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A Multiscale Model of Photosynthesis

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nature of periodic photonic nanostructure results in this enhancement, nonetheless, it will inevitably accompany with light capture efficiency reduction in the photonic band gap spectrum range. Enhancement or reduction of light capture efficiency depends on the coupling condition between the electric field spatial variation and the lamellar structures. This work will provide insight about how photonic band gap wavelength of the lamellae can be regulated and the possibility in correlation between this regulation and different strategies from nature for environmental adaptation. Most of the plants with iridescent chloroplasts dwell in understorey environment, low light coherence condition might affect the predicted efficiency enhancement, and some results will be presented. These results will offer new perception about the formation of lamellar structure become a better tactic than accumulate more chlorophyll (or other light absorbing materials) molecules together for obtaining better light harvesting efficiency.

2578-Pos Board B594

Identification of Red Pigments in the Photosystem I Complex of Oxygenic Photosynthesis

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Oxygenic photosynthesis powers our biosphere using two large reaction centers, photosystem I and photosystem II (PSI and PSII). Both photosystems are composed of hundreds of light harvesting pigments, mainly chlorophylls, coordinated by several transmembrane protein subunits. All chlorophylls are not equivalent due to their interactions with their environment, either amino acids side chains, lipids, or other chlorophylls. The absorption maxima of some chlorophylls in the core antenna of PSI is tuned to very low levels, lower than that of the final photochemical trap in the complex. Because of this low excitation maximum, these red pigments play a crucial role in the path of excitation energy through the core PSI antenna. The location of these red pigments within the PSI antenna is unknown. Using chimeric PSI complexes in cyanobacteria we identified the first red pigment in the PSI antenna. We show that a single added red pigment and can greatly affect energy migration in the core of PSI, which contain more than 90 other chlorophylls. We also determined the structure of chimeric PSI and observe the configuration of the added red site.

2579-Pos Board B595

A Multiscale Model of Photosynthesis

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Photosynthetic light harvesting, the conversion of photons into chemical energy, is responsible for all food and atmospheric oxygen on earth. Understanding the design principles underpinning light harvesting from the atomic to cellular length scales offers the potential of rationally engineering increased photosynthetic yield. The challenge, however, is bridging the large range of length and timescales involved. We have developed a model of excitation energy transfer and light harvesting that accurately spans from isolated pigment-protein complexes to the 100 nm length scale of the photosystem II (PSII) enriched portion of the thylakoid membrane. We explore the emergent features of PSII light harvesting in the presence of quenchers and demonstrate that the phenomenological models used historically fail to capture essential features of regulation by non-photochemical quenching, a process important for plant fitness. This work connects the structure of pigment-protein complexes to the resulting properties of photosystem II light harvesting in vivo, providing a first step towards a predictive model of photosynthesis.

2580-Pos Board B596

Molecular Dynamcis of Light-Harvesting Complex II Embedded in the Thylakoid Membrane

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Plant chloroplasts contain considerable amounts of the antenna protein light-harvesting complex II (LHCII) which is a key player in natural photosynthesis. It is associated to the photosystem II (PSII) and occurs as trimer. Each monomer contains a variety of different cofactors: 8 chlorophyll a, 6 chlorophyll b, and 4 carotenoid molecules. They are responsible for capturing photons and transmitting the excitation energy towards the PSII reaction center. This challenging task requires a highly precise arrangement of the involved chromophores resulting in a specifically fine-tuned ordering of the energy levels and chromophore couplings. Moreover, LHCII can switch between two states: a low light state which allows for efficient excitation transport and a non-photochemically quenched state which protects the thylakoids from too many excitations.
We built a coarse-grained model of LHCII using the Martini force field. Based thereon, we investigated the dynamics of LHCII monomers and trimers in an ordinary dipalmitoylphospatidylcholine (DPPC) bilayer as well as in the thylakoid membrane. The latter constitutes the natural environment of LHCII and contains a large amount of glycolipids. We discuss the differences between the monomeric and the trimeric form as well as the impact of the membrane composition on the properties of LHCII. In addition, we simulated LHCII trimers under low and high light conditions by adapting the protonation state of several residues exposed to the thylakoid lumen. Our simulations capture small configurational changes and provide insight into the exchange of violaxanthin by zeaxanthin by switching from low to high light conditions. This is in agreement with experiments and provides a molecular view on this important process.

2581-Pos Board B597

Increase in Dynamical Collectivity and Directionality of Orange Carotenoid Protein in the Photo-Protective State

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Photo-protection is crucial for photosynthesis efficiency. Cyanobacteria have evolved a unique photo-protection mechanism mediated by Orange Carotenoid Protein (OCP). OCP binds a single ketocarotenoid as the chromophore, essential to its photo-protective function. Under strong green-blue (or white) illumination or high chaotrope concentration, OCP converts from the orange state OCP^O to the activated or photo-protective red state OCP^R. The OCP^R facilitates dissipation of excess energy via direct interaction with allophycocyanin (APC) cores of the light-harvesting antenna Phycobilisome (PB). Picosecond intramolecular dynamics are critical to the photo-protective conformational switching, energy transfer between the APC and OCP, and energy dissipation. In particular intramolecular vibrations at THz frequencies can both provide efficient access to intermediate state conformations and couple to embedded chromophore vibrations for energy dissipation. Here we characterize global picosecond flexibility using temperature dependent terahertz spectroscopy on OCP solutions. The THz absorbance decreases and structural resilience increases in the photoactive state. The dynamical turn on temperature for picosecond dynamics shifts from 200K in OCP^O to 250K in OCP^R, signifying a substantial increase in vibrational collectivity and structural stability. To characterize the nature of the intramolecular vibrations in more detail, we employ our recently developed technique Polarization-Varying Anisotropic Terahertz Microscopy (PV-ATM). The technique isolates specific vibrational bands associated with long range collective motions of the protein structure. For the first time we demonstrate intramolecular vibrational changes with photoexcitation. In particular we find an increase in vibrational directionality in the photo-activated OCP in the 60-72 cm^{-1} and 85-100 cm^{-1} bands. In addition, the orientation of the vibrational motions switches for the 38-48 cm^{-1} band. We suggest that the increased dynamical collectivity and directionality changes with photo-state contribute to OCP efficiently binding and interacting with the APC complex to optimize photo-protective function.

2582-Pos Board B598

Single-Molecule Measurements of Quenching and Photophysical Heterogeneity in Phycobiliproteins

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Phycobilisomes, the membrane-associated light-harvesting antenna system of cyanobacteria, dynamically adjust to changing irradiation by modulating energy capture and transfer over a few seconds or longer, for example by genetic regulation, structural reorganization, or non-photochemical quenching by Orange Carotenoid Protein (OCP). Recent observation of excitation-dependent photodynamics in single intact surface-immobilized phycobilisomes, including ‘‘blinking’’ to dark or dim states, suggests that the phycobilisome itself