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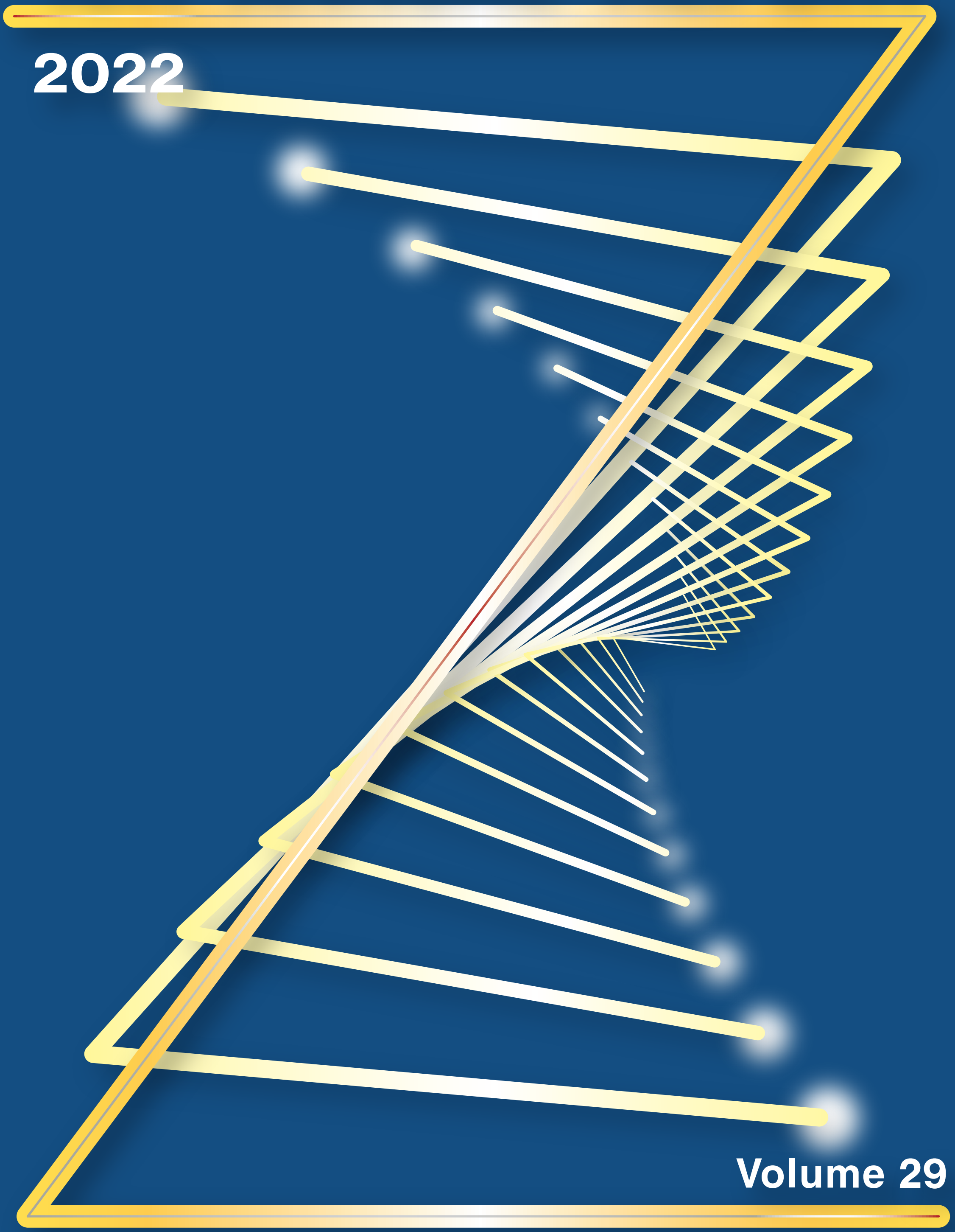
ICR ANNUAL REPORT

2022



Volume 29

Institute for Chemical Research
Kyoto University

ICR ANNUAL REPORT 2022 (Volume 29) - ISSN 1342-0321 -

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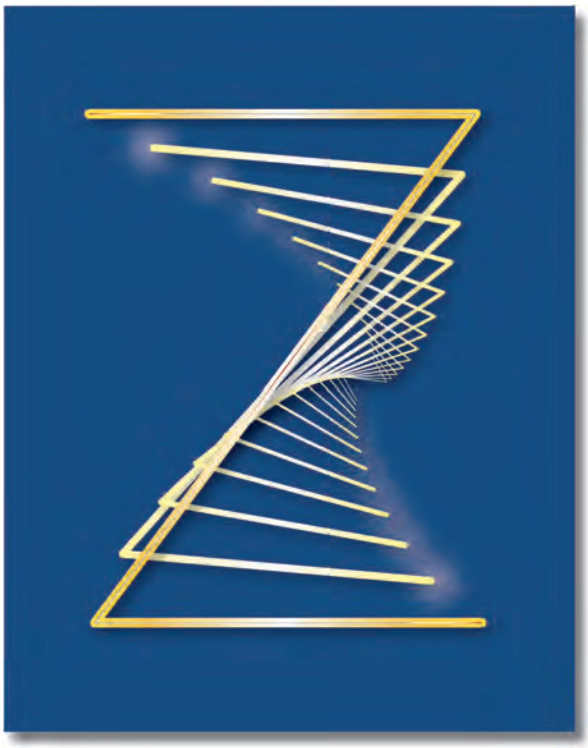
Request for Cooperation to the ICR's 100th Anniversary Fund

ICR has established a fund called "The ICR's 100th Anniversary Fund," which is a part of the Kyoto University Fund. Its aims are to hold the 100th anniversary event in 2026, to enhance the educational and research environments at ICR, and to promote social contribution activities. We ask for your kind understanding and cooperation.

■ http://www.kikin.kyoto-u.ac.jp/contribution/chemical/

ICR ANNUAL REPORT 2022



Institute for Chemical Research
Kyoto University

Volume 29

Preface

The history of the Institute for Chemical Research (ICR) dates back to 1915, when the Specialized Center for Chemical Research, the predecessor of ICR, was established for research and production of Salvarsan and other pharmaceutical chemicals at the Faculty of Science, Kyoto Imperial University. In 1926, ICR was formally established as the first research institute in Kyoto University, with the founding philosophy “To Excel in the Investigation of Basic Principles of Chemistry and Their Applications.” ICR has promoted pioneering studies with a focus on basic sciences ever since. Our staffs include 120 faculty members, 200 graduate students including 50 from foreign countries, and 60 researchers. These scientists are grouped into 30 laboratories divided into five research divisions—Synthetic Chemistry, Materials Chemistry, Biochemistry, Environmental Chemistry, and Multidisciplinary Chemistry—and three research centers—Advanced Research Center for Beam Science, International Research Center for Elements Science, and Bioinformatics Center. The laboratories are diversely affiliated with the graduate schools of science, engineering, agriculture, pharmaceutical sciences, medicine, and informatics.

The research activity of ICR encompasses a wide range of scientific disciplines, including physics, biology, and informatics as well as chemistry. ICR members are conducting cutting-edge research not only in fields of their own specific disciplines but also in interdisciplinary and innovative fields. Some of outstanding research achievements in 2022 are as follows: *1) A Carlactonoic Acid Methyltransferase that Contributes to the Inhibition of Shoot Branching in Arabidopsis; 2) A Triple Photoredox/Cobalt/Brønsted Acid Catalysis Enabling Markovnikov Hydroalkoxylation of Unactivated Alkenes; 3) Size-Controlled Quantum Dots Reveal the Impact of Intraband Transitions on High-Order Harmonic Generation in Solids; 4) Field-Free Superconducting Diode Effect in Noncentrosymmertic Superconductor/Ferromagnet Multilayers; 5) Nitrogen Reduction by the Fe Sites of Synthetic [*Mo_3S_4Fe*] Cubes; 6) Harnessing Infrared Solar Energy with Plasmonic Energy Upconversion; 7) Synthesis of Twisted [N]Cycloparaphenylene by Alkene Insertion.* Other distinctive achievements were presented also in the 122nd ICR Annual Symposium on December 9, 2022.

ICR collaborates with other research institutions as a key member of MEXT Inter-University Collaborative Project “Integrated Consortium on Chemical Synthesis”, MEXT Large-scale Scientific Research Project “Spintronics Research Network of Japan”, and the Kyoto University Research Coordination Alliance. We have also been engaged in over 60 international collaborations with overseas universities and research institutions. In 2018, based on our strong global activity in chemistry-oriented fields, ICR was certified by MEXT as an International Joint Usage/Research Center. In 2019, we established an On-site Laboratory, the “Kyoto University Shanghai Lab” in Shanghai, China under the MEXT’s Designated National University program. To foster and secure young researchers we have initiated several programs to support research and graduate education, including an in-house annual grant system, “ICR Grant for Promoting Integrated Research.” These collaborative achievements highlight our commitment to promoting ICR as a global research core in chemistry-oriented fields.

The environment surrounding us is now experiencing a wave of changes. The growing economy has exposed various worldwide problems including climate change and social inequity. For a just and sustainable society, science and technology must become a credible beacon of light. ICR contributes towards this goal by providing leadership and expertise in scientific research, promoting multidisciplinary, chemistry-related communities, and developing new and technologically important innovations. We hope this Annual Report will serve to update you on the progress of our research activities and globalization. We appreciate your continued encouragement and support.

January 2023

Takashi Aoyama

AOYAMA, Takashi
Director

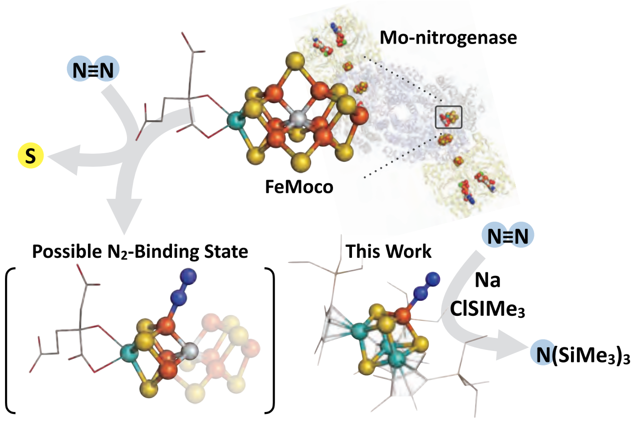
ICR News 2022

Recently Published in *Nature*!
“Nitrogen Reduction by the Fe Sites of Synthetic $[Mo_3S_4Fe]$ Cubes”

■ Prof OHKI, Yasuhiro

In July 2022, our research paper was published in Nature. This study, entitled “Nitrogen reduction by the Fe sites of synthetic $[Mo_3S_4Fe]$ cubes”, demonstrates the first catalytic reduction of N_2 by synthetic metal-sulfur compounds and provides clues on how N_2 is captured by the enzyme in nature and why the protein matrix around the N_2-binding site is needed.

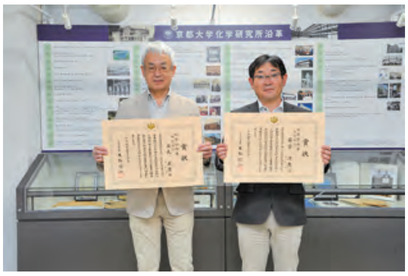
The reduction of N_2 is the key elementary step to provide nitrogen atoms in amino acids and DNA and is hence indispensable for every form of life. Nitrogenase is the enzyme for this process, and at an atomic level, FeMoco (top in the figure) consisting of iron (Fe)-molybdenum (Mo)-sulfur (S)-carbon (C) is in charge of the difficult N_2 reduction. Due to the structural complexity of FeMoco, the key elements of N_2 reduction have remained unresolved. In this study, Ohki *et al.* predicted the structure of N_2-bound FeMoco (left bottom of the figure) and the function of the protein, and synthesized cubic Mo-Fe-S compounds as simplified models (right bottom of the figure). This study not only represents the first step toward N_2 reduction by artificial metal-sulfur compounds, but also a good example of how the utilities of metal-sulfur compounds can be expanded by learning from enzymes and applying appropriate molecular design.



Remarkable Awards!
“The Commendation for Science and Technology by MEXT”

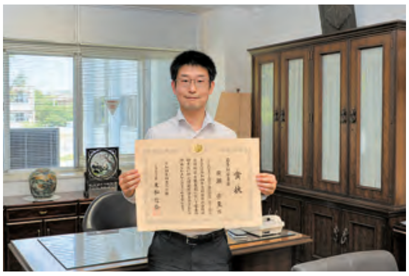
Four Professors, Institute for Chemical Research were awarded “The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology” for AY2022, to honor those who have made noteworthy contributions either to the research and development of science and technology, or to advancing the understanding of science. Prof. ONO, Prof. WAKAMIYA and Prof. KANEMITSU received Awards for Science and Technology. Assoc. Prof. HIROSE received the Young Scientists’ Award.

Prof ONO, Teruo
(Nanospintronics)



Prof WAKAMIYA, Atsushi
(Molecular Aggregation Analysis)

Prof KANEMITSU, Yoshihiko
(Nanophotonics)



Assoc Prof HIROSE, Takashi
(Structural Organic Chemistry)

Green Innovation Fund Project

■ Prof WAKAMIYA, Atsushi

With the goal of achieving “carbon neutrality by 2050”, the Ministry of Economy, Trade, and Industry (METI) created the Green Innovation Fund Project (total 2 trillion yen) to support research and development over a 10-year period as part of the New Energy and Industrial Technology Development Organization (NEDO). A research team including Prof. Atsushi Wakamiya, Prof. Yoshihiko Kanemitsu, and Prof. Takeshi Hasegawa at our institute (ICR) was selected in partnership with Enecoat Technologies, Co., Ltd. to lead one of the priority areas of the Green Innovation Fund Project, “The Development of Next Generation Solar Cells”. This project aims to commercialize lightweight, flexible, and high-performance perovskite solar cells for installation in locations where traditional solar cells cannot be used, such as factory roofs and building walls with low load-bearing capacity.

TSK Corporation Bonding the People, Materials, and Nature with Chemistry

■ Prof NAKAMURA, Masaharu

TSK Corporation was established on July 1, 2021. TSK is an acronym for Tetsu Shokubai Kagaku【鐵触媒化学】. Tetsu【鐵】is the old Chinese character for iron, “the king of metals. Shokubai Kagaku【触媒化学】is catalytic chemistry. In 1996, I started researching “Iron-Catalyzed Precise Organic Synthetic Reactions” during the last year of my Dr course study. In 2006, I was appointed as a professor at the Institute for Chemical Research, Kyoto University, where I met the current CEO of TSK, Dr. Euncheol Son (then D3 in Tamao Group). Dr. Son later worked at Sekisui Chemical and Samsung Display before going independent in 2019. In 2016, I met Mr. Matsuura, the TSK COO, at an industry-academia exchange meeting at the Uji Campus. This team was selected for the 2020 Incubation Program (IPG) of Kyoto University. Under its support, Mr. Matsuda and Mr. Avena, talented synthetic organic chemists, have joined, establishing a new iron-catalyzed methodology for synthesizing organic electronic materials. At the start of 2023, Ms. Yamada, Mr. Imai, and Mr. Allys have also joined the company, and we all are pursuing New Material Resource Revolution (NMR2)” This new Chemistry will gently and joyfully re-bond nature and humanity. We are running full speed toward such a future!

CONTENTS

International Research Center for Elements Science

Bioinformatics Center

Abbreviations used in the columns

Prof Em	Professor Emeritus
Prof	Professor
Vis Prof	Visiting Professor
Assoc Prof	Associate Professor
Vis Assoc Prof	Visiting Associate Professor
Senior Lect	Senior Lecturer
Assist Prof	Assistant Professor
Lect (pt)	Lecturer (part-time)
Specially Appointed Prof	Specially Appointed Professor
Program-Specific Assoc Prof	Program-Specific Associate Professor
Program-Specific Senior Lect	Program-Specific Senior Lecturer
Program-Specific Assist Prof	Program-Specific Assistant Professor
Program-Specific Res	Program-Specific Researcher
Techn Staff	Technical Staff
Assist Res Staff	Assistant Research Staff
Assist Techn Staff	Assistant Technical Staff

Guest Scholar	Guest Scholar
Guest Res Assoc	Guest Research Associate
SPD (JSPS)	Special Post-Doctoral Research Fellow (JSPS)
PD	Post-Doctoral Research Fellow
Res	Researcher
Res Support Staff	Research Support Staff
Proj Res	Project Researcher
RF	Research Fellow
D 1~3	Doctoral Course (Program) 1~3
M 1~2	Master’s Course (Program) 1~2
RS	Research Student
UG	Undergraduate Student
D Sc	Doctor of Science
D Eng	Doctor of Engineering
D Agr	Doctor of Agricultural Science
D Pharm Sc	Doctor of Pharmaceutical Science
D Med Sc	Doctor of Medical Science
D Inf	Doctor of Informatics
D Human & Envirnmtl. Studies	Doctor of Human and Environmental Studies
D Energy Sc	Doctor of Energy Science
Ph D	Doctor of Philosophy
(pt)	part-time

ORGANIZATION

Institute for Chemical Research

5 Divisions and 3 Centers | **Laboratories**

Research Divisions

- **Division of Synthetic Chemistry**
  - Organoelement Chemistry
  - Structural Organic Chemistry
  - Synthetic Organic Chemistry
  - Advanced Inorganic Synthesis
- **Division of Materials Chemistry**
  - Chemistry of Polymer Materials
  - Polymer Controlled Synthesis
  - Inorganic Photonics Materials
  - Nanospintronics
- **Division of Biochemistry**
  - Biofunctional Design-Chemistry
  - Chemistry of Molecular Biocatalysts
  - Molecular Biology
  - Chemical Biology
- **Division of Environmental Chemistry**
  - Molecular Materials Chemistry
  - Hydrospheric Environment Analytical Chemistry
  - Chemistry for Functionalized Surfaces
  - Molecular Microbial Science
- **Division of Multidisciplinary Chemistry**
  - Polymer Materials Science
  - Molecular Rheology
  - Molecular Aggregation Analysis

Research Centers

- **Advanced Research Center for Beam Science**
  - Particle Beam Science
  - Laser Matter Interaction Science
  - Electron Microscopy and Crystal Chemistry
  - Atomic and Molecular Structures
- **International Research Center for Elements Science**
  - Synthetic Organotransformation
  - Advanced Solid State Chemistry
  - Organometallic Chemistry
  - Nanophotonics
  - Structural Organic Chemistry
  - Biofunctional Design-Chemistry
- **Bioinformatics Center**
  - Chemical Life Science
  - Mathematical Bioinformatics
  - Bio-knowledge Engineering
  - GenomeNet Project Management Office

- Visiting Divisions
- International Joint Usage/Research Center
- Supercomputer System
- Low Temperature Laboratory

TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

Division of Synthetic Chemistry
– Organoelement Chemistry –

http://oec.kuicr.kyoto-u.ac.jp/~tokitohlab/index_e.html

Assoc Prof
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Assist Prof
YUKIMOTO, Mariko
(D Sc)

Techn Staff*
HIRANO, Toshiko

*Re-employed Staff

PD
NISHINO, Ryohei
(D Sc)

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TSUJI, Shingo (D3)
GARCIA, Julius (D3)
YANG, Yi (D2)
IJICHI, Wataru (M2)
UCHIDA, Daichi (M2)
NAKANISHI, Taiki (M2)
AOKI, Takamasa (M1)
REN, Zhe (M1)

Guest Scholars

SMITS, Preslav	University of Groningen, Kingdom of the Netherlands, 9 May 2022–31 August 2022
BREHM, Philipp	Institut für Anorganische Chemie der Universität Bonn, Germany, 15 June 2022–13 July 2022

Guest Res Assoc

WATERMAN, Rory (D Sc) Department of Chemistry, University of Vermont, United States, 15 August 2022–14 May 2023

Scope of Research

Organic chemistry has mainly developed with the use of second-row elements such as carbon, oxygen, and nitrogen, while the synthesis and isolation of the heavier congeners of typical organic molecules as stable compounds has been a dream for organic chemists. Our main research interest is the elucidation of the similarities and differences in structures and reactivities between organic compounds and the corresponding heavier congeners. These studies are interesting and important from the standpoints of fundamental chemistry, and open the way to the more extensive application of main group chemistry.

KEYWORDS

Steric Protection
Low-Coordinated Species
Transition Metal Complexes
Kinetic Stabilization
Heteroatom

Recent Selected Publications

Garcia, J. A.; Yasui, Y.; Yukimoto, M.; Mizuhata, Y.; Tokitoh, N., Synthesis of a Kinetically Stabilized 2,2-Dihydrosilene, *Chem. Lett.*, **51,** 898-901 (2022).

Jun-i, Y.; Mizuhata, Y.; Tokitoh, N., Convergent Synthesis of *E*-Disilene by the Reduction of Diastereomerically Separable 1,2-Dichlorodisilanes, *Eur. J. Inorg. Chem.*, **2022(5),** e202100962 (2022).

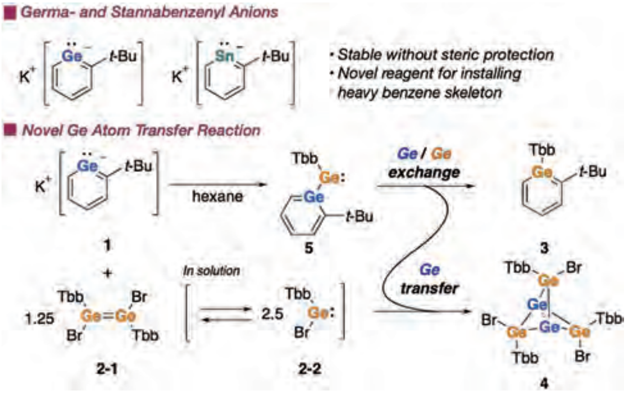
Oshiro, T.; Mizuhata, Y.; Tokitoh, N., 2-Germaazulene: Synthesis and Properties of 2-Heteraazulene Containing a Germanium Atom as a Skeletal Element, *Chem. Lett.*, **51,** 312-316 (2022).

Fujimori, S.; Mizuhata, Y.; Tokitoh, N., Stannabenzenylpotassium: The First Isolable Tin-Containing Benzene Derivative, *Chem. Eur. J.*, **24,** 17039-17045 (2018).

Mizuhata, Y.; Fujimori, S.; Sasamori, T.; Tokitoh, N., Germabenzenylpotassium: A Germanium Analogue of a Phenyl Anion, *Angew. Chem. Int. Ed.*, **56,** 4588-4592 (2017).

Novel Germanium-Atom-Transfer Reaction Using Germabenzenyl Anion

"Single atom" is regarded as the simplest building block of all molecules. Although its potential high versatility, limited generation method and extremely high reactivity prevent its application to organic synthesis. In recent years, the synthesis and isolation of "metallylone" which can be described as a central E(0) atom with Lewis bases have been reported. Some of the compounds are expected to be utilized as the synthon of group 14 elements. We have successfully synthesized the germa- and stannabenzenyl anions, the heavier Group 14 element (E = Ge, Sn) analogues of phenyl anion as an isolable compound. These germa- and stannabenzenyl anions can be used to introduce a heavy benzene skeleton, and we have already succeeded in the synthesis of several types of new germabenzenyl derivatives. Additionally, when germabenzenyl potassium **1** was reacted with dibromodigermene **2-1**, the novel germanium-atom-transfer reaction was observed. In the reaction, germabenzene **3** and pentagerma[1.1.1]propellane **4** were obtained. According to the various additional experiments and quantum chemical calculations, it was revealed that the reaction underwent the Ge atom exchange on the germabenzenyl ring to the germylene-derived Ge atom and transfer of the extruded Ge atom to bromogermylene **2-2** *via* germabenzenylgermylene **5**. The findings of this research are expected to provide a novel synthetic method of molecular germanium clusters, which attract much attention due to their unique electronic and bonding situation as well as the similarity to the allotrope of elemental germanium.



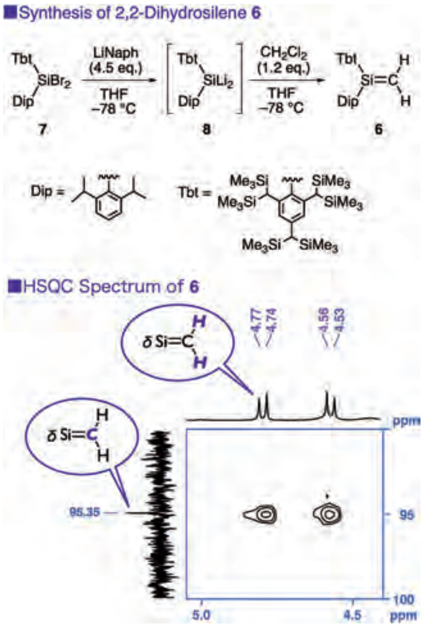
Kinetically Stabilized 2,2-Dihydrosilene

Siliconcarbon doubly bonded compounds, also known as "silenes", are generally difficult to isolate due to the instability caused by the poor 3p(Si)-2p(C) orbital overlap as well as high reactivity towards oligomerization driven by their polar, zwitterionic character ($Si^{\delta+}=C^{\delta-}$).

We succeeded in synthesis of 2,2-dihydrosilene **6**. The formation of **6** was confirmed by multinuclear NMR studies and extensive theoretical calculations. Although the successful identification of **6** by X-ray crystallographic analysis was achieved, it was not suitable for discussion because the obtained crystal contained trace amount. of an impurity.

Dibromosilane **7** was treated with 4.5 equiv. of lithium naphthalenide in THF at –78 °C to give the corresponding dilithiosilane **8**, to which was added 1.2 equiv. of CH_2Cl_2 to afford a crude product containing approximately 36% of **6**, as judged by ^{1}HNMR. Further purification of the crude product to isolate **6** proves to be extremely challenging at this stage despite several attempts to recrystallize the crude product with various solvents and conditions. Nevertheless, the characteristic NMR signals of **6** were sufficiently determined. ^{29}Si NMR spectrum of **6** showed a sharp resonance at 90.5 ppm, which is characteristic of a doubly bonded silicon atom. Furthermore, a signal at 95.4 ppm ($^1J_{C\text{-}H}$ = 146 Hz) in the ^{13}C NMR was assigned to that of the sp^2-carbon atom based on DEPT-135 measurement. In the ^{1}H NMR spectrum, two doublet signals were observed for the two geminal protons at around 4.76 ($^2J_{H\text{-}H}$ = 9.4 Hz) and 4.55 ppm ($^2J_{H\text{-}H}$ = 9.4 Hz). This assignment was further complemented with ^{1}H-^{13}C HSQC.

The silene **6** was found to be stable in solution and in the solid state at room temperature for a long period of time, suggesting that the protection used was sufficient. Further investigations towards the properties of **6** as well as its reactivity are currently in progress.



Division of Synthetic Chemistry
– Structural Organic Chemistry –

https://www.scl.kyoto-u.ac.jp/~kouzou/en/index.html


Prof
MURATA, Yasujiro
(D Eng)


Assoc Prof
HIROSE, Takashi
(D Eng)


Assist Prof
HASHIKAWA, Yoshifumi
(D Eng)

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HUANG, Guanglin (D3)
ZHANG, Zheng (D2)
HU, Weizhe (D2)
GU, Jiajian (D1)
SADAI, Shumpei (M2)
MIYAKE, Yuya (M2)
ZENG, Yuting (M2)
LIU, Zhibo (M2)

Guest Scholar

DUAN, Deliang (Ph D) Yunnan University, China, 19 September 2022–19 September 2023

Scope of Research

Fundamental studies are being conducted for the creation of new functional π-systems with novel structures and properties, and for evaluation of their application as organic semiconducting materials for photovoltaic and electroluminescent devices. The major subjects are: 1) organochemical transformation of fullerenes C_{60} and C_{70}, specifically organic synthesis of endohedral fullerenes by the technique of molecular surgery; 2) generation of ionic fullerene species and their application for the synthesis of functional material; 3) synthesis of new carbon-rich materials by the use of transition metal complex; and 4) creation of new functional π-materials with unique photoelectric properties.

KEYWORDS
π-Conjugated Systems
Functional Materials
Radical Species
Endohedral Fullerenes
Helical Structures

Recent Selected Publications

Hashikawa, Y.; Fujikawa, N.; Murata, Y., π-Extended Fullerenes with a Reactant Inside, *J. Am. Chem. Soc.*, **144(51),** 23292-23296 (2022).
Huang, G.; Hasegawa, S.; Hashikawa, Y.; Ide, Y.; Hirose, T.; Murata, Y., An H_2O_2 Molecule Stabilized inside Open-Cage C_{60} Derivatives by a Hydroxy Stopper, *Chem. Eur. J.*, **28**, e202103836 (2022).
Hashikawa, Y.; Kawasaki, H.; Murata, Y., π-Backbonding in Group 9 Metal Complexes Bearing an η^2-($H_2O@C_{60}$) Ligand, *Organometallics*, **41**, 354-359 (2022).
Hashikawa, Y.; Okamoto, S.; Sadai, S.; Murata, Y., Chiral Open-[60]Fullerene Ligands with Giant Dissymmetry Factors, *J. Am. Chem. Soc.*, **144**, 18829-18833 (2022).
Nakakuki, Y.; Hirose, T.; Matsuda, K., Logical Design of Small HOMO–LUMO Gap: Tetrabenzo[*f,jk,mn,r*][7]helicene as a Small-Molecule Near-Infrared Emitter, *Org. Lett.*, **24**, 648-652 (2022).
Nakakuki, Y.; Hirose, T.; Sotome, H.; Gao, M.; Shimizu, D.; Li, R.; Hasegawa, J.-y.; Miyasaka, H.; Matsuda, K., Doubly Linked Chiral Phenanthrene Oligomers for Homogeneously π-Extended Helicenes with Large Effective Conjugation Length, *Nat. Commun.*, **13**, 1475 (2022).

π-Backbonding in Group 9 Metal Complexes Bearing an η^2-($H_2O@C_{60}$) Ligand

As a measure of d-π* back-donation, IR stretching modes are, in general, used for metal carbonyl compounds. Once the ligand is replaced with olefins (metal–arene complexes), it can be analyzed crystallographically unless otherwise the C–C bond length falls into values within standard deviation. Herein, we propose a novel measure using an η^2-($H_2O@C_{60}$) ligand in group 9 metal–fullerene complexes, in which the stronger d-π* backbonding causes enhanced sp3-character on the coordinated olefinic bond and consequently leads to the restricted rotation for the H2O molecule as detectable by the ^{1}H NMR relaxation time. The π-backbonding strengths were, therefore, found to follow the ascending order of atomic numbers (Co < Rh < Ir) in CpM(CO)(η^2-$H_2O@C_{60}$) (Cp = cyclopentadienyl), associated with the anodic shift on oxidation potentials and hypsochromic shift on absorption edges.

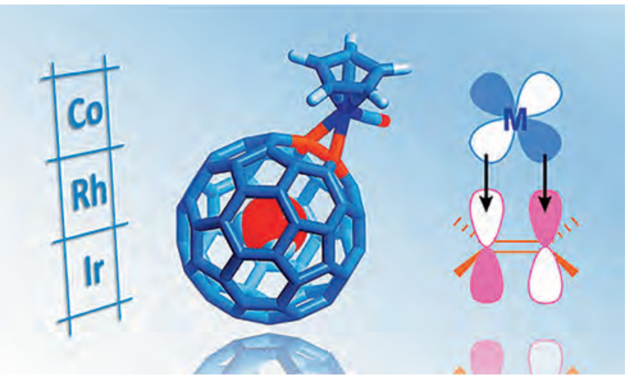

Figure 1. Group 9 metal complexes with a [60]fullerene ligand.

Chiral Open-[60]Fullerene Ligands with Giant Dissymmetry Factors

The optical resolution of open-[60]fullerenes has been limited to only one example since 1998, while the recent advances revealed the excellence of fullerenes as revisited chiral functional materials. Different from conventional chiral induction on [60]fullerene by a multiple-functionalization, a random disruption of the spherical π-conjugation is avoidable for open-[60]fullerenes. Moreover, the macrocyclic orifices enable a metal coordination which endows modulated electronic structures on chiral chromophores. Herein, we showcase Li+-coordination behavior and optical resolution of three chiral open-[60] fullerene ligands, showing a giant dissymmetry factor up to 0.20 owing to a congenital topology of the spherical π-conjugation.

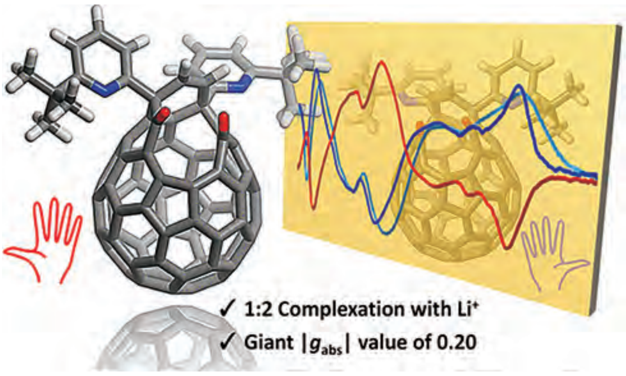

Figure 2. Chiral open-[60]fullerene ligands.

Homogeneously π-Extended Helicenes with Large Effective Conjugation Length as Helical Molecular Wires

π-Conjugated molecules with large effective conjugation length (ECL) are potentially applicable to conductive materials in the nanometer scale, which are called molecular wires. Linear molecular wires have been developed, however, chiral molecular wires with helical structures have been largely undeveloped at the moment. Herein, we report the synthesis of per-*peri*-perbenzo[*n*]helicenes (*n* = 5, 7, and 9), whose HOMO−LUMO gap of the π-extended helicenes decreased significantly from 2.14 to 1.15 eV with increasing helical length. The large ECL of π-extended helicenes is attributed to the large orbital interactions between the phenanthrene subunits at the 9- and 10-positions, which form a polyene-like electronic structure.

