Title of Project : Aqua planetology

Yasuhito Sekine
(The University of Tokyo, Graduate School of Science,
Associate Professor)

Research Project Number : 17H06454 Researcher Number : 60431897

【Purpose of the Research Project】

Recent advances in spacecraft explorations have revealed the present/past existence of liquid water on planetary bodies beyond Earth in the Solar system, which include Mars, icy satellites, and planetesimals in the protoplanetary disk.

Our research project proposes a new field of research – aqua planetology – that aims at comprehensive understanding on the roles of liquid water in the origin and evolution of planets and on habitability there. This requires research interactions among geology, geochemistry, biosphere science, astronomy, and planetary science. We try to achieve this goal both by constructing a theory of chemical reactions and hydrological cycles on planetary bodies and by collecting observational evidence through spacecraft missions, such as Hayabusa2, and geochemical analyses of extraterrestrial samples.

【Content of the Research Project】

On a planet that can hold liquid water, similar physicochemical processes occur (Fig.). These include photolysis of water/ice and oxidization on the surface, and water-rock reactions providing reductants and metallic ions to water in the subsurface. These components are connected through hydrological cycles, which in turn results in chemical gradients on the planet and could provide energy for chemotrophic life. To construct a theory of hydrological and geochemical cycles on planets, we set the following research subgroups: A01 water-rock reactions, A02 water-ice interactions, and A03 modeling of cycles.

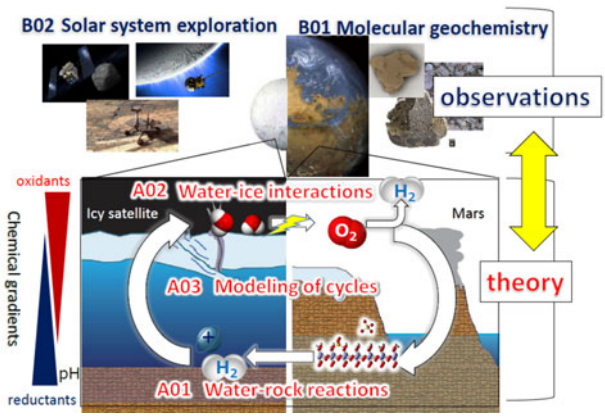

Figure. A conceptual image of this research project.

Based on this theory, we will interpret observational data provided by spacecraft and molecular geochemical analyses of samples. In particular, we focus on revealing chemical properties and physical conditions of water beyond Earth. To this end, we also set the following research subgroups: B01 molecular geochemistry and B02 Solar system exploration.

【Expected Research Achievements and Scientific Significance】

The expected achievements of our research project include 1) understanding of hydrological and geochemical cycles within planetesimals and the factors that control water volume of Earth, and 2) revealing the evolution of aqueous environments and prediction of biosphere on Mars and icy satellites. The former allows to treat the fate of water in planetary formation theory and thus to predict probability of formation of Earth-like aqua planets in the Solar system and beyond. The latter enables us to predict biomarker and biomass on Mars and icy satellites.

These knowledge will be critical in the upcoming ages of both astronomical observations of Earth-like exoplanets and space missions to find life in the Solar system. Aqua planetology will be a unique science to address fundamental questions – Are there any Earth-like planets in the Universe? Is there life beyond Earth?

【Key Words】

Water-rock reactions: Chemical reactions between liquid water and rock materials, including ion exchanges, dissolution, and alterations.
Hayabusa2: Japanese spacecraft mission to C-type asteroid, Ryugu. The spacecraft launched in 2014, and will arrive at the asteroid in 2018. Collected samples will return to Earth in 2020.

【Term of Project】 FY2017-2021

【Budget Allocation】 1,079,400 Thousand Yen

【Homepage Address and Other Contact Information】

http://www-sys.eps.s.u-tokyo.ac.jp/aqua-planetology
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Title of Project : Discrete Geometric Analysis for Materials Design

Motoko Kotani
(Tohoku University, Graduate School of Science, Professor)

Research Project Number: 17H06460　Researcher Number: 50230024

【Purpose of the Research Project】

Creating materials with outstanding functions supports our affluent life and can change our lifestyles and values. Japan is a world leader in materials science and industry, but creation of new materials is due to trial and error based on the experience and intuition of researchers and developers, and takes 20-30 years.

