Synthesis of Molecular Catalysts for Interconversion of Water and Oxygen

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【Outline of survey】

Plant photosynthesis is the most frequently occurring chemical process on earth wherein solar energy is harnessed for reduction of carbon dioxide and oxidation of water to produce carbohydrates, which function as reservoirs of chemical energy. Plants use water as an electron source (a reducing agent) and produce dioxygen as a byproduct. The process of respiration is complementary to photosynthesis. Dioxygen is reduced to water with electrons obtained via combustion of carbohydrates. The concomitant generation of chemical energy is used to sustain life. These natural complementary reactions that occur between water and dioxygen were optimized over a very long period of biochemical evolution and provide the ultimate means for energy storage and utilization. These highly efficient reactions are enabled by large and precisely structured metalloenzymes, whose mechanisms of action are highly complex. In this study, we synthesize and investigate the function of chemical models of the active sites of metalloenzymes that act as mimics of the active sites of enzymes involved in reactions contributing to the interconversion of dioxygen and water with the objective of understanding how metalloenzymes catalyze these reactions. Results are expected to provide guidelines for the design of new, efficient and environmentally friendly molecular catalysts for energy conversions involving interconversion of water and dioxygen.

【Expected results】

Electrons obtained via oxidation of water in a manner similar to that of photosynthesis may be used for hydrogen production in electrolysis of water and proton reduction in industrial fuel cells provides energy in a manner similar to that of respiration. Selection of the most energy efficient of the multi-electron conversions is a significant technical challenge in development of industrial catalysts. Thus, in addition to providing a greater understanding of the fundamental biochemical processes of photosynthesis and respiration, this research project is also designed to provide insight into design of catalysts for the future hydrogen economy based on fuel cell technologies that use hydrogen as a clean and renewable energy source.

【References by the principal researcher】

"An Elaborate Functional Model of Cytochrome *c* Oxidase Active Site Displaying a Unique Conversion of a Heme-m-peroxo-Cu^{II} Species to a Heme-superoxo/Cu^{I}", *Angew. Chem. Int. Ed.* 2005, *44* (12), 1836-1840.

"Characterization of a Dinuclear Mn^{V}=O Complex and Its Efficient O_2 Evolution in the Presence of Water", *Angew. Chem. Int. Ed.* 2004, *43* (1), 98-100.

【Term of project】 FY 2005 - 2009	【Budget allocation】 79,700,000 yen
【Homepage address】 http://narutalab.ifoc.kyushu-u.ac.jp	