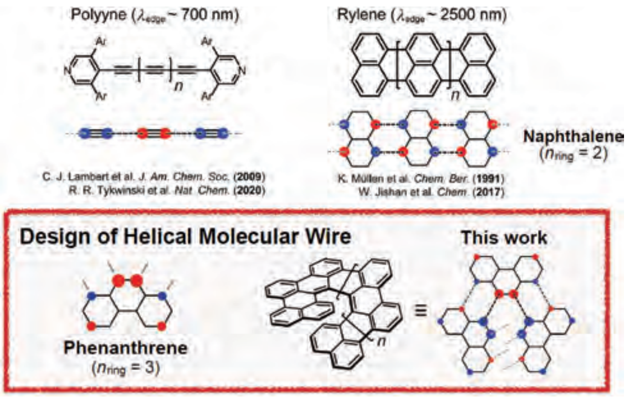

Figure 3. Design of helical molecular wires based on doubly-linked chiral phenanthrene oligomers.

Division of Synthetic Chemistry
– Synthetic Organic Chemistry –

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Prof
OHMIYA, Hirohisa
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Assist Prof
UEDA, Yoshihiro
(D Pharm Sc)


Assist Prof
NAGAO, Kazunori
(D Sc)

Students

SATO, Yukiya (D2)
SHIBUTANI, Shotaro (D2)
FUJIMURA, Kouki (D2)
OTA, Kenji (D1)

Scope of Research

Our group has been carrying out innovative research on the organic synthesis by designing catalysts and chemical reactions as well as molecules. Our current research projects include (1) radical-mediated organocatalysis such as N-heterocyclic carbene catalysis or organophotoredox catalysis; (2) reductive umpolung reactions; and (3) boron-based new molecules.

KEYWORDS
Synthetic Reactions
Photoredox Catalysis
Organocatalysis
Radical Reaction
Boron Molecule

Recent Selected Publications

Kodo T.; Nagao K.; Ohmiya H., Organophotoredox-Catalyzed Semipinacol Rearrangement via Radical-Polar Crossover, *Nat. Commun.*, **13,** 2684 (2022).

Nakagawa M.; Matsuki Y.; Nagao K.; Ohmiya H., A Triple Photoredox/Cobalt/Brønsted Acid Catalysis Enabling Markovnikov Hydroalkoxylation of Unactivated Alkenes, *J. Am. Chem. Soc.*, **144,** 7953-7959 (2022).

Matsuki Y.; Ohnishi N.; Kakeno Y.; Takemoto S.; Ishii T.; Nagao K.; Ohmiya H., Aryl Radical-Mediated N-Heterocyclic Carbene Catalysis, *Nat. Commun.*, **12,** 3848 (2021).

Sato Y.; Nakamura K.; Sumida Y.; Hashizume D.; Hosoya T.; Ohmiya H., Generation of Alkyl Radical through Direct Excitation of Boracene-Based Alkylborate, *J. Am. Chem. Soc.*, **142,** 9938-9943 (2020).

Shibutani S.; Kodo T.; Takeda M.; Nagao K.; Tokunaga N.; Sasaki Y.; Ohmiya H., Organophotoredox-Catalyzed Decarboxylative C(sp^3)–O Bond Formation, *J. Am. Chem. Soc.*, **142,** 1211-1216 (2020).

A Triple Photoredox/Cobalt/Bronsted Acid Catalysis Enabling Markovnikov Hydroalkoxylation of Unactivated Alkenes

We demonstrate Markovnikov hydroalkoxylation of unactivated alkenes using alcohols through a triple catalysis consisting of photoredox, cobalt, and Brønsted acid catalysts under visible light irradiation. The triple catalysis realizes three key elementary steps in a single catalytic cycle: (1) Co(III) hydride generation by photochemical reduction of Co(II) followed by protonation, (2) metal hydride hydrogen atom transfer (MHAT) of alkenes by Co(III) hydride, and (3) oxidation of the alkyl Co(III) complex to alkyl Co(IV). The precise control of protons and electrons by the three catalysts allows the elimination of strong acids and external reductants/oxidants that are required in the conventional methods.

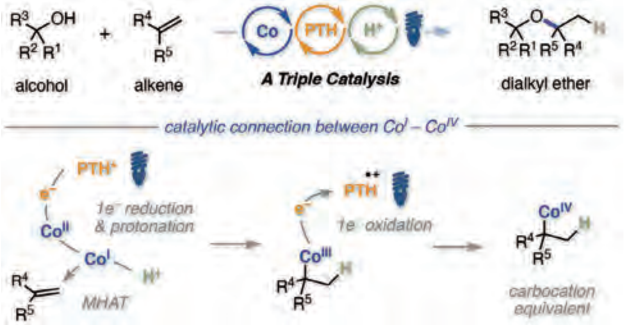

Figure 1. A Triple Photoredox/Cobalt/Bronsted Acid Catalysis Enabling Markovnikov Hydroalkoxylation of Unactivated Alkenes.

Organophotoredox-Catalyzed Semipinacol Rearrangement via Radical-Polar Crossover

Over the past century, significant progress in semipinacol rearrangement involving 1,2-migration of α-hydroxy carbocations has been made in the areas of catalysis and total synthesis of natural products. To access the α-hydroxy carbocation intermediate, conventional acid-mediated or electrochemical approaches have been employed. However, the photochemical semipinacol rearrangement has been underdeveloped. Herein, we report the organophotoredox-catalyzed semipinacol rearrangement via radical-polar crossover (RPC). A phenothiazine-based organophotoredox catalyst facilitates the generation of an α-hydroxy nonbenzylic alkyl radical followed by oxidation to the corresponding carbocation, which can be exploited to undergo the semipinacol rearrangement. As a result, the photochemical approach enables decarboxylative semipinacol rearrangement of β-hydroxycarboxylic acid derivatives and alkylative semipinacol type rearrangement of allyl alcohols with carbon electrophiles, producing α-quaternary or α-tertiary carbonyls bearing *sp*^{3}-rich scaffolds.

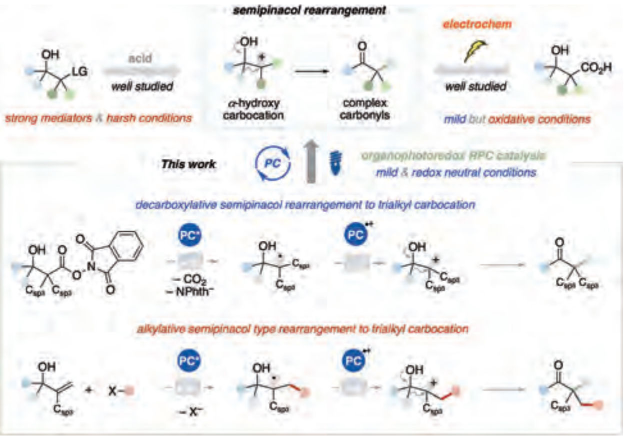

Figure 2. Organophotoredox-catalyzed semipinacol rearrangement via radical-polar crossover.

Organic Photoredox-Catalyzed Silyl Radical Generation from Silylboronate

A visible-light-driven silyl radical generation method from silylboronates has been developed. The activation of silylboronates with a catalytic amount of mild base promoted the single-electron oxidation process to form silyl radicals. Facile single electron transfer for the borate form readily occurred without hydrogen atom transfer for hydrosilane in the presence of various photoredox catalysts. Combining this protocol with radical-mediated N-heterocyclic carbene catalysis enabled the acylsilylation of alkenes *via* a radical relay process with silyl radical generation. Furthermore, the recent advanced methods for the synthesis of silylboronates significantly improved the utility of this silyl radical generation process.

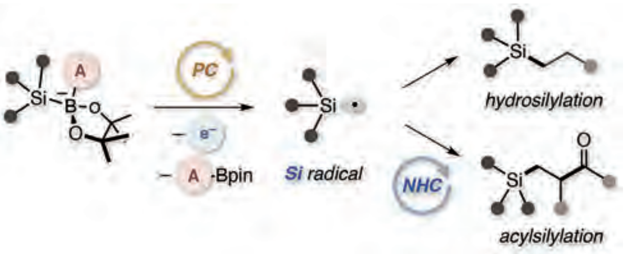

Figure 3. Organic Photoredox-Catalyzed Silyl Radical Generation from Silylboronate.

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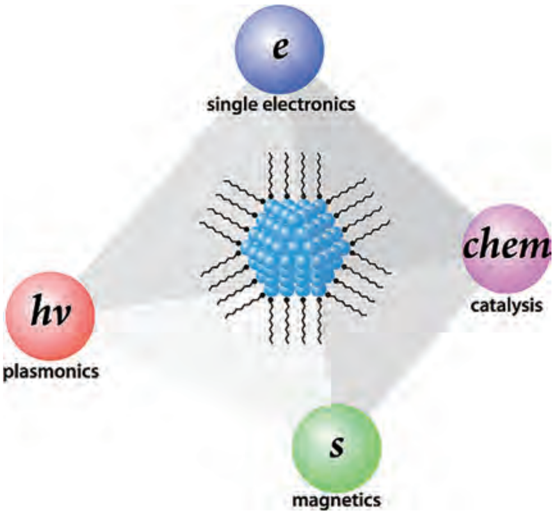
Scope of Research

We are focusing on the precise synthesis of inorganic nanoparticles by controlling the primary (size, shape, composition, *etc.*) and secondary (spatial arrangement) structures to tune properties such as electron confinement, carrier oscillation, spin, and catalysis. These high-quality inorganic nanoparticles are applied to both high-performance nanodevices (*e.g.*, single electron transistor, plasmon waveguide, and nanocomposite magnet) and photo-energy conversion materials (*e.g.*, overall water splitting and solar cell).



KEYWORDS

Inorganic Nanoparticles
Single Electronics
Plasmonics
Nanocomposite Magnet
Photocatalysts

Recent Selected Publications

Saruyama M.; Sato R.; Teranishi T., Transformations of Ionic Nanocrystals via Full and Partial Ion Exchange Reactions, *Acc. Chem. Res.*, **54,** 765-775 (2021).

Li Z.; Saruyama M.; Asaka T.; Tatetsu Y.; Teranishi T., Determinants of Crystal Structure Transformation of Ionic Nanocrystals in Cation Exchange Reactions, *Science,* **373,** 332-337 (2021).

Inter-Element Miscibility Driven Stabilization of Ordered Pseudo-Binary Alloy

The crystal structure is a crucial factor for determining the physical and chemical properties, which indicates that an exploration of new-type crystal structures can give us a chance for the development of well-known properties or the discovery of new functions. An infinite number of crystal structures in a multicomponent alloy with a specific atomic ratio can be geometrically possible, although only thermodynamically-stable phases can be formed. For instance, in the case of the $FePd_3$ alloy system, only $L1_2$ (Cu_3Au-type) phase and $A1$ (*fcc*-type solid–solution) phase have been experimentally obtained. Therefore, a synthetic strategy of stabilizing new-type crystal structures is deserved. Here, we experimentally showed the first example of a layer-structured pseudo-binary alloy, theoretically called $Z3$-$FePd_3$. This $Z3$ structure is achieved by adding a small amount of In, which is immiscible with Fe but miscible with Pd and consists of an alternate $L1_0$ (CuAu-type)-PdFePd trilayer and Pd–In ordered alloy monolayer along the *c* axis (Figure 1). First-principles calculations strongly support that the specific inter-element miscibility of In atoms stabilizes the thermodynamically-unstable $Z3$-$FePd_3$ phase without significantly changing the original density of states of the $Z3$-$FePd_3$ phase. Our results demonstrate that the specific inter-element miscibility can switch stable structures and manipulate the material nature with a slight composition change.

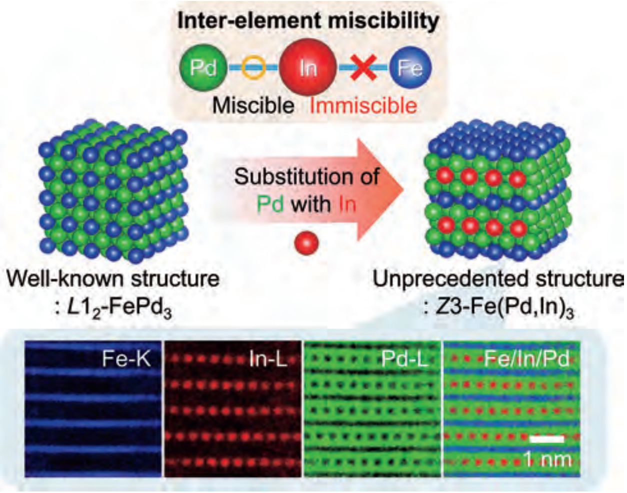


Figure 1. (a) Model of the phase change from well-known ($L1_2$) to unprecedented ($Z3$) structures driven by the specific inter-element miscibility of In atoms and atomic-resolution energy dispersive X-ray spectroscopy (EDX) elemental maps of $Z3$-type $Fe(Pd,In)_3$.

Revealing the Determinants of Crystal Structure Transformation of Ionic Nanocrystals in Cation Exchange Reactions

Ionic NCs have been widely utilized as photo-functional materials, whose properties are determined by the constituent elements and crystal structures. Cation exchange reaction can easily modulate the composition of ionic NCs to prepare a variety of functional nanomaterials. However, it has been believed that cation exchange hardly changes the crystal structure of parent ionic NCs. We applied the cation exchange reaction to hexagonal-prism-shaped $Cu_{1.8}S$ NCs with 16 kinds of height and width using Co^{2+}. It was discovered that crystal system of resultant CoS_x NCs depends on the height of parent $Cu_{1.8}S$ NCs, in which the original hexagonal-close-packed (hcp) crystal system of $Cu_{1.8}S$ NCs with thicker or thinner than about 10 nm yielded cubic-close-packed (ccp) Co_9S_8 or hcp CoS NCs, respectively (Figure 2). The ab-initio calculation revealed the surface energy of side surface is larger than that of basal plane in hcp CoS, suggesting unfavored large side surface area of thick hcp CoS NCs induced the phase transformation into more stable ccp Co_9S_8. Other incoming cations (Mn^{2+}, Zn^{2+}, and Ni^{2+}) modulated the phase transformation trend in cation exchange reactions by various means, such as volume, thermodynamic stability, and coordination environment. This discovery could lead to the phase control of ionic NCs under mild condition, which enables the synthesis of unexplored functional ionic nanomaterials.

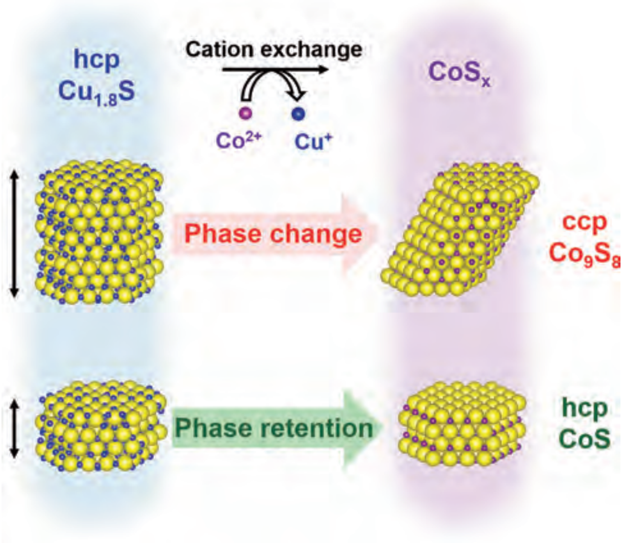


Figure 2. Height of hexagonal-prism $Cu_{1.8}S$ NCs determines the crystal structure of products after Co^{2+} cation exchange.

Division of Materials Chemistry
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Scope of Research

We perform kinetic and mechanistic analyses toward understanding chemical and physicochemical reactions occurring in polymerization systems and better routes for synthesis of well-defined polymers. In particular, new well-defined polymers or polymer assemblies are prepared by living polymerization techniques, and their structure–properties relationships are precisely analyzed. Projects in progress include: 1) kinetics and mechanisms of living radical polymerization (LRP); 2) synthesis of new polymeric materials by living polymerizations and their structure/properties studies; and 3) synthesis, properties, and applications of concentrated polymer brushes (CPB).

KEYWORDS

Precision Polymerization
Polymer Brush
Hybrid Materials
Living Radical Polymerization
Tribology

Recent Selected Publications

Nakanishi, Y.; Sakakibara, K.; Nakamichi, K.; Ohno, K.; Morinaga, T.; Sato, T.; Sagawa, T.; Tsujii, Y., Concentrated-Polymer-Brush-Modified Silica Nanoparticles Self-Assembled in Ionic Liquid Containing Iodide/Triiodide (I^-/I_3^-)-Redox System as Quasi-Solid Electrolytes for Dye-Sensitized Solar Cells, *ACS Appllied Nano Materials*, **4,** 6620-6628 (2021).

Sakakibara, K.; Ishida, H.; Kinose, Y.; Tsujii, Y., Regioselective Synthesis of Cellulosic Janus Bottlebrushes with Polystyrene and Poly(ε-Caprolactone) Side Chains and Their Solid-State Microphase Separation, *Cellulose*, **28,** 6857-6868 (2021).

Kinose, Y.; Sakakibara, K.; Sato, O.; Tsujii, Y., Near-Zero Azimuthal Anchoring of Liquid Crystals Assisted by Viscoelastic Bottlebrush Polymers, *ACS Appl. Mater.*, **3,** 2618-2625 (2021).

Sakakibara, K.; Maeda, K.; Yoshikawa, C.; Tsujii, Y., Water Lubricating and Biocompatible Films of Bacterial Cellulose Nanofibers Surface-Modified with Densely Grafted, Concentrated Polymer Brushes, *ACS Appl. Nano Mater.*, **4,** 1503-1511 (2021).

Maguire, S. M.; Krook, N. M.; Kulshreshtha, A.; Bilchak, C. R.; Brosnan, R.; Pana, A.-M.; Rannou, P.; Maréchal, M.; Ohno, K.; Jayaraman, A.; Composto, R. J., Interfacial Compatibilization in Ternary Polymer Nanocomposites: Comparing Theory and Experiments, *Macromolecules.*, **54,** 797-811 (2021).

Study on Shear-Induced Wearing of Swollen Concentrated Polymer Brushes via Fluorescence Detection of Mechanoradicals

The reduction of friction and wear in materials brings to a significant improvement in energy efficiency, product lifetime, and environmental sustainability. As a novel soft material realizing this, a concentrated polymer brush (CPB), an assembly of polymer chains sufficiently densely end-grafted on a solid surface, has received considerable attention. Especially, a thick CPB of a mm-order thickness successfully synthesized by surface-initiated controlled radical polymerization under a high-pressure condition exhibits an excellent low-friction performance in a good solvent even under a macro-scale contact. The key to its social implementation lies in understanding the mechanism of its wearing under severe conditions. In this study, we have developed a novel method to detect chain-scission events of a CPB by trapping thereby generated mechano-radicals with fluorescent monomers and hence observing its wear state using fluorescence microscopy with high sensitivity and resolution. Figs 1 and 2 show an example of fluorescence-microscopic images and its histogram of fluorescence intensity of the CPB layer, which was slid using a glass lens in an ionic liquid containing a fluorescent monomer and then washed with a solvent. We suggest that the obtained wear image can be classified into three regions of different fluorescence intensity and hence different wear state. The area of weak fluorescence intensity was observed almost all along the sliding track, the moderate-intensity area dendritically spread mainly around a defect, and the strong-intensity area was distributed along the sliding direction beyond the moderate-intensity region. Along with the thickness data obtained by a scanning laser microscope, we have discussed the mechanism of CPB wearing especially from the viewpoint of different modes of wear progression toward durability improvement and practical application.

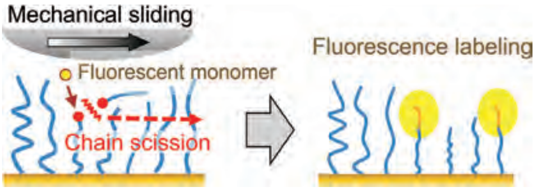

Figure 1. Schematic illustration of CPB wearing by shear force and its fluorescent labeling.

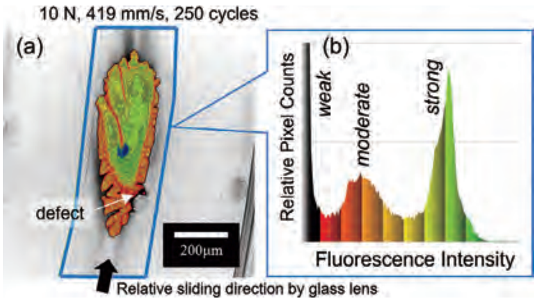

Figure 2. A fluorescence-microscopic image and (b) its histogram of a CPB of poly(methyl methacrylate) worn by mechanical sliding in a lubricant.

Anchoring Property of Liquid Crystal on Bottlebrush Polymer Film Fabricated by Langmuir Blodgett Method

Although liquid crystals (LCs) in bulk can be aligned by external fields such as electric and magnetic fields, the change in the direction of LCs near a surface is restricted by the interaction between LCs and the surface, which is known as the anchoring effect. Previously, it was reported for a bottlebrush comprised of poly(hexyl methacrylate) (PHMA) that LC molecules at the interface of its spin-coated film could easily rotate in the plane according to the external field, which is called the zero-azimuthal anchoring property. In the film fabricated by the spin-coating method, the bottlebrush molecules could be randomly oriented in the film. In this study, we have applied the Langmuir Blodgett (LB) method to control the structure of a film at the molecular level and investigated the anchoring properties of the LB film of the PHMA bottlebrush. The azimuthal anchoring coefficients A_2 on the multilayered LB and spin-coated films was estimated, from the voltage–transmittance curves, to be almost the same (Fig. 3). In contrast, they showed different characteristics in controlling the easy axis of LCs. The LB film maintained an easy axis of LCs perpendicular to the dipping direction even after the studied LC cell was once heated above the nematic-isotropic transition temperature. The alignment-regulating power of the multilayered LB film was stronger than that of the unevenness of a comb electrode (Fig. 4). The reason for this characteristic property of the LB film is discussed from the viewpoints of the orientation of bottlebrush molecules and/or the surface microstructure created during the multilayer-film formation: the detailed mechanism is under investigation.

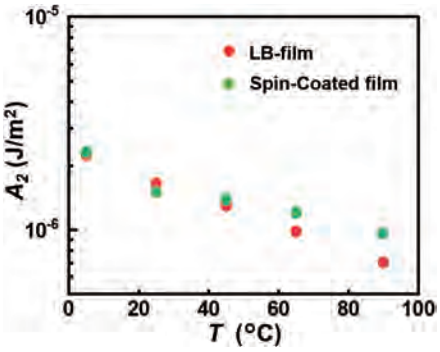

Figure 3. Temperature dependence of A_2 of LB and spin-coated films.

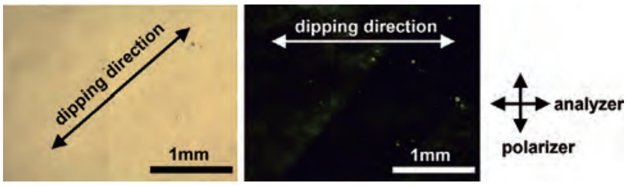

Figure 4. Polarization-microscopic images of LC cell with LB films.

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Scope of Research

Our research focuses on creation of new organic molecules with potential as key reagents and materials for future science and technologies. Furthermore, we have been developing new organic and polymeric materials based on our tailor-made molecules. For example, we are developing a new living radical polymerization method using heavier heteroatom compounds as controlling agents. Another topic is the synthesis of cycloparaphenylenes, hoop-shaped π-conjugated molecules, based on new synthetic strategies. We also study various condensed states of polymers by both static and dynamic methods to understand the relationship between structure and physical properties.

KEYWORDS

Organic Synthesis
Polymer Synthesis
Living Radical Polymerization
Polymer Properties
Curved π-Conjugated Molecules

Recent Selected Publications

Jiang, Y.; Fan, W.; Tosaka, M.; Yamago, S., Controlled Synthesis of High-Molecular-Weight Polystyrene and Its Block Copolymers by Emulsion Organotellurium-Mediated Radical Polymerization, *ACS Macro Lett.*, **11(12)**, 1331-1335 (2022).

Park, B.; Tosaka, M.; Yamago, S., Crystallization of Isotactic Poly(*N,N*-diethyl acrylamide) Synthesized by Ytterbium Triflate/H_2O Catalyzed Stereoselective Radical Polymerization, *Polym. J.*, **53,** 533-538 (2021).

Jiang, Y.; Fan, W.; Tosaka, M.; Cunningham, M. F. ; Yamago, S., Fabrication of Structurally Controlled Poly(n-Butyl Acrylate) Particles by ab initio Emulsion Organotellurium-mediated Radical Polymerization. Synthesis of High Molecular Weight Homo and Block Copolymers, *Macromolecules*, **54,** 10691-10699 (2021).

Imamura, Y.; Yamago, S., Role of Lewis Acids in Preventing the Degradation of Dithioester-Dormant Species in the RAFT Polymerization of Acrylamides in Methanol to Enable the Successful Dual Control of Molecular Weight and Tacticity, *Polym. Chem.*, **12**, 5336-5341 (2021).

Li, X.; Ogihara, T.; Nakamura, Y.; Yamago, S., Evidence for Polarity- and Viscosity-Controlled Pathways in the Termination Reaction in the Radical Polymerization of Acrylonitrile, *Macromolecules*, **54,** 4497-4506 (2021).

Synthesis of Twisted [N]Cycloparaphenylene by Alkene Insertion

By fusing CPP precursors and alkene or *ortho*-phenylene groups via coupling reactions, mono-alkene-inserted [*N*] cycloparaphenylenes **1** [(ene)-[*N*]CPP] with *N* = 6, 8, and 10, mono-*ortho*-phenylene-inserted [6]CPP **2**, and di-alkene-inserted [*N*]CPP **3** [$(\text{ene})_2$-[*N*]CPP] with *N* = 4, 6, and 8 were synthesized. Single-crystal X-ray diffraction analyses revealed that the strips formed by the π-surfaces of **1** and **2** exhibited a Möbius topology in the solid state. The Möbius topology in the parent **1** and **2** in a solution was lost due to the free rotation of the paraphenylene unit even at low temperatures. On the other hand, ene- [6]CPP **4** with eight 1-pyrrolyl groups preserved the Möbius topology even in a solution. Despite a twist, **1** has in-plane conjugation and possesses a unique size dependence of the electronic properties; i.e., the opposite size dependency of the HOMO-LUMO energy relative to conventional π-conjugated molecules.

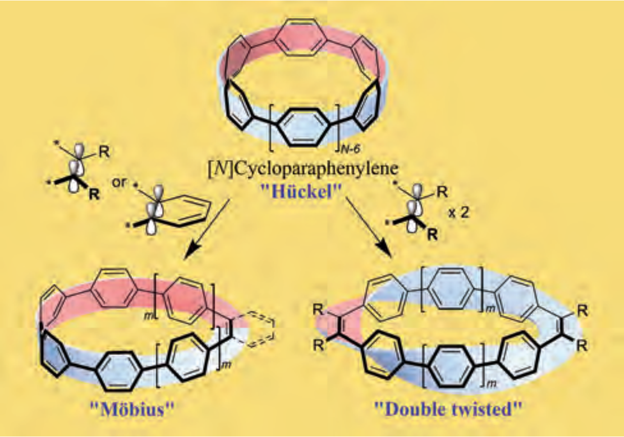

Figure 1. Insertion of alkene or *ortho*-phenylene units into a CPP skeleton.

Controlled Synthesis of High-Molecular-Weight Polystyrene and Its Block Copolymers by Emulsion Organotellurium-Mediated Radical Polymerization

Despite recent developments in reversible-deactivation radical polymerization, the synthesis of high-molecular-weight (HMW) polymers, particularly polystyrenes (PSts) and block copolymers, has been a formidable challenge. We have successfully synthesized structurally controlled HMW PSts and block copolymers consisting of HMW PSt segments by emulsion organotellurium-mediated radical polymerization (TERP). The hydrophilicity of the organotellurium group of TERP chain transfer agents (CTAs) was found to be important for successful control of molecular weight; CTAs **1b** and **1c** with di- and tetra-ethylene glycol units were suitable. By using **1b** and **1c** along with hexadecyltrimethylammonium bromide (CTAB) as the surfactant, PSts with MWs over 1 million and with low dispersity ($Đ < 1.6$) were synthesized with monomer conversion exceeding 96%. Because of the high monomer conversion, high end-group fidelity, and rapid monomer diffusion to polymer particles, we could successfully synthesize also HMW block copolymers with low dispersity by the addition of a second monomer after converting the first monomer without isolating the macroinitiators. This method provides a valuable route for fabricating polymer materials based on HMW PSts.

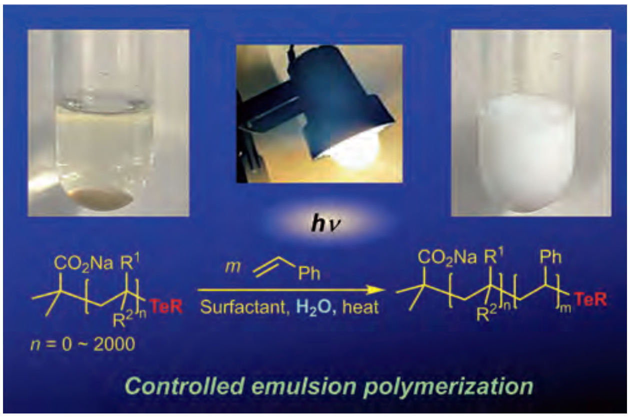

Figure 2. Emulsion TERP giving high molecular weight homo ($M_n > 1 \times 10^6$) and block copolymer ($M_n > 4 \times 10^5$) with narrow dispersity ($Đ < 1.6$).

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Scope of Research

NV centers in diamond have been extensively interested because a single spin of the NV center can be manipulated and detected at room temperature. Furthermore, a spin-coherence time of the NV center is very long. The spin-coherence time is the time to retain coherence (superposition state) and directly relates to the sensitivity of sensors of magnetic field, electric field and temperature. Therefore, the unique and excellent properties of the NV center are expected to be applied for quantum computing, quantum communication, bio-imaging, and high-sensitive sensor with nano-scale resolution.

KEYWORDS
Diamond
NV Center
Quantum Information Science
Quantum Materials
Quantum Sensing

Recent Selected Publications

Nishikawa, T.; Morioka, N.; Abe, H.; Morishita, H.; Ohshima, T.; Mizuochi, N., Electrical Detection of Nuclear Spin via Silicon Vacancy in Silicon Carbide at Room Temperature, *Appl. Phys. Lett.*, **121,** 184005 (2022).

Kawase, R.; Kawashima, H.; Kato, H.; Tokuda, N.; Yamasaki, S.; Ogura, M.; Makino, T.; Mizuochi, N., *n*-Type Diamond Synthesized with *tert*-Butylphosphine for Long Spin Coherence Times of Perfectly Aligned NV Centers, *J. Appl. Phys.*, **132,** 174504 (2022).

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Fujiwara, M.; Uchida, G.; Ohki, I.; Liu, M.; Tsurui, A.; Yoshikawa, T.; Nishikawa, M.; Mizuochi, N., All-Optical Nanoscale Thermometry Using Silicon-Vacancy Centers in Detonation Nanodiamonds, *Carbon*, **198,** 57-62 (2022).

Ultra-Long Coherence Times Amongst Room-Temperature Solid-State Spins

Solid-state single spins are promising resources for quantum sensing, quantum-information processing and quantum networks, because they are compatible with scalable quantum-device engineering. However, the extension of their coherence times proves challenging. Although enrichment of the spin-zero ^{12}C and ^{28}Si isotopes drastically reduces spin-bath decoherence in diamond and silicon, the solid-state environment provides deleterious interactions between the electron spin and the remaining spins of its surrounding. Here we demonstrate, contrary to widespread belief, that an impurity-doped (phosphorus) n-type single-crystal diamond realises remarkably long spin- coherence times. Single electron spins show the longest inhomogeneous spin-dephasing time ($T_2^* \approx 1.5$ ms) and Hahn-echo spin-coherence time ($T_2 \approx 2.4$ ms) ever observed in room-temperature solid-state systems, leading to the best sensitivities (amongst others such as temperature), which we confirmed for AC magnetic fields. From the analysis of the noise spectrum, the elongation of T_2 could be realised by optimising the phosphorus concentration and by continuing to decrease the paramagnetic impurities and defects.

The extension of coherence times in diamond semiconductor may allow for new applications in quantum technology.

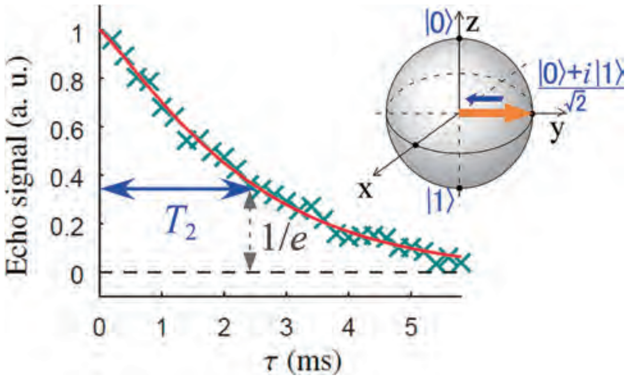

Figure 1. Echo signal of the single NV centre at room temperature. (Insert) Bloch sphere to show the coherence (superposition state).

Extension of the Coherence Time by Generating MW Dressed States in a Single NV Centre in Diamond

Nitrogen-vacancy (NV) centres in diamond hold promise in quantum sensing applications. A major interest in them is an enhancement of their sensitivity by the extension of the coherence time (T_2). In this report, we experimentally generated more than four dressed states in a single NV centre in diamond based on Autler-Townes splitting (ATS). We also observed the extension of the coherence time to $T_2 \sim 1.5$ ms which is more than two orders of magnitude longer than that of the undressed states. Numerical estimations show the sensitivity of the quantum sensing with the dressed states can be enhanced at least one-order of magnitude with experimentally observed $T_{2\rho}$ and T_2. Thus, we believe that the quantum sensing with the dressed states can be applicable for improving the sensitivity of a quantum sensing. As an example of a quantum application using these results we propose a protocol of quantum sensing, which shows more than an order of magnitude enhancement in the sensitivity.