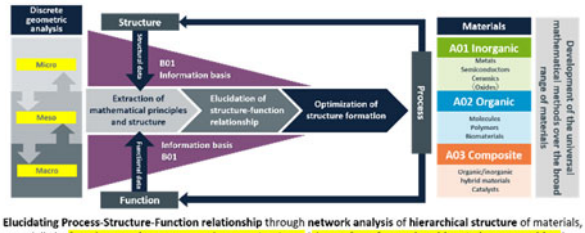
So major data-driven materials design projects applying information science have started in the US, Germany, China, etc. (e.g. Materials Genome Initiative). Computers use findings for search and classifying and material structures are screened for functional materials. But material structure and function correlations are complex, multiscale and involve multiphysics, so getting results with just information science is difficult.

To get meaning from masses of data, scientists must organize information with "good descriptors" that stimulate the imagination. A foundation for realizing and validating materials design is needed to describe layered structures intuitively and reveal the "structure, functions, processes correlation principle" that is key to material creation.

In this context we propose a universal and mathematical materials science through collaboration between mathematics and materials science in which Japan is strong.

【Content of the Research Project】

The aim is to understand the key structure, functions, processes correlation principle and develop geometric methods for that. We apply the latest findings of discrete geometric analysis to **disordered systems** and **multilayered hierarchical systems**, to clarify micro/mesoscopic structure and macroscopic property relationships, to change materials development from a **forward problem** to an **inverse problem**. We use discrete geometric analysis connecting discrete and continuous to find structures hidden behind diversity, and build a foundation for a unified understanding of complex materials.



Elucidating Process-Structure-Function relationship through network analysis of hierarchical structure of materials, especially by focusing on micro, meso, and macro structures (change from forward problem to inverse problem)

We work on the following research based on collaboration between mathematics and materials science.

- **A01 (inorganic): topological materials**
- **A02 (organic): polymeric materials using network analysis**
- **A03 (composite): dynamic structure formation of minimal surfaces and nano-structures**

In particular, we use discrete geometric analysis to **expand the unified theory from ordered to disordered systems (random and complex) and from static control to dynamic control**.

【Expected Research Achievements and Scientific Significance】

In academia the structure-function-process correlation principle is deepening, and new phase materials are being created using the power of information science and data science. In mathematics discrete geometric analysis and discrete dynamical systems that understand complex and multiscale structures hierarchically and study the correlation of discrete and continuous are making great progress. These contribute to materials development and human resources development for the big data society.

【Key Words】

Discrete geometric analysis: The discrete form of geometric analysis analyzing macroscopic geometric structure is discrete geometric analysis. The relationship of discrete and continuous is understood by developing a technique to find the continuous structure behind the discrete data.

Data-driven materials design: If conventional materials development is the forward problem of finding functions from structure, aiming to use data analysis techniques to solve the inverse problem of finding structures that have the required functions is data-driven materials design. It is also called materials informatics.

【Term of Project】 FY2017-2021

【Budget Allocation】 1,002,900 Thousand Yen

【Homepage Address and Other Contact Information】

https://www.math-materials.jp/

Title of Project : Soft Crystals: Science and Photofunctions of Flexible Response Systems with High Order

Masako Kato
(Hokkaido University, Faculty of Science, Professor)

Research Project Number : 17H06366 Researcher Number : 80214401

【Purpose of the Research Project】

This project aims to establish a new science concerning "Soft Crystals", which responds to macroscopic gentle stimuli (e.g. vapor exposure, rubbing, and rotation) that exhibit visually remarkable changes such as luminescence and optical properties. This project also aims to develop novel functional materials on the basis of the scientific achievements. "Soft Crystals" are regulated solids with stable and highly ordered structures. However, they are characteristic of facile structural transformations and phase transitions in response to weak but particular stimuli (Fig. 1). One of scientifically most important challenges is to clarify the phenomena of the formation and phase-transition of "Soft Crystals". Through the scientific research, we aim to create a new area, which can provide new materials beyond the conventional hard crystals and/or soft matters.

