Theory of light-harvesting in photosynthesis

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In photosynthesis, light energy absorbed in light-harvesting pigment-protein complexes is transferred via an exciton mechanism to the reaction center where it is used to drive electron transfer reactions. The quantum efficiency of the transfer is close to 100 percent, that is, almost all excitons created reach the reaction center. In order to bridge the gap between the crystal structures of these light-harvesting proteins and optical experiments probing their function, two essential problems need to be solved. On one hand, theories of optical spectra and excitation energy transfer have to be developed that take into account the pigment-pigment (excitonic) and the pigment-protein (exciton-vibrational) coupling on an equal footing. On the other hand, the parameters entering these theories need to be calculated from the structural data. I will give a summary of recent approaches to solve the above problems using tools from non-equilibrium statistical mechanics, like non-Markovian density matrix theory, for the derivation of expressions for optical lineshape functions and rate constants for excitation energy transfer and a combination of quantum chemical, electrostatic and normal mode simulations for the parameters of the Hamiltonian of the pigment-protein complex. Small model systems like the water-soluble chlorophyll-binding protein are used to test different theories and calculation schemes. Application of the methods to larger complexes like the Fenna Matthews Olson complex of green sulfur bacteria and photosystem II of cyanobacteria and higher plants reveals different strategies developed in these systems for efficient light-harvesting.