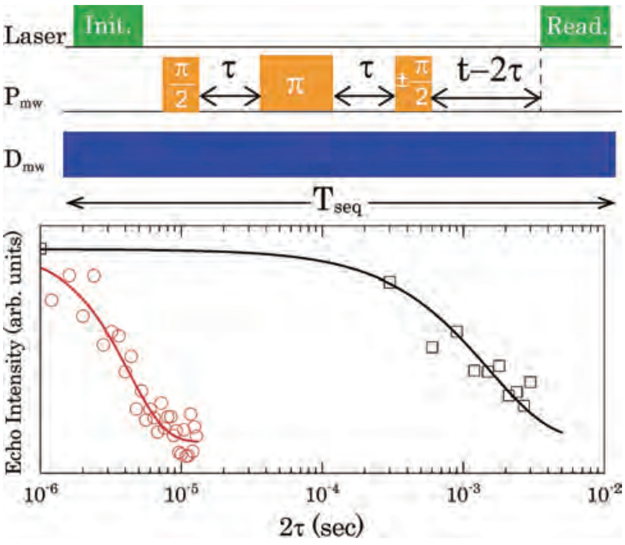

Figure 2. (Top) Pulse sequence to observe $T_{2\rho}$ and T_2 with applying a phase cycle to the final π/2 pulse. (Bottom) Black and red plots show the results of $T_{2\rho}$ and T_2 measurements, respectively. They are fitted by exponential decay curves described by black and red solid lines.

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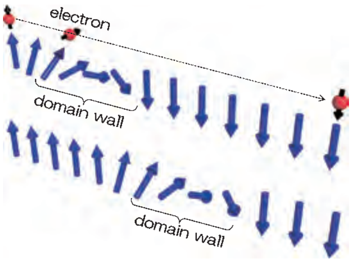
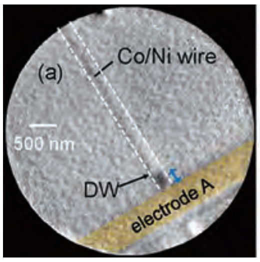
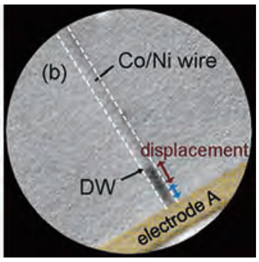
Scope of Research

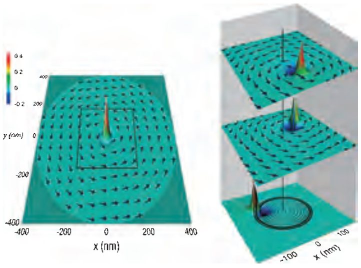
Conventional electronics uses only the charge of electrons, while traditional magnetic devices use only the spin degree of freedom of electrons. Aiming at complete control of both charge and spin in single solid-state devices, an emerging field called spintronics is rapidly developing and having an impact on information technologies. By combining the atomic-layer deposition with nanofabrication, we focus on the development of spin properties of various materials and the control of quantum effects in mesoscopic systems for novel spintronics devices.

KEYWORDS
Spintronics
Magnetism
Magnetic Materials









Recent Selected Publications

Ando, F.; Miyasaka, Y.; Li, T.; Ishizuka, J.; Arakawa, T.; Shiota, Y.; Moriyama, T.; Yanase, Y.; Ono, T., Observation of Superconducting Diode Effect, *Nature*, **584,** 373-376 (2020).

Moriyama, T.; Hayashi, K.; Yamada, K.; Shima, M.; Ohya, Y.; Ono, T., Tailoring THz Antiferromagnetic Resonance of NiO by Cation Substitution, *Phys. Rev. Materials*, **4,** 074402 (2020).

Ishibashi, M.; Shiota, Y.; Li, T.; Funada, S.; Moriyama, T.; Ono, T., Switchable Giant Nonreciprocal Frequency Shift of Propagating Spin Waves in Synthetic Antiferromagnets, *Sci. Adv.*, **6,** eaaz6931 (2020).

Iwaki, H.; Kimata, M.; Ikebuchi, T.; Kobayashi, Y.; Oda, K.; Shiota, Y.; Ono, T.; Moriyama, T., Large Anomalous Hall Effect in $L1_2$-Ordered Antiferromagnetic Mn_3Ir Thin Films, *Appl. Phys. Lett.*, **116,** 022408 (2020).

Okuno, T.; Kim, D.-H.; Oh, S.-H.; Kim, S.-K.; Hirata, Y.; Nishimura, T.; Ham, W.-S.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Tserkovnyak, Y.; Shiota, Y.; Moriyama, T.; Kim, K.-J.; Lee, K.-J.; Ono, T., Spin-Transfer Torques for Domain Wall Motion in Antiferromagnetically Coupled Ferrimagnets, *Nat. Electron.*, **2,** 389-393 (2019).

Realization of the Field-Free Superconducting Diode Effect

The diode effect is fundamental to electronic devices and is widely used in rectifiers and AC–DC converters. At low temperatures, however, conventional semiconductor diodes possess a high resistivity, which yields energy loss and heating during operation. The superconducting diode effect (SDE), which relies on broken inversion symmetry in a superconductor may mitigate this obstacle: in one direction a zero-resistance supercurrent can flow through the diode, but for the opposite direction of current flow, the device enters the normal state with ohmic resistance. The application of a magnetic field can induce SDE in Nb/V/Ta superlattices with a polar structure, in superconducting devices with asymmetric patterning of pinning centres, or in superconductor/ferromagnet hybrid devices with induced vortices. The need for an external magnetic field limits their practical application. Here, we present implementation of zero-field SDE using noncentrosymmetric $[Nb/V/Co/V/Ta]_{20}$ multilayers. The magnetic layers provide the necessary symmetry breaking and we can tune the SDE by adjusting the structural parameters, such as the constituent elements, film thickness, stacking order, and number of repetitions. We control the polarity of the SDE through the magnetization direction of the ferromagnetic layers. Energy-loss-free SDEs as presented in this work may therefore enable novel non-volatile memories and logic circuits with ultralow power consumption.

Spin-Transfer-Torque-Driven Magnetic Domain Wall Motion in Antiferromagnetically Coupled Ferrimagnets

Magnetic domain wall (DW) racetrack memory is a next-generation, non-volatile and high-density magnetic memory, where the magnetic domain walls work as information bits and they are controlled by electric current via the effect of spin transfer torque (STT). However, to enhance thermal stability while keeping low driven current is difficult in traditional domain wall (DW) motion devices. The increasing of energy barrier for thermal stability inevitably results in the enhancement of driven current. We numerically investigate depinning field (H_{depin}) and critical current density (J_c) for DW motion as a function of uniaxial magnetic anisotropy (K_u) in vertical DW motion memory with artificial ferromagnet. It is found that H_{depin} and J_c show different K_u dependence. The results indicate that it is promising to simultaneously achieve high thermal stability and low driven current in artificial ferromagnet based DW motion devices.

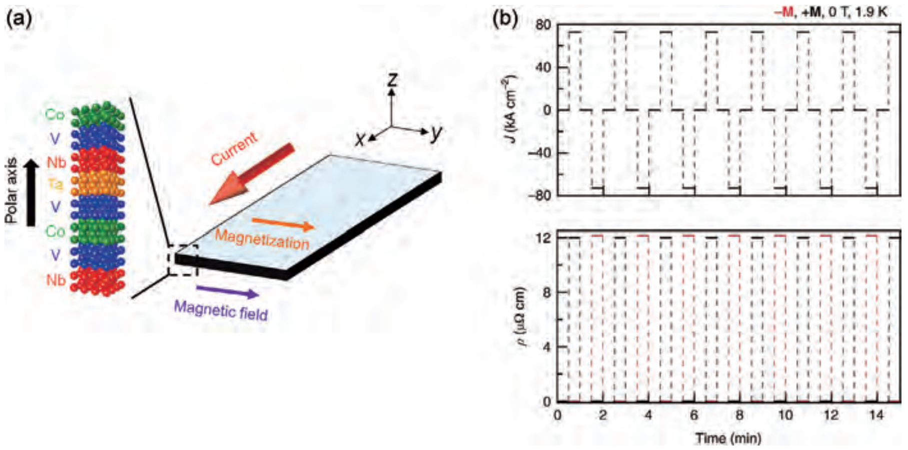


Figure 1. (a) Schematic of the SDE and measurement configuration. The magnetic field is applied perpendicular to both the polar axis and the electrical current. (b) Non-volatile SDE at 1.9 K. Red and black dots represent the results for negative magnetization (-**M**) and positive magnetization (+**M**), respectively. Current densities J = 72.7 kA cm-^{2} and J = −72.7 kA cm-^{2} at 1.9 K without a magnetic field were repeatedly applied. The device shows a superconducting state or normal conducting state depending on the polarity of the current. Note that the polarity of SDE depends on the direction of magnetization. The -**M** or +**M** state is achieved after sweeping the magnetic field in the order of +0.5, 0, −0.15, 0 T or −0.5, 0, +0.15, 0 T.

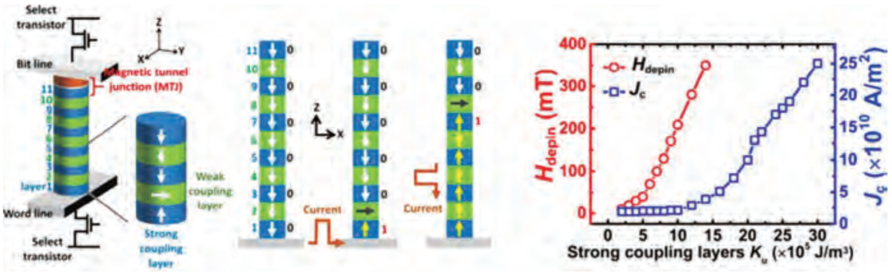


Figure 2. (a) Schematic illustration of the experimental setup. (b) The STT-induced DW velocity as a function of temperature. The dotted orange line represents the angular momentum compensation temperature T_A.

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Scope of Research

The ultimate goal of our research is the regulation of cellular functions by designed peptides and proteins. Current research subjects include (1) development of novel intracellular delivery systems aiming at elucidation and control of cellular functions using designed membrane permeable peptide vectors, (2) elucidation of the DNA or RNA binding modes of nucleic acid binding proteins, and design of artificial regulators of gene expression, (3) elucidation and control of membrane curvature, and (4) design of stimulation-responsible artificial peptides and proteins.

KEYWORDS

Membrane-Permeable Peptides
Intracellular Delivery
Peptide Design
DNA/RNA Binding Protein
Membrane Curvature

Recent Selected Publications

Kuriyama M.; Hirose H.; Masuda T.; Shudou M.; Arafiles J.V.V.; Imanishi M.; Maekawa M.; Hara Y.; Futaki S., Piezo1 Activation Using Yoda1 Inhibits Macropinocytosis in A431 Human Epidermoid Carcinoma Cells, *Sci. Rep.*,**12,** 6322 (2022).

Hirose H.; Hirai Y.; Sasaki M.; Sawa H.; Futaki S., Quantitative Analysis of Extracellular Vesicle Uptake and Fusion with Recipient Cells, *Bioconjug. Chem.*, **33,** 1852-1859 (2022).

Nakagawa Y.; Arafiles J.V.V.; Kawaguchi Y.; Nakase I.; Hirose H.; Futaki S., Stearylated Macropinocytosis-Inducing Peptides Facilitating the Cellular Uptake of Small Extracellular Vesicles, *Bioconjug. Chem.*, **33,** 869-880 (2022).

Yoshida A.; Oyoshi T.; Suda A.; Futaki S.; Imanishi M., Recognition of G-quadruplex RNA by a Crucial RNA Methyltransferase Component, METTL14, *Nucleic Acids Res.*, **50,** 449-457 (2022).

Nagano Y.; Arafiles J.V.V.; Kuwata K.; Kawaguchi Y.; Imanishi M.; Hirose H.; Futaki S., Grafting Hydrophobic Amino Acids Critical for Inhibition of Protein-Protein Interactions on a Cell-Penetrating Peptide Scaffold, *Mol. Pharm.*, **19,** 558-567 (2022).

Topics

Piezo1 Activation Using Yoda1 Inhibits Macropinocytosis

Macropinocytosis is a type of endocytosis accompanied by actin reorganization-driven membrane ruffling, followed by the formation of large vesicles called macropinosomes. Because macropinosomes (0.2–10 μm in diameter) are considerably larger than vesicles produced by other endocytic pathways (~100 nm in diameter), micropinocytosis can supply cells with large amounts of amino acids and proteins that are important for cell growth. Especially, it is well known that cancer cells with oncogenic RAS mutations promote micropinocytosis and efficiently acquire nutrients for their growth through macropinocytosis. Thus, inhibition of macropinocytosis is a promising way for cancer therapy. However, few specific agents that inhibit macropinocytosis have been developed because macropinocytosis-specific functional proteins and lipids have not been identified. Macropinocytosis is accompanied by large membrane deformations, but it is not known whether mechanosensitive channels that sense membrane tension are involved in macropinocytosis. In this study, we focused on Piezo1, one of the the mechanosensitive ion channels, and investigated if Piezo1 activation affects micropinocytosis (Fig. 1) [1]. We found that Yoda1, a specific Piezo1 agonist, potently inhibits macropinocytosis induced by epidermal growth factor (EGF) in A431 cancer cells. Treatment with Yoda1 efficiently inhibited membrane ruffle induction and subsequent macropinosome formation. The inhibition of ruffle formation by Yoda1 was dependent on the extracellular Ca^{2+} influx through Piezo1. Piezo1 activation aberrantly activated the calcium-activated potassium channel KCa3.1 and inhibited Rac1 activation which is crucial for membrane ruffle formation. These results suggest that Ca^{2+} ions can regulate EGF-stimulated macropinocytosis. This study paves the way for the development of methods to manipulate macropinocytosis by regulating Ca^{2+} channel activity such as mechanosensitive channels using chemical tools.

References

[1] Kuriyama, M. *et al*., *Sci. Rep.*, **12,** 6322. (2022).

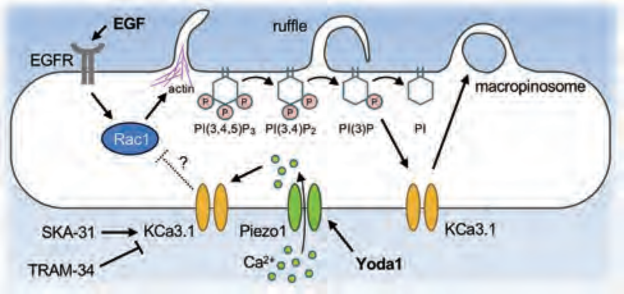

Figure 1. Proposed mechanism of macopinocytosis inhibition by Piezo1 activation. Reprinted from [1].

G-Quadruplex Specific Binding of the METTL14 RGG Domain

RNA G-quadruplexes (rG4s) are non-canonical four-stranded structures formed by G-rich sequences. Previous reports have shown the importance of rG4s in various biological processes. Recent bioinformatics analyses pointed out that potential RNA G4-forming sequences and *N*6-methyladenosines (m6A) are colocalized in viral RNA (ZIKV and HIV)[2]. m6A is the most abundant RNA modification which involves in various important aspects of RNA metabolism. The m6A modification is catalyzed by the m^{6}A writer complex composed of the METTL3/METTL14 heterodimer and additional adaptor proteins. So far, the mechanism of the relationship between rG4 and RNA adenosine methylation has not been elucidated at all. Here, we focused on the RNA binding property of METTL3/METTL14 methyltransferase heterodimer, especially the RNA binding specificity of the RGG repeats of METTL14 to RNA G-quadruplexes.

Methyltransferase domain (MTD) heterodimer of METTL3 and METTL14 with the RGG repeats of METTL14, MTD3/MTD14-RGG, were prepared. Gel mobility shift assays demonstrated that the RNA binding affinities of MTD3/MTD14-RGG to G4-forming RNAs were higher than those to non-G4 forming RNAs in K$^+$ buffer but comparable in Li$^+$ buffer. These results indicate that MTD3/MTD14-RGG specifically recognized G4-structured RNAs. In addition, *in vitro* methylation assays in the mixtures of G4 forming RNA and non-G4 forming RNA in the presence of HeLa total RNA showed that MTD3/MTD14-RGG selectively methylated adenosines close to rG4. These results provide a possible process for recruiting METTL3/METTL14 to G4 forming regions and a new insight of rG4 in epitranscriptomic regulation (Fig. 2) [3].

Reference

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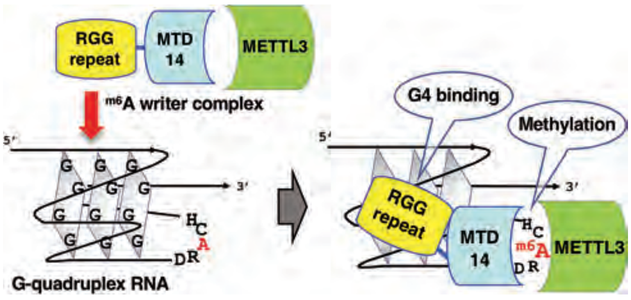

Figure 2. m6A writer complex binds to G-quadruplex RNA.

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Scope of Research

Plant hormones are a group of small molecules that are synthesized by plants and control their growth, development and environmental responses. This laboratory aims at elucidating how plant hormones are made and act in plants. Towards this goal, we combine chemical (organic chemistry, biochemistry, and analytical chemistry) and biological (molecular genetics, physiology, molecular biology, genomics) approaches. We are also looking for new hormone-like compounds by using mutant plants that show morphological phenotypes.

KEYWORDS
Plant Hormone
Strigolactone
Biosynthesis
Cytochrome P450
Receptor

Recent Selected Publications

Mashiguchi, K.; Seto, Y.; Onozuka, Y.; Suzuki, S.; Takemoto, K.; Wang, Y.; Dong, L.; Asami, K.; Noda, R.; Kisugi, T.; Kitaoka, N.; Akiyama, K.; Bouwmeester, H.; Yamaguchi, S., A Carlactonoic Acid Methyltransferase That Contributes to the Inhibition of Shoot Branching in Arabidopsis. *Proc. Natl. Acad. Sci. U.S.A.*, **119(14),** e2111565119 (2022).

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Seto, Y.; Yasui, R.; Kameoka, H.; Tamiru, M.; Cao, M.; Terauchi, R.; Sakurada, A.; Hirano, R.; Kisugi, T.; Hanada, A.; Umehara, M.; Seo, E.; Akiyama, K.; Burke, J.; Takeda-Kamiya, N.; Li, W.; Hirano, Y.; Hakoshima, T.; Mashiguchi, K.; Noel, J. P.; Kyozuka, J.; Yamaguchi, S., Strigolactone Perception and Deactivation by a Hydrolase Receptor DWARF14, *Nat. Commun.*, **10,** [191-1]-[191-10] (2019).

The Mechanism for Strigolactone Perception and Deactivation by a DWARF14 Receptor

Strigolactones (SLs) have been identified as root-derived signals for parasitic and symbiotic interactions in the rhizosphere. In addition to these functions as allelochemicals, SLs are now known as endogenous plant hormones that regulate many aspects of plant growth such as outgrowth of axillary shoots, root development and leaf senescence.

Recently, the perception mechanism for SLs has been a subject of debate because their receptor, DWARF14 (D14), is an α/β-hydrolase that can cleave SLs. In the study of Seto *et al.* (2019), we first conducted time-course analyses of SL binding and hydrolysis by Arabidopsis D14 (AtD14) by using differential scanning fluorimetry (DSF) experiments and hydrolysis assays (Figure 1). In these analyses, we found that the level of uncleaved GR24, a synthetic SL analog, strongly correlates with the induction of the melting temperature (Tm) shift of AtD14, suggesting that SLs trigger the active state of D14 before their hydrolysis.

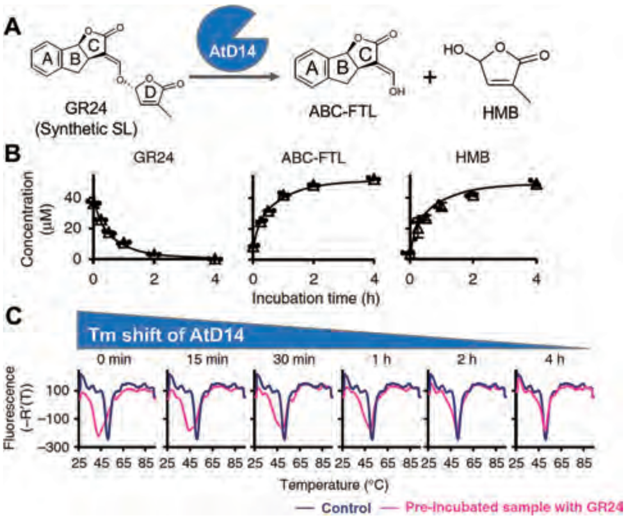

Figure 1. The time-course analyses of SL binding and hydrolysis by AtD14. (A) Hydrolysis reaction of SL (GR24) by AtD14. (B) Quantification of the hydrolysis reaction of GR24 (40 µM) by AtD14. (C) The Tm shift of AtD14 incubated with GR24 (40 µM) in DSF analysis. The maximum Tm shift was observed at initial incubation (0 min).

We next analyzed the catalytic triad mutants of AtD14. Among them, interestingly, the AtD14^{D218A} mutant completely complemented the hyper-branching phenotype of the *atd14* mutant though it lacks the hydrolase activity (Figure 2). Moreover, we found that the AtD14^{D218A} mutant could interact with SMXL7, a negative regulator of SL signaling, in an SL-dependent manner in yeast two hybrid experiments (Figure 2). These findings suggest that the hydrolase reaction catalyzed by D14 is not necessary for the signal transducing role.

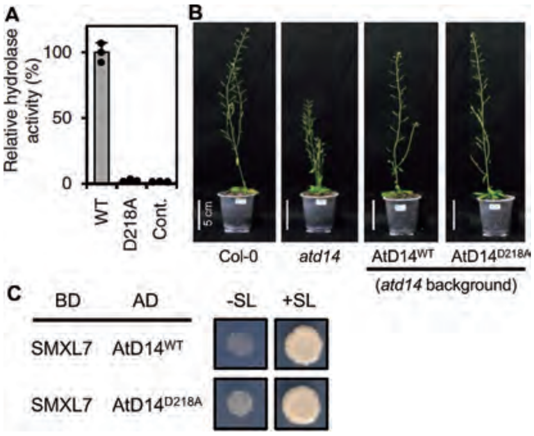

Figure 2. Functional analysis of the AtD14^{D218A} mutant. (A) The SL hydrolysis activities of maltose binding protein (MBP)-tagged wild-type of AtD14 protein (AtD14^{WT}) and the AtD14^{D218A} mutant. MBP was used in the control reaction. (B) The branching phenotype of Arabidopsis transgenic plants expressing AtD14^{WT} and AtD14^{D218A}. (C) The SL-dependent interaction of SMXL7 with AtD14^{WT} and AtD14^{D218A} in yeast.

Moreover, we showed that overexpression of the AtD14^{R183H} mutant, which could not interact with SMXL7 in the presence of SLs, but could hydrolyze SLs like AtD14^{WT}, resulted in an increased shoot branching phenotype (data not shown). These results support the idea that the hydrolase reaction catalyzed by D14 would be a deactivating step of SLs after transducing the signal.

From these lines of evidence, we conclude that the intact SL molecules trigger the D14 active signaling state, and that D14 deactivates bioactive SLs by hydrolysis after signal transmission. Together, our results revealed that D14 is a dual-functional receptor, responsible for both the perception and deactivation of bioactive SLs (Figure 3).

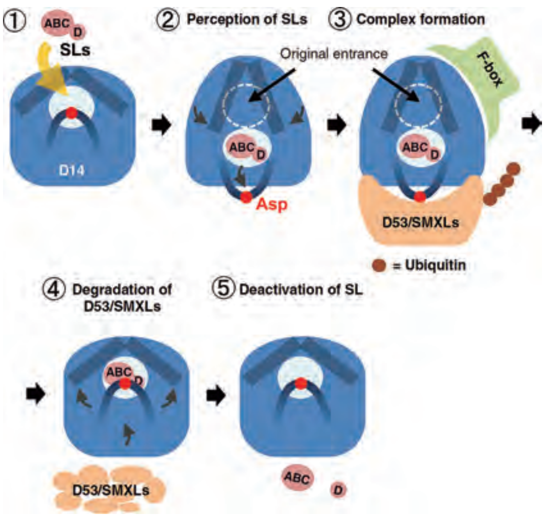

Figure 3. A proposed model of D14 in SL signaling. Bioactive SLs induce the conformational changes of D14, which triggers complex formation with the signaling partners. After the degradation of negative regulators of SL signaling (D53/SMXLs) and transmission of the SL signal, D14 reconstructs the catalytic triad to inactivate the bioactive SL.

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Scope of Research

This laboratory aims at clarifying molecular bases of regulatory mechanisms for plant development, especially plant morphogenesis, with techniques of forward and reverse genetics, molecular biology, and biochemistry. Current major subjects are: 1) phospholipid signaling in cell morphogenesis, 2) the transcriptional network for cytokinin responses, 3) COP9 signalosome modulating signal transduction in the nuclei, and 4) the endoreduplication cell cycle in cell differentiation.

KEYWORDS

Morphogenesis
Phospholipid Signaling
mRNA Processing
Signal Transduction
COP9 Signalosome

Recent Selected Publications

Watari, M.; Kato, M.; Blanc-Mathieu, R.; Tsuge, T.; Ogata, H.; Aoyama, T., Functional Differentiation among the Arabidopsis Phosphatidylinositol 4-Phosphate 5-Kinase Genes *PIP5K1*, *PIP5K2* and *PIP5K3*, *Plant Cell Physiol.*, **63,** 635-648 (2022).

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Aki, S. S.; Yura, K.; Aoyama, T.; Tsuge, T., SAP130 and CSN1 Interact and Regulate Male Gametogenesis in *Arabidopsis thaliana*, *J. Plant Res.*, **134,** 279-289 (2021).

Genetic Research of Plant PIP5K Genes

Phosphatidylinositol (4,5)-bisphosphate [PtdIns(4,5)P_2], a phosphoinositide serving as a lipid signal interacting with its effector proteins, modulates various cellular processes including cytoskeletal organization, membrane trafficking, and signal transduction for gene expression. Although the metabolic pathways of phosphoinositides are elaborately linked to one another, phosphatidylinositol 4-phosphate 5-kinase (PIP5K), which produces PtdIns(4,5)P_2 by phosphorylating PtdIns(4)P, is thought to be a key enzyme responsible for the spatiotemporal pattern of PtdIns(4,5)P_2 in higher plant cells. Higher plants encode a large number of PIP5Ks compared with animals and fungi. The model plant *Arabidopsis thaliana* encodes eleven PIP5Ks. Of these, nine can be classified into three subgroups – PIP5K1–3, PIP5K4–6, and PIP5K7–9 – belonging to different type B clades while PIP5K10 and PIP5K11 are classified as type A PIP5Ks. Genetic and molecular biological studies have revealed that the PIP5K4–6, PIP5K7–9 and PIP5K10–11 subgroup genes redundantly function in pollen tube growth, cell adaptation to stressful conditions, respectively, while *PIP5K10* and *PIP5K11* are exclusively expressed in pollen and thought to be redundantly involved in actin cytoskeletal reorganization during pollen tube growth.

With regard to the PIP5K1–3 subgroup genes, a common function to all genes has not been found so far. The loss of *PIP5K2* function affects auxin-related phenomena including root gravitropism and lateral root development. The *pip5k1pip5k2* double mutation causes sever dwarfism accompanied by sieve-element defects. In contrast, *PIP5K3*, which produces a protein localized to the plasma membrane at elongating root hair apices and sites where root hair bulges are about to form, is involved in root hair elongation. Although PIP5K3 belongs to a clade closely related with but distinct from that of PIP5K1 and PIP5K2 in the molecular phylogenetic tree of plant PIP5Ks, it is unknown how the PIP5K1–3 subgroup genes differ in their expression patterns and protein functions.

We performed comparative analyses of the PIP5K1–3 subgroup genes to determine their conserved and/or differentiated functions. Genetic analysis revealed that *PIP5K1* and *PIP5K3* have distinct functions – total plant growth and root hair elongation, respectively – whereas *PIP5K2* redundantly has both functions. This pattern of functional redundancy well coincides with the overlapping pattern of their promoter activities. In transformation rescue experiments with promoter-swapped transgenes, PIP5K1 could completely substitute for PIP5K3 in terms of protein functions (Figure 1), but only partial substitution could be achieved in the reverse case (Figure 2). Phylogenetic analysis of angiosperm type B PIP5Ks revealed that PIP5K3 orthologs have evolved faster than have PIP5K1/2 orthologs. These findings suggest that during the evolution of the PIP5K1–3 subgroup genes, *PIP5K3* differentiated to specialize in promoting root hair elongation and lost some of the ancestral protein-encoded functions conserved in PIP5K1 and PIP5K2, whereas *PIP5K1* and *PIP5K2* differentiated from each other only in their promoter-directed expression patterns.

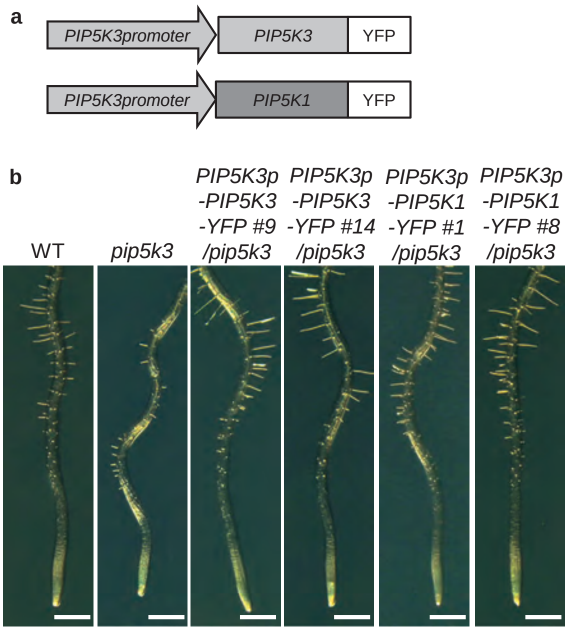

Figure 1. Rescue of the short-root-hair phenotype in *pip5k3* by *PIP5K3p-PIP5K1-YFP*. (a) Structures of the transgene *PIP5K3p-PIP5K3-YFP* and the promoter-swapped transgene *PIP5K3p-PIP5K1-YFP* are schematically illustrated. (b) Primary roots at 5 days after germination are shown for the wild type (WT), *pip5k3*, and the transformation lines harboring *PIP5K3p-PIP5K3-YFP* (lines #9 and #14) or *PIP5K3p-PIP5K1-YFP* (lines #1 and #8) in the *pip5k3* background. Bars = 1 mm

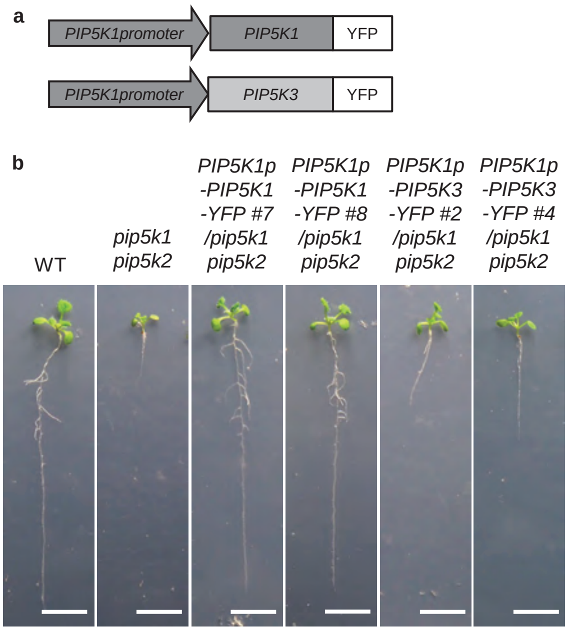

Figure 2. Partial rescue of the severe dwarf phenotype in *pip5k1pip5k2* by the promoter-swapped transgene *PIP5K1p-PIP5K3-YFP*. (a) Structures of the transgene *PIP5K1p-PIP5K1-YFP* and the promoter-swapped transgene *PIP5K1p-PIP5K3-YFP* are schematically illustrated. (b) Seedlings at 10 days after germination are shown for the wild type (WT), *pip5k1pip5k2*, and the transformation lines harboring *PIP5K1p-PIP5K1-YFP* (lines #8 and #7) or *PIP5K1p-PIP5K3-YFP* (lines #2 and #4) in the *pip5k1pip5k2* background. Bars = 1 mm

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Scope of Research

Chemical biology is an interdisciplinary field of study that is often defined as “chemistry-initiated biology.” As biological processes all stem from chemical events, it should be possible to understand or manipulate biological events using chemistry. Our laboratory has been discovering or designing unique organic molecules that modulate fundamental processes in human cells. Such synthetic organic molecules often serve as tools for basic cell biology. Discovery or design of small molecules with unique biological activities permits small-molecule-initiated exploration of complex cellular events. Our mission is to create a new world of bioactive synthetic molecules: new modes of activity, new shapes, and new sizes. We hope that these basic studies open new avenues for small-molecule applications in a range of fields.

KEYWORDS
Chemical Biology
Self-Assembly
Chemical Library
Chemical Genetics
Immunology

Recent Selected Publications

Toh, K.; Nishio, K.; Nakagawa, R.; Egoshi, S.; Abo, M.; Perron, A.; Sato, S.; Okumura, N.; Koizumi, N.; Dodo, K.; Sodeoka, M.; Uesugi, M., Chemoproteomic Identification of Blue-Light-Damaged Proteins, *J. Am. Chem. Soc.*, **144,** 20171-20176 (2022).

Jin, S.; Zhuo, S.; Takemoto, Y.; Li, Y.; Uesugi, M., Self-Assembling Small-Molecule Adjuvants as Antigen Nano-Carriers, *Chem Commun.*, **58,** 12228-12231 (2022).