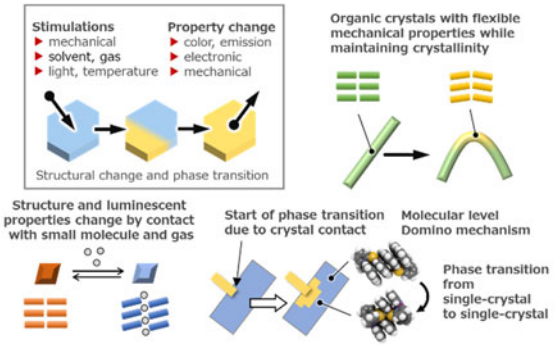


Fig. 1. Soft Crystals: features and examples of flexible new materials with high order.

【Contents of the Research Project】

In this research area, the following three research items are promoted cooperatively to establish a new fusion area with the concept of Soft Crystals.

- Research Item A01: Development of Soft Crystals through molecular design & synthesis
- Research Item A02: Development of Soft Crystals with novel structure & morphology
- Research Item A03: Development of Soft Crystals with superior physical properties & functions

For all three items, several experimental and theoretical research groups will collaborate closely with each other for effective studies. Intensive studies will also be performed collaboratively over these research items.

【Expected Research Achievements and Scientific Significance】

Recently, there are successive reports concerning new crystals which exhibit sensitive changes in luminescence and/or optical properties in response to gentle stimuli. However, those discoveries owe the serendipity or screening because those phenomena are influenced by many complicated factors. It would be essential to understand various factors that govern the formation and phase-transition phenomena of molecular crystals constructed by various intermolecular interactions. Through close collaborations concerning material creation, structural control, physical measurements, theoretical studies, and functionalization, we will achieve the establishment of a new scientific arena, Soft Crystals for the first time to the world. The deep understanding of such complex systems will lead the development of novel materials such as sophisticated responsive materials or those with special functions (Fig.2).

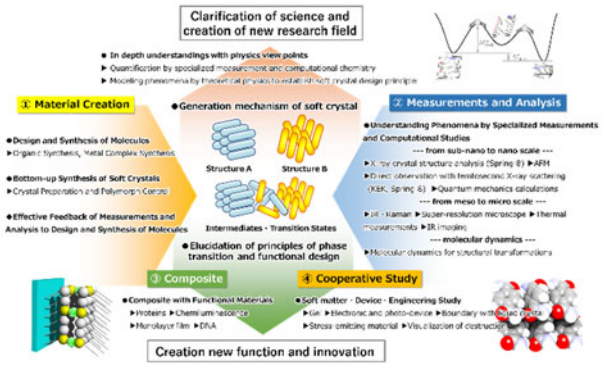


Fig. 2. Research strategy and expected achievements for Soft Crystals.

【Key Words】

Soft Crystals: Crystalline materials with flexibility and high order, which exhibit visual changes such as luminescence and optical properties in response to gentle stimuli.

【Term of Project】

FY2017-2021

【Budget Allocation】

1,012,200 Thousand Yen

【Homepage Address and Other Contact Information】

https://www.softcrystal.org

Title of Project : Chemistry for Multimolecular Crowding Biosystems

Itaru Hamachi
(Kyoto University, Graduate School of Engineering, Professor)

Research Project Number : 17H06347 Researcher Number : 90202259

【Purpose of the Research Project】

Live cells and tissues are multimolecular crowding biosystems consisting of many kinds of biological molecules densely condensed in the closed small spaces. However, conventional biochemical researches ignored such complicated environments where biological molecules reside, and most experiments have been conducted in a purified and diluted solution. Therefore, there are concerns that the obtained results are discrepant with the real functions of biomolecules working in life systems, and also the artificial probes or modulators selected from the pure systems often cannot function in natural biological systems. The purpose of our research project is to establish new chemical approaches available for functional analysis and artificial regulation of biological molecules in the multimolecular crowding biosystems. Accumulating cutting-edge findings from a broad range of research fields (chemical biology, synthetic biology, biophysical chemistry, nano-bioengineering, etc.), we aim to quantitatively describe the multimolecular crowding biosystems and to devise new molecules and methods, which contribute to innovate on bioimaging, drug discovery and disease diagnosis. We envision that our researches could create a new trend for biofunctional chemistry.

