低温度周りに適応可能な光合成色素の理論的探索：中心金属による物理化学的特性の調整

Theoretical search for photosynthetic pigments applicable around low temperature stars: Modulation of physical-chemical properties by central metals

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A lot of extrasolar planets have been discovered in the habitable zone, and the number of samples will be increasing in future. In order to discover planets which harbour lives, it will be a significant achievement to identify potential biosignatures, which are traces of life from planetary spectra. Gaseous molecules such as oxygen and ozone and spectral features in surface vegetation called as "vegetation red edge (VRE)" are considered as biosignatures. In current observations, planets around M dwarfs, lower temperature stars than the Sun, have been focused, and there are large uncertainties in how assumed photosynthetic organisms evolve in the planets and how they would exhibit spectral features. Recently, it has been shown that the Earth-type photosynthesis can be evolved even around M dwarfs, considered lighting conditions in shallow water and how phototrophs can adapt to it (Takizawa, K., et al.: 2017, *Scientific Reports*, **7**, 7561). Moreover, an interesting example has been discovered that a cyanobacteria, which are categorized into oxygenic photosynthetic bacteria, becomes to utilize longer wavelength radiation for photochemistry than previously known, after grown under near infrared light, 750 nm (Nürnberg, D. J. et al.: 2018, *Science*, **360**, 1210.). Accumulating such knowledges and benchmarks from various points of view would lead to implications for future observations.

We investigate thoroughly by quantum chemical calculations the properties of photosynthetic pigments like and artificial pigments which might form on early Earth or other planets to unravel the red limit of the pigment. Photosynthetic pigments play a central role to convert available light energies into chemical energies. Chlorophyll has a tetrapyrrole ring with a metal ion such as Mg in the center of the ring. The ring structure can encapsulate a variety of metals to have a modulation of physical-chemical properties. Starting with the tetrapyrrole, we search for the pigments which are applicable around M dwarfs by calculating their basic structures, functional groups, central metals and solvents to determine the absorption wavelength and other properties. At first, we focused on the role of the central metal. Metals *M={H2, Mg, Ca, Ni, Cu, Zn, Sr, Cd, Hg, Pb, ...}* are put in the center of rings and are evaluated. According to our calculations, the wavelength of the first excited state is slight long in *M=Ni* in chlorophylls *a* and *b* and bacteriochlorophylls *a* and *b*. Additionally, binding eneries for metals into the rings in solvent conditions, molecular orbitals and reactivities (ionization potential and electron affinity) are analyzed for each pigment.

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