

## Theoretical investigation on the absorption spectrum of photosystem for the biomarker of extrasolar planets

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Over 800 extrasolar planets have been discovered, and more than 20,000 candidates have been detected. Planets in habitable zone have been observed, and the discovery of Earth-like planets is expected. Great attentions have been paid to the detection of life in extrasolar planets. For the detection, various indices have been proposed as biomarkers. One of the indicators is red edge[1], which is a characteristic steep gradient observed in the near-infrared region of around 750 nm in plant's reflection spectra [2]. In fact, red edge can be observed in the reflection spectrum of the Earth via the Moon (earthshine [3]). Since red edge is affected by many factors, its precise predictions is not simple. However, a leaf chlorophyll absorption is thought to be the major factor of red edge [2].

On Earth, photosynthetic organisms have evolved through the collection of sunlight. On the other hand for the extrasolar planets, whose surrounding space environment has different spectrum from their primary star, photosystems should be different in many parts, such as pigment types and arrangements even though the environment is similar to the Earth.

Before predictions of biomarkers of extrasolar planets, we examine the basic characters of chlorophylls in photosystems. It is also important for the study of the diverse photosystems on Earth. Chlorophylls are concentrated in a chloroplast, and form pigments-protein complexes in the photochemical systems.

The purpose of this research is to characterize the absorption spectrum of chlorophylls in a photosystem. First of all, we calculated the absorption spectrum of the pigment in methanol using DFT based polarization continuum model (PCM) method, and confirmed the validity of our calculation method. Then, quantum mechanics/molecular mechanics (QM/MM) calculations were performed for the absorption spectra of the photosystem. Each chlorophyll was included in the QM region. We found that the absorption wavelengths are shifted about +10 nm by the effects of the protein environment. Similar influence was observed by the effect of amino acid coordination to the central Mg ion in the chlorophyll. These calculated results indicate a fine modulation character of the adsorption wavelength for the photosystem. This character is important for photosystems in extrasolar planets as well as in extreme conditions on Earth.

[1] N. Y. Kiang et al., *Astrobiology*, 7 (1), 252, 2007

[2] S. Seager et al., *Astrobiology*, 5 (3), 372, 2005

[3] L. Arnold et al., *Astronomy&Astrophysics*, 392, 231, 2002

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