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Protein-Controlled Electronic Energy Transfer in PSI

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Photosystem I (PSI) is the most efficient light-to-energy conversion apparatus. To reach and maintain high quantum yield, all processes in PSI, including electronic energy transfer (EET) between the pigments, must be exceptionally rapid. After the absorption, excitation energy can be transferred to the nearby pigment over tens of angstroms. Such dynamics is determined by inter-pigment couplings J_{mn}, described in terms of the electronic transition densities [1], that can be replaced by the atomic transition charges [2]. We have investigated the excitation dynamics in four complexes of PSI light-harvesting antenna LHCI (see Fig. 1). The structure of the antenna was obtained from the PDB (PDB ID: 5L8R) [3]. We used the aforementioned approach to obtain the chlorophyll-chlorophyll coupling energies in vacuum and in protein environment. For accounting for the protein environment, we used similar approach to our previous research [4]. We have also accounted for the solvent screening effect [5] and compared the properties of EET with the effects of protein and solvent screening and without (vacuum).

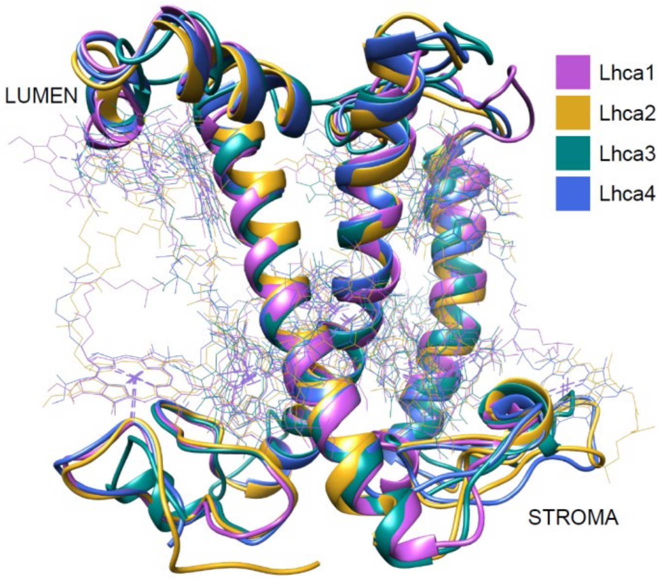

Fig. 1. Lhca1-4 complex structures mapped on top of each other.

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