlorophyll; the photocurrent decreases or disappears with the application of 3-(3',4'-dichlorophenyl)-1,1-dimethylurea as an inhibitor. A new finding of a peak in the photocurrent as a function of the concentration C_{BQ} of electron mediator para-benzoquinone (p-BQ) has been reported here. It is found that the photocurrent measured increases at small C_{BQ}, and a maximum current is obtained at C_{BQ} approximately equal to 1.8-2 mM and decreases with further increase in C_{BQ}. A simplistic model has been proposed to explain the peak. The effect of bias voltage applied between the electrodes on photocurrent is studied as well.

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Environmental Effects in the FMO and PE545 Photosynthetic Complexes

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In most natural photosynthetic systems, light energy is absorbed by antenna pigment-protein complexes and subsequently transferred to a reaction center for conversion to a more stable form. Recent experimental findings in some light-harvesting complexes suggest the existence of long-lived quantum coherences between the individual pigments. A combination of molecular dynamics, quantum chemistry and dynamics can be employed to theoretically contribute to the questions of environmental coupling, spatial correlations between the chromophores, and two-dimensional spectra.

Long-lived quantum coherences were observed in the Fenna-Matthews-Olson (FMO) light-harvesting complex as well as in the PE545 complex and have steered considerable effort to explain these findings. Along molecular dynamics trajectories, electronic structure calculations for the vertical excitation energies of the individual bacteriochlorophylls have been performed for different light-harvesting complexes. In addition, the electronic couplings between the pigments have been determined in a time-dependent manner as well. In a first step, the distribution of energies and couplings have been analyzed together with possible spatial correlations. In subsequent steps, ensemble-averaged wave packet dynamics are used to determine the exciton dynamics in the system. Finally, the time-dependent Hamiltonian is used to determine linear and two-dimensional spectra. This allows a direct comparison with experiment. In conclusion, atomistic simulations can be employed to directly determine