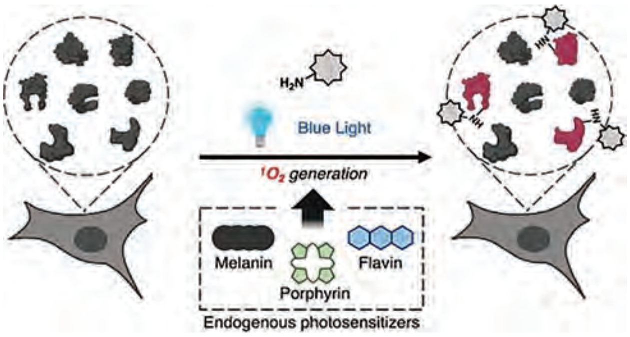
Nishio, K.; Toh, K.; Perron, A.; Goto, M.; Abo, M.; Shimakawa, Y.; Uesugi, M., Magnetic Control of Cells by Chemical Fabrication of Melanin, *J. Am. Chem. Soc.*, **144,** 16720-16725 (2022).

Ado, G.; Noda, N.; Vu, H.; Perron, A.; Mahapatra, A.; Arista, K.; Yoshimura, H.; Packwood, D.; Ishidate, F.; Sato, S.; Ozawa, T.; Uesugi, M., Discovery of a Phase-Separating Small Molecule That Selectively Sequesters Tubulin in Cells, *Chemical Science*, **13,** 5760-5766 (2022).

Mendoza, A.; Takemoto, Y.; Cruzado, K.; Masoud, S.; Nagata, A.; Tantipanjaporn, A.; Okuda, S.; Kawagoe, F.; Sakamoto, R.; Odagi, M.; Mototani, S.; Togashi, M.; Kawatani, M.; Aono, H.; Osada, H.; Nakagawa, H.; Higashi, T.; Kittaka, A.; Nagasawa, K.; Uesugi, M., Controlled Lipid β-Oxidation and Carnitine Biosynthesis by a Vitamin D Metabolite, *Cell Chemical Biology*, **29,** 660-669 (2022).

Chemoproteomic Identification of Blue-Light-Damaged Proteins

Visible light, particularly in the blue region of the spectrum, can cause cell dysfunction through the generation of singlet oxygen, contributing to cellular aging and age-related pathologies. Although photooxidation of nucleic acids, lipids, and amino acids has been extensively studied, the magnitude and span of blue-light-induced protein damages within proteome remain largely unknown. The Uesugi group took a chemoproteomic approach to mapping blue-light-damaged proteins in live mammalian cells by exploiting a nucleophilic alkyne chemical probe. A gene ontology enrichment analysis revealed that cell surface proteins are more readily oxidized than other susceptible sets of proteins, including mitochondrial proteins. In particular, the integrin family of cell surface receptors (ITGs) was highly ranked in the mammalian cells tested, including human corneal endothelial cells. The blue-light-oxidized ITGB1 protein was functionally inactive in promoting cell adhesion and proliferation, suggesting that the photodamage of integrins contributes to the blue-light-induced cell dysfunction. Further application of our method to various cells and tissues should lead to a comprehensive analysis of light-sensitive proteins.



Magnetic Control of Cells by Chemical Fabrication of Melanin

Melanin is an organic material biosynthesized from tyrosine in pigment-producing cells. The Uesugi group developed a simple method to generate tailored functional materials in mammalian cells by chemically fabricating intracellular melanin. Our approach exploits synthetic tyrosine derivatives to hijack the melanin biosynthesis pathway in pigment-producing cells. Its application was exemplified by synthesizing and using a paramagnetic tyrosine derivative, m-YR, which endowed melanoma cells with responsiveness to external magnetic fields. The mechanical force generated by the magnet-responsive melanin forced the cells to elongate and align parallel to the magnetic power lines. Critically, even non-pigment cells were similarly remote-controlled by external magnetic fields once engineered to express tyrosinase and treated with m-YR, suggesting the versatility of the approach. The present methodology may potentially provide a new avenue for mechanobiology and magnetogenetic studies and a framework for magnetic control of specific cells.

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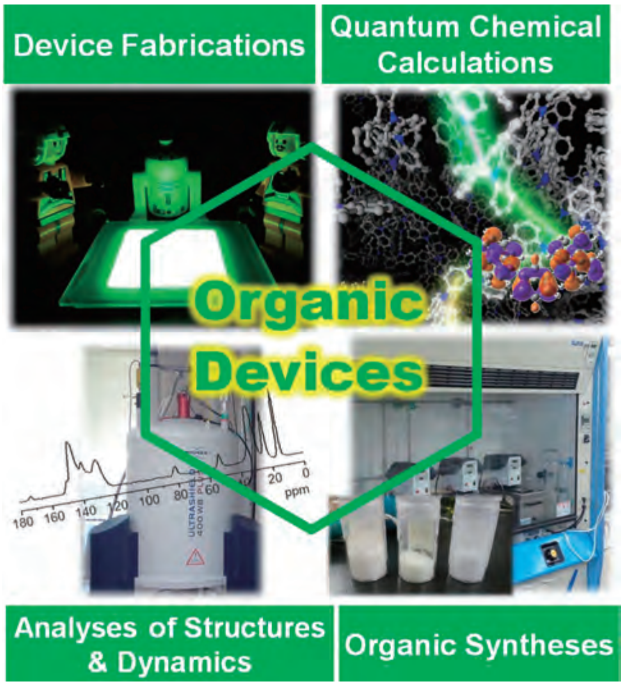
YASUDA, Yuka (UG)

Scope of Research

Our research goal is to develop high-performance organic electroluminescence devices, organic solar cells, and polymer materials. Toward this, we carry out syntheses, device fabrications, precise structure characterizations, and quantum chemical calculations for high functional organic materials. Along with exploring novel synthetic routes and novel devices, we perform detailed analyses of structures and dynamics, mainly by sophisticated solid-state NMR spectroscopy, in order to obtain structure–dynamics–property relationships.



KEYWORDS

Organic Light-Emitting Diodes
Solid-State NMR
Quantum Chemical Calculation
Amorphous Materials
Dynamic Nuclear Polarization Enhanced NMR

Recent Selected Publications

Kusakabe, Y.; Wada, Y.; Misono, T.; Suzuki, K.; Shizu, K.; Kaji, H., Imidazole Acceptor for Both Vacuum-Processable and Solution-Processable Efficient Blue Thermally Activated Delayed Fluorescence, *ACS Omega*, **7,** 16740-16745 (2022).

Shizu, K.; and Kaji, H., Comprehensive Understanding of Multiple Resonance Thermally Activated Delayed Fluorescence via Quantum Chemistry Calculations, *Commun. Chem.*, **5**, 53(1-6), (2022).

Ren, Y.; Nakagawa, H.; Suzuki, K.; Kaji, H., Near-Infrared-Red-Orange Thermally Activated Delayed Fluorescence Emitters Using a Strong Tetracoordinated Difluoroboronated Acceptor, *Jpn. J. Appl. Phys.*, **61**, [081001-1]-[081001-5] (2022).

Theoretical Determination of Rate Constants for Materials Screening

Theoretical prediction of rate constants has attracted great attention because of its relevance to materials chemistry. We report a cost-effective method of theoretically predicting electronic transition rate constants from the excited states of molecules. Our method is based on quantum chemical calculations of electronic states and the Fermi golden rule. We apply the method to the excited-state decay mechanism of photoexcited benzophenone and show that calculated rate constants, including radiative (fluorescence) and nonradiative decays from S_1 to S_0, radiative decay (phosphorescence) from T_1 to S_0, and intersystem crossing from S_1 to T_2, are quantitatively in good agreement with the experimental ones. From the calculated population kinetics, a stepwise $S_1 \rightarrow T_2 \rightarrow T_1 \rightarrow S_0$ transition is found to be the predominant decay pathway. The direct $S_1 \rightarrow T_1$ transition is suppressed owing to a fast $S_1 \rightarrow T_2$ intersystem crossing. Our method of predicting rate constants is useful for accelerating materials screening.

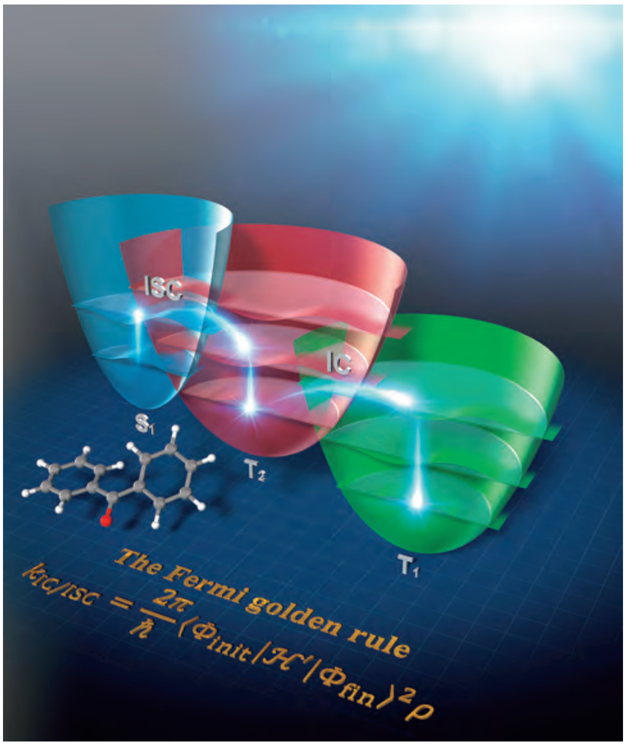


Figure 1. A stepwise $S_1 \rightarrow T_2 \rightarrow T_1$ decay mechanism of photoexcited benzophenone.

Imidazole Acceptor for Both Vacuum-Processable and Solution-Processable Efficient Blue Thermally Activated Delayed Fluorescence

The members of the imidazole family have been widely used for electron transporting, host, conventional fluorescent, and phosphorescent materials. Although the imidazole core also has great potential as an acceptor segment of deep-blue thermally activated delayed fluorescence (TADF) owing to its high triplet energy, the emission color of imidazole-based TADF organic light-emitting diodes (OLEDs) has so far been limited to blue to green. In this work, four acridan-imidazole systems are theoretically designed aiming for deep- or pure-blue emitters. All four emitters exhibit deep-blue to blue emission owing to the high energy levels of the lowest excited singlet states, exhibiting y coordinates of Commission Internationale de l'Eclairage coordinates between 0.06 and 0.26. The molecule composed of a trifluoromethyl-substituted benzimidazole acceptor in combination with a tetramethyl-9,10-dihydroacridine donor (named MAc-FBI) achieves a high maximum external quantum efficiency (EQEMAX) of 13.7% in its application to vacuum-processed OLEDs. The emitter has high solubility even in ecofriendly nonhalogenated solvents, which motivates us to fabricate solution-processed MAc-FBI-based OLEDs, resulting in an even higher EQEMAX of 16.1%.

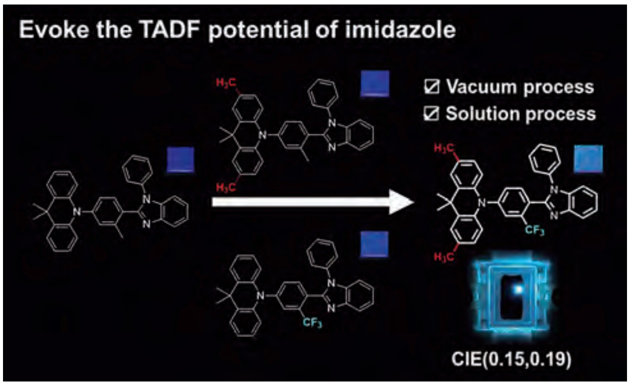


Figure2. Imidazole Acceptor for Both Vacuum-Processable and Solution-Processable Efficient Blue TADF emitters.

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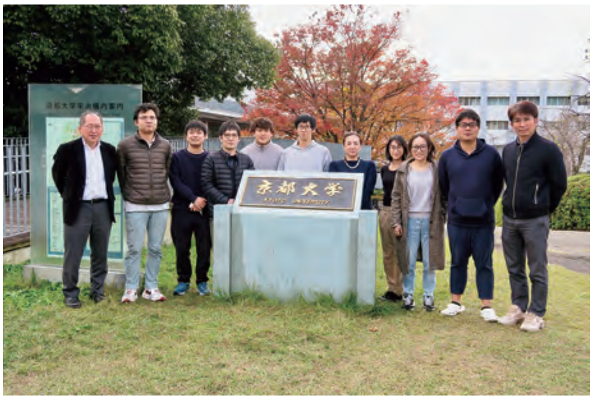
Scope of Research

(i) Biogeochemistry of trace elements in the hydrosphere: Novel analytical methods are developed for trace metals and their isotopes. Distribution of trace elements in the hydrosphere and their effects on the ecosystem are investigated. The study also covers hydrothermal activity, deep biosphere, and paleocean. (ii) Ion recognition: Novel ligands and ion recognition system are designed, synthesized, and characterized.



KEYWORDS

Marine Chemistry
Analytical Chemistry
Trace Elements
Stable Isotopes
Metal Ion Recognition

Recent Selected Publications

Zheng, L.; Minami, T.; Takano, S.: Sohrin, Y., Distributions of Aluminum, Manganese, Cobalt, and Lead in the Western South Pacific: Interplay between the South and North Pacific, *Geochim. Cosmochim. Acta.*, **338,** 105-120 (2022).

Sohrin, Y., Geochemical Study of Trace Metals in the Hydrosphere Based on Stoichiometry and Stable Isotope Ratios, *Chikyukagaku*, **56,** 21-28 (2022) (in Japanese).

Takano, S.; Liao, W.-H.; Ho, T.-Y.: Sohrin, Y., Isotopic Evolution of Dissolved Ni, Cu, and Zn along the Kuroshio through the East China Sea, *Mar. Chem.*, **243,** 104135 (2022).

Nakaguchi, Y.; Sakamoto, A.; Asatani, T.; Minami, T.; Shitashima, K.; Zheng, L.; Sohrin, Y., Distribution and Stoichiometry of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in the Seas of Japan and Okhotsk, *Mar. Chem.*, **241,** 104108 (2022).

Alam, M.; Tripti, M.; Gurumurthy, G. P.; Sohrin, Y.; Tsujisaka, M.; Singh, A. D.; Takano, S.; Verma, K., Palaeoredox Reconstruction in the Eastern Arabian Sea since the late Miocene: Insights from Trace Elements and Stable Isotopes of Molybdenum ($\delta^{98/95}$Mo) and Tungsten ($\delta^{186/184}$W) at IODP Site U1457 of Laxmi Basin, *Palaeogeogr. Palaeoclimatol. Palaeoecol.*, **587,** 110790 (2022).

Distribution and Stoichiometry of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in the Seas of Japan and Okhotsk

Trace metals play an important role in marine biogeochemistry. However, the detailed distribution of trace metals in the Seas of Japan and Okhotsk remain unknown. Herein, we report the full-depth and section distributions of the dissolved (d), total dissolvable (td), and labile particulate (lp) phases of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in seawater samples collected from the Seas of Japan and Okhotsk during the GEOTRACES-Japan program. High lpM/tdM ratios suggest active scavenging in the Seas of Japan and Okhotsk. The lpAl and lpFe species were dominant in tdAl and tdFe, showing a strong positive correlation to each other in the both the Seas of Japan and Okhotsk. The maximum lpAl, lpFe, lpMn, and lpCo concentrations were observed at σ_0 = 26.8–27.0 for dense shelf water (DSW) in the Sea of Okhotsk, implying that a metal source is laterally transported to the western subarctic North Pacific. The high enrichment factors of dMn, dCo, dNi, dCu, dZn, dCd, and dPb in the surface water of the Sea of Japan were attributed to anthropogenic emissions of these metals. In addition, temporal variations of the trace metals were examined in the Sea of Japan. The distribution of dCd did not change significantly during 1984–2010; however, data suggest that lpMn and lpFe exhibited dynamic temporal and spatial variations. This is a collaborative study with the group of Prof. Nakaguchi, Kindai University.

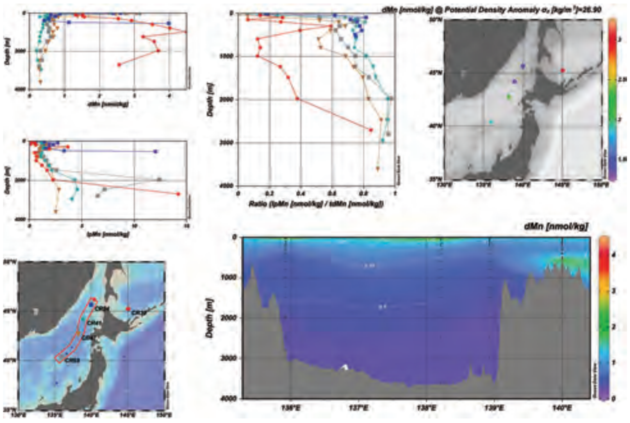


Figure 1. Distribution of dissolved Mn (dMn), labile particulate Mn (lpMn), and the lpMn/total dissolvable Mn (tdMn) ratio in the Seas of Japan and Okhotsk.

Isotopic Evolution of Dissolved Ni, Cu, and Zn along the Kuroshio through the East China Sea

We have investigated the evolution of concentrations and isotope ratios of dissolved Ni, Cu, and Zn from the North Equatorial Current in the western North Pacific to the Kuroshio in the East China Sea. The concentrations and isotope ratios for Ni, Cu, and Zn in the deep water of the East China Sea are similar to those of the western North Pacific. The concentrations of Ni, Cu, and Zn in the Changjiang diluted water (<34.0 of salinity) are 3.0–4.1 nmol/kg, 2.0–2.7 nmol/kg, and 0.5–1.1 nmol/kg, respectively, which are significantly higher than those in the surface water of the western North Pacific, thereby indicating the impact of the riverine input. In the Changjiang diluted water, isotope ratios of Ni range from +0.8 to +1.4‰, which is lower than +1.7‰ observed in the surface water (<150 m) of the western North Pacific. The distribution of concentrations and isotope ratios for dissolved Ni fit with simple mixing among the three endmembers, Changjiang diluted water, Kuroshio surface water, and deep water in the western North Pacific. A mixing model using isotope ratios and concentrations for Ni quantitatively evaluates the sources of dissolved Ni in the East China Sea. The ranges of the isotope ratios are +0.4 to +0.5‰ for Cu and −0.1 to +0.2‰ for Zn in the Changjiang diluted water, which are similar to those in the surface water of the Okinawa Trough but lower than those in the distal ocean, such as the central Pacific. Compared with published data from the global ocean, dissolved Ni, Cu, and Zn are isotopically lighter in the surface water of some coastal regions than in the pelagic regions, indicating that isotopically light Ni, Cu, and Zn are supplied from the continents. This is a collaborative study with the group of Dr. Ho, Academia Sinica, Taiwan.

Figure 2. Seawater sampling during the GEOTRACES Japan KH-15-3 cruise of R/V Hakuho Maru.

Division of Environmental Chemistry
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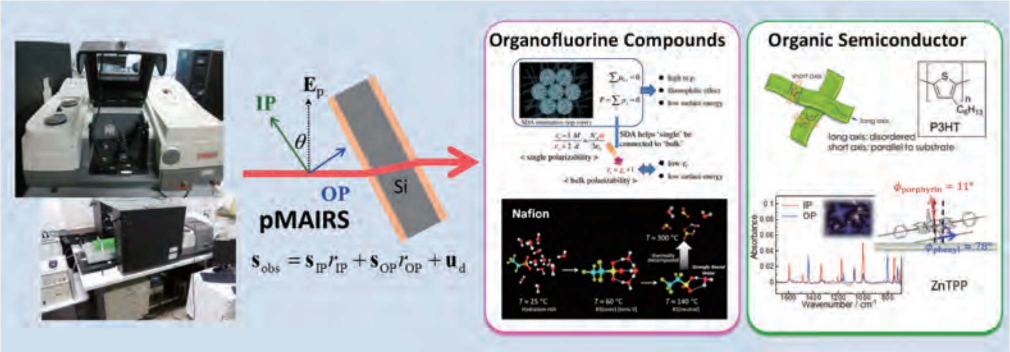
Scope of Research

To understand the chemical structure and properties of a molecular aggregated system, the keywords of molecular interactions and orientation are focused on, and the molecular aggregates are investigated by using originally developed spectroscopic techniques. The current major topics are: (1) perfluoroalkyl-specific properties in a condensed system; (2) controlling factors of molecular packing and orientation in a thin film of an organic semiconductor compound; (3) development of new molecular orientation analytical technique “MAIRS2.”

KEYWORDS

Infrared and Raman Spectroscopy
Surface and Interface Chemistry
Perfluoroalkyl Compounds
Organic Semiconductors
pMAIRS and MAIRS2



Recent Selected Publications

Shioya, N.; Yoshida, M.; Fujii, M.; Shimoaka, T.; Miura, R.; Maruyama, S.; Hasegawa, T., Conformational Change of Alkyl Chains at Phase Transitions in Thin Films of an Asymmetric Benzothienothiophene Derivative, *J. Phys. Chem. Lett.*, **13,** 11918-11924 (2022).

Shioya N.; Fujii M.; Shimoaka T.; Eda K.; Hasegawa T., Stereoisomer-Dependent Conversion of Dinaphthothienothiophene Precursor Films, *Sci. Rep*., **12,** 4448 (2022).

Tomita K.; Shioya N.; Shimoaka T.; Wakioka M.; Hasegawa T., Control of Supramolecular Organizations by Coordination Bonding in Tetrapyridylporphyrin Thin Films, *Chem. Commun.*, **58,** 2116-2119 (2022).

Shimoaka T.; Fukumi A.; Shioya N.; Hasegawa T., Perfluoroalkanes Remain on Water Surface Even after Volatilization: Affinity Analysis of Fluorinated Solvent with Water Surface, *J. Colloid Interf. Sci.*, **611,** 390-396 (2022).

Stereoisomer-Dependent Conversion of Dinaphthothienothiophene Precursor Films

Soluble precursor materials of organic semiconductors are employed for fabricating solution-processable thin film devices. While the so-called precursor approach has already been tried for various organic electronic devices such as transistors and solar cells, understanding of the conversion process in the film lags far behind. Here, we report that molecular aggregation of the precursor compound significantly influences the thermal conversion reaction in the film. For this study, two stereoisomers of a dinaphthothienothiophene (DNTT) precursor that are the endo- and exo-DNTT-phenylmaleimide monoadducts are focused on. This study reports that the endo-isomer is readily converted to DNTT in the film by heating, whereas the exo-isomer exhibits no reaction at all (Figure 1). This finding shows a new direction of controlling the on-surface reaction.

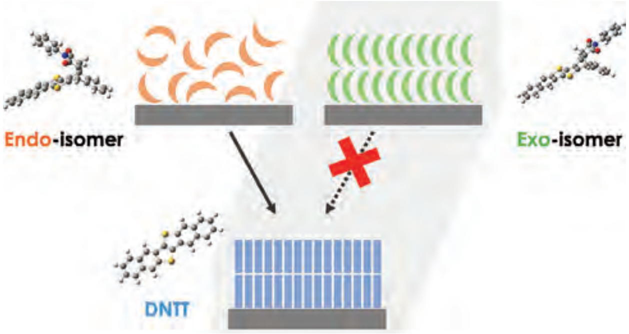


Figure 1. Stereoisomer-dependent conversion reaction of dinaphthothienothiophene precursor films.

Control of Supramolecular Organizations by Coordination Bonding in Tetrapyridylporphyrin Thin Films

Coordination bonding has been employed to control molecular orientation in thin films and is demonstrated by using tetrapyridylporphyrin. Changing the central metal ion of porphyrin controls the balance of the coordination bonding and hydrogen bonding, and edge-on orientation has been realized for the first time as well as face-on orientation (Figure 2). The mechanism of the film structure formation is comprehensively explained based on the electron configuration of the central metal ion. In this manner, the present study presents a novel strategy to control 2D supramolecular structures using coordination bonding.

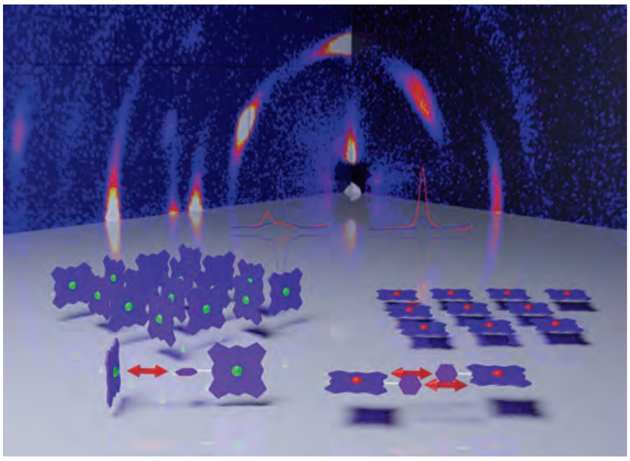


Figure 2. The edge-on and face-on orientations of tetrapyridylporphyrin are selectively obtained in thin films by changing the central metal ion of the porphyrin ring.

Perfluoroalkanes Remain on Water Surface Even after Volatilization

Perfluoroalkyl (R_f) compounds are known to have a poor solubility for most solvents except fluorinated solvents, which is known as a fluorous property. On the other hand, a single R_f chain with a short length such as C_6F_{13} is known to exhibit a totally different character from a condensed matter to have a strong affinity to a water molecule on the water surface via the dipole–dipole interaction, which is known as the dipole interactive (DI) property. On considering the DI property, the solvents of perfluoro-*n*-alkanes would remain on water for a long time. In the present study, details of a liquid layer of perfluoro-*n*-alkanes on water are investigated by using infrared external reflection spectrometry. Although the perfluoro-*n*-alkanes are highly volatile, the relevant vibration bands did not disappear even after two hours, which means that they remain on the water surface (Figure 3).

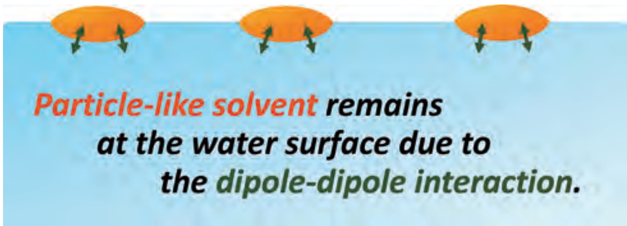


Figure 3. Schematic image of fluorinated solvents remaining on the water surface.

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Scope of Research

Microorganisms are found almost everywhere on Earth. They have a great diversity of capacities to adapt to various environments, including chemically and physically unusual environments. Our main subject is to clarify the molecular basis of environmental adaptations of microorganisms and their application. Specific functions of proteins and lipids with essential roles in environmental adaptation of extremophilic microorganisms are of our particular interest. We also undertake mechanistic analysis of microbial enzymes, in particular, those involved in unique metabolic pathways, and their application.

KEYWORDS

Extremophiles
Phospholipid Acyltransferase
Bacterial Cold-Adaptaion Mechanism
Extracellular Membrane Vesicle
Polyunsaturated Fatty Acid

Recent Selected Publications

Kawamoto, J.; Kurihara, T., Membrane Vesicles Produced by *Shewanella vesiculosa* HM13 as a Prospective Platform for Secretory Production of Heterologous Proteins at Low Temperatures, *Methods Mol. Biol.*, **2414**, 191-205 (2022).

Casillo, A.; Di Guida, R.; Cavasso, D.; Stellavato, A.; Rai, D.; Yokoyama, F.; Kamasaka, K.; Kawamoto, J.; Kurihara, T.; Schiraldi, C.; Kulkarni, S.; Paduano, L.; Corsaro, M. M., Polysaccharide Corona: The Acetyl-Rich Envelope Wraps the Extracellular Membrane Vesicles and the Cells of *Shewanella vesiculosa* Providing Adhesiveness, *Carbohydr. Polym.*, **297,** 120036 (2022).

Ogawa, T.; Kuboshima, M.; Suwanawat, N.; Kawamoto, J.; Kurihara, T., Division of the Role and Physiological Impact of Multiple Lysophosphatidic Acid Acyltransferase Paralogs, *BMC Microbiol.*, **22**, 241 (2022).

Chen, C.; Kawamoto, J.; Kawai, S.; Tame, A.; Kato, C.; Imai, T.; Kurihara, T., Isolation of a Novel Bacterial Strain Capable of Producing Abundant Extracellular Membrane Vesicles Carrying a Single Major Cargo Protein and Analysis of Its Transport Mechanism, *Frontiers in Microbiology*, **10,** 3001 (2020).

Ogawa, T.; Hirose, K.; Yusuf, Y.; Kawamoto, J.; Kurihara, T., Bioconversion from Docosahexaenoic Acid to Eicosapentaenoic Acid in the Marine Bacterium *Shewanella livingstonensis* Ac10, *Frontiers in Microbiology*, **11,** 1104 (2020).

Capsular Polysaccharide-Mediated Cargo Loading to Extracellular Membrane Vesicles of *Shewanella vesiculosa* HM13

Shewanella vesiculosa HM13, a Gram-negative bacterium isolated from fish intestine, secretes a large amount of extracellular membrane vesicles (EMVs) compared to the related strains and *Escherichia coli*, and the EMVs carry a functionally unknown protein, P49, as a single major cargo. This strain has been expected to be a clue to understanding the molecular mechanism of bacterial vesiculation and the EMV-targeted cargo transfer. A whole genome analysis of this strain demonstrated that the P49-coding gene is included in a gene cluster consisting of genes coding for protein secretion machinery and polysaccharide synthesis. An O-antigen-related flippase, Wzx, found in the gene cluster is a key protein for the cargo loading of P49 to EMVs and the synthesis of capsular polysaccharide (CPS) of the EMV surface. To verify whether CPS synthesized by the Wzx-dependent pathway interacts with P49, *in vitro* binding assay using purified P49 and P49-free EMVs was conducted. When EMVs harboring CPS were used, P49 bound to the EMVs. In contrast, P49 did not interact with EMVs collected from the *wzx*-less mutant. In the absence of CPS, no changes in the secondary structure of P49 were observed. These results revealed that CPS mediates the superficial interaction between P49 and EMVs. This system can be applied to the surface engineering of EMVs without modifying membrane components such as phospholipids.

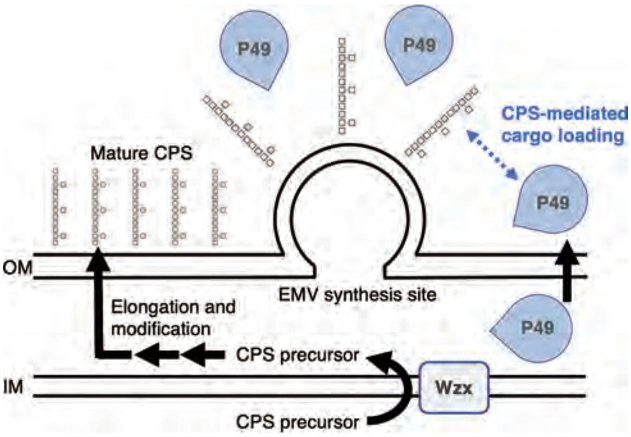

Figure 1. Schematic illustration of the capsular polysaccharide-mediated cargo loading.
An O-antigen flippase, Wzx, translocates a precursor of CPS from the inner leaflet to the outer leaflet of the inner membrane. After the elongation and maturation, CPS localizes at the surface of the cells and EMVs. P49 secreted to the surface of the cells by the function of a bacterial Type II-like secretion machinery interacts with CPS and is loaded onto the EMV surface.

A Novel and Second Lysophosphatidic Acid Acyltransferase YihG in *Escherichia coli*

A biological membrane largely comprises of glycerophospholipids, of which a fatty acyl group at the *sn*-2 position is introduced by a lysophosphatidic acid acyltransferase (LPAAT). For more than 30 years, PlsC had been believed to be a sole LPAAT in *Escherichia coli*, which is a well-studied, model Gram-negative bacterium. However, we demonstrated that an uncharacterized protein YihG is a second LPAAT in *E. coli*. We found some differences of the two LPAATs; PlsC is an essential LPAAT, whereas YihG is dispensable; YihG produces phospholipids that are distinct from ones generated by PlsC; and YihG, but not PlsC, controls the motility of *E. coli* cells. To gain further insights into the functions of YihG and how YihG controls cell physiology, we comparably analyzed the membrane proteome and transcriptome of wild-type and *yihG*-deficient cells. As a result, many genes required for cell motility (*e.g.* flagella formation and chemotaxis) were 2.2−40 times up-regulated in the mutant cells compared with the wild-type cells. This is in line with the enhanced motility of *yihG*-deficient cells. On the other hand, genes responsible for Glu-dependent acid resistance and biofilm formation were down-regulated in the mutant (up to 28-folds). As these genes and motility-related ones are known to be inversely controlled by regulatory factors such as a histone-like nucleoid structuring protein (H-NS) and a cAMP receptor protein (CRP), it is supposed that YihG affects the action of some transcriptional factors to modulate acid resistance and biofilm formation, in addition to cell motility.

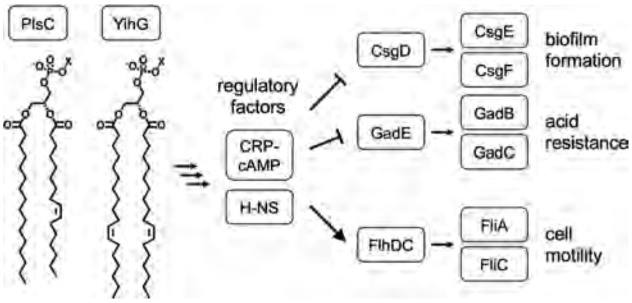

Figure 2. Proposed mechanism of how YihG controls cell physiology.

Division of Multidisciplinary Chemistry
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Scope of Research

The structure and molecular motion of polymer substances are studied, mainly using scattering methods such as X-ray, neutron, and light with intent to solve fundamentally important problems in polymer science. The main projects are studied on 1) the morphologies and the dynamics of self-assembling processes in block copolymers, 2) the hierarchical structures in crystalline polymer and rubber-filler systems, 3) the viscoelastic effects in glassy materials, 4) formation processes and ordering structures in polymer thin films.

