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Energy transfer in the photosynthetic unit of green sulphur bacterium

Juha M. Linnanto
University of Tartu, Estonia

Statement of the problem: Photosynthesis is the most important biological energy conservation pathway on the Earth, and oxygenic photosynthesis produces most of the oxygen we breathe. Photosynthetic organisms make use of solar energy to create free chemical energy that is used in their metabolic reactions. For light energy to be store by photosynthesis, it must first be absorbed by pigment molecules associated with the photosynthetic apparatus. The Light-Harvesting (LH) antenna systems collect sunlight and transfer excitation energy rapidly to the photosynthetic Reaction Centers (RCs), where the energy is trapped in an electron-transfer reaction. Photosynthetic Units (PSUs) of phototrophic organisms have such structural architecture that light energy absorbed by an LH antenna is transferred to a RC through efficient Energy Transfer (ET). To investigate these processes both experimental and theoretical methods are needed. There are available only a few experimentally solved atomic-resolution X-ray LH and RC structures. Thus, different computational methods together with experimental structural and spectroscopic information are needed to generate three-dimensional pigment-protein LH antenna model structures. The purpose of this study is to generate atomistic model for the PSU of Green Sulphur Bacteria (GSB) and to explain solar energy transfer processes in this system. Experimental X-ray, electron microscopy, and cryo-electron microscopy LH and RC structures of GSB are used as initial structure models in this study. The PSU of GSB is very interesting system because it contains both self-aggregated pigment oligomer LH complexes as also pigment-protein LH complexes. All of these complexes have their own specific absorption spectrum and energy levels. The PSU of the GSB allows some of GSB to live in extraordinarily low light conditions under which no other photosynthetic organisms can grow, such as in the bottom of stratified lakes, deep in the sea and near geothermal vents.

Methods: Classical and quantum chemical methods together with experimental data were used to generate macroscopic PSU complex of GSB. Both semi empirical and density functional method were used to optimize local protein environment and to find out correct pigment conformations. Conformation of pigment has been shown to have an significant effect on the transition energies and transition dipoles of the pigments. Indicating that molecular conformation has strong role in the function of molecular complexes. Absorption and circular dichroism spectra of the complex were calculated by using molecular exciton theory to verify quality of the model. At the end, energy transfer rates were calculated by using molecular exciton theory to model energy funneling processes in the system.

Finding: Local protein environment is able to modify conformation of the pigment molecule. These different conformers have different spectroscopic properties and this has an effect on the spectroscopic and ET properties of the LH and PSU complexes. Architecture of the PSU–energy transfer donor and acceptor states are physically close to each other–allows effective energy transfer processes towards to the RC.

Conclusion: The study demonstrates that modern computational methods allow producing high quality pigment-protein model structures. It indicates that photosynthetic organisms are able to fine tuning the light-harvesting and energy transfer properties by modifying local protein geometry/structure. In such a way Nature is able to build up PSU complex with optimal intra-complex and inter-complex ET flowing process. This study giving important information needed to design self-assembled molecular nanowires those might be primary elements of future artificial photosynthetic devises.

Biography

Juha Matti Linnanto is from the Institute of Physics, University of Tartu, Estonia. He is computational/theoretical chemist. His research interest cover various aspects of theory and modeling of electronic, optical, structural and transport properties of photosynthetic pigments, pigment-protein complexes, self-aggregates, dendrimers and metal-organic compounds. His computation competence includes classical molecular mechanic methods; molecular dynamic methods; semi-empirical quantum chemical methods; density functional methods; ab-initio methods; configuration interaction methods; time-dependent Hartree-Fock/density functional methods; and molecular exciton theory. He has published >50 articles in international peer-review journals, has >1400, H index 24 (Web of Science). Currently he is an associate professor (Laboratory of Biophysics) at the Institute of Physics of Tartu University.

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