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Light absorption and energy transfer in photosynthesis: Toward extending our current biosignatures

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In the recent success in detecting for extrasolar planets, several habitable planets, which can sustain liquid water, have already been discovered. From reflection spectra on exoplanets, what and how to detect signs of life, biosignatures, have been controversial (Kiang et al. 2007). One of proposed biosignatures is vegetation red edge (VRE), which is observed from reflectance spectra on the Earth. VRE is identified as a sharp contrast in about 700 - 750 nm due to the absorption in visible region by photosynthetic pigments like chlorophylls and the reflection in NIR region. However, VRE is an effective as biosignature only if exovegetation shows the same spectral feature to that on the Earth (Seager et al. 2005). Therefore, the criterion as biosignature needs to be extended when the primary stars are totally different. Because in future missions searching for a second earth, the M type stars (cooler than Sun) will be the main targets, as the first step, we focused on the fundamental properties of purple bacteria which absorbs longer wavelength radiation (1025 nm).

We investigated light absorptions and excitation energy transfers (EETs) based on quantum dynamics simulations for light harvesting complexes (LHCs), which contain array of photosynthetic pigments. After light reaches in LHCs, effective EET is accomplished by corporative electronic excitation of the pigments. We used theoretical models for LHCs in purple bacteria (LH2s). LH2 is made of 2 rings: inner ring (B850) and the outer (B800), as shown in Figure. In our model, a dipole-dipole approximation was used for the electronic excitations. The low-lying electronic excited states of a LH2 were computed by using transition dipole moment of first excited state of each pigment calculated at time-dependent density functional theory. Corresponding to the light absorption process, the oscillator strength in the system could be computed. The oscillator strength of one LH2 was in a good agreement with the experimental value. Subsequently, quantum dynamics simulations were performed by Liouville equation to examine the EET process. In this model, the densities relaxed according to energy gradient. This treatment corresponded with the EET process. The relaxation parameters were determined based on the energy transfer time from B800 to B850 (0.8 ps). The calculated transfer time between two LH2s was determined to 2.72 - 3.67 ps in good agreement with the experiment values (2.0 - 10.0 ps). In order to deal with more realistic system, we calculated at a macro structural model. The calculated systems were composed of 7 LH2s and 19 LH2s, where LH2s were aligned in triangle lattice. As the system size increases, the oscillator strength shifted longer and the transfer velocity became faster. In photosynthesis, collected energies are efficiently transferred to lower energy sites where redox reactions take place, very efficiently by EET. When two pigments in central LH2 in the system were exchanged to pigments absorbed longer wavelength radiation (850 nm to 890 nm), the transfer velocities became faster. Moreover, in order to examine for what environments the absorption spectra of purple bacteria were optimized, the absorption efficiency was calculated from blackbody spectra expected in typical extrasolar planets. As a result, the absorption efficiency was maximum at the emission spectrum of a black body at around 200 K. Furthermore, the Light absorptions and EETs in purple bacteria, cyanobacteria and plants will be examined by using our methodology.

Keywords: biosignatures, extrasolar planets, photosynthesis, quantum chemical calculation, light harvesting, purple bacteria