KEYWORDS

Polymer Physics
Self Assembly
Hierarchical Structure
Polymer Properties
Softmatter

Recent Selected Publications

Jeon, J.; Doi, K.; Kim, H. D.; Ogawa, H.; Takenaka, M.; Ohkita, H., Correlating the Structures and Photovoltaic Properties in Phase-Separated Blends of Conjugated Donor Polymers and Accepters, *Polym. J.*, doi: 10.1038/s41428-022-00718-9 (2022).

Ogawa, H.; Aoki, M.; Ono, S.; Watanabe, Y.; Yamamoto, S.; Tanaka, K.; Takenaka, M., Spatial Distribution of the Network Structures in Epoxy Resin via the MAXS-CT Method, *Langmuir*, **38,** 11432-11439 (2022).

Arakawa, M.; Kishimoto, M.; Nakanishi, Y.; Mita, K.; Takenaka, M., Spatial Inhomogeneity of Chain Orientation Associated with Strain-Induced Density Fluctuations in Polyethylene, *Polym. J.*, **54,** 243-248 (2022).

Nakanishi, Y.; Uchida, K.; Mita, K.; Kamitani, K.; Kojio, K.; Takahara, A., Morphological Study of Isotactic Polypropylene Thin Films on Different Substrates Using Grazing Incidence Wide-Angle X-Ray Diffraction, *Polymer*, **245,** 124665-1-124665-9 (2022).

Topics

Spatial Inhomogeneity of Chain Orientation Associated with Strain-Induced Density Fluctuations in Polyethylene

We found the spatial inhomogeneity of chain orientation on the submicron scale in polyethylene (PE) under strain by scanning transmission X-ray microscopy (STXM). Strain is expected to induce the spatial inhomogeneity of chain orientation as well as density fluctuations, and the spatial inhomogeneity might also affect the mechanical behavior. However, wide-angle X-ray scattering can be used to explore the spatially averaged local structure, and the spatial inhomogeneity of chain orientation on the submicron scale has not yet been investigated. To clarify the spatial inhomogeneity of chain orientation, we observed near-edge X-ray absorption fine structure (NEXAFS) spectra at the carbon K-edge of stretched PE, with a resolution on the order of 10 nm, by STXM and investigated the spatial inhomogeneity of chain orientation as well as density fluctuations. The intensity of the NEXAFS spectra revealed that the chains were more oriented in the low-density region under stretching. The orientation was induced by the stretching of the polymer chains mechanically melted.

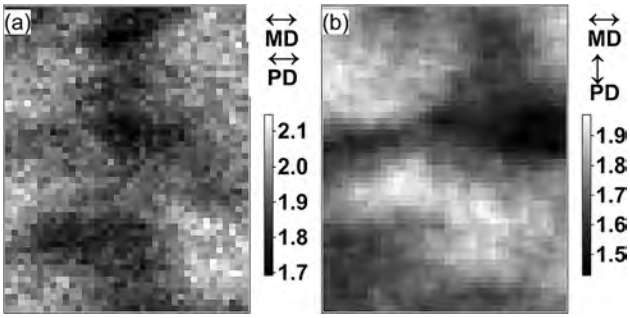

Figure 1. Optical density images of HDPE at 287.5 ± 0.2 eV corresponding to the peak of the C–H bond. The polarization direction (PD) of the incident X-rays was set to be (a) parallel and (b) perpendicular to the stretching direction (MD).

Spatial Distribution of the Network Structures in Epoxy Resin via the MAXS-CT Method

We have succeeded in visualizing the spatial heterogeneity of the reaction ratio in epoxy resins by combining medium-angle X-ray scattering (MAXS) and computed tomography (CT). The reaction ratio is proportional to the degree of cross-linking between epoxy and amine in epoxy resins. The reaction ratio and its spatial inhomogeneity affects the toughness of epoxy resins. However, there has been no non-destructive method to measure the spatial inhomogeneity of the reaction ratio although we can measure only the spatially averaged reaction ratio by FT-IR. We found that the scattering peak reflected the cross-linking structures in the *q* region of MAXS and that the peak intensity is proportional to the reaction ratio. By reconstructing CT images from this peak intensity, we visualized the spatial heterogeneity of the reaction ratio. The application of this method may not be limited to epoxy resins but may extend to studying the heterogeneity of cross-linked structures in other materials.

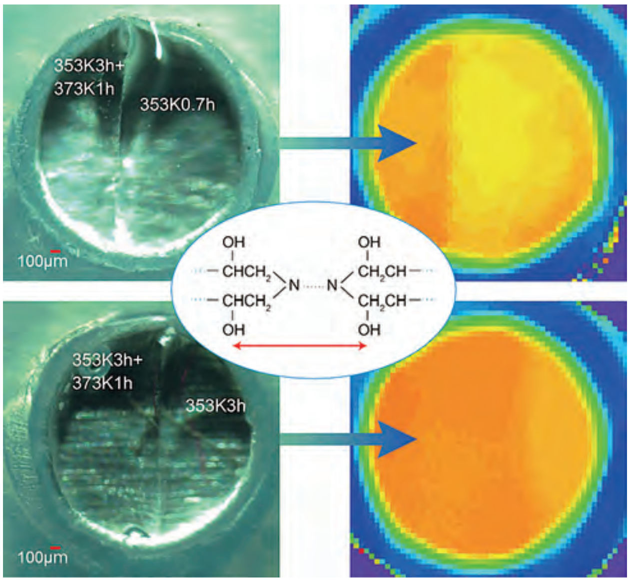

Figure 2. Optical microscopy and MAXS-CT images of samples with different cross-linking reaction ratios in epoxy resin.

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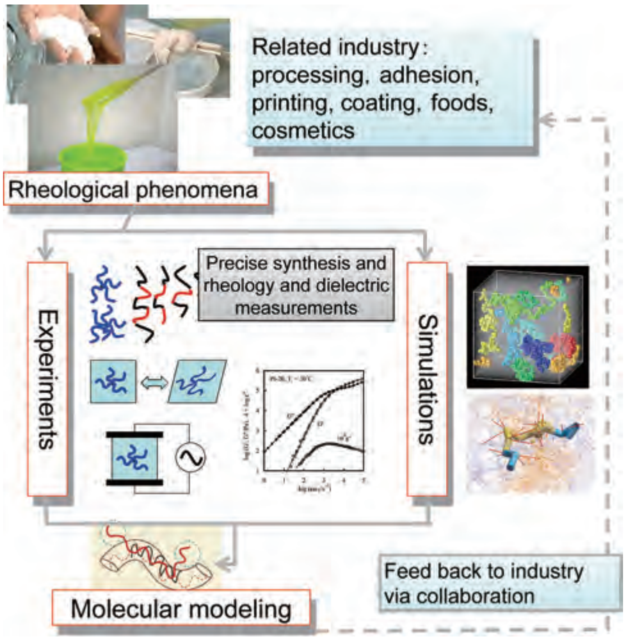
Scope of Research

Research focus is placed on the molecular origin of rheological properties of various materials. Depending on time and temperature, homogeneous polymeric materials exhibit typical features of glass, rubber, and viscous fluid while heterogeneous polymeric systems exhibit plasticity in addition to these features. For basic understanding of these features, the molecular motion and structures at various scales are studied for polymeric systems in deformed state. Rheological measurements are performed with various rheometers. Auto-correlation of the molecular orientation is also investigated with dynamic dielectric spectroscopy. Analysis of rheological and dielectric behavior elucidates a new aspect of softmatter physics.



KEYWORDS

Rheology	Dielectric Spectroscopy
Soft Matter	Mesoscopic Model

Recent Selected Publications

Sato, T.; Matsumiya, Y.; Watanabe, H., Experimental Study of Phase Separation in Dynamically Asymmetric Unentangled Polymer Blend, *J. Chem. Phys.*, **157,** 224908 (2022).

Matsumiya, Y.; Sato, T.; Chen, Q.; Watanabe, H., Rheo-Dielectric Behavior of Unentangled Poly(butylene oxide) under Steady Shear: Preliminary Evaluation of Non-Equilibrium Parameters at the Onset of Nonlinearity, *Nihon Reoroji Gakkaishi*, **50(5),** 371-385 (2022).

Sato, T.; Larson, R. G., Nonlinear Rheology of Entangled Wormlike Micellar Solutions Predicted by a Micelle-Slip-Spring Model, *J. Rheol.*, **66,** 639-656 (2022).

Sato, T.; Matsumiya, Y.; Watanabe, H., Rheo-Dielectrics and Diffusion of Type-A Rouse Chain under Fast Shear Flow: Method of Evaluation of Non-equilibrium Parameters, *Nihon Reoroji Gakkaishi*, **50,** 253-268 (2022).

Sato, T., Modeling Techniques for the Rheology of Wormlike Micellar Solutions, *Nihon Reoroji Gakkaishi*, **50,** 9-13 (2022).

Rheo-Dielectric Behavior of Unentangled Poly(butylene oxide) under Steady Shear: Preliminary Evaluation of Non-Equilibrium Parameters at the Onset of Nonlinearity

For a type-A Rouse chain, a recent study derived an analytical expression of its dielectric loss ε” under steady shear in terms of the Rouse parameters, the spring strength κ, the friction coefficient $\boldsymbol{\zeta}$, and the mean-square Brownian force intensity **B**, all being allowed to arbitrarily change with the Weissenberg number *Wi* (i.e., shear rate multiplied by the longest relaxation time at equilibrium) and the latter two having a tensorial form. Here, we have conducted a rheo-dielectric test for a type-A unentangled melt, poly (butylene oxide) to measure ε_y” in the velocity gradient (y) direction as well as the viscosity η and the first normal stress difference coefficient Ψ_1. Both dielectric relaxation time and intensity were found to decrease on an increase of *Wi* up to the onset of rheological nonlinearity where η and Ψ_1 exhibited moderate thinning, but the dielectric relaxation mode distribution was not affected by this increase of *Wi*. Analyzing those ε_y”, η, and Ψ_1 data on the basis of the above expressions, we found that κ increases moderately but the off-diagonal components of $\boldsymbol{\zeta}$ remains negligibly small on that increase of Wi. We also found that the diagonal components ζ_{xx} (with x being the velocity direction) and B_{yy} hardly change but ζ_{yy} decreases moderately. These results serve as a starting point for deeper investigation of κ, $\boldsymbol{\zeta}$, and **B**.

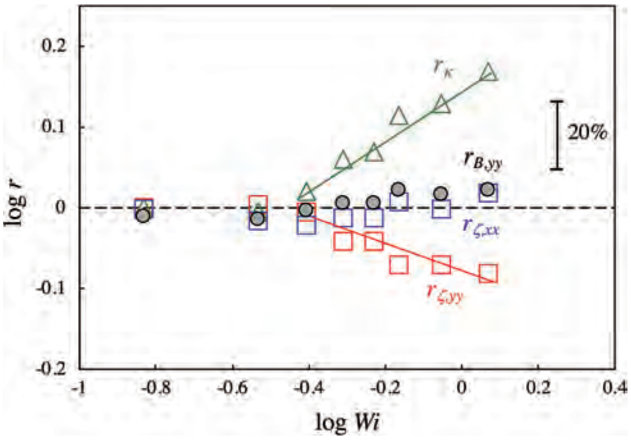


Figure 1. Changes of non-equilibrium parameters r’s with the Weissenberg number *Wi* defined with respect to the longest viscoelastic relaxation time in the LVE regime.

Experimental Study of Phase Separation in Dynamically Asymmetric Unentangled Polymer Blend

We examined a phase separation process of a dynamically asymmetric blend of unentangled polyisoprene (PI) and poly(4-ethylstyrene) (PC2St) exhibiting the upper critical solution temperature (UCST). PI having the type-A dipole was the dielectrically active fast component, whereas PC2St was the dielectrically inert slow component whose dynamics can be detected by rheological measurements. To precisely model the phase separation process, it is important to estimate the composition-dependence of the mobility which is needed to describe the phase separation dynamics. For that purpose, we conducted dielectric and rheological measurements to determine the friction coefficient of each component in a homogeneous state sufficiently above the phase separation temperature. The temperature dependence of the friction coefficient of each component was reasonably expressed by the Williams-Landel-Ferry (WLF) equation. Extrapolating this dependence obtained for blends of various compositions to the test temperature T^* below the phase separation temperature, we were able to estimate the friction coefficient of the chain at T^* as a function of the composition. This friction coefficient was then used to determine the mobility Λ defined for the material fluxes at T^*. The time-dependent Ginzburg-Landau (TDGL) equation incorporating this Λ well described the experimentally observed phase separation dynamics. In particular, the 2D TDGL simulation with this Λ qualitatively captured the phase-separated structure observed with the optical microscope as well as broad dielectric mode distribution of the blend at T^*.

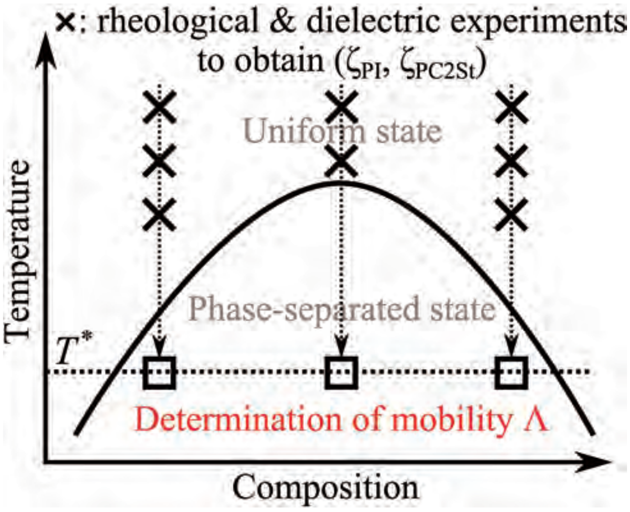


Figure 2. Schematic illustration of the experimental strategy to obtain the mobility.

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Scope of Research

We design and synthesize unique electronic materials with sophisticated device applications in mind. These materials have novel solid-state aggregation structures or well-defined interface orientation that promote efficient electrical current flow or enhance device lifetime. Electronic devices based on these new materials are then evaluated using advanced measurement techniques, and the results are used to inform the next direction of the materials chemistry. We call this synergistic approach for achieving our research goals “Needs Inspired Fundamental Science”.

KEYWORDS

Molecular Design and Synthesis
Molecular Aggregation
Functional Materials
Semiconductors
Perovskite Solar Cells

Recent Selected Publications

Hu, S.; Pascual, J.; Liu, W.; Funasaki, T.; Truong, M. A.; Hira, S.; Hashimoto, R.; Morishita, T.; Nakano, K.; Tajima, K.; Murdey, R.; Nakamura, T.; Wakamiya, A., A Universal Surface Treatment for p-i-n Perovskite Solar Cells, *ACS Appl. Mater. Interfaces*, **14,** 56290-56297 (2022).

Nakamura, T.; Otsuka, K.; Hu, S.; Hashimoto, R.; Morishita, T.; Handa, T.; Yamada, T.; Truong, M. A.; Murdey, R.; Kanemitsu, Y.; Wakamiya, A., Composition-Property Mapping in Bromide-Containing Tin Perovskite Using High-Purity Starting Materials, *ACS Appl. Energy Mater.*, **5,** 14789-14798 (2022).

Murdey, R.; Ishikura, Y.; Matsushige, Y.; Hu, S.; Pascual, J.; Truong, M. A.; Nakamura, T.; Wakamiya, A., Operational Stability, Low Light Performance, and Long-Lived Transients in Mixed-Halide Perovskite Solar Cells with a Monolayer-Based Hole Extraction Layer, *Sol. Energy Mater. Sol. Cells*, **245,** 111885 (2022).

Hu, S.; Otsuka, K.; Murdey, R.; Nakamura, T.; Truong, M. A.; Yamada, T.; Handa, T.; Matsuda, K.; Nakano, K.; Sato, A.; Marumoto, K.; Tajima, K.; Kanemitsu, Y.; Wakamiya, A., Optimized Carrier Extraction at Interfaces for 23.6% Efficient Tin-Lead Perovskite Solar Cells, *Energy Environ. Sci.*, **15,** 2096-2107 (2022).

Optimized Carrier Extraction at Interfaces for 23.6% Efficient Tin–Lead Perovskite Solar Cells

Carrier extraction in mixed tin–lead perovskite solar cells is improved by modifying the top and bottom perovskite surfaces with ethylenediammonium diiodide and glycine hydrochloride, respectively. Trap densities in the perovskite layers are reduced as a result of surface passivation effects and an increase in film crystallinity. In addition, the orientated aggregation of the ethylenediammonium and glycinium cations at the charge collection interfaces result in the formation of surface dipoles, which facilitate charge extraction. As a result, the treated mixed tin–lead perovskite solar cells showed improved performance, with a fill factor of 0.82 and a power conversion efficiency up to 23.6%. The unencapsulated device also shows improved stability under AM1.5G, retaining over 80% of the initial efficiency after 200 h continuous operation in inert atmosphere. Our strategy is also successfully applied to centimeter-scale devices, with efficiencies up to 21.0%.1)

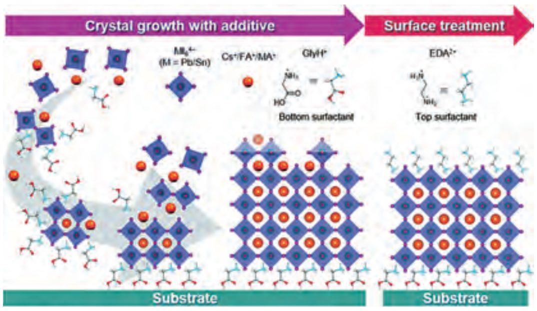

Figure 1. Tin-Lead perovskite films with top and bottom interface modification.

Operational Stability, Low Light Performance, and Long-Lived Transients in Mixed-Halide Perovskite Solar Cells with a Monolayer-Based Hole Extraction Layer

Due to their tunable bandgap and low manufacturing cost, metal halide perovskite solar cells are attractive for ambient/indoor light-harvesting applications. In this work, we evaluate p-i-n perovskite solar cells fabricated with MeO-2PACz, a molecular monolayer hole extraction layer, as potential candidates for ambient light- harvesting applications. Two triple-cation mixed halide lead perovskite absorbers are compared, one with high bromide content (Br/I ratio 1:2, bandgap 1.72 eV, 16.1% power conversion efficiency) and one with low bromide content (Br/I ratio 1:11, bandgap 1.57 eV, 19.1% power conversion efficiency). Both materials demonstrated good stability while operating under simulated sunlight at the maximum power point for 100 h, a cumulative light dose comparable to over two years of ambient use. After 100 h operation, however, the measured device efficiency fell temporarily due to a transient loss of output current before returning to the nominal level after a long recovery period in the dark. These transient losses were more apparent in the wide bandgap device under strong light and were likely caused by light-induced halide segregation. After recovery, both devices retained good performance under a wide range of light intensities. Under a simulated ambient light source (835 lx white LED), the power conversion efficiency of the wide bandgap device reached 30.4%.2)

Composition-Property Mapping in Bromide-Containing Tin Perovskite Using High Purity Starting Materials

The wide band gaps of bromide-containing tin perovskites, $ASnI_{3-x}Br_x$, make them attractive materials for use as the top-layer absorber in tandem solar cells, as well as in single junction solar cells for indoor applications. In the present work, a series of $ASnI_{3-x}Br_x$ films was systematically fabricated by varying the A-site (FA^+, MA^+, Cs^+) and X-site (I^-, Br^-) ions. The use of solvent-coordinated $SnBr_2$ complex as a high purity source of bromide combined with Sn(IV) scavenging treatment helps to ensure that the optimal film quality across the compositional space is realized. The energy levels and electronic properties of the films were characterized by photoemission yield spectroscopy and photoluminescence (PL) measurements. The films with long PL lifetime and favorable energy level alignment resulted in superior device efficiency when evaluated in standard single junction solar cells. The best power conversion efficiency of 7.74% was obtained when the composition was $FA_{0.75}MA_{0.25}SnI_{2.25}Br_{0.75}$.3)

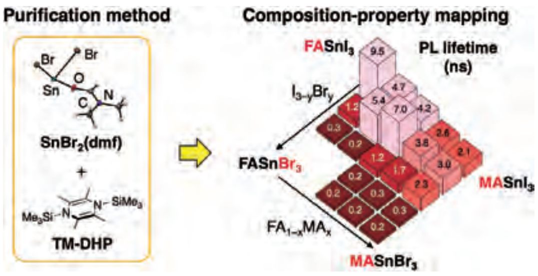

Figure 2. Composition-property mapping in bromide -containing tin perovskite using high purity starting materials.

References

1) S. Hu, K. Otsuka, R. Murdey, T. Nakamura, M. A. Truong, T. Yamada, T. Handa, K. Matsuda, K. Nakano, A. Sato, K. Marumoto, K. Tajima, Y. Kanemitsu, A. Wakamiya, *Energy Environ. Sci.* **2022**, *15*, 2096.
2) R. Murdey, Y. Ishikura, Y. Matsushige, S. Hu, J. Pascual, M. A. Truong, T. Nakamura, A. Wakamiya, *Sol. Energy Mater. Sol. Cells* **2022**, *245*, 111885.
3) T. Nakamura, K. Otsuka, S. Hu, R. Hashimoto, T. Morishita, T. Handa, T. Yamada, M. A. Truong, R. Murdey, Y. Kanemitsu, A. Wakamiya, *ACS Appl. Energy Mater.* **2022**, in press (DOI: 10.1021/acsaem.2c02144).

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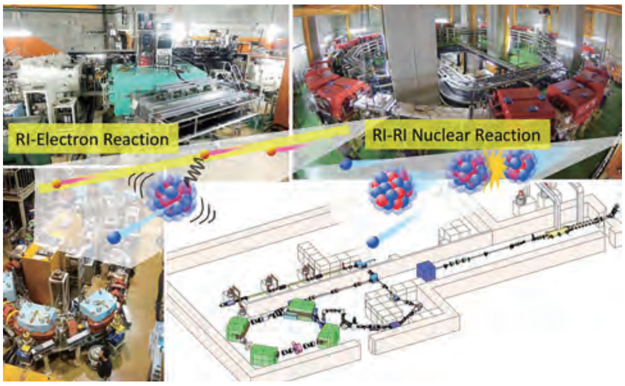
Scope of Research

One of our research is an experimental research for unstable nuclear structures by means of the electron and heavy-ion accelerators. We address the technical development in an RI beam production driven by a high-energy electron beam, an electron scattering from the RI's in combination with the RI target inserted in an electron storage ring, and the precision mass measurement for extremely short-lived and rare exotic nuclei using a heavy-ion storage ring. We will address some technical development aiming at a nuclear photo-absorption cross-section measurement and the beam recycling in a heavy-ion storage ring to study the nuclear reactions involving rare exotic nuclei.

KEYWORDS

Beam Physics	Accelerator Physics
Unstable Nuclear Physics	Storage Ring
Electron Linac	



Recent Selected Publications

Li, H. F.; Naimi, S.; Sprouse, T. M.; Mumpower, M. R.; Abe, Y.; Yamaguchi, Y.; Nagae, D.; Suzaki, F.; Wakasugi, M.; Arakawa, H.; Dou, W. B.; Hamakawa, D.; Hosoi, S.; Inada, Y.; Kajiki, D.; Kobayashi, T.; Sakaue, M.; Yokoda, Y.; Yamaguchi, T.; Kagesawa, R.; Kamioka, D.; Moriguchi, T.; Mukai, M.; Ozawa, A.; Ota, S.; Kitamura, N.; Masuoka, S.; Michimasa, S.; Baba, H.; Fukuda, N.; Shimizu, Y.; Suzuki, H.; Takeda, H.; Ahn, D. S.; Wang, M.; Fu, C. Y.; Wang, Q.; Suzuki, S.; Ge, Z.; Litvinov, Yu. A.; Lorusso, G.; Walker, P. M.; Podolyak, Zs.; Uesaka, T., First Application of Mass Measurements with the Rare-RI Ring Reveals the Solar r-Process Abundance Trend at A = 122 and A = 123, *Phys. Rev. Lett.*, **128,** 152701 (2022).

Kusumoto, T.; Inoue, S.; Ogawara, R.; Kodaira, S., Measurement of the Energy Spectrum of Laser-Accelerated Protons Using FNTD: Development of an Easy and Quick Method for Energy Spectrometry, *Radiat. Meas.*, **151,** 106715 (2022).

F. Sakuma *et al.*, Summary of the $K^{-}pp$ Bound-State Observation in E15 and Future Prospects, *EPJ Web Conf.*, **262,** 01008 (2022).

Nagae, D.; Abe, Y.; Okada, S.; Omika, S.; Wakayama, K.; Hosoi, S.; Suzuki, S.; Moriguchi, T.; Amano, M.; Kamioka, D.; Ge, Z.; Naimi, S.; Suzaki, F.; Tadano, N.; Igosawa, R.; Inomata, K.; Arakawa, H.; Nishimuro, K.; Fujii, T.; Mitsui, T.; Yanagisawa, Y.; Baba, H.; Michimasa, S.; Ota, S.; Lorusso, G.; Litvinov, Yu. A.; Ozawa, A.; Uesaka, T.; Yamaguchi, T.; Yamaguchi, Y.; Wakasugi, M., Development and Operation of an Electrostatic Time-of-Flight Detector for the Rare RI Storage Ring, *Nucl. Instrum. Meth. A*, **986,** 164713 (2021).

Omika, S.; Yamaguchi, T.; Tadano, N.; Abe, Y.; Amano, M.; Ge, Z.; Kamioka, D.; Moriguchi, T.; Nagae, D.; Naimi, S.; Ozawa, A.; Suzaki, F.; Suzuki, S.; Suzuki, T.; Uesaka, T.; Wakasugi, M.; Wakayama, K.; Yamaguchi, Y., Development of a New in-Ring Beam Monitor in the Rare-RI Ring, *Nucl. Instrum. Meth. B*, **463,** 241 (2020).

Analytical Formalization of Beam Recycle Operation at RUNBA

A compact heavy ion storage ring RUNBA (Recycled Unstable Nuclear Beam Accumulator) is under construction at the RIKEN RI Beam Factory in collaboration with ICR. It aims to develop beam recycling techniques, which will provide a new tool for precise nuclear reaction studies, especially for rare radioactive nuclides (RIs). It is assumed that a few RIs are accumulated in a RUNBA with an internal target and the RIs hit the target many times until a nuclear reaction occurs. This is a beam recycling, which is established by compensating the energy loss, energy straggling, and angular straggling. Therefore, the RUNBA will be equipped with a radio-frequency cavity, an energy dispersion corrector (EDC) and an angular diffusion corrector (ADCh, ADCv). These devices correctly modulate the beam motion in 6D phase space on a turn-by-turn basis. Assuming a thin internal target, beam information such as the timing and position of the beam as it passes through the target can be obtained. The beam information is converted into correction signals, which are transported to each corrector in synchronization with the arrival of the beam. As this is the first time such a process has been attempted in a storage ring, we formulate analytical equations describing the beam motion under the above configuration and situation.

The beam motion is described by a Hamiltonian with canonical variables q and p, and the invariant of motion is defined as $W(q, p)$. The target changes the variables stochastically and the correctors change them compensatory manner. Including those effect, the change of the invariants is expressed as $\Delta W = W(q+\Delta q, p+\Delta p) - W(q, p)$. The time differential equation is obtained from it divided by the revolution time T. Assuming the probability density function $\Psi(\Delta p)$ for straggling at the target and $\phi(\delta)$ for uncertainty in the beam information measurement, averaged differential coefficient is expressed as

$$\langle\frac{dW}{dt}\rangle = \frac{1}{T}\iint \Delta W \psi(\Delta p)\phi(\delta)d\Delta p d\delta \quad .$$

The numerical values in (q, p) phase space are shown in Fig. 1(a) for transverse case and Fig. 2(a) for longitudinal. Since this value depends on the position (q, p), it should be averaged in the acceptance of RUNBA as

$$\Lambda(\kappa) = \frac{1}{S}\iint \langle\frac{dW}{dt}\rangle dqdp \quad ,$$

where S is a volume of the acceptance and κ is a parameter of the correction at EDC and/or ADC. An example of $\Lambda(\kappa)$ for transverse motion is shown in Fig. 1(b) and that for longitudinal motion is shown in Fig. 2(b) in the case of 10-MeV/u $^{12}C^{6+}$ beam accumulated in RUNBA with 10^{18}/cm^2-thick ^{12}C target. The calculations show that the minimum correction required to maintain beam circulation is κ - 3 μrad/mm and that a technically realistic ADC field of 2 kV/m gives an adequate correction.

We formulated the Fokker-Planck equation for the beam recycling process to reveal the time evolution of the probability density distribution $f(W, t)$ of circulating particles in phase space. That for transverse motion is expressed as

$$\frac{\partial f(W,t)}{\partial t} = -\frac{\partial f(W,t-\Delta t)}{\partial W}F(W,\kappa) + \frac{\partial^2 f(W,t-\Delta t)}{\partial W^2}D(W,\kappa) \text{ ,}$$

where β is a beta function at the target, $V(\kappa)$ a function of the correction parameter, σ_t a standard deviation of the straggling. The friction term is expressed as $F(W, \kappa) = \{\beta\sigma_t^2 + V(\kappa)W\} / T$, and the diffusion coefficient as $D(W, \kappa) = \{3\beta^2\sigma_t^4 + 2\beta\sigma_t^2 V(\kappa)W + V(\kappa)^2 W^2\} / 2T$. This formulation completely generalizes the beam recycle process, which is new concept.

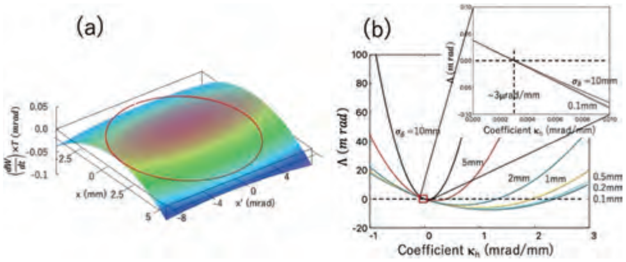


Figure 1. (a) Numerically calculated averaged time differential coefficient <*dW* / *dt*> in transverse phase space and (b) Λ(*κ*) values as a function of ADC correction in some cases of beam information measurement uncertainty.

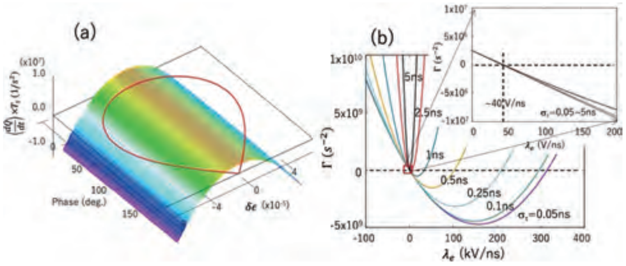


Figure 2. (a) Numerically calculated averaged time differential coefficient <*dQ* / *dt*> in longitudinal phase space and (b) Γ(*κ*) values as a function of EDC correction in some cases of beam information measurement uncertainty.

Advanced Research Center for Beam Science
– Laser Matter Interaction Science –

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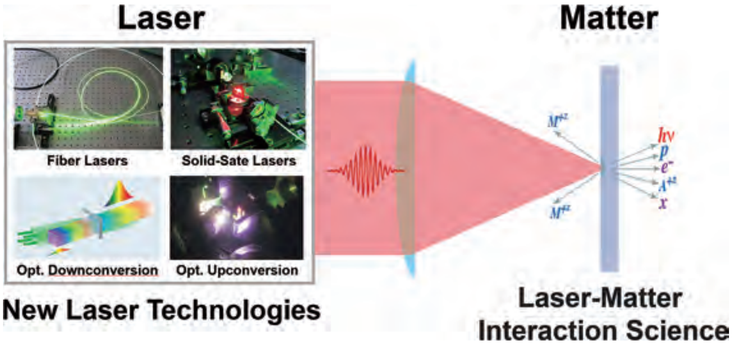
Scope of Research

We are developing cutting-edge high-intensity laser sources and studying experimental research on the laser interaction with matter by using the new laser sources. We are promoting cross-disciplinary research based on high-intensity laser technologies such as development of high-intensity mid-infrared solid-state lasers and fiber lasers, research on particle acceleration and wavelength conversion with plasmas produced by high-intensity ultrafast lasers, development of laser isotope separation method for neutrino research, and search for dark matter using high-intensity lasers.

KEYWORDS
High Power Laser Optics
Ultrafast Laser Physics
Laser Plasma Interaction Physics
Laser Nano-Ablation Physics
Femtosecond Laser Prosessing



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Yokoyama, N.; Morioka, Y.; Murata, T.; Honda, H.; Serita, K.; Murakami, H.; Tonouchi, M.; Tokita, S.; Ichikawa, S.; Fujiwara, Y.; Hikosaka, T.; Uemukai, M.; Tanikawa, T.; Katayama, R., Second Harmonic Generation in GaN Transverse Quasi-Phase-Matched Waveguide Pumped with Femtosecond Laser, *Appl. Phys. Express*, **15,** 112002 (2022).

Sekine, T.; Kurita, T.; Hatano, Y.; Muramatsu, Y.; Kurata, M.; Morita, T.; Watari, T.; Iguchi, T.; Yoshimura, R.; Tamaoki, Y.; Takeuchi, Y.; Kawai, K.; Zheng, Y.; Kato, Y.; Kurita, N.; Kawashima, T.; Tokita, S.; Kawanaka, J.; Kodama, R., 253 J at 0.2 Hz, LD Pumped Cryogenic Helium Gas Cooled Yb:YAG Ceramics Laser, *Opt. Express*, **30,** 44385-44394 (2022).

Takenaka, K.; Hashida, M.; Sakagami, H.; Masuno, S.; Kusaba, M.; Yamaguchi, S.; Iwamori, S.; Sato, Y.; Tsukamoto, M., Uniformity Evaluation of Laser-Induced Periodic Surface Structures Formed by Two-Color Double-Pulse Femtosecond Laser Irradiation, *Rev. Sci. Instrum.*, **93,** 093001 (2022).

