【International Leading Research】

Dynamic Element-Effect Design for Unconventional Molecular Functions

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Purpose and Significance of the Research

●Producing superior molecular functionality from the perspective of "dynamic element-effect design"

In the context of the sustainable development of modern society, the role of chemistry becomes ever more important. In this program, we will tackle three subjects, i) the development of catalysis systems to realize the highly efficient synthesis of useful substances, ii) the creation of functional materials that will bring about innovative advances in materials and life science, and iii) control over the functionality of biomolecular systems. We will approach these subjects from the perspective of "dynamic element-effect design." It should be noted that most molecular functionality is essentially determined by combinations of element-specific properties, as well as by various inter- or intramolecular interactions. An essential issue is to precisely understand how these "element effects" change, synergistically interact with each other, and ultimately produce a given function in a certain environment or energy state. In this context, we will try to understand the correlation between dynamic changes in the element effects and molecular functionality, and through design of the "dynamic elemental effects", we will aim to produce superior catalytic/materials/biomolecular functionality.

● Three key approaches to establish the "dynamic element-effect design"

We will establish the concept of "dynamic element-effect design" through three different approaches, i.e.,: i) precise design of the reaction space to create highly efficient catalyst systems, ii) control over the excited-state space to pursue molecular photo-functionality, and iii) utilization of specific nanospaces, such as metal–organic framework (MOF) and protein nanospace, to acquire unconventional molecular functionality. Among these researches, we identify the development of "photo-induced catalysts" and "hetero-pi-electron systems" as our high-priority projects. To make this approach successful, we have assembled a highly complementary research team that allows interdisciplinary collaborations including not only synthetic chemistry and high-precision quantum-chemical calculations, but also catalysis, photo-chemistry, materials chemistry, protein engineering, and biochemistry.

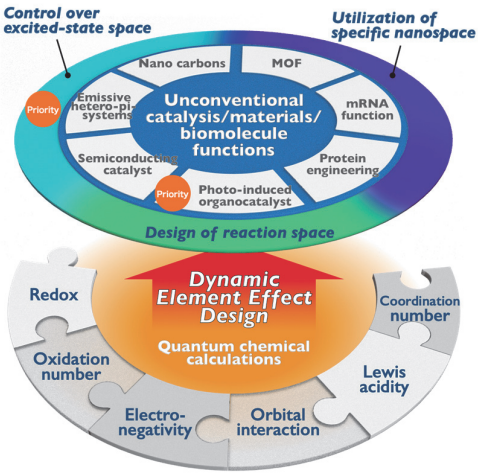

Fig.1 Schematic representation of dynamic element effects design for acquiring unconventional catalysis/ materials/biomolecular functions.

Organization of the Project Team

● A highly complementary team based on a robust collaborative platform

Our team consists of 20 research groups from the Nagoya University, the University of Münster (Germany), the Institut Català d'Investigació Química (ICIQ, Spain), and the University of Frankfurt (Germany). The strength of our team is based on the fact that we have already established a robust collaborative research platform among the participating universities. In particular, the Nagoya University and the University of Münster have a robust history of collaboration over nearly two decades, in which we have accepted a total of 70 German students, and these exchanges have resulted in nearly 80 peer-reviewed papers. We now renew the members from the past for the PIs at the Nagoya University and the University of Münster, so as to be optimized to pursue the catalytic, materials, and biological molecular functionality targeted in this study. The addition of the PIs from the ICIQ and the University of Frankfurt reinforces to pursue the two high-priority projects, *i.e.,* the development of photo-induced catalysts and hetero-pi-electron systems.

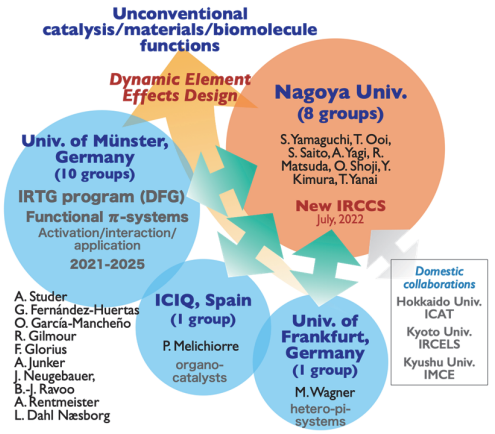

Fig.2 Institutions and members in the international leading research.

Plan for Fostering Early-career Researchers

●Fostering the self-reliance of early-career

The six postdocs (including a postdoc supported by JSPS postdoctoral fellowships) or designated assistant professors will participate to this program. They will go abroad in one-year intervals in the period of 3–4 years. In addition, 18 doctoral students in a steady state with six new D1 students in every academic year for the period 2023–2028 will join this program from the Nagoya University. Each doctoral student will be dispatched to one of the counterpart institutes for at least three months. We expect that three early-career researchers and six to eight doctoral students will stay abroad per year. To support their research activities, the following opportunities will be provided.

Collaborative-research-proposal Awards: Financially supports will be given for the young researchers to conduct their independent researches.

Japanese–German buddy system: Our students will make a pair with the students from Münster students to conduct co-working on their research.

Interdisciplinary tutorial courses: A series of high-quality tutorial courses will be periodically provided to introduce various research areas.

One-on-one discussions with overseas PIs will be set on the occasion of our joint symposium to foster the independence and internationality of the doctoral students.

This program will be conducted as one of the key projects of the Integrated Research Consortium on Chemical Sciences (IRCCS), which has been launched in 2022 in Nagoya University to accelerate collaborative researches over four universities (Hokkaido, Kyoto, Kyushu, and Nagoya). IRCCS will periodically hold young-researcher workshops, to which our young researchers will participate to form a tight network.

Homepage Address, etc.	https://irccs.nagoya-u.ac.jp