【Content of the Research Project】

This research project consists of three teams (A01 – A03) to promote individual researches on their specific topics. Meanwhile, the project highly encourages collaborative researches between the teams. A01 team focuses on design and synthesis of artificial probes and modulators for analyzing and regulating biomolecules available in cells and tissues. A02 team focuses on quantitative analysis and description of multimolecular crowding biosystems based on biophysical and computational chemistry. A03 team focuses on creation of new nanobio-devices for analyzing and diagnosing specific biological molecules (biomarkers) in cells and tissues.
This project also plans to establish Center for Integrated Biomolecular Chemistry (CIBIC) as a hub that underpins and promotes collaborative research between the joining members.

【Expected Research Achievements and Scientific Significance】

Development of artificial probes, sensors and modulators capable of visualizing and regulating biological systems will lead to figure out their new functions and unknown interactive networks in live cell systems (chemical biology research). Quantitative and precise description of multimolecular crowding biosystems will facilitate the rational explanation of such new findings and also greatly accelerate the rational design of functional molecules useful in the crowding biosystems. From the viewpoint of fundamental science, these approaches will promote comprehensive understanding of living cells and organisms as multimolecular crowding systems, which allows for constructing tight and strong bridges between biology and chemistry. Great progress in our research project will also bring technical innovation in precise bio-imaging and highly efficient drug discovery. The innovative nanobio-devices designed by our tools and parameters are expected to provide new methodologies applicable to highly sensitive and rapid medical diagnosis in crude tissues and *in vivo*. Ultimately, establishment of such new chemistry for living systems would contribute to many aspects of progress in life science, life chemistry and medical engineering of Japan.

【Key Words】

Chemical Biology : Chemical research to uncover structure and function of biological molecules and their network systems by exploiting molecular probe and modulator.
Multimolecular crowding biosystems : Biological environments where a variety of biomolecules such as protein, DNA, sugar, ions and small molecules etc., densely exist in a small space.
Nanobio-divice : nano- or microfabricated devices (such as microsensor tip) capable of analyzing a trace of biological molecules with high sensitivity.

【Term of Project】 FY2017-2021

【Budget Allocation】 1,215,500 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Gravitational wave physics and astronomy: Genesis

Takahiro Tanaka
(Kyoto University, Graduate School of Science, Professor)

Research Project Number : 17H06357 Researcher Number : 40281117

【Purpose of the Research Project】

The first direct detection of gravitational waves (GWs) was announced by LIGO in 2016. KAGRA, Japanese GW detector, is going to start operation in full configuration from 2019. We have advantages in GW data analysis, multi- messenger observations of the GW counterparts, and a long history of theoretical research. The purpose of this area is to extract the synergy effects and push forward the new trend of GW physics / astronomy.

【Content of the Research Project】

Currently, we are at the very beginning of GW observation. The impact of this completely new observational probe on the progress of physics and astronomy is high. The task of this innovative area is to conduct world-leading researches in exploiting the research fields that are rapidly expanding.

Fig.1 Image of the expanding research area

As past heritage, preparations for basic data analysis and organizations of follow-up observation teams have been already completed. Taking the advantage of this opportunity, we promote GW physics and astronomy from the following two aspects:

(1) Comprehensive analysis of GWs

Theoretical and data analysis researches closely cooperate to develop new GW data analysis methods beyond the standard framework and extract valuable information.

(2) New physics and astronomy spreading out of GW detection

By the close collaboration of observational and theoretical researches, we promote research fields that are directly driven by GW observations. We will organize and promote research projects focusing on the themes that expect drastic progress in near future.

【Expected Research Achievements and Scientific Significance】

(1) Comprehensive analysis of GWs

For the development of GW physics and astronomy, it is required to extract maximum information from weak GW signals, and the following results are expected: Actual detection of GWs by the KAGRA data analysis team members participating in this innovative area. Proposing and implementing advanced GW data analysis method for the test of gravity (A01). Obtaining restrictions on the equation of state and internal structure of high density matter from binaries including neutron stars (B01). Giving a quantitative theoretical prediction of the GW waveform from supernovae based on state-of-the-art simulations (C01).