Collaborative Development of Compact High-Power Femtosecond Lasers for Micromachining

In the recent industrial field of automobiles, semiconductors, medical equipment, etc., it is required to develop/supply products with higher performance and smaller sizes, and accordingly, downsizing their components is also required. For this purpose, one of the crucial technologies is microfabrication on the order of several tens of microns for metals, ceramics, resins, glass, and their composite materials. Recently, ultrafast lasers, which have extremely short pulse durations of picoseconds to femtoseconds, are expanding their use in a wide range of fields as crucial tools that enable high-speed and precise microfabrication. Currently, with the rapid growth of the laser microfabrication market, the global market size for ultrafast laser oscillators has reached 420 billion yen in 2018 and is expected to expand to more than 1.2 trillion yen. The presence of Japanese companies in the ultrafast laser market, however, is extremely low, and they are far behind European and American companies.

In the present project, to enhance the presence of Japan in this expanding industrial field, novel high-performance femtosecond lasers will be developed based on a collaboration by our laboratory, which is one of the centers of excellence in high-power laser studies, and Spectronics Co., Ltd., which is the only manufacturer/seller of picosecond laser oscillators for microfabrication in Japan. The existing femtosecond lasers have lower power efficiency and more complicated structures compared with general nanosecond/picosecond lasers, and therefore their sizes inevitably become large, and the prices are not competitive. By combining the state-of-the-art technologies in mode-locked fiber oscillators and chirp pulse amplification, and through optimizing the structure of the laser systems as well as the materials of their housing in detail, we have developed next-generation femtosecond, lasers that realize high power output, an ultra-compact size, and ultra-lightness in weight, simultaneously (Fig. 1).

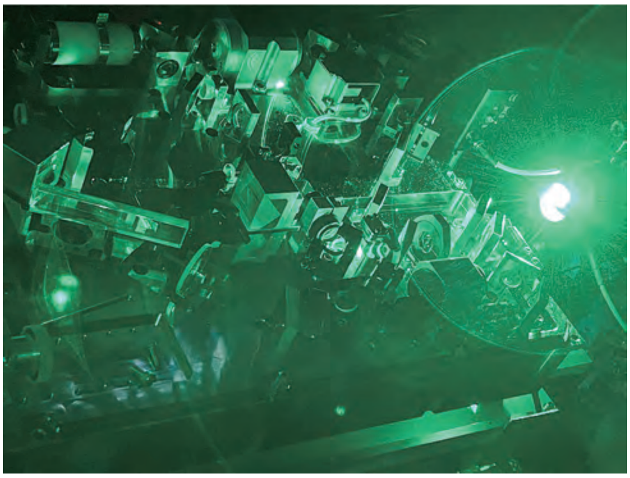

Figure 1. The developed high-power and compact laser emitting intense green femtosecond pulses for laser microfabrication.

Uniformity Evaluation of Laser-Induced Periodic Surface Structures Formed by Two-Color Double-Pulse Femtosecond Laser Irradiation

In order to evaluate the uniformity of a laser-induced periodic surface structure (LIPSS) we have proposed a Perpendicular Period and Phase Scanning (P^3S) method. P^3S assesses the uniformity of LIPSS using the standard deviation of the peak period and the average of the phase difference in the direction perpendicular to LIPSS. The P^3S method demonstrates that LIPSS formed by two-color double-pulse irradiation is reduced to a quarter of the period dispersion, and the average phase difference of LIPSS is also reduced compared to the single-pulse irradiation. In addition, a three-dimensional electromagnetic particle-in-cell simulation was performed to evaluate the possibility of an improved uniformity of LIPSS. The results confirm that the two-color double-pulse irradiation produces a uniform LIPSS and validates the effectiveness of the P^3S method to assess the uniformity of LIPSS.

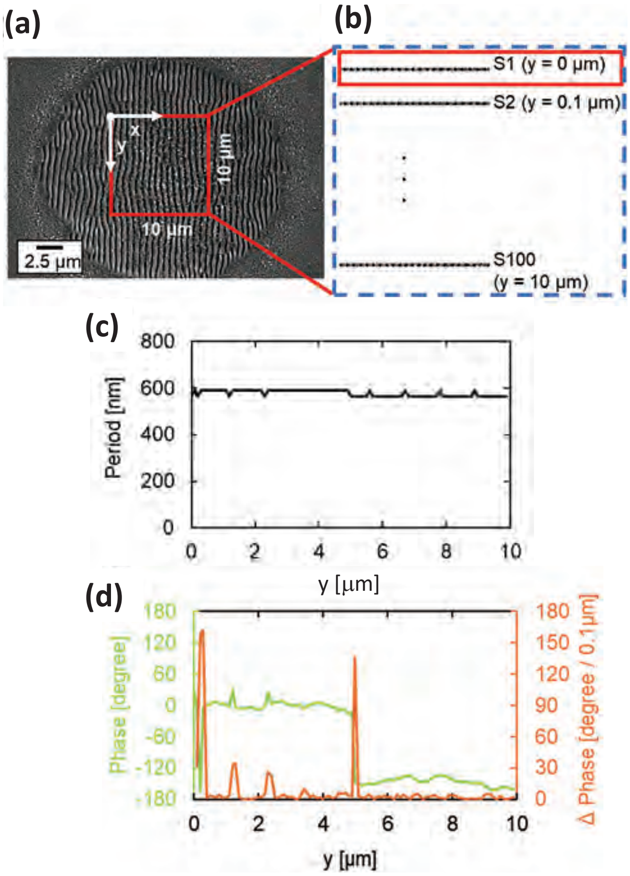

Figure 2. Schematic of P^3S method for evaluating the LIPSS uniformity. (a) SEM image is divided into (b) S1–S100 segments. Then segment of S1 is performed by 1-D Fast Fourier transform (FFT), and the peak period of 1-D FFT and the peak phase are evaluated. Standard deviation (SD) of the period and the average of the Δ phase are determined by calculating (c) the period, and (d) the phase, and the Δ phase for each y-coordinate, the SD of the period, and the average of the Δ phase.

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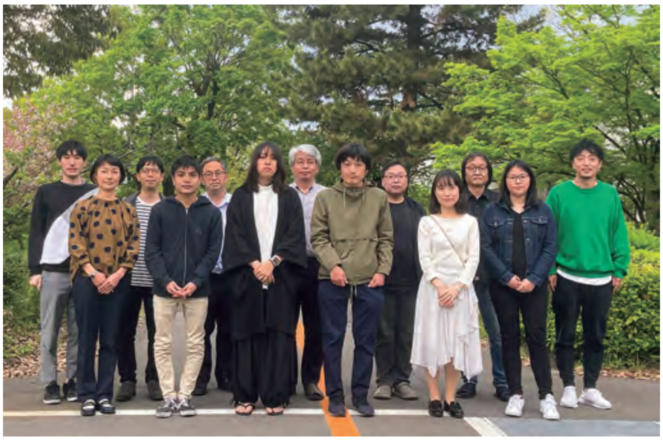
Scope of Research

We study crystallographic and electronic structures of materials and their transformations through direct imaging of atoms or molecules by high-resolution electron spectromicroscopy, which realizes energy-filtered imaging and electron energy-loss spectroscopy as well as high-resolution imaging. By combining this with scanning probe microscopy, we cover the following subjects: 1) direct structure analysis, electron crystallographic analysis, 2) elemental analysis and electronic states analysis, 3) structure formation in solutions, and 4) epitaxial growth of molecules.



KEYWORDS
STEM-EELS ELNES Spectrum Imaging Electron Orbital Multiple Frame Acqusition

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Haruta, M.; Kikkawa, J.; Kimoto, K.; Kurata, H., Comparison of Detection Limits of Direct-Counting CMOS and CCD Cameras in EELS Experiments, *Ultramicroscopy*, **240,** [113577-1]-[113577-6] (2022).

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Haruta, M.; Nii, A.; Hosaka, Y.; Ichikawa, N.; Saito, T.; Shimakawa, Y.; Kurata, H., Extraction of the Local Coordination and Electronic Structures of FeO_6 Octahedra Using Crystal Field Multiplet Calculations Combined with STEM-EELS, *Appl. Phys. Lett.*, **117,** [132902-1]-[132902-5] (2020).

Yamaguchi, A.; Nemoto, T.; Kurata, H., Study of C K-Edge High Energy Resolution Energy-Loss Near-Edge Structures of Copper Phthalocyanine and Its Chlorinated Molecular Crystals by First-Principles Band Structure Calculations, *J. Phys. Chem. A*, **124,** 1735-1743 (2020).

Electron Orbital Mapping of $SrTiO_3$ Using Electron Energy-Loss Spectroscopy (EELS)

The visualization of electron orbitals in real space is expected as a next-generation technique that has been evolved from high spatial resolution electron microscopy. Although its possibility has recently theoretically reported by using an energy-filtered energy-loss near-edge structure (ELNES) mapping, the experimental demonstration has been quite challenging because of the low signal-to-noise ratio (SNR). Here, we present the visualization of 2*p* electron orbitals of oxygen in $SrTiO_3$ in real space using STEM-EELS combined with newly developed our multi-frame acquisition approach that dramatically improves the SNR.

The experiment was carried out using a spherical aberration corrected STEM (JEOL; JEM-ARM200F) with an EELS spectrometer (Gatan; GIF Quantum ERS). Spectrum imaging (SI) data of about 100 × 1000 pixels were obtained. Image distortion due to sample drift was suppressed as much as possible by measuring the SI data in a horizontally narrow scan area with a short acquisition time of 2ms per pixel. Individual SI data was applied the subtraction of ultra-high-quality dark reference spectrum obtained from the average of 20 000 dark spectra and then the original gain-correction. To improve the SNR of the spectrum and to correct the image distortion, 7762 SI data were summed using the multi-frame non-rigid registration combined with a template matching technique. Spectral deconvolution by zero-loss peak was applied to improve the energy resolution. In the present experiment, in order to minimize sample drift and obtain high signal intensity, we prioritized the acquisition of SI data in a short time using a high-current incident probe rather than the acquisition of high-energy resolution spectra. Finally, weighted-principal component analysis (W-PCA) was used to remove spectral noise.

Figure 1(b) shows the oxygen *p*-partial density of states (PDOS) of unoccupied bands at the O1 site and simulated O K-ELNES. Figure 1(c) shows the experimental O K-ELNES. It is suggested that peaks a and d are mainly composed of a single component of $p_{x,y}$ (hybridized with Ti $3d(t_{2g})$ forming a π*-bond), while peaks b and e are composed of p_z (hybridized with Ti $3d(e_g)$ forming a σ*-bond) orbitals. Figures 2(a) and 2(b) show ground state charge density maps projected along the [110] axis for the unoccupied states of π*- and σ*-bonds, respectively. The distribution at oxygen sites is anisotropic, which reflects the orientation of the 2*p* orbitals. In the oxygen map in Fig. 2(d), oxygen atoms were not observed in the Sr-O columns because the atomic density of oxygen is half compared to the pure oxygen columns. Figures 2(e)–2(h) show O K-ELNES maps using the intensities of peaks a, b, d, and e. Figures 2(e) and 2(g) show vertically elongated ellipses, while Figs. 2(f) and 2(h) show lateral ellipses. These orientations agree well with those of the calculated charge density distribution showing oxygen *p*-orbitals. In summary, we experimentally demonstrated the visualization of 2*p* electron orbitals of oxygen in the $SrTiO_3$ [110] projection in real space. Although orbital mapping has been a challenge due to the SNR problem with spectra, improvement of the SNR for a core-loss spectrum measured with atomic resolution has made it possible to observe electron orbitals using electron microscopy.

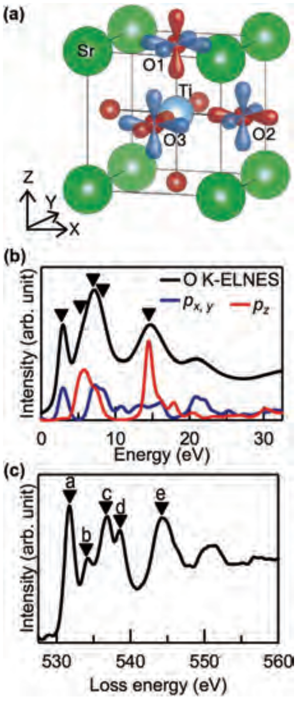

Figure 1. PDOS and oxygen K-ELNES of $SrTiO_3$. (a) Structural model of $SrTiO_3$. The O 2*p* orbitals can be classified into two groups: the blue orbitals distributed in the Sr–O plane, hybridized with the Ti 3*d* orbitals with t_{2g} symmetry, and the red orbitals distributed in the direction of the Ti–O–Ti bond, hybridized with Ti 3*d* orbitals with e_g symmetry. (b) Simulated O K-ELNES (black) and oxygen *p* PDOS for O1 sites (blue and red). (c) Experimental O K-ELNES.

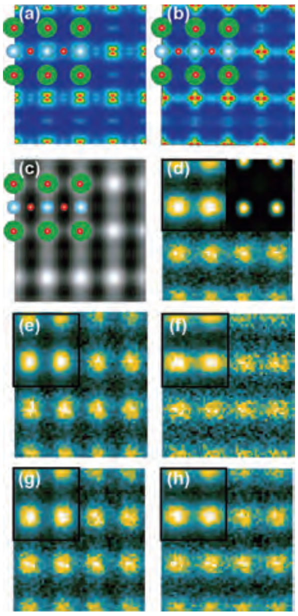

Figure 2. Projection along the [110] axis. Charge density maps for the unoccupied state of the (a) π*-bond (3–4 eV) and (b) σ*-bond (5–6 eV). (c) Accumulated HAADF image along the [110] axis. (d) Oxygen elemental map using an energy window of 26 eV from the threshold of the O K-edge. O-ELNES mappings using (e) peak a, (f) peak b, (g) peak d, and (h) peak e. The upper left insets in (d)–(h) are the results of W-PCA. The upper right inset in (d) is a simulated elemental mapping.

Advanced Research Center for Beam Science
– Atomic and Molecular Structures –

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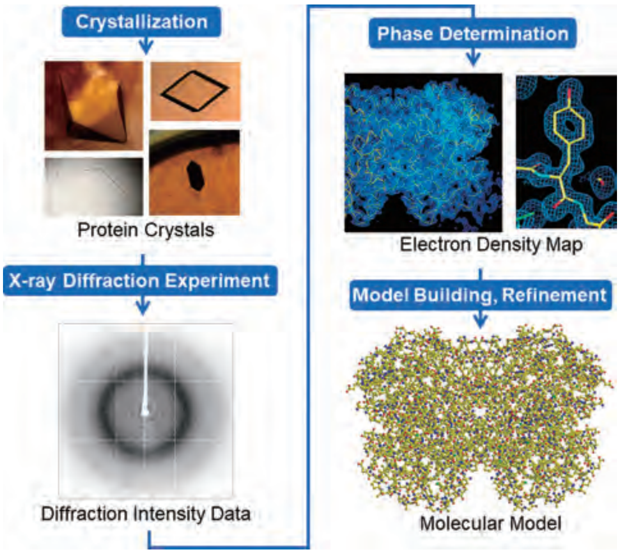
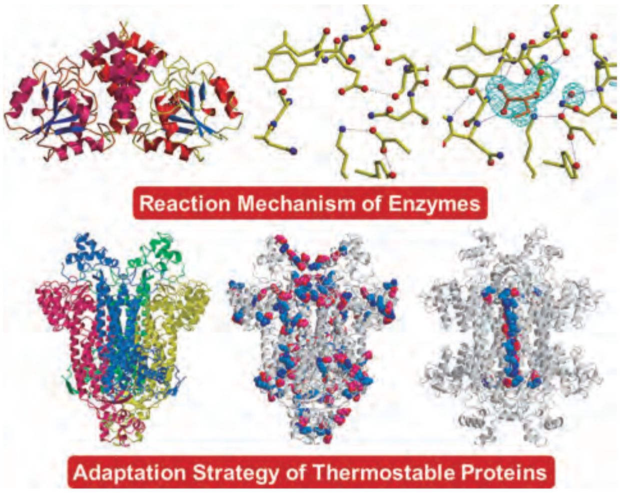
Scope of Research

This laboratory analyzes X-ray crystallographic structures of biological macromolecules and studies the structural biology about the relationships between protein structures and their functions and properties based on the crystal structures. The main research themes are elucidation of the reaction mechanism of enzymes, the relationship between the multiform conformation and the functional variety of proteins, the structural basis for the domain-arrangements of multi-domain proteins or protein-protein interactions, structure determination for structure-based protein engineering and industrial application, and the adaptation strategy of proteins from thermophilic or cold-adapted bacteria.

KEYWORDS

Crystal
X-ray Crystallographic Analysis
Structural Biology
Protein Crystallography
Structure and Function





Recent Selected Publications

Fujii, T.; Sato, A.; Okamoto, Y.; Yamauchi, T.; Kato, S.; Yoshida, M.; Oikawa, T.; Hata, Y., The Crystal Structure of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005 Provides Insights into the Reaction Mechanism of Enzymes in Its Original Family, *Proteins: Structure, Function, and Bioinformatics*, **84,** 1029-1042 (2016).

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Fujii, T.; Goda, Y.; Yoshida, M.; Oikawa, T.; Hata, Y., Crystallization and preliminary X-ray Diffraction Studies of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **64,** 737-739 (2008).

Fujii, T.; Oikawa, T.; Muraoka, I.; Soda, K.; Hata, Y., Crystallization and Preliminary X-ray Diffraction Studies of Tetrameric Malate Dehydrogenase from the Novel Antarctic Psychrophile *Flavobacterium frigidimaris* KUC-1, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **63,** 983-986 (2007).

Fujii, T.; Sakai, H.; Kawata, Y.; Hata, Y., Crystal Structure of Thermostable Aspartase from *Bacillus* sp. YM55-1: Structure-based Exploration of Functional Sites in the Aspartase Family, *J. Mol. Biol.*, **328,** 635-654 (2003).

Refined Crystal Structure of the Oxygenase Component (GraA) of Resorcinol Hydroxylase

Resorcinol hydroxylase is involved in the first step of the resorcinol catabolic pathway and catalyzes the hydroxylation of resorcinol to hydroxyquinol. This enzyme belongs to the two-component flavin-diffusible monooxygenase (TC-FDM) family and comprises two components: an oxygenase and a flavin reductase. It uses molecular oxygen and reduced flavin for hydroxylation and NAD(P)H for flavin reduction. The smaller component, flavin reductase, generates reduced flavin to allow the oxygenase component to oxygenate the substrate. Thus, the enzymatic reaction is executed in two steps. However, hydroxylation activity requires cooperation between both the components. To understand the structural basis of the catalytic mechanism, we performed a crystal structure analysis of the apo-form of the oxygenase component (GraA) from *Rhizobium* sp. strain MTP-10005. GraA is a tetramer, and its subunit consists of 409 amino acid residues with a mass of 43,305 Da.

N-terminal His-tagged GraA was used for crystallization. The protein solution consisted of 5 mg/ml GraA and 50 mM Tris-HCl pH 8.0. Crystals with suitable sizes for X-ray diffraction experiments were obtained over several days by a sitting drop vapor diffusion method, with a reservoir solution consisting of 17% (w/v) PEG3350 and 0.2 M K_2HPO_4. They belonged to the tetragonal space group $I4_122$ with unit cell dimensions of $a = b = 101.6$ Å, $c = 319.8$ Å and contained one GraA subunit in asymmetric unit. Diffraction data were collected up to 1.9 Å resolution under cryogenic conditions at beamline BL5A, PF, Tsukuba, Japan. The structure was determined by molecular replacement and refined at 1.9 Å resolution up to $R = 0.162$ and $R_{\mathrm{free}} = 0.185$.

GraA is a tetramer of four identical subunits related to one another by three molecular two-fold axes which are identical to crystallographic two-fold axes (Figure 1). A given pair of two subunits in the molecule forms a close dimer and two of the close dimers form a loose dimer. The GraA tetrameric molecule adopts the structure of a dimer of dimers. The subunit consists of three domains (Figure 2). The N-terminal domain (residues Met1–Ala121) has an α-structure mainly of antiparallel α-helices, the central domain has a β-structure of two β-sheets stacked together, and the C-terminal domain (residues Phe218–Tyr409) has a four-helix-bundle structure of long antiparallel α-helices involved in tetramer formation. The part of PEG3350 used as a precipitating agent for the crystallization is located in the space that is encompassed by these three domains (Figure 2). The PEG binds to both the binding site of a portion of isoalloxazine ring of FAD in the GraA-FAD complex and the putative substrate binding site (Figure 3). The loop region of 13 residues (residues Gly271–Asn283), which is ordered and covers the FAD of another subunit in the GraA-FAD complex, is disordered in this apo-form (Figures 2 and 3).

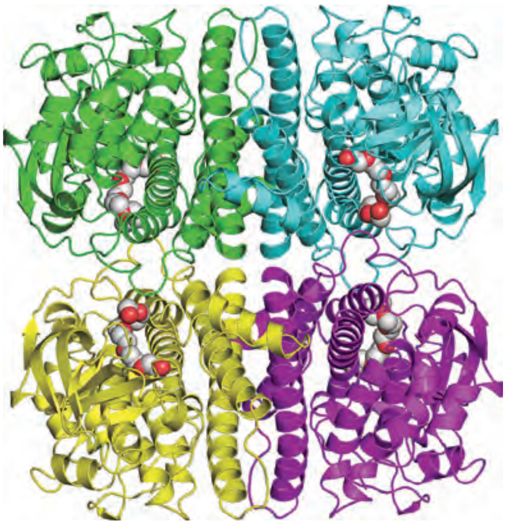

Figure 1. Tetrameric molecular structure of the apo-form of the oxygenase component of resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 with bound PEG.

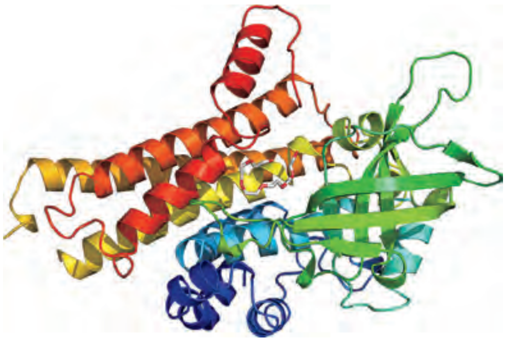

Figure 2. Subunit structure of the apo-form of the oxygenase component of resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 with bound PEG.

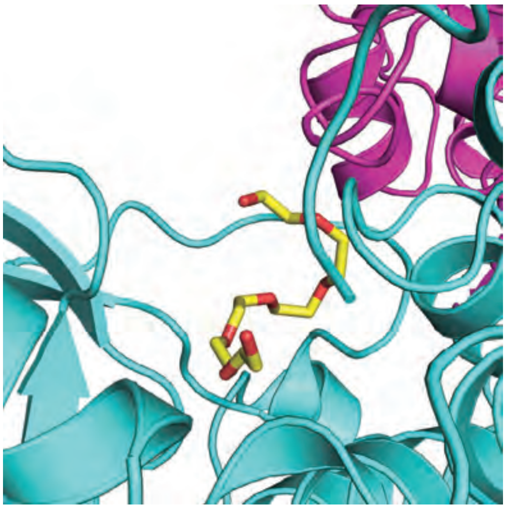

Figure 3. Structure of the active site cleft of the apo-form of the oxygenase component of resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 with bound PEG.

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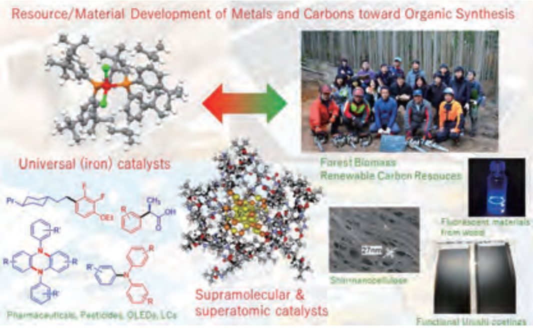
Scope of Research

Our research activity focuses on the development of new molecular transformations, which can contribute to better or ideal synthesis of functional molecules as well as to exploitation of new chemical (metal and carbon) resources. The present research subjects are (1) metal-catalyzed carbon–carbon and carbon–heteroatom bond forming reactions by using universal metals such as iron (2) development of small metallic nanocluster catalysts based on supramolecular approaches (3) utilization of woody biomass as the renewable carbon resources by mild catalytic transformations of wood molecules into useful compounds and materials.



KEYWORDS

Iron Catalysis Organotransformation Woody Molecular Transformation Supramolecular & Superatomic Catalysis

Recent Selected Publications

Isozaki, K.; Ueno, R.; Ishibashi, K.; Nakano, G.; Yin, H.; Iseri, K.; Sakamoto, M.; Takaya, H.; Teranishi, T.; Nakamura, M., Gold Nanocluster Functionalized with Peptide Dendron Thiolates: Acceleration of the Photocatalytic Oxidation of an Amino Alcohol in a Supramolecular Reaction Field, *ACS Catal.*, **11,** 13180-13187 (2021).

Adak, L.; Jin, M.; Saito, S.; Kawabata, T.; Itoh, T.; Ito, S.; Sharma, A. K.; Gower, N. J.; Cogswell, P.; Geldsetzer, J.; Takaya, H.; Isozaki, K.; Nakamura, M., Iron-Catalysed Enantioselective Carbometalation of azabicycloalkenes, *Chem. Commun.*, **57,** 6975-6978 (2021).

Iwamoto, T.; Okuzono, C.; Adak, L.; Jin, M.; Nakamura, M., Iron-Catalysed Enantioselective Suzuki-Miyaura Coupling of Racemic Alkyl Bromides, *Chem. Commun.*, **55,** 1128-1131 (2019).

Agata, R.; Takaya, H.; Matsuda, H.; Nakatani, N.; Takeuchi, K.; Iwamoto, T.; Hatakeyama, T.; Nakamura, M., Iron-Catalyzed Cross Coupling of Aryl Chlorides with Alkyl Grignard Reagents: Synthetic Scope and FeII/FeIV Mechanism Supported by X-Ray Absorption Spectroscopy and Density Functional Theory Calculations, *Bull. Chem. Soc. Jpn.*, **92,** 381-390 (2019).

Adak, L.; Kawamura, S.; Toma, G.; Takenaka, T.; Isozaki, K.; Takaya, H.; Orita, A.; Li, H. C.; Shing, T. K. M.; Nakamaura, M., Synthesis of Aryl C-Glycosides via Iron-Catalyzed Cross Coupling of Halosugars: Stereoselective Anomeric Arylation of Glycosyl Radicals, *J. Am. Chem. Soc.*, **139,** 10693-10701 (2017).

Iron-Catalyzed Organic Synthesis

Transition-metal-catalyzed carbon–carbon and carbon–heteroatom bond forming reactions are powerful tools for the synthesis of functional molecules. Our group focuses on use of iron as a catalyst, and so far developed a variety of iron-catalyzed cross-coupling reactions, some of which can’t be achieved by conventional transition-metal catalysts such as palladium. As a recent representative example, we developed the iron-catalyzed enantioselective carbometalation of azabicycloalkenes (Figure 1a), which is of significant interest due to the facile installation of four stereocenters retaining the azabicyclic skelton. By the combination of X-ray absorption spectroscopy and DFT calculation, we proposed a catalytic cycle of diaryliron complex involving coordination of azabicyclic alkene, olefin insertion, and transmetalation steps (Figure 1b).

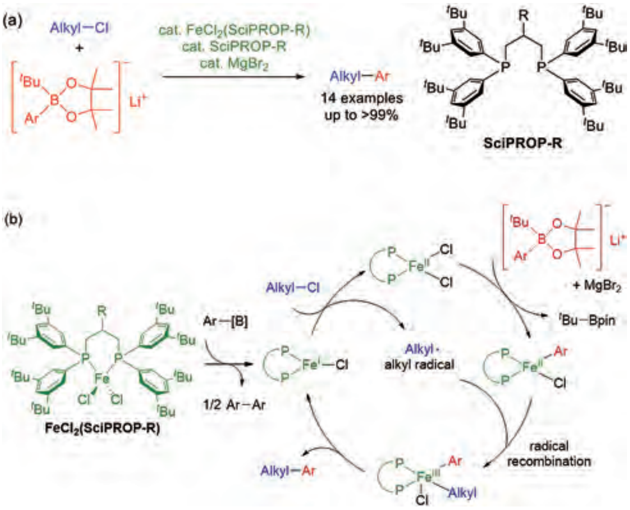


Figure 1. Iron-catalyzed Suzuki-type cross coupling between alkyl chlorides and arylboronates. (a) General reaction scheme and (b) proposed catalytic cycle.

Supramolecular & Superatomic Catalysis

This project focuses on development of smart materials based on synergistic effect of various metals on artificial peptides. Based on this concept, we have developed novel ruthenium complex bound with norvaline, which catalyze efficient and selective oxidation of several methoxybenzene analogues to quinones. Now we are trying further modification of the catalysts toward investigation of future chemical resources.

Wood Molecular Transformation

Woody biomass is renewable and the most abundant carbon resouce on the earth, thus expected to utilize as a feedstock to chemicals and energy toward a sustainable society. This project focuses on the chemical transformation of woody biomass into useful materials under mild catalytic conditions. To achieve this purpose, we have developed two key technologies; 1) direct transformation of woody lignin to fluorescent molecules, 2) one-pot disintegration of wood powder into nanocellulose. As a recent representative example, we reported the development of artificial urushi-coating materials by installing trienyl side chains from natural linolenic acid to the bio-renewable phenoxypropanone compounds obtained from enzymatic degradatio of woody lignin.

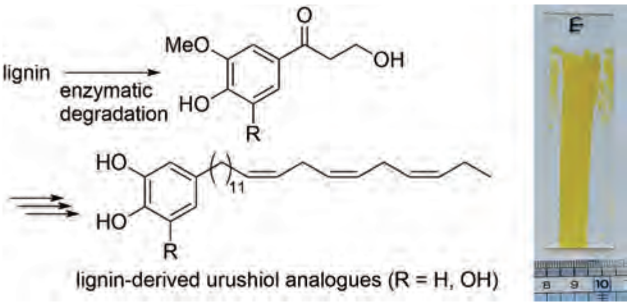


Figure 2. Artificial urushi-coating materials derived from renewable woody lignin.

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Scope of Research

Transition metal oxides have a wide variety of interesting and useful functional properties, including electronic conduction, superconductivity, ferroelectricity, and ferromagnetism. In fact, some of these oxides are used in current electronic devices. Our research mainly focuses on perovskite-structured transition metal oxides with novel functional properties due to complex couplings between their lattices, charges and spins. We are currently exploring such functional oxides with advanced oxide-synthesis techniques such as high-pressure synthesis and epitaxial thin film growth.

KEYWORDS

Solid State Chemistry
High Pressure Synthesis
Heterointerface
Functional Metal Oxides
Epitaxial Thin Film Growth

Recent Selected Publications

Patino, M. A.; Romero F. D.; Koo, H. -J.; Avdeev, M.; Injac, S. D. A.; Goto, M.; Whangbo, M. -H.; Shimakawa, Y., Orthogonal Antiferromagnetism to Canted Ferromagnetism in $CaCo_3Ti_4O_{12}$ Quadruple Perovskite Driven by Underlying Kagome Lattices, *Commun. Mater.*, **3,** 51 (2022).

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Isoda, Y.; Kan, D.; Ogura, Y.; Majima, T.; Tsuchiya, T.; Shimakawa, Y., Electrochemical Control and Protonation of the Strontium Iron Oxide $SrFeO_y$ by Using Proton-Conducting Electrolyte, *Appl. Phys. Lett.*, **120,** 091601 (2022).

Guo, H.; Patino, M. A.; Ichikawa N.; Saito, T.; Watanabe, R.; Goto, M.; Yang, M.; Kan D.; Shimakawa Y., Oxygen Release and Incorporation Behaviors Influenced by A-Site Cation Order/Disorder in $LaCa_2Fe_3O_9$ with Unusually High Valence $Fe^{3.67+}$, *Chem. Mater.*, **34,** 345-350 (2022).

Geometrical Spin Frustration and Monoclinic-Distortion-Induced Spin Canting in the Double Perovskites Ln_2LiFeO_6 (Ln = La, Nd, Sm,and Eu) with Unusually High Valence Fe^{5+}

Exploring materials containing transition-metalions with unusual valence states could lead to finding exotic properties and functionalities. Fe in oxides typically has valence states between +2 and +3, as seen in the Fe2+ of Wustite FeO, and in the Fe^{3+} of α-hematite α-Fe_2O_3. Unusually high valence Fe^{5+} is much rare. Recently, we discovered a Fe^{5+} example in the B-site-ordered double perovskite La_2LiFeO_6, which is stable in the air. Importantly, Fe^{5+} in the B-site-ordered double perovskite structure makes a face-centered cubic (fcc.) arrangement of Fe^{5+}, and thus geometrically spin frustration arises if the magnetic interaction between the Fe^{5+} spins is antiferromagnetic.

After this discovery, we extended our material exploration to related B-site-ordered double perovskites Ln_2LiFeO_6 (Ln =Nd, Sm, and Eu) and systematically studied the Fe^{5+}-spin frustration effects in the fcc lattice. Our experimental and theoretical results show the presence of most likely unusually high valence Fe5+ ions in all of the compounds. In particular, Ln_2LiFeO_6 (Ln = La, Nd, Sm) are the first examples adopting purely and octahedrally oxygen-coordinated Fe^{5+}. We also elucidated the structure–property relationships in the geometrically frustrated system. All of the compounds we synthesized were found to be highly frustrated due to the Fe fcc arrangements. In contrast, the crystal structure and magnetic ground state depend on the Ln ion. Indeed, while La_2LiFeO_6 adopts a rhombohedral structure, the others adopt monoclinic structures, and the monoclinic distortion largely increases for Ln = Sm and Eu. Associated with the monoclinic distortion, only Ln = Sm and Eu adopt spontaneous magnetization, which is most likely due to the Dzyaloshinskii-Moriya interaction. We believe that the present results will further stimulate research for materials containing transition metal ions with unusual valence states such as Fe^{5+}, which could lead to finding novel exotic properties and functionalities.

