Theory of light-harvesting in photosynthesis: A bottom up approach

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The modelling of light-harvesting in pigment-protein complexes requires on one hand to develope theories that take into account the pigment-pigment (excitonic) and the pigment-protein (exciton-vibrational) interaction in a way that goes beyond standard perturbation theories that assume one type of interaction to be weak compared to the other. On the other hand, the parameters entering these theories have to be calculated directly from the crystal structure data, in order to make meaningful predictions and to understand the molecular building principles of these complexes. We developed theory for the calculation of optical spectra and excitation energy transfer and structure-based calculation schemes for excitonic couplings, local optical transition energies of the pigments in their binding site in the protein, and the spectral density characterizing the modulation of site energies and excitonic couplings by the protein dynamics. Here I will present recent applications of the theory and calculation schemes to various photosynthetic pigment-protein complexes and discuss the following questions: Which molecular mechanisms can be used to create excitation energy funnels? Why is there such a large diversity in light-harvesting antennae? Are the reaction centers really so similiar as their structure suggests at first glance and how do the small differences influence the light-harvesting antennae? Why do purple bacteria use the pigment-pigment coupling to create an excitation energy funnel and plants do not possess a simple energy funnel? How is the site energy funnel, realized in green sulfur bacteria related to the dissipation of exciton's excess energy by the proteins and the decay of coherences?