(2) Expanding frontiers of GW physics/astronomy

Accelerating the new research trend stimulated by GWs, we expect to obtain the following results: Identification of GW sources and follow-up observation. Testing extended gravity theories and cosmological scenarios (A02). Providing a quantitative prediction on the evolution of massive black hole binaries to be compared with GW observations (A03). Clarifying the radiation mechanism of the counterparts of GW sources, and the formation history of black holes and neutron stars by X-ray and gamma-ray observations (B02). Identification and observation of the optical and infrared counterparts of GW sources. Identification of the production site of r-process elements in the universe (B03). Obtaining new restrictions on background neutrino quantity and average energy from distant supernova origin. Realizing theoretical calculation of more precise supernova explosion based on it (C02).

【Key Words】

Gravitational waves: Space-time ripples predicted by Einstein's general relativity.
Multi-messenger observation: Observing one astrophysical event by infrared, visible light, neutrino, GWs, etc. simultaneously to obtain detailed information.

【Term of Project】 FY2017-2021

【Budget Allocation】 1,079,000 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Frontier research on chemical communications

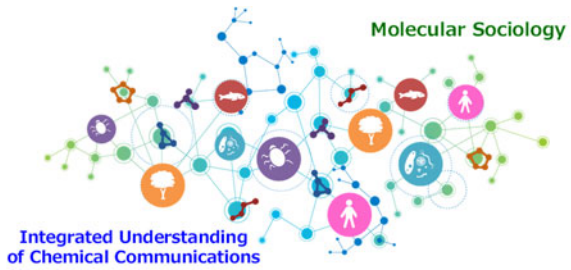
Hideaki Kakeya
(Kyoto University, Graduate School of Pharmaceutical Sciences, Professor)

Research Project Number : 17H06400 Researcher Number : 00270596

【Purpose of the Research Project】

Many natural products have served as pharmaceuticals, agrochemicals, and their leads because of the structural and biological diversity. However, essential roles of natural products as chemical communication molecules among microbes, animals, plants, et cetera have not been fully elucidated. Integrated understanding of various kinds of chemical communications could therefore accelerate functional regulation by utilizing chemical communication molecules.

This research project aims at not only developing innovative high-order analysis platforms, but also at clarifying essential roles of natural products as chemical communication molecules in the natural environment, leading to development of useful chemical tools as well as pharmaceuticals/agrochemicals leads. In addition, this research project would contribute to the advancement in medical, agricultural, and food sciences, as well as open up a new discipline, "Molecular Sociology", which would focus on the frontiers in chemical communications in a variety of biological species.



【Contents of the Research Project】

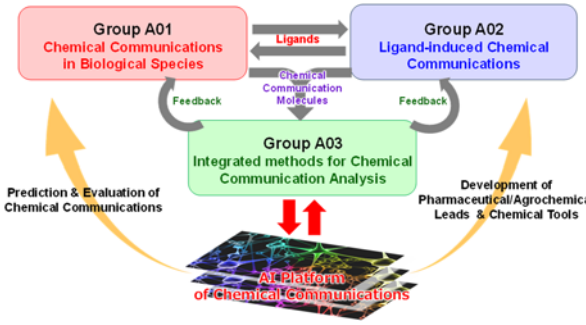
In this research area, the following three research groups interact closely with each other.

Group A01 (Chemical Communications in Biological Species): Screening and development of bioactive natural products as chemical communication molecules by a target-based phenotypic screening approach.

Group A02 (Ligand-induced Chemical Communications): Development of bioactive synthetic ligands as chemical communication molecules by theoretical design & synthesis and physicochemical approach.

Group A03 (Integrated Methods for Chemical Communication Analysis): Development and application of integrated platforms for identifying chemical communication molecules and analyzing their modes of action.

Proposal with synergistic, transversal, and applied perspectives will be openly recruited for these research items.



【Expected Research Achievements and Scientific Significance】

This research project will establish a new scientific principle of "Molecular Sociology" in regard to chemical communications in the natural environment, which will result in the paradigm shift not only in natural product chemistry but also in chemical biology. Moreover, a new class of useful chemical tools as well as pharmaceutical and agrochemical leads will be developed, contributing greatly to human welfare in the future.

We also focus on international collaboration among interdisciplinary research fields, leading to international network development and bringing up young scientists broader views and higher expertise.