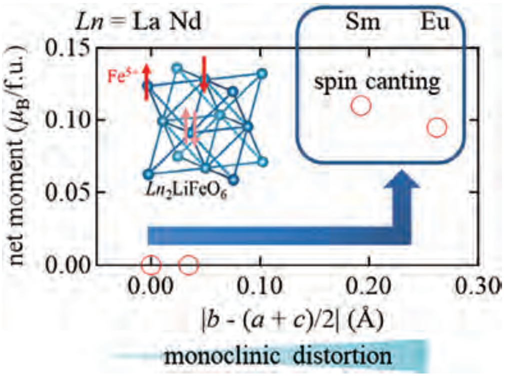

Figure 1. Net moment of Ln_2LiFeO_6 (Ln =La, Nd, Sm, and Eu) as a function of the magnitude of monoclinic distortion.

Electrochemical Control and Protonation of the Strontium Iron oxide SrFeOy by Using Proton-Conducting Electrolyte

Utilizing electrochemical redox reactions and modulating transition metals' valence states enable one to electrically control structural and physical properties of transition metal oxides. Fabricating electric-field-effect transistor structures with gate insulators of electrolytes is a way for electrically inducing redox reactions in channels of oxide films and for electrochemically controlling oxides' physical properties.

In the work reported here, we used the proton-conducting solid electrolyte Nafion, which contains a large amount of water and protons, as a gate insulator and demonstrated electrochemical control and protonation of oxygen-deficient iron oxide $SrFeO_y$ (SFO). Structural and electrical transport properties of SFO are known to depend on oxygen concentration y that ties with the Fe valence state (or the carrier density). When SFO is oxidized and y is close to 3, the oxygenated SFO ($SrFeO_3$) containing Fe^{4+} exhibits metallic transport properties with low electrical resistivity. On the other hand, when oxygen vacancies are introduced and y is lowered to 2.5, SFO is transformed to the insulating brownmillerite $SrFeO_{2.5}$ containing only Fe^{3+}. Given that SFO is integrated as a channel layer in transistor structures having a gate insulator of Nafion, as shown in Figure 2, electrical properties of the SFO channels are expected to be controlled by electrochemical redox reactions. When a positive gate bias V_{GS} is applied, protons are injected into the channel, and the SFO layers would be electrochemically reduced. When a negative V_{GS} is applied, protons are removed from the channel, and the SFO layers are expected to be oxidized. In fact, as we expected, we show that fabricating transistor structures with Nafion as a gate insulator and applying electric-field redox reactions to SFO film channels enables nonvolatile and reversible control of channels' resistance. Furthermore, electrochemically reducing the channels is found to implant protons into SFO, leading to the formation of proton-accumulated oxide $H_xSrFeO_{2.5}$ that has not been seen so far.

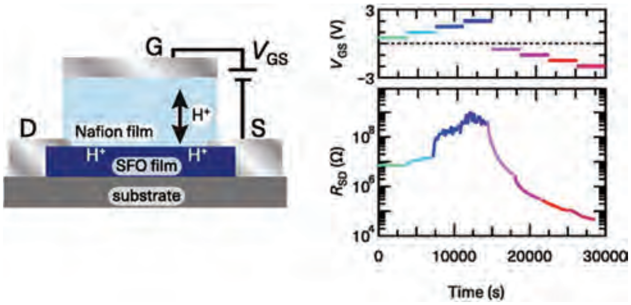

Figure 2. (left) Schematic illustration of electrochemical transistor device in which the proton-conducting solid electrolyte Nafion is used as a gate insulator. (right) Gate voltage V_{GS} dependence of the $SrFeO_y$ channel resistance R_{SD}.

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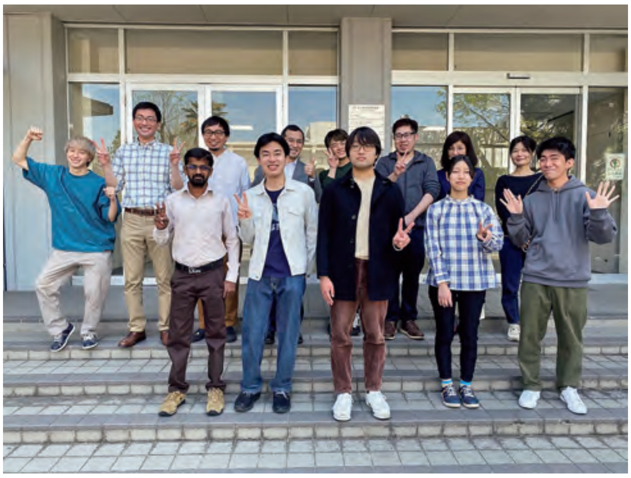
Scope of Research

Developing efficient energy storage systems and innovative material production processes is a significant challenge for chemists to contribute to a sustainable society. We plan to approach these problems by using *transition metal clusters* of which multiple metal atoms work together as catalysts and functional materials. Our laboratory focuses explicitly on creating a new method to synthesize the clusters with atomic precision and applying the obtained clusters to difficult reactions such as the reduction of CO_2 and N_2.

KEYWORDS

Transition Metal Clusters
Homogeneous Catalysis
Nitrogen Fixation
Bioinorganic Chemistry



Recent Selected Publications

Ohki, Y.; Munakata, K.; Matsuoka, Y.; Hara, R.; Kachi, M.; Uchida, K.; Tada, M.; Cramer, R. E.; Sameera, W. M. C.; Takayama, T.; Sakai, Y.; Kuriyama, S.; Nishibayashi, Y.; Tanifuji, K., Nitrogen Reduction by the Fe Sites of Synthetic [Mo_3S_4Fe] Cubes, *Nature*, **607,** 86-90 (2022).

Lee, C. C.; Kang, W.; Jasniewski, A. J.; Stiebritz, M. T.; Tanifuji, K.; Ribbe, M. W.; Hu, Y., Evidence of Substrate Binding and Product Release via Belt-Sulfur Mobilization of the Nitrogenase Cofactor, *Nat. Catal.*, **5,** 443-454 (2022).

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Tanifuji, K.; Jasniewski, A. J.; Villarreal, D.; Stiebritz, M. T.; Lee, C. C.; Wilcoxen, J.; Ohki, Y.; Chatterjee, R.; Bogacz, I.; Yano, J.; Kern, J.; Hedman, B.; Hodgson, K. O.; Britt, R. D.; Hu, Y.; Ribbe, M. W., Tracing the Incorporation of the “Ninth Sulfur” into the Nitrogenase Cofactor Precursor with Selenite and Tellurite, *Nat. Chem.*, **13,** 1228-1234 (2021).

Tanifuji, K.; Ohki, Y., Metal-Sulfur Compounds in N_2 Reduction and Nitrogenase-Related Chemistry, *Chem. Rev.*, **120,** 5194-5251 (2020).

Catalytic N_2 Silylation by the Fe Sites of Cuboidal $[Mo_3S_4Fe]$ Clusters

Biological N_2 fixation is conducted by nitrogenase that employs a unique Fe/Mo-S-C cluster as its catalytic site (FeMoco, [(*R*-homocitrate)$MoFe_7S_9C$]). Synthetic counterparts of the FeMoco, metal-sulfur clusters, demonstrated capturing N_2 on rare occasions; nevertheless, the catalytic conversion of this stable molecule has not been achieved despite its relevance to the biological N_2 fixation. This study focuses on capture, activation, and catalytic conversion of N_2 by an Fe atom incorporated into our $[Mo_3S_4]$ incomplete-cubane platform bearing bulky Cp ligands. Treatment of these clusters with excess Na and $ClSiMe_3$ under a N_2 atmosphere gave $N(SiMe_3)_3$ with up to 248 eq. per cluster. This work exemplifies the N_2-reducing capability of Fe atoms in a S-rich environment, which biological systems have selected to achieve a similar purpose. Further studies are ongoing to unveil the effect of an incorporated metal atom (Fe vs Co or Ni) on catalytic N2 silylation.

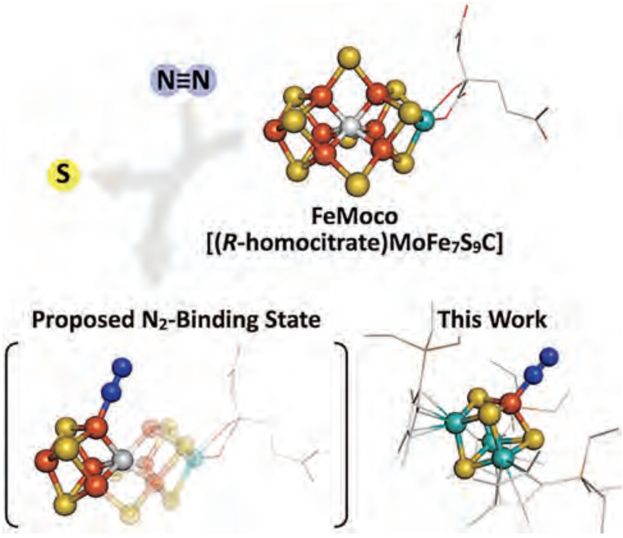

Figure 1. Proposed N_2 binding state of FeMoco and a N_2-bound Mo-Fe-S cluster.

Tracing the S Incorporation into the Nitrogenase Cofactor Precursor

FeMoco is arguably one of the most complex metallocofactors in Nature. Its biosynthetic pathway is correspondingly complicated and remains unclear, which hampers applications of this enzyme toward artificial N_2 fixation. In this study, we investigated an enzymatic process by which FeMoco precursor (L-cluster, $[Fe_8S_9C]$) is generated from two $[Fe_4S_4]$ clusters on the protein by using a *semi-synthetic* approach. The study revealed that this process includes a S atom uptake from SO_3^{2-} and that the S atom is replaceable with homologous elements (Se, Te). Moreover, we succeeded in selective observation of the incorporated elements and theoretical simulations supporting the reactions' feasibility. These results show that nitrogenase requires an S source as an external substrate for its function.

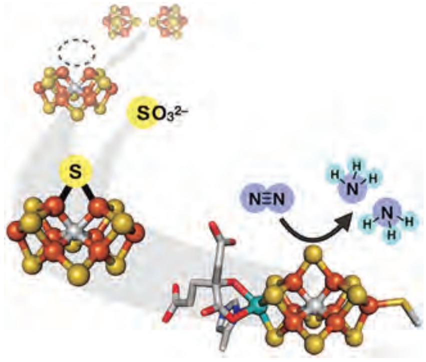

Figure 2. Schematic description of a sulfur uptake from sulfite (SO_3^{2-}) in the biosynthetic pathway of FeMoco.

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Scope of Research

Our research interest is to understand optical and quantum properties of nanometer-structured materials and to establish opto-nanoscience for creation of innovative functional materials. Space- and time-resolved laser spectroscopy is used to study optical properties of semiconductor quantum nanostructures and strongly correlated electron systems in low-dimensional materials. The main subjects are as follows: 1) investigation of optical properties of single nanostructures through the development of a high-resolution optical microscope, 2) ultrafast optical spectroscopy of excited states of semiconductor nanostructures, 3) photophysics of solar cell materials, 4) engineering material properties with lights.

KEYWORDS

Femtosecond Laser Spectroscopy
Semiconductor Nanoparticles
High Harmonic Generation
Single Photon Spectroscopy
Perovskites

Recent Selected Publications

Nakagawa, K.; Hirori, H.; Sato, S. A.; Tahara, H.; Sekiguchi, F.; Yumoto, G.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Size-Controlled Quantum Dots Reveal the Impact of Intraband Transitions on High-Order Harmonic Generation in Solids, *Nature Phys.*, **18,** 874-878 (2022).

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Sanari, Y.; Otobe, T.; Kanemitsu, Y.; Hirori H., Modifying Agular and Polarization Selection Rules of High-Order Harmonics by Controlling Electron Trajectories in k-Space, *Nature Commun.*, **11,** [3069-1]-[3069-7] (2020).

Ultrafast Spatiotemporal Dynamics of Exciton Spins in a Two-Dimensional Layered Halide Perovskite at Room Temperature

Along with their excellent optoelectronic properties, two-dimensional (2D) layered halide perovskites (LHPs) have unique spintronic properties. 2D LHPs have stable excitons with spins of ±1 and exhibit substantial exciton-exciton interactions and relatively long exciton spin relaxation times at room temperature. These properties provide potential for realizing room-temperature exciton spin transport. To investigate the spatiotemporal evolution of exciton spins, we developed polarization-resolved pump-probe microscopy with millidegree, submicrometer, and subpicosecond resolutions and performed time-resolved Faraday rotation imaging of room-temperature spin-polarized excitons in 2D LHP single crystals of $(C_4H_9NH_3)_2(CH_3NH_3)_3Pb_4I_{13}$. Under strong photoexcitation conditions, we observed that as the pump-probe delay time increases, a ring-like spatial pattern emerges in the spin-polarized exciton population and simultaneously ultrafast exciton spin transport occurs. Furthermore, we found that the anomalous spatiotemporal dynamics of the exciton spins originates from exciton-exciton exchange interactions. Our findings reveal the potential of 2D LHPs for room-temperature spin-optoelectronic applications.

Observation of High-Order Harmonic Generation from Semiconductor Quantum Dots

High-order harmonic generation (HHG) is attracting much attention as a new spectroscopic tool for understanding ultrafast carrier dynamics under strong electric fields and has a great potential for a coherent light source in the extreme ultraviolet region. Recently, the intensive studies on HHG from solids have been conducted both theoretically and experimentally and it is known that the mechanism of HHG from solids is completely different from that from gases. The HHG mechanism in solids is theoretically discussed in terms of two processes, the intraband and interband transitions, but there have been no experimental studies on the control of these two processes. To clarify the role of two transitions in the HHG efficiency, we investigated HHG from CdSe and CdS quantum dots. We can control the intraband transition process by utilizing the quantum confinement effects of dots. We observed that the high-order harmonic (HH) intensity increases with the dot size (Fig. 1). Our findings reveal that the intraband transitions play an important role in HHG from solids.

Exciton-Phonon and Trion-Phonon Couplings in Single $CsPbBr_3$ Perovskite Nanocrystals

Lead halide perovskite nanocrystals (NCs) are attracting significant attention as light-emitting device materials because of their superior optical properties such as high photoluminescence (PL) quantum yields and bandgap tunability. In these NCs, exciton-phonon couplings strongly affect their optical properties. However, the mechanism of exciton-phonon coupling in perovskite NCs remains unclear. Very narrow PL lines at low temperatures in the NCs enable LO-phonon-mode-resolved analysis of exciton-phonon couplings. We studied the PL spectra of single $CsPbBr_3$ NCs by using single-dot spectroscopy at 5.5 K to evaluate the strengths of exciton-phonon couplings (the Huang-Rhys factors). We observed that PL of trions becomes more dominant than that of excitons under strong photoexcitation conditions and LO-phonon replicas of trions clearly appear in addition to those of excitons (Fig. 2). Both the Huang-Rhys factors of excitons and trions become larger for smaller NCs. We also found that the size dependence of the Huang-Rhys factors for trions are weaker than that for excitons. These results are caused by the difference in the charge distributions of excitons and trions in the NCs.

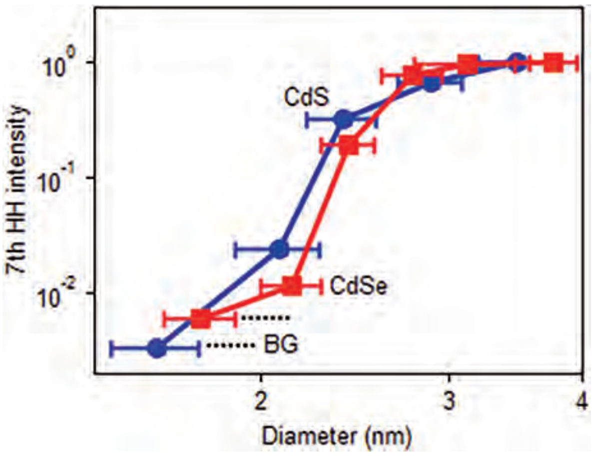

Figure 1. Diameter dependence of 7th HH intensity.

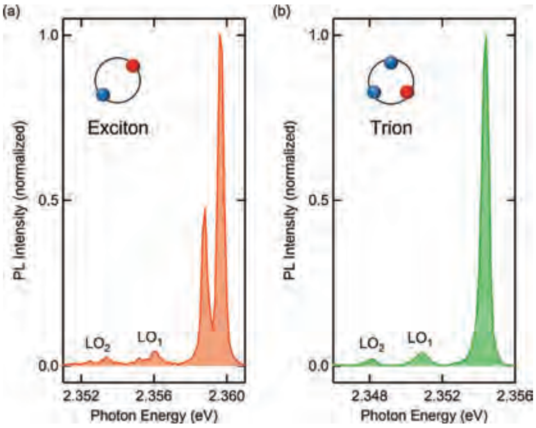

Figure 2. PL peaks of (a) exciton and (b) trion with their LO-phonon replicas.

Bioinformatics Center
– Chemical Life Science –

https://cls.kuicr.kyoto-u.ac.jp/en/


Prof
OGATA, Hiroyuki
(D Sc)


Assoc Prof
ENDO, Hisashi
(D Environmental Science)


Assist Prof
OKAZAKI, Yusuke
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SHIH, Chi-Yu
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(D Agr)

*1 National Taiwan Ocean University, Taiwan, 23 August 2021–31 July 2022
*2 JSPS International Fellowships for Research in Japan, USA, 26 May 2022–25 May 2023
*3 Hubei University of Technology, China, 23 May 2022–11 May 2023

Students

XIA, Jun (D3)
BAN, Hiroki (D2)
ZHANG, Ruixuan (D1)
YANG, Qingwei (D1)
FANG, Yue (M2)
WU, Junyi (M2)
ZHANG, Liwen (M1)
CHEN, Jingjie (M1)
LIU, Wenwen (RS)
ZHAO, Hongda (RS)
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Proj Res

NGUYEN, Thi Tuyen

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PRODINGER, Florian (D Sc)

Assist Techn Staff

ZHU, Mengdi
OGATA, Yuki

Guest Res Assoc

PRONDZINSKY, Paula	Tokyo Institute of Technology, Japan, 4 April 2022–21 May 2022
GAIA, Morgan Thibaud (Ph D)	Commissariat à l'Energie Atomique (CEA / Atomic Energy Commission) – Genoscope, France, 20 June 2022–4 July 2022
CHAFFRON, Samuel (Ph D)	CNRS, Nantes University, France, 22 October 2022–31 October 2022
GAUDIN, Marinna	CNRS, Nantes University, France, 14 October 2022–4 November 2022
SALCHER, Michaela Maria (Ph D)	The Czech Academy of Sciences, Czech Republic, 16 September 2022–5 October 2022

Scope of Research

We are interested in understanding the functioning and evolution of biological systems at varying scales from tiny microbes up to the Earth's environment, by leveraging rapidly accumulating big data in life science and bioinformatics approaches. We currently focus on 1) the evolution of viruses and their links to the origin of life, 2) microbial ecology in different ecosystems, and 3) the development of bioinformatics methods and biological knowledge resources for biomedical and industrial applications. To fuel these research activities, we take part in environmental sampling campaigns such as *Tara* Oceans. Our resources and developed tools are accessible through GenomeNet (www.genome.jp) to scientific communities and the public.

KEYWORDS

GenomeNet Bioinformatics Environmental Genomics Virology Molecular Evolution

Tight Association Discovered between *Imitervirales* and Their Microbial Eukaryotic Host Communities in the Arctic Ocean

Imitervirales is an order belonging to phylum *Nucleocytoviricota*, or so-called giant viruses. The microbial eukaryotic community hosts various *Imitervirales*, and play an important role in marine ecosystem. To explore the association between them in the Arctic Ocean, we sampled microbial DNA from surface water of 21 stations during a cruise in the summer of 2018. Two types of water (NECS: northeastern Chukchi Sea; AS: adjacent seas) can be separated according to temperature and salinity. In AS sites, eukaryotic community was strongly correlated with physicochemical factors, while in the oligotrophic NECS sites it showed a loose association (Fig. 1). In contrast, *Imitervirales* community were consistently correlated with eukaryotic community, and correlation coefficients were rarely influenced by environmental factors in both of NECS and AS sites (Fig. 1). At the individual amplicon sequence variant (ASV) level in all sites, positive associations (above 37% eukaryotic ASVs and 25% *Imitervirales* ASVs) between *Imitervirales* and eukaryotic community were then discovered by co-occurrence analysis. These results support that *Imitervirales* community actively interacted and co-varied with eukaryotic community, even in the oligotrophic and homogeneous environment in the Arctic Ocean. This work has been published in Xia et al., Limnol. Oceanogr., 2022, doi: 10.1002/lno.12086.

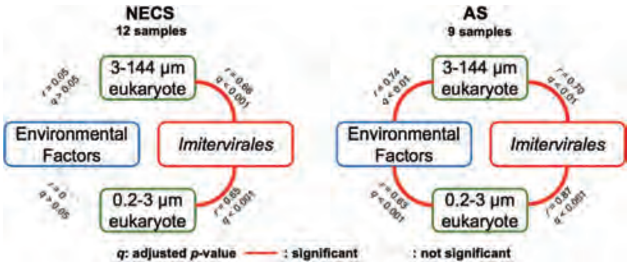

Figure 1. Mantel test result between microbial eukaryotic community, environmental factors, and *Imitervirales* community.

"*Mamonoviridae*", a New Virus Family of the Phylum *Nucleocytoviricota*

Large DNA viruses of phylum *Nucleocytoviricota* are widespread in the ecosystems around the globe and show a great genetic and morphological diversity. Medusavirus is a group of viruses in this phylum, which was first represented by Acanthamoeba castellanii medusavirus J1 isolated from a hot spring. With the development of culture-independent techniques such as metagenomics, many related viral genomes have been identified so far. However, the current taxonomy rank of medusaviruses is not officially defined by the International Committee on Taxonomy of Viruses. The creation of new taxonomic ranks is thus warranted to capture the diversity of this group of viruses. We assessed the morphological, genomic, and gene content similarities within the two isolated medusaviruses and compared them with other large DNA viruses. Our results show that medusaviruses clearly differ from members of other families in this phylum in terms of all used metrics. We thus propose to create the family "*Mamonoviridae*" within the phylum *Nucleocytoviricota*. This work has been accepted by the journal Archive of Virology.

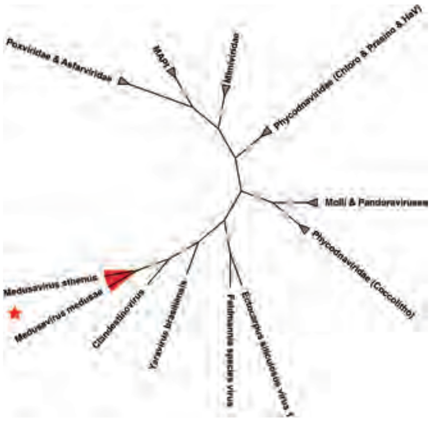

Figure 2. Phylogenetic tree based on concatenated core genes of viruses of the phylum *Nucleocytoviricota* based on a maximum-likelihood framework. Blue circles represent supports that passed confidence cutoff for branches. The red background color along branches and the star indicate medusaviruses.

Recent Selected Publications

Xia, J.; Kameyama, S.; Prodinger, F.; Yoshida, T.; Cho, K.-H.; Jung, J.; Kang, S.-H.; Yang, E.-J.; Ogata, H.; Endo, H., Tight Association between Microbial Eukaryote and Giant Virus Communities in the Arctic Ocean, *Limnol. Oceanogr.*, **67,** 1343-1356 (2022).

Da Cunha, V.; Gaia, M.; Ogata, H.; Jaillon, O.; Delmont, T.O.; Forterre, P., Giant Viruses Encode Actin-Related Proteins, *Mol. Biol. Evol.*, **39,** msac022 (2022).

Prodinger, F.; Endo, H.; Takano, Y.; Li, Y.; Tominaga, K.; Isozaki, T.; Blanc-Mathieu, R.; Gotoh, Y.; Hayashi, T.; Taniguchi, E.; Nagasaki, K.; Yoshida, T.; Ogata, H., Year-Round Dynamics of Amplicon Sequence Variant Communities Differ among Eukaryotes, Imitevirales, and Prokaryotes in a Coastal Ecosystem, *FEMS Microbiol. Ecol.*, **97,** fiab167 (2022).

Zhang, R.; Endo, H.; Takemura, M.; Ogata, H., RNA Sequencing of Medusavirus Suggests Remodeling of the Host Nuclear Environment at an Early Infection Stage, *Microbiol. Spectr.*, **9,** e0006421 (2021).

Kijima, S.; Delmont, T.O.; Miyazaki, U.; Gaia, M.; Endo, H.; Ogata, H., Discovery of Viral Myosin Genes With Complex Evolutionary History Within Plankton, *Front. Microbiol.*, **12,** 683294 (2021).

Bioinformatics Center
– Mathematical Bioinformatics –

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Prof
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Assoc Prof
TAMURA, Takeyuki
(D Inf)


Assist Prof
MORI, Tomoya
(D Inf)


Guest Scholar*
SONG, Jiangning
(Ph D)

*Monash University, Australia, 28 June 2022–25 February 2023

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TAKAGI, Motoshige (D3)
LI, Ruiming (D3)
OHTOMO, Masahiro (D3)
NAKASHIMA, Shogo (D3)
MU, Lixuan (D3)
SHIOTA, Koji (D2)
LIU, Chunting (D2)
MA, Yier (D1)
FUJITA, Satoki (D1)
GHAFOOR, Mamoona (D1)
CUI, Yan (M1)

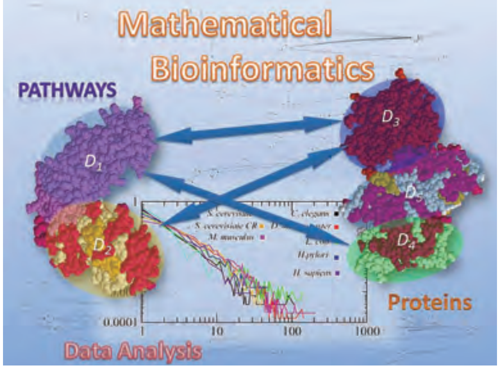
Guest Res Assoc

ZHANG, Bin	South China University of Technology, China, 23 May 2022–17 November 2022
SUN, Liangjie	The University of Hong Kong, China, 10 June 2022–25 August 2022

Scope of Research

Due to the rapid progress of genome sequencing technology, whole genome sequences of organisms ranging from bacteria to human have become available. In order to understand the meaning behind the genetic code, we have been developing algorithms and software tools for analyzing biological data based on advanced information technologies such as theory of algorithms, artificial intelligence, and machine learning. We are currently studying the following topics: systems biology, scale-free networks, protein structure prediction, the inference of biological networks, chemo-informatics, and discrete and stochastic methods for bioinformatics.

KEYWORDS
Complex Networks
Boolean Networks
Neural Networks
Chemical Graphs
Protein Informatics



Recent Selected Publications

Guo, S.; Liu, P.; Ching, W-K.; Akutsu, T., On the Distribution of Successor States in Boolean Threshold Networks, *IEEE Transactions on Neural Networks and Learning Systems*, **33,** 4147-4159 (2022).

Kumano, S.; Akutsu, T., Comparison of the Representational Power of Random Forests, Binary Decision Diagrams, and Neural Networks, *Neural Computation*, **34,** 1019-1044 (2022).

Münzner, U.; Mori, T.; Krantz, M.; Klipp, E.; Akutsu, T., Identification of Periodic Attractors in Boolean Networks Using a Priori Information, *PLoS Computational Biology*, **18,** [e1009702-1]-[e1009702-27] (2022).

Sugihara, R.; Kato, Y.; Mori, T.; Kawahara, Y., Alignment of Single-Cell Trajectory Trees with CAPITAL, *Nature Communications*, **13,** [5972-1]-[5972-11] (2022).

Tamura, T., L1 Norm Minimal Mode-based Methods for Listing Reaction Network Designs for Metabolite Production, *IEICE Transactions on Information and Systems*, **104,** 679-687 (2021).

On the Compressive Power of Autoencoders Using Linear Threshold Activation Functions

Artificial neural networks have recently been extensively applied to bioinformatics. Among various models of artificial neural networks, autoencoders attract much attention because of their power to generate new objects such as protein sequences and chemical structures. An autoencoder is a layered neural network (Figure 1) consisting of an encoder which compresses an input vector to a lower dimensional vector, and a decoder which transforms the low-dimensional vector back to the original input vector (or one that is very similar). Although it is often mentioned that autoencoders perform dimensionality reduction, a kind of data compression, how data are compressed is not yet very clear. Therefore, we study the numbers of nodes and layers that are required to ensure that each vector in a given set of distinct input binary vectors is transformed back to its original using a autoencoder model with linear threshold activation functions. We show that for any set of distinct vectors there exists a seven-layer autoencoder with the optimal compression ratio, but that there is a set of vectors for which there is no three-layer autoencoder with a middle layer of the same size. We also study the numbers of nodes and layers required only for encoding, and the results suggest that decoding is more difficult than encoding.

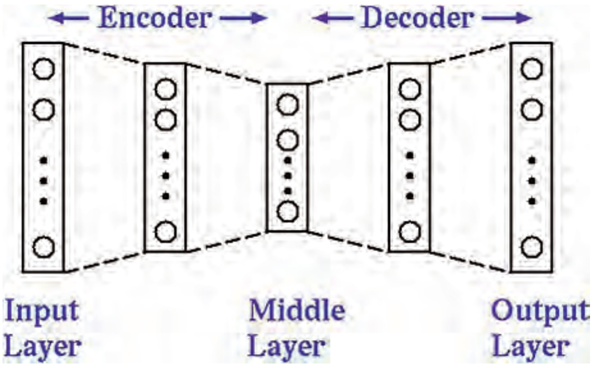


Figure 1. Architecture of an autoencoder.

Gene Deletion Algorithms for Minimum Reaction Network Design by Mixed-Integer Linear Programming for Metabolite Production in Constraint-based Models: gDel_minRN

Genome-scale constraint-based metabolic networks play an important role in the simulation of growth coupling, which means that cell growth and target metabolite production are simultaneously achieved. To achieve growth coupling, a minimal reaction-network-based design is known to be effective. However, the obtained reaction networks often fail to be realized by gene deletions due to conflicts with gene-protein-reaction relations.

Here, we developed gDel_minRN that determines gene deletion strategies using mixed-integer linear programming to achieve growth coupling by repressing the maximum number of reactions via gene-protein-reaction relations. Computational experiments were conducted in which gDel_minRN was applied to iML1515, a genome-scale model of *Escherichia coli*. The target metabolites were three vitamins that are highly valuable and require cost-effective bioprocesses for economics and the environment. gDel_minRN successfully calculated gene deletion strategies that achieve growth coupling for the production of biotin (vitamin B7), riboflavin (vitamin B2), and pantothenate (vitamin B5).

Since gDel_minRN calculates a constraint-based model of the minimum number of gene-associated reactions without conflict with gene-protein-reaction relations, it helps biological analysis of the core parts essential for growth coupling for each target metabolite. The source codes are implemented in MATLAB, CPLEX, and COBRA Toolbox. The obtained data and source codes are available on
https://github.com/taketam/gDel-minRN

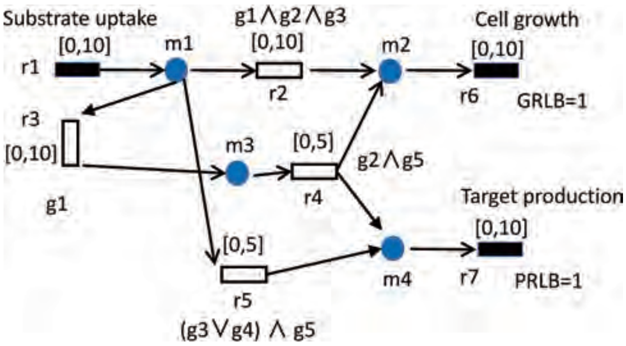


Figure 2. A toy example of the constraint-based model. Circles and rectangles represent metabolites and reactions, respectively. Black and white rectangles are external and internal reactions.

Bioinformatics Center
– Bio-knowledge Engineering –

https://www.bic.kyoto-u.ac.jp/pathway/index.html

Prof
MAMITSUKA, Hiroshi
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Senior Lect
NGUYEN, Hao Canh
(D Knowledge Science)

Guest Res Assoc*
PETSCHNER, Peter
(Ph D)

*Semmelweis University, Hungary, 28 November 2020–15 November 2022

Students

NGUYEN, Duc Anh (D3)

Guest Scholars

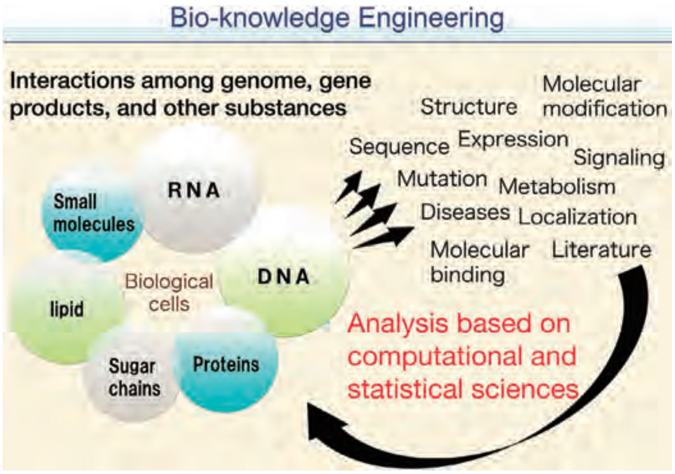
KLIPP, Edda (Ph D)	Humboldt University Berlin, Germany, 12 April 2022–15 May 2022
RAUN, Rune Linding (Ph D)	Humboldt University Berlin, Germany, 22 April 2022–6 May 2022
MALHI, Avleen Kaur (Ph D)	Bournemouth University, UK, 2 June 2022–18 August 2022

Guest Res Assoc

LI, Yufei	Xi’an Jiaotong University, China, 2 May 2022–23 April 2023
GOLDENBOGEN, Björn	Humboldt University Berlin, Germany, 4 April 2022–20 May 2022
GECSE, Kinga	Semmelweis University, Hungary, 13 August 2022–22 October 2022

Scope of Research

We are interested in graphs and networks in biology, chemistry, and medical sciences, including metabolic networks, protein-protein interactions and chemical compounds. We have developed original techniques in machine learning and data mining for analyzing these graphs and networks, occasionally combining with table-format datasets, such as gene expression and chemical properties. We have applied the techniques developed to real data to demonstrate the performance of the methods and find new scientific insights.



