



**Title of Project : Stimuli-responsive Chemical Species for the
Creation of Functional Molecules**

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【Purpose of the Research Project】

Recent developments in the field of “elemental science” based on the efficient utilization of the intrinsic character of each element are remarkable. A variety of fascinating compounds having unusual bonding schemes and structures have been spectroscopically characterized or even isolated owing to the creative design of ligands and substituents. Representative examples include those containing silicon-silicon triple bonds, π -single bonds, five- and six-coordinate carbons, and nucleophilic borons. A notable point is that most of them are highly stimuli-responsive molecules and are thus readily converted to high-energy species that possess high potential for molecular functions.

In this project, we aim to establish the fundamentals and explore applications of such “stimuli-responsive chemical species” through joint studies between leading chemists in various research fields including organic, inorganic, materials, theoretical, and biological chemistry, with the goal of creating new types of functional molecules.

【Content of the Research Project】

The valence shell of main group elements of the third and lower rows of the periodic table is distant from the nuclei and high in energy. In addition, the size of the s-orbital and the p-orbitals is very different. Thus, the hybridization of these orbitals is generally difficult. This partially contributes to the transition metal-like properties of such elements. Innovative functional molecules are to be created by joint research involving main-group element and transition metal chemistry. Indeed, main group elements of the third row and transition metals are known to play important cooperative roles at the active sites of enzymes in essential biological processes.

Molecular compounds with new functionality derived from characteristics inherent to each element are targets in this Scientific Research on Innovative Areas project. New reactions, molecules with new functions, and new catalysts are to be developed through joint research studies, and the elucidation of enzyme reaction mechanisms and the development of artificial enzymes are to be achieved. To advance the

scientific research project, we have set up the following four sub-projects.

A01: Stimuli-Responsive Chemical Species for the Development of Functional Reagents. Highly polarized chemical bonds using main-group elements are to be designed and prepared. The stimuli-responsive chemical bonds are expected to activate inert small molecules such as CO₂.

A02: Stimuli-Responsive Chemical Species for the Development of Functional Materials. Compounds with unusual π -bonds such as silicon-silicon triple bonds and π -single bonds are to be designed and synthesized using kinetic stabilization methods.

A03: Stimuli-Responsive Chemical Species for the Development of Functional Catalysts. New types of molecular catalysts are to be developed and new ligands designed utilizing electronically flexible main-group elements.

A04: Stimuli-Responsive Chemical Species for the Elucidation of Enzymatic Processes. The discovery of new stimuli-responsive chemical species and their application for the elucidation of enzyme reactions are to be explored using methods of advanced structural biochemistry and quantum chemical calculations.

【Expected Research Achievements and Scientific Significance】

The invention of new functional molecules is one of the utmost important tasks of chemistry. With the clear-cut concept of “stimuli-responsive chemical species”, it is highly anticipated that the newly discovered reactions, properties, and functions will provide the basis for breakthroughs in socially important issues including renewable energy and environmental problems.

【Key Words】

Stimuli-responsive Chemical Species, High-energy Species, Functional Molecules.

【Term of Project】 FY2012-2016

【Budget Allocation】 1,118,200 Thousand Yen

【Homepage Address and Other Contact Information】

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