【Key Words】

Chemical Communications, Chemical Signal, Molecular Sociology, Natural Product Chemistry, Bioactive Ligand, Chemical Biology, Chemical Genomics, Chemical Ecology, Cheminformatics, Artificial Intelligence (AI), Bioinformatics

【Term of Project】 FY2017-2021

【Budget Allocation】 1,108,700 Thousand Yen

【Homepage Address and Other Contact Information】

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Title of Project : Hybrid Catalysis for Enabling Molecular Synthesis on Demand

Motomu Kanai
(The University of Tokyo, Graduate School of Pharmaceutical Sciences, Professor)

Research Project Number : 17H06441 Researcher Number : 20243264

【Purpose of the Research Project】

Organic synthesis has been consistently developed and refined up to the present, but several important issues remain unresolved. One such issue is the practical synthesis of high-value-added complex molecules through streamlined multicatalytic reactions starting from readily-available, abundant molecules. Nature utilizes multicatalytic (i.e., multienzymatic) systems for the biosynthesis of natural products. The most effective artificial multicatalyst system in a flask so far, however, promotes only two or three reactions at most.

With this in mind, the purpose of our research project is to develop hybrid catalysis, a multicatalytic system involving catalysts with distinct individual functions. Integrating the functions of multiple catalysts, hybrid catalysis will enable molecular synthesis of high efficiency, flexibility, and adaptability on demand, starting from abundant organic molecules such as hydrocarbons and other carbon feedstocks (Figure).

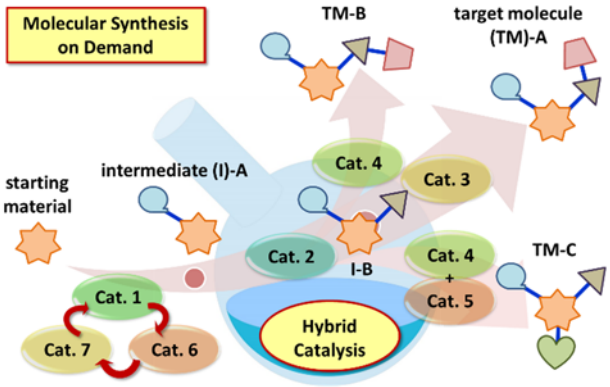

Figure. Molecular Synthesis on Demand Based on the Development of Hybrid Catalysis, Integrating Functions of Multiple Catalysts

【Content of the Research Project】

Based on the interdisciplinary research ranging from physics to chemistry, we intend to develop conceptually new catalyses leading to innovative organic synthesis. The following three research aspects, A01, A02, and A03, work together to cultivate the supremely high-level research only possible with this project framework.

A01 (Activation): Identification of hybrid catalyses activating stable and abundant organic molecules, including hydrocarbons and other carbon feedstocks.

A02 (Control): Identification of selective hybrid catalyses that precisely control multiple reaction parameters, including regio-, functional-group, and stereoselectivity, with high flexibility and adaptability.

A03 (Continuity): Identification of domino catalyses rapidly increasing structural complexity, starting from simple molecules to produce multifunctional molecules.

【Expected Research Achievements and Scientific Significance】

The following ground-breaking achievements are expected: 1) efficient conversion of stable and abundant carbon feedstocks, such as hydrocarbons, to valuable organic molecules; 2) on-demand synthesis of a specific target molecule among structurally diverse molecules; 3) practical synthesis of target molecules without restriction due to structural complexity. Inducing innovation in molecular synthesis, this project will vastly expand the structural variety of organic molecules available to human beings. This project will markedly influence the various fields that require organic molecules, such as the pharmaceutical sciences, agriculture, and industry. This project will in the long term benefit human healthcare, well-being, and the advancement of civilization and society.

【Key Words】

Hybrid catalysis, molecular synthesis on demand, activation of organic molecules, carbon feedstock, reaction control, regioselectivity, functional-group selectivity, stereoselectivity, domino catalysis, organic synthesis, metal complex catalyst, organocatalyst, solid catalyst, photocatalyst, polymerization catalyst

【Term of Project】 FY2017-2021

【Budget Allocation】 1,224,600 Thousand Yen

【Homepage Address and Other Contact Information】

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hybrid_catalysis@mol.f.u-tokyo.ac.jp