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ENVIRONMENT-DEPENDENT CHLOROPHYLL-CHLOROPHYLL CHARGE TRANSFER STATES IN Lhca4 PIGMENT-PROTEIN COMPLEX

Gabrielė Rankelytė[1,2], Jevgenij Chmeliov[1,2], Andrius Gelzinis[1,2], Leonas Valkunas[1,2]

[1]Institute of Chemical Physics, Faculty of Physics, Vilnius University, Lithuania
[2]Department of Molecular Compound Physics, Centre for Physical Sciences and Technology, Vilnius, Lithuania
gabriele.rankelyte@gmail.com

Photosynthesis is one of the most important processes on Earth. The most efficient organisms that carry out photosynthesis are land plants. In the thylakoid membrane of chloroplasts there are two systems that carry out photosynthesis – Photosystem I (PSI) and Photosystem II (PSII), both with their own light harvesting complexes - LHCI and LHCII. PSI is the most efficient light-to-energy conversion apparatus with quantum yield almost equal to 1 [1]. One of the conditions needed for high efficiency is very fast energy transfer between the molecules in light harvesting complex. Light-harvesting complex of PSI absorbs and emits light at the longest wavelengths compared to other pigment-protein complexes. In plants light harvesting antenna of PSI is composed of four species of LHCI complexes. They all have very similar structure, however, their spectral properties are different. The most red-shifted peak (at around 733 nm) is observed in the fluorescence spectrum of Lhca4 light harvesting sub-complex [2].

The excitation dynamics in LHCI is highly affected by the charge-transfer (CT) states that occur between two or more pigments (chlorophylls or carotenoids). Some sites in which CT states occur in LHCI are known, however, they do not completely explain the spectral properties of this antenna, such as the red-shifted peak in fluorescence spectrum. The energy of the excited states of pigments (including the CT states) are highly affected by the surrounding environment, consisting of other pigments and the protein chain. Therefore, it is necessary to account for the environment in order to model light-harvesting complexes properly.

The structure of Lhca4 was obtained as the 4th chain of PSI supercomplex structure, freely accessible on Protein Data Bank (PDB) [3]. We performed quantum chemical calculations to obtain energies of chlorophyll dimer CT states in vacuo. We then included the environment (single chlorophylls, carotenoids and the protein chain molecules in their ground state) in our calculations by obtaining atomic partial charges of both environmental blocks and dimers of interest and evaluating the electrostatic interaction between these charges (see Figure [fig:Energy-level-diagram]). In case of the protein chain, we estimated the most probable protonation pattern in neutral solution and also looked into other possible protonation patterns. The energy shifts caused by the environment were calculated considering 9 different possible protonation patterns of the protein and were compared to those obtained when the protein chain was considered to be in its most probable (estimated) protonation state.

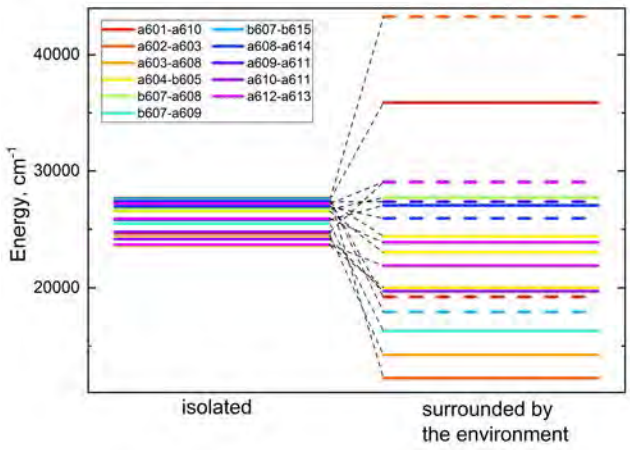

Fig. 1. Energy level diagram of dimer CT state energies.

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