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The energy transfer calculation of light harvesting systems for detecting biomarker on extrasolar planets

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A large number of extrasolar planet candidates have been detected by Kepler. Moreover the planets in habitable zone have already been detected, and ELP (Earth-like planet) is expected to be discovered. As detecting signs of life from the spectrum of ELPs in future, several indicators called as biomarkers or biosignatures were proposed [1]: (1) molecule absorption line, such as O_2, CH_4, and (2) red edge, which is a strong contrast in NIR (~700-750 nm) that derives from plant's feature. Red edge comes from absorption in visible by the chlorophyll, which is one of the photosynthetic pigments, and reflectance in NIR due to the structural features such as cell wall, air space of leaf and so on. The spectrum considered as red edge is observed by remote sensing or earthshine [2].

However, it is not guaranteed that red edge on extrasolar planets is detected as same wavelength on Earth. In fact, the photosynthetic organisms on Earth harvest light according to the surrounding environments to efficiently use light having a variety of wavelength that reaches, and of course their spectrum varies. In case of photosynthesis in extrasolar planets, photosynthetic organisms should evolve as optimized to utilize their principal star. We focus on the fundamental light harvesting mechanism and aim to propose how to detect the spectrum of the planet orbiting the different spectrum types of star otherwise Sun. At first, we adopted our models to photosynthetic organisms on Earth and compared with the experimental data. The light harvesting antenna in these organisms differs from kinds of pigments and their conformations.

We investigated the mechanism how the organisms harvest light by quantum mechanical calculation. However, because of the cost difficulty, we introduced an approximation instead of calculating all the electrons in the system. First, we calculated the excitation energies and the transition moments from the ground state to the excited states in the pigments by TDDFT (time-dependent density functional theory) [3]. Then, by introducing the transition moments of each pigment to the antenna, which consists of several kinds of pigments (other environment: proteins, solvent,...), we assume as an approximation that one pigment has the excited energy and interacts with the other pigments by the dipole-dipole interaction. When the light, as it seems to be considered as traveled from a star to a surface of an extrasolar planet, induces the system, we traced the time evolution of the energy transfer by solving Liouvile equation. We dealt the light with an external potential. By this method, we can calculate the spectral intensity and energy efficiency.

In certain types of bacteria, the contrast like red edge can be detected, although the contrast is weaker than that of plants. In purple bacteria, red edge is not detected or emerges in longer wavelength (~1013-1025 nm). In addition, its structure of the antenna is simple so that we adopted easily our model to the bacteria. The calculated spectrum has a good agreement with the experimental result from purple bacteria. We will extend our model to the other species. By comparing the light harvesting mechanisms showing red edge and no red edge, we can examine how red edge emerges in photosynthetic organisms. For the other inducing light condition, we will survey the light harvesting mechanism optimized to extrasolar planets.

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