【Grant-in-Aid for Transformative Research Areas（A）】

The Pursuit of Functionality Woven by π-Molecular Complexity

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Purpose and Background of the Research

●Outline of the Research

The exploration of molecular photo- and electronic functions not only offers solutions to current energy and environmental issues, through the development of technologies such as energy-saving light-emitting devices and flexible solar cells, but also drives advances in biology and medicinal science through the progress of fluorescence imaging technologies. Thus, the chemistry of designing sophisticated π-conjugated molecules stands at the heart of functional molecular science. However, the creation of scientifically intriguing π-skeletons does not necessarily lead to the development of epoch-making materials. Bridging this gap remains a major issue in the field.

In this context, we focus our attention on the term "molecular complexity", which describes the inherent richness of molecular structures, encompassing factors such as the variety of functional groups, bonding modes, symmetry, and stereochemistry. However, when we turn our attention to molecular photo- and electronic-functions, the essential elements of complexity differ significantly. In this research project, we propose the concept of "*π-molecular complexity*," and through a distinctive hierarchical approach, we take on the challenge of pioneering new molecular functionalities and advancing transformative molecular technologies (Figure 1). Specifically, by combining "structural complexity," which generates new classes of molecules, with "state complexity," which brings about exceptional physical properties and responsiveness, we seek to create advanced π-molecules that forge new frontiers in science. Furthermore, by incorporating "functional-field complexity" optimized for these molecules, we will elaborate advanced π-molecular systems, paving the way toward a diverse array of functional molecular science. By integrating quantum chemical understanding with advanced exploration methodologies, we aspire to establish a new integrated design principle for weaving π-molecular complexity.

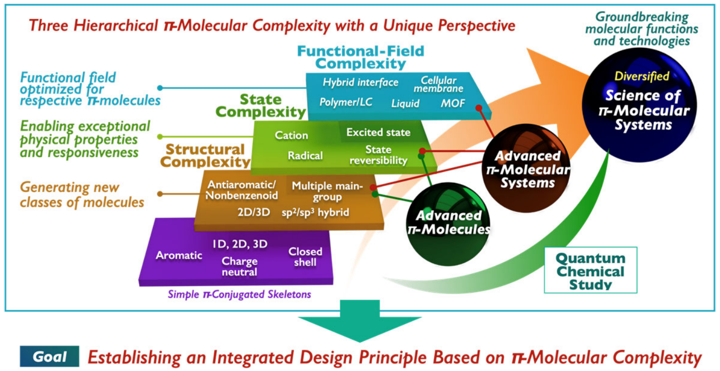

Figure 1. Hierarchical π-molecular complexity: A new paradigm for scientific advancement.

Expected Research Achievements

●Research Strategies in This Research Area

This research area aims to bring about a transformation through two key approaches: (1) the pursuit of π-molecular complexity to create advanced π-molecules at the forefront of chemistry, and (2) achieving groundbreaking molecular functions and technologies, contributing to the advances in science and society beyond the boundaries of chemistry. To this end, we have organized four research groups, A01–A04, and will tackle this challenge through interdisciplinary fusion across 11 distinct fields (Figure 2). The initiatives of each group are outlined below.

A01 Structural complexity: We aim to create unprecedented π-skeletons through diverse approaches, such as harnessing antiaromaticity and non-benzenoid frameworks, introducing novel bonding modes and main-group-based unsaturated bonds, and hybridizing 2D and 3D structures.

A02 State complexity: We aim to realize and control outstanding properties by employing π-molecules bearing charge or spin, precise management of excited states, and reversible control between multiple states utilizing molecular flexibility.

A03 Functional-field complexity: We aim to create novel molecular functions and technologies by optimizing the properties and behaviors of molecules under specific environments, such as device, biological systems, interfaces of multiple materials or phases, and other unique conditions.

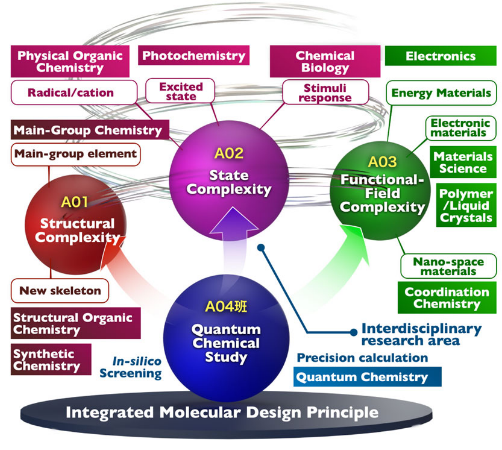

Figure 2. Interdisciplinary fusion in this research area.

A04 Quantum chemical understanding and screening: We aim to systematize insights into advanced π-molecular systems by combining high-precision quantum chemical analysis with in-silico screening of chemical space.

●What do we achieve?

To develop exceptional functional molecule, the key lies in a needs-inspired perspective, accurately identifying fundamental challenges and designing molecular structures that solve them. Indeed, our team has demonstrated the untapped potential of p-molecules through breakthroughs such as fluorescent probes for visualizing previously inaccessible intracellular phenomena and useful molecular systems for solar cells (Figure 3). We aim to pioneer next-generation molecular systems and establish the design principles that underpin them.

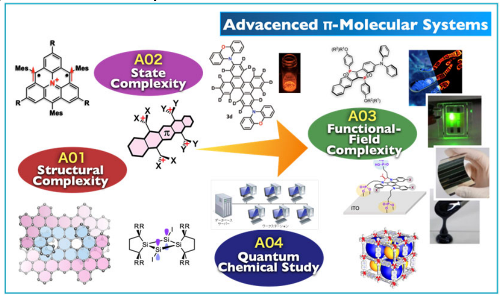

Figure 3. Development of advanced π-molecular systems.

Homepage Address, etc.	https://pi-molecular-complexity.jp