KEYWORDS

Bioinformatics
Data Mining
Machine Learning
Artificial Intelligence
Systems Biology

Recent Selected Publications

Nguyen, D. A.; Nguyen, C. H.; Petschner, P.; Mamitsuka, H., SPARSE: A Sparse Hypergraph Neural Network for Learning Multiple Types of Latent Combinations to Accurately Predict Drug-Drug Interactions, *Bioinformatics*, **38** *(Supplement 1) (Proceedings of the 30th International Conference on Intelligent Systems for Molecular Biology (ISMB 2022))*, i333-i341 (2022).

You, R.; Qu, W.; Mamitsuka, H.; Zhu, S., DeepMHCII: A Novel Binding Core-Aware Deep Interaction Model for Accurate MHC II-peptide Binding Affinity Prediction, *Bioinformatics*, **38** *(Supplement 1) (Proceedings of the 30th International Conference on Intelligent Systems for Molecular Biology (ISMB 2022))*, i220-i228 (2022).

Nguyen, C.H.; Mamitsuka, H., Learning on Hypergraphs with Sparsity, *IEEE Transactions on Pattern Analysis and Machine Intelligence*, **43,** 2710-2722 (2021).

Nakamura, A.; Takigawa, I.; Mamitsuka, H., Efficiently Enumerating Substrings with Statistically Significant Frequencies of Locally Optimal Occurrences in Gigantic String, *Proceedings of the AAAI Conference on Artificial Intelligence (AAAI 2020)*, **34(4),** 5240-5247 (2020).

Nguyen, D. H.; Nguyen, C. H.; Mamitsuka, H., ADAPTIVE: learning DAta-dePendenT, concIse molecular VEctors for fast, accurate metabolite identification from tandem mass spectra, *Bioinformatics*, **35(14),** *(Proceedings of the 27th International Conference on Intelligent Systems for Molecular Biology (ISMB/ECCB 2019))*, i164-i172 (2019).

An Advanced Deep Learning Model for Predicting Side Effects of Drug-Drug Interactions

A drug-drug interaction (DDI) is a reaction between two drugs, whereby the effects of one drug are modified by the concomitant use of the second drug. A DDI might cause side effects, which are unwanted effects and are responsible for significant patient morbidity and mortality. Hence predicting side effects of drug-drug interactions is a very important task in pharmacology. Given known DDI data, a prominent approach is to use machine learning models to obtain highly accurate and fast DDI predictions.

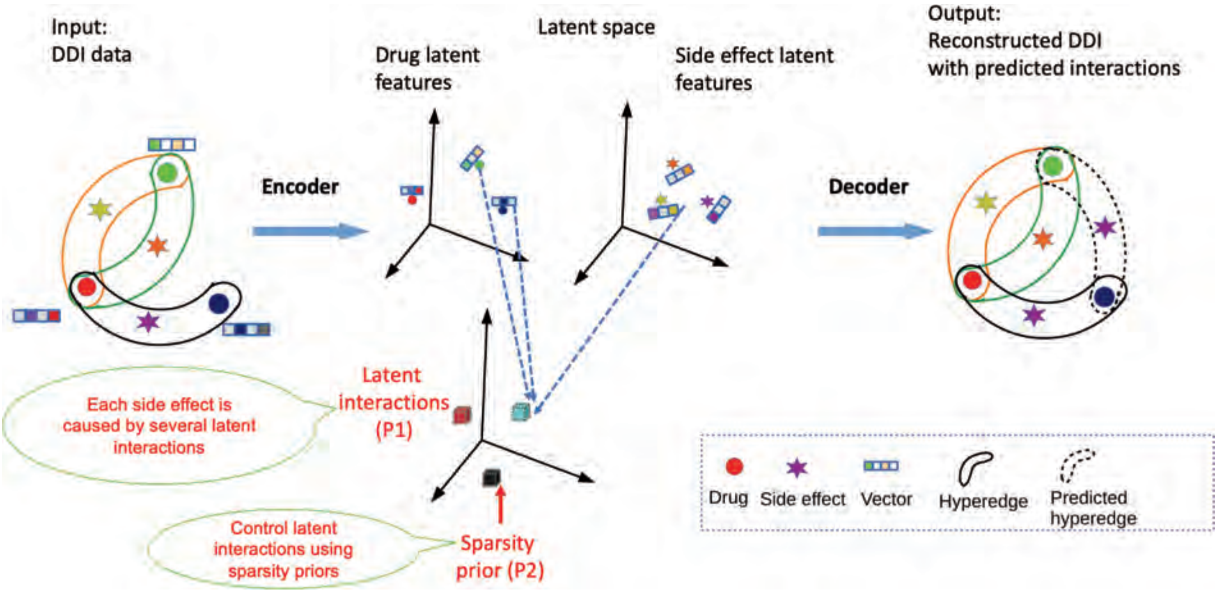
Recent state-of-the-art models assume that each side effect is caused by a unique combination of properties of the corresponding interacting drugs. However, there still exist two remaining problems that have not been addressed: (P1) in reality, a side effect might have multiple mechanisms that cannot be represented by a single combination of drug properties, and (P2) DDI data is sparse with a very few percentages of known DDIs, which might impair the model performances.

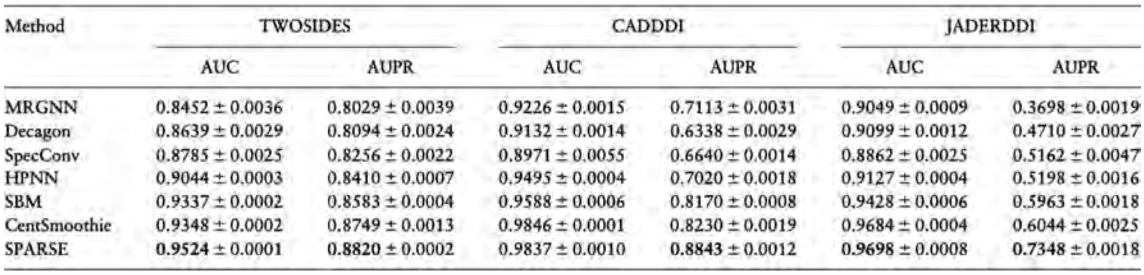
To address the above two problems, we proposed SPARSE, an advanced deep learning model for predicting drug-drug interactions with an illustration as in Figure 1. For problem (P1), we assumed that each side effect is caused by different combinations of drug properties. For problem (P2), we used a sparsity control to guide the model to fit with the sparse data.

We conducted experiments on the three real-world DDI benchmark datasets to show the advantage of the prediction performance of our proposed method. We compared SPARSE with other state-of-the-art methods under two commonly used measures: AUC (area under the ROC curve) and AUPR (area under the precision-recall curve). The results were shown in Figure 2. The figure shows that our method (SPARSE) outperformed other methods in both AUC and AUPR, suggesting that our method was suitable for drug-drug interaction prediction.

Reference

Duc Anh Nguyen, Canh Hao Nguyen, Peter Petschner, Hiroshi Mamitsuka, SPARSE: a sparse hypergraph neural network for learning multiple types of latent combinations to accurately predict drug–drug interactions, Bioinformatics, Volume 38, Pages i333-i341, https://doi.org/10.1093/bioinformatics/btac250.





Method	TWOSIDES		CADDDI		JADERDDI	
	AUC	AUPR	AUC	AUPR	AUC	AUPR
MRGNN	0.8452 ± 0.0036	0.8029 ± 0.0039	0.9226 ± 0.0015	0.7113 ± 0.0031	0.9049 ± 0.0009	0.3698 ± 0.0019
Decagon	0.8639 ± 0.0029	0.8094 ± 0.0024	0.9132 ± 0.0014	0.6338 ± 0.0029	0.9099 ± 0.0012	0.4710 ± 0.0027
SpecConv	0.8785 ± 0.0025	0.8256 ± 0.0022	0.8971 ± 0.0055	0.6640 ± 0.0014	0.8862 ± 0.0025	0.5162 ± 0.0047
HPNN	0.9044 ± 0.0003	0.8410 ± 0.0007	0.9495 ± 0.0004	0.7020 ± 0.0018	0.9127 ± 0.0004	0.5198 ± 0.0016
SBM	0.9337 ± 0.0002	0.8583 ± 0.0004	0.9588 ± 0.0006	0.8170 ± 0.0008	0.9428 ± 0.0006	0.5963 ± 0.0018
CentSmoothie	0.9348 ± 0.0002	0.8749 ± 0.0013	0.9846 ± 0.0001	0.8230 ± 0.0019	0.9684 ± 0.0004	0.6044 ± 0.0025
SPARSE	**0.9524** ± 0.0001	**0.8820** ± 0.0002	0.9837 ± 0.0010	**0.8843** ± 0.0012	**0.9698** ± 0.0008	**0.7348** ± 0.0018

Figure 2. Comparisons on prediction performance.

HAKUBI RESEARCHERS' ACTIVITIES IN ICR

Hakubi Project: Fosterage and Support of Young Researchers, Kyoto University

Research Topic

Optoelectronic Energy Recycling and Quantum Cooperative Effects in Semiconductor Nanostructures

Program-Specific Assoc Prof
TAHARA, Hirokazu
(D Sc)

Host Laboratory Laboratory of Nanophotonics

Host Professor KANEMITSU, Yoshihiko

Outline of Research

Semiconductor nanostructures are attractive materials that provide a platform to enhance quantum effects. In nanomaterials, strongly-confined electrons and holes form unique quantum states such as multiexcitons, which are hardly generated in bulk semiconductors. Since multiexcitons consist of a few electrons and holes, their generation and dissociation processes have a great potential to increase electric signals in photon-to-current conversion. My research focuses on applications of quantum effects and control of photon-to-current conversion processes in semiconductor nanostructures. I will clarify the microscopic mechanism of photocarrier generation processes in coupled nanostructures and establish a way to recycle thermal and radiative energies.

ACTIVITIES OF INTERNATIONAL JOINT USAGE/RESEARCH CENTER

iJURC Cooperative Research Subjects 2022

(1 April 2022 ~ 31 March 2023)

STARTING-UP SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY iJURC)

Synthesis and Optical Characterization of Helical Gold Nanowires with Branches
NAKAGAWA, Makoto, Osaka Research Institute of Industrial Science and Technology
Host in iJURC KURATA, Hiroki

Development of New Nano-Structure Target for ISOL
OHNISHI,Tetsuya, SCRIT Team, Instrumentation Development Group, Nishina Center for Accelerator Based Science, RIKEN
Host in iJURC WAKASUGI, Masanori

Verification of Radiochemical Reaction Mechanism for FLASH Radiotherapy with Electron Beams
KODAIRA, Satoshi, Radiation Measurement Group, Department of Radiation Measurement and Dose Assessment, National Institute of Radiological Sciences, National Institutes for Quantum Science and Technology
Host in iJURC OGAWARA, Ryo

Computational Mechanistic Study on the Co-Catalyzed Nitrogenase Model Reactions
SAMEERA, W. M. C., Department of Chemistry, University of Colombo
Host in iJURC OHKI, Yasuhiro I

High-Pressure Synthesis and Ionic Conducting Study of Novel Na-Antiperovskites Containing Hydride and Cluster Anions as Solid Electrolytes in Batteries
KOEDTRUAD, Anucha, Chinese Academy of Science (CAS), Institute of High Energy Physics (IHEP), Chinese Spallation Neutron Source (CSNS),
Host in iJURC SHIMAKAWA, Yuichi I

Synthesis of Fe-Containing Phosphorus Ligands and Their Application in the Preparation of Metal-Cluster Molecules
OGASAWARA, Masamichi, Graduate School of Technology, Industrial and Social Sciences, Tokushima University
Host in iJURC OHKI, Yasuhiro

Synthesis of Self-Assembled Organoboran Compounds, Elucidation of Self-Assembly Process, and Creation of New Functions
WAKABAYASHI, Shigeharu, Department of Clinical Nutrition, Faculty of Health Science, Suzuka University of Medical Science
Host in iJURC OHKI, Yasuhiro

Synthesis of Alkyl Ethers Using Two Different Alcohols Catalyzed by Organosilane Compound
HASHIMOTO,Toru, Faculty of Engineering, Sanyo-Onoda City University
Host in iJURC NAKAMURA, Masaharu

Development of Heteroacenes with Excellent Photophysical and Electrochemical Properties
MITSUDO, Koichi, Graduate School of Natural Science and Technology, Okayama University
Host in iJURC WAKAMIYA, Atsushi

A Study on Statistical Machine Learning for Efficient Graph Structured Data Analysis
KARASUYAMA, Masayuki, Department of Computer Science, Nagoya Institute of Technology
Host in iJURC MAMITSUKA, Hiroshi I

Revealing Evolution Mechanism of Adaptation to High Temperature Based on Omics Data and Flux Balance Analysis
KISHIMOTO, Toshihiko, Faculty of Science, Biomolecular Science, Toho University
Host in iJURC TAMURA, Takeyuki

Control and Analysis of Complex Networks via Probabilistic Minimum Dominating Sets
NACHER, Jose C., Department of Information Science, Faculty of Science, Toho University
Host in iJURC AKUTSU, Tatsuya

Microbial Ecology in the Dark Sea
YOSHIDA,Takashi, Division of Applied Biosciences, Graduate School of Agriculture, Kyoto University
Host in iJURC OGATA, Hiroyuki

Investigations into Catalytic and Biochemical Behaviors of Nitrogenase Fe Protein Using ^{57}Fe Labeling
RIBBE, Markus W., Department of Molecular Biology and Biochemistry, University of California, Irvine
Host in iJURC TANIFUJI, Kazuki I

Precise Synthesis and Viscoelastic Properties of Ring Polymers with High Purity and High Molecular Weight
TAKANO, Atsushi, Department of Molecular and Macromolecular Chemistry, Nagoya University
Host in iJURC MATSUMIYA, Yumi I

Developing Bioinspired Molecular Catalysts for Materials Science and Medicinal Chemistry
OHTA, Takehiro, Department of Applied Chemistry, Faculty of Engineering, Sanyo-Onoda City University
Host in iJURC OHKI, Yasuhiro

Dinitrogen Fixation Based on Nickel→Z-Type (σ-Electron Acceptor) Ligand Interaction
KAMEO, Hajime, Department of Chemistry, Graduate School of Science, Osaka Prefecture University
Host in iJURC OHKI, Yasuhiro

Evaluation an Effect of Structure in Chiral Silica on Molecular Recognition
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Host in iJURC TAKENAKA, Mikihito

Development of Organometallic n-Type Materials with High Electrical Conductivity
MURATA, Michihisa, Department of Applied Chemistry, Osaka Institute of Technology
Host in iJURC MURATA, Yasujiro

I : International Joint Research
F : Female PI

Non-Linear Viscoelasticity of Unentangled Polymers
IANNIRUBERTO, Giovanni, Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale, Università degli Studi di Napoli "Federico II"
Host in iJURC SATO, Takeshi I

Nonlinear Extensional Rheology of Entangled Poly(n-alkyl methacrylate) Melts with Fixed Number of Entanglements and Kuhn Segments per Chain
WU, Shilong, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences (CAS)
Host in iJURC MATSUMIYA, Yumi I

Control of Mechanical Properties in Polymer Blend Materials by Hydrogen Bonding Interaction
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Host in iJURC MATSUMIYA, Yumi I

Effect of Microplastics on Distribution of Trace Heavy Metals in Seawater
NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kindai University
Host in iJURC SOHRIN, Yoshiki

Exploration of Liquid Membrane Transportation of Metal Ions with a Polymer Membrane Containing Ionic Liquid by Use of Electric Field Response of Ions
MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education
Host in iJURC SOHRIN, Yoshiki

Conformation Analysis on Polymer in Food-Grade Oil
OSAKA, Noboru, Okayama University of Science
Host in iJURC TAKENAKA, Mikihito

Physicochemical Characterization of Novel Hybrid Partially Fluorinated Phospholipid Bilayers
SONOYAMA, Masashi, Faculty of Science and Technology, Gunma University
Host in iJURC HASEGAWA, Takeshi

Identification of Active Gibberellins in the Basal Land Plant Marchantia Polymorpha
KOHCHI, Takayuki, Graduate School of Biostudies, Kyoto University
Host in iJURC YAMAGUCHI, Shinjiro

Investigation on High Efficient Spin-Orbit Torque Effect in Multilayers with Combine Anisotropy and DMI
OGNEV, Alexey, Department of General and Experimental Physics, Institute of High Technologies and Advanced Materials, Far Eastern Federal University
Host in iJURC ONO, Teruo I

Demonstration of Topological Phase Control in Chalcogenide Superlattices
MOROTA, Misako, Device Technology Research Institute, National Institute of Advanced Industrial Science and Technology (AIST)
Host in iJURC ONO, Teruo F

Research and Development of Magnon Quantum Logic Gate Devices Using Synthetic Antiferromagnets
ISHIBASHI, Mio, Department of Physics, Faculty of Science & Graduate School of Science, The University of Tokyo
Host in iJURC ONO, Teruo F

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY iJURC)

Crystal Structure Analysis of GraE from Root-Nodule-Forming Bacterium
OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University
Host in iJURC FUJII, Tomomi

Enhanced Production of Fast Ions by TNSA with Pre-Pulse Laser
HANAYAMA, Ryohei, The Graduate School for the Creation of New Photonics Industries
Host in iJURC WAKASUGI, Masanori

Design and Tailoring Advanced Functional Materials: Symmetry Operation and High Pressure Synthesis
CHEN, Wei-Tin, Center for Condensed Matter Sciences, National Taiwan University
Host in iJURC SHIMAKAWA, Yuichi I

Carboboration and Carbosilylation by Merging Iron and Visible-Light Photocatalysis
HAJRA, Alakananda, Department of Chemistry, Visva-Bharati University
Host in iJURC NAKAMURA, Masaharu I

Development and Device Evaluation of New D-π-A Emitters Based on Rigidified Triarylborone Acceptors
MARDER, Todd B., Julius-Maximilians-Universität Würzburg, Institut für Anorganische Chemie
Host in iJURC KAJI, Hironori I

High Pressure Synthesis of Novel Hexagonal Perovskite Oxides Containing Unusually High-Valence Fe Ions and Investigation of Their Magnetic Properties
TAN, Zhenhong, Institute of High Energy Physics (IHEP) of the Chinese Academy of Sciences, China Spallation Neutron Source (CSNS)
Host in iJURC SHIMAKAWA, Yuichi I

Preparation and Characterization of Novel Magnetic Quadruple Perovskites by High Pressure
AMANO PATINO, Midori Estefani, Institut Charles Gerhardt Montpellier (ICGM, CNRS), D4: Chemistry of Materials, Nanostructures, Materials for Energy
Host in iJURC SHIMAKAWA, Yuichi I F

Small Molecule Activation Using Anionic Crypto-FLPs
STREUBEL, Rainer, Institute for Inorganic Chemistry, University of Bonn
Host in iJURC TOKITOH, Norihiro I

Development of Unsymmetrical π-Electron Systems of Heavier Main Group Elements and Elucidation of Their Property
IWAMOTO, Takeaki, Department of Chemistry, Tohoku University
Host in iJURC MIZUHATA, Yoshiyuki I

Development of 1,4-Addition Reactions via Iron Catalysis
ADAK, Laksmikanta, Department of Chemistry, Indian Institute of Engineering Science and Technology
Host in iJURC NAKAMURA, Masaharu I

Peptide Bolaamphiphile Anchored Nickel-Based Metallohydrogel as Electrocatalyst for Hydrogen Production
DAS, Apurba K., Department of Chemistry, Indian Institute of Technology Indore
Host in iJURC NAKAMURA, Masaharu I

Highly Efficient Solution-Processed Organic Light-Emitting Diodes Employing Multiple Resonance-Induced Thermally Activated Delayed Fluorescence Emitter
ODA, Susumu, Department of Chemistry, Graduate School of Science and Technology, Kwansei Gakuin University
Host in iJURC KAJI, Hironori

Synthesis and Its Catalysis of Dinuclear Complexes Utilizing a Pincer-Type N,N,P Ligand
YAMAGUCHI, Yoshitaka, Graduate School of Engineering, Yokohama National University
Host in iJURC NAKAMURA, Masaharu

Creation of Effective Oxidation Scavenger for Efficient Perovskite-Based Solar Cells
SASAMORI, Takahiro, Faculty of Pure and Applied Sciences, University of Tsukuba
Host in iJURC WAKAMIYA, Atsushi

Developing Machine Learning Approaches for Prediction of Protein Stability Changes upon Missense Mutations
SONG, Jiangning, Biomedicine Discovery Institute, Monash University
Host in iJURC AKUTSU, Tatsuya I

Integrating Omics Data and Module-Based Network with Deep Learning to Develop Cancer Type Predictive Models
YANG, Jinn-Moon, Department of Biological Science and Technology, Institute of Bioinformatics & Systems Biology, National Yang Ming Chiao Tung University
Host in iJURC AKUTSU, Tatsuya I

Evolution of Giant Viruses and Relationships with the Origin of Life
MORGAN, Gaïa, Genoscope - Centre National de Séquençage, Institut François Jacob - CEA
Host in iJURC OGATA, Hiroyuki I

Revealing Marine Microbial-Viral Interactions Through Community Interactome Analyses
CHAFFRON, Samuel, Laboratoire des Sciences du Numérique de Nantes (LS2N), CNRS and Université de Nantes
Host in iJURC ENDO, Hisashi I

Development of a Comprehensive Detection Method for Coronaviruses Originated in Wildlife
WATANABE, Tokiko, Research Institute for Microbial Diseases (RIMD), Osaka University
Host in iJURC OGATA, Hiroyuki F

Effective Molecular Network Analysis and Application to Medical and Agricultural Research
KAYANO, Mitsunori, Research Center for Global Agromedicine, Obihiro University of Agriculture and Veterinary Medicine
Host in iJURC MAMITSUKA, Hiroshi

Precise Synthesis and Controlling Higher Order Structure of Tadpole-Like Janus Cellulose Nanocrystal
GOTO, Atsushi, School of Physical & Mathematical Sciences, Division of Chemistry & Biological Chemistry, Nanyang Technological University
Host in iJURC KINOSE, Yuji I

Exploration of Perovskite Solar Cell Composition: Correlating Device Performance and Fundamental Property
SAEKI, Akinori, Department of Applied Chemistry, Graduate School of Engineering, Osaka University
Host in iJURC WAKAMIYA, Atsushi I

Exploration of Cycloaddition Properties of Guanidine Functionalized Isatins
MARGETIC, Davor, Division of Organic Chemistry and Biochemistry, Laboratory for Physical Organic Chemistry, Rudjer Boskovic Institute
Host in iJURC MURATA, Yasujiro I

Synthesis of Novel Nanotube Molecules with Different Hole Directions by Introducing a Double Heptalene Structure
CHAOLUMEN, College of Chemistry and Chemical Engineering, Inner Mongolia University (IMU)
Host in iJURC HASHIKAWA, Yoshifumi I

Synthesis of Functional Vinyltellurides Using Flow Reactors
NAGAKI, Aiichiro, Faculty of Science, Hokkaido University
Host in iJURC YAMAGO, Shigeru

Host-Guest Complexation of Cyclohexa-2,7-Anthrylene Ethynylene Derivatives with [n]CPP
KOBAYASHI, Kenji, Research Institute of Green Science and Technology, Shizuoka University
Host in iJURC KAYAHARA, Eiichi

Elucidation of the Lubrication Properties of Hyperbranched Polymers and Their Optimization
TAKAHASHI, Yutaka, New Industry Creation Hatchery Center, Tohoku University
Host in iJURC TOSAKA, Masatoshi

Synthesis of Highly Strained Macrocyclic π-Conjugated Molecules via a Multinuclear Au(I)-Pt(II) Complex
TSUCHIDO, Yoshitaka, Department of Chemistry, Faculty of Science Division I, Tokyo University of Science
Host in iJURC KAYAHARA, Eiichi

Synthesis and Applications of Novel Azaazulene Trimer toward Electronic materials
KUROTOBI, Kei, National Institute of Technology, Kurume College
Host in iJURC MURATA, Yasujiro

Isolation of Ultra-Unstable Chemical Species toward Unprecedented Element Strategy
UENO, Hiroshi, Frontier Research Institute for Interdisciplinary Sciences, Tohoku University
Host in iJURC MURATA, Yasujiro

Trace Metal Elemental and Isotopic Composition in the North Pacific Ocean: Sources and Internal Cycling (3)
HO, Tung-Yuan, Research Center for Environmental Changes, Academia Sinica
Host in iJURC SOHRIN, Yoshiki I

Resolving the Structure-Dynamics-Property Relationship in Polymer Nanocomposites under Uniaxial Stretching-II
KOGA, Tadanori, Department of Material Science and Chemical Engineering, Stony Brook University
Host in iJURC TAKENAKA, Mikihito I

High Frequency Response of Polymeric Liquids: Rheology and Dielectric Relaxation
SUKUMARAN, Sathish K., Graduate School of Organic Materials Science, Yamagata University
Host in iJURC SATO, Takeshi I

Analyzing Structural Fluctuation in Thermally Activated Delayed Fluorescence Materials with Ultralow-Frequency Raman Spectroscopy
SATOME, Hikaru, Graduate School of Engineering Science, Osaka University
Host in iJURC KAJI, Hironori

Nano-Scale Structure Characterization of Organosulfur Polymer
FUJIWARA, Akihiko, School of Engineering, Kwansei Gakuin University
Host in iJURC TAKENAKA, Mikihito

Construction of Theoretical Guidelines for Designing Plasmonic Nanoalloys
IIDA, Kenji, Institute for Catalysis, Hokkaido University
Host in iJURC TERANISHI, Toshiharu

Characteristics of Quantum Magnon in Magnetic Insulators
KIM, Kab-Jin, Department of Physics, Korea Advanced Institute of Science and Technology
Host in iJURC ONO, Teruo I

Observation of Orbital Hall Effect in Transition Metal Dichalcogenides.
KIM, Sanghoon, Department of Physics, University of Ulsan
Host in iJURC ONO, Teruo I

Research on the Efficiency Enhancement of the NV Centers Creation in Nanodiamond
SEGAWA, Takuya F., Laboratory for Physical Chemistry, ETH Zürich
Host in iJURC MIZUOCHI, Norikazu I

Research toward Stable NV Centers at Shallow Region and Spin Dynamics in Diamond
BALASUBRAMANIAN, Gopalakrishnan, Leibniz Institute for Surface Engineering, Leipzig, Germany
Host in iJURC MIZUOCHI, Norikazu I

Research of Surface State for Diamond Quantum Information Device
TOKUDA, Norio, NanoMaterials Research Institute, Kanazawa University
Host in iJURC MIZUOCHI, Norikazu

Research of Quantum Technology and Diamond Synthesis for Higher Sensitivity of NV Quantum Sensor
MAKINO, Toshiharu, Advanced Power Electronics Research Center, National Institute of Advanced Industrial Science and Technology
Host in iJURC MIZUOCHI, Norikazu

STARTING-UP SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Intracellular Delivery of Biofunctional Proteins Using Artificial Protein Nanocages
AZUMA, Yusuke, Małopolska Center of Biotechnology, Jagiellonian University
Host in iJURC FUTAKI, Shiroh I

Real-Time Visualization of Cellular Phase-Separating Proteins
KIKUCHI, Kazuya, Tokyo University of Science
Host in iJURC UESUGI, Motonari

Remote Control of Cells by Synthetic Small Molecules
NISHIKAWA, Makiya, Tokyo University of Science
Host in iJURC UESUGI, Motonari

Fabrication of Luminescent Thin Films Using Amphiphilic Lanthanide Complexes
MIEDA, Eiko, Department of Chemistry, Graduate School of Science, Osaka City University
Host in iJURC HASEGAWA, Takeshi F

Molecular Characterization of Fluoropolymer at Frictional Interface
KASUYA, Motohiro, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University
Host in iJURC HASEGAWA, Takeshi

Construction of Heterologous Protein Secretion System at Low Temperatures by Using Cold-Adapted Microorganisms
DAI, Xianzhu, College of Resources and Environment, Southwest University
Host in iJURC KURIHARA, Tatsuo I F

Analysis of Novel Transporters for Strigolactones or Their Biosynthetic Intermediates
ZHAO, Yunde, Department of Cell and Developmental Biology, Division of Biological Sciences, University of California San Diego
Host in iJURC MASHIGUCHI, Kiyoshi I

Verification and Development of Dynamic Stiction Theory
NAKANO, Ken, Faculty of Environment and Information Sciences, Yokohama National University
Host in iJURC TSUJII, Yoshinobu I

Regulatory Role of Phytohormone Cytokinin on Leaf Epidermal Cell Differentiation
AKI, Shiori, Graduate School of Science and Technology, NAIST (Nara Institute of Science and Technology)
Host in iJURC AOYAMA, Takashi F

Establishment of the Thermally Activated Delayed Fluorescence Kinetics Incorporating the Dynamical Effects
URATANI, Hiroki, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University
Host in iJURC KAJI, Hironori

Analysis of Membrane Lipid-Dependent Fermentation Stress Response in Acetic Acid Bacteria
TOYOTAKE, Yosuke, Department of Biotechnology, College of Life Sciences, Ritsumeikan University
Host in iJURC KURIHARA, Tatsuo

Thermal Conduction of Pseudo-Ordered Oxide Glasses
MASUNO, Atsunobu, Graduate School of Science and Technology, Hirosaki University
Host in iJURC SHIMAKAWA, Yuichi

Novel Functional Properties of Metal Oxides Explored by Electrochemical Proton Insertion
TSUCHIYA, Takashi, International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS)
Host in iJURC KAN, Daisuke

Syntheses of Novel Fluoride-Ion Conductors Using High pressures
SAITO, Takashi, High Energy Accelerator Research Organization (KEK)
Host in iJURC SHIMAKAWA, Yuichi

Metal Separation by Solvent Impregnated Resin Using Surfactant
KURAHASHI, Kensuke, Environmental and Materials Chemistry Course, College of Technology, Osaka Prefecture University
Host in iJURC SOHRIN, Yoshiki

Development of bi-Functional Catalysts by Modification of Supported Metal Surface with Metal Oxide Clusters
YAMAZOE, Seiji, Department of Chemistry, Graduate School of Science, Tokyo Metropolitan University
Host in iJURC TERANISHI, Toshiharu

Simultaneous Observation of Electron Transport Property and Phase Transition of a Single 3D Quantum Dot Superlattice in an Electron Microscope
ASAKA, Toru, Frontier Research Institute for Materials Science, Nagoya Institute of Technology
Host in iJURC SARUYAMA, Masaki

Development of Efficient Conversion Method of Woody Biomass, Renewable Biological Resources, to Advanced Chemical Materials
HATANO, Osamu, Fuculty of Medicine, Nara Medical University
Host in iJURC NAKAMURA, Masaharu

Study and Experiment of the High-Pressure Gas Generation by the High-Power Laserirradiation to the Stacked CNT Target
MATSUI, Kotaro, Graduate School of Energy Science, Kyoto University
Host in iJURC WAKASUGI, Masanori

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Self-Assembling Adjuvant-Built-In Vaccines for Cancer Immune Therapy
LI, Yan-Mei, Department of Chemistry, Tsinghua University
Host in iJURC UESUGI, Motonari I F

Evaluation of $CaCO_3$ Dissolution Rates in Deep-Sea Sediments by a Novel Tracer Method
CAI, Pinghe, Department of Marine Chemistry and Geochemistry, Xiamen University
Host in iJURC SOHRIN, Yoshiki I

Advanced Oxygen – Mediated Flow Chemistry
THOMAS, Wirth, School of Chemistry, Cardiff University
Host in iJURC NAKAMURA, Masaharu I

Novel Strategy for Intracellular Delivery of Nanomedicines
PUJALS, Sílvia, Nanoscopy for Nanomedicine Group, Institute for Bioengineering of Catalonia (IBEC)
Host in iJURC FUTAKI, Shiroh I F

Structural and Functional Analysis of Curvature-Inducing Peptides and Application
ULRICH, Anne S., Institute of Organic Chemistry (IOC) and Institute of Biological Interfaces (IBG-2), Karlsruhe Institute of Technology (KIT)
Host in iJURC FUTAKI, Shiroh I F

In-Depth Analysis of Efficiency Roll-Off in Highly Efficient TADF-Based Organic Electroluminescence Devices
NAMDAS, Ebinazar B., School of Mathematics and Physics, Centre for Organic Photonics & Electronics, The University of Queensland
Host in iJURC KAJI, Hironori I

Construction of Two-Dimensional Donor-Acceptor Systems by the Collaboration of Organic Synthesis, Single-Molecule Measurement, and Computational Chemistry.
KIMURA, Kensuke, Surface and Interface Science Laboratory, RIKEN
Host in iJURC KAJI, Hironori

Design of Intracellular Delivery Systems for Extracellular Vesicles
NAKASE, Ikuhiko, Graduate School of Science, Osaka Metropolitan University
Host in iJURC FUTAKI, Shiroh

Investigation of Cellular Uptake Mechanism Using Extracellular Vesicles
EGUCHI, Akiko, Department of Gastroenterology and Hepatology, Graduate School of Medicine, Mie University
Host in iJURC FUTAKI, Shiroh F

Role of *PIP5K* Genes in Pollen Tube Development
QU, Li-Jia, School of Life Sciences, Peking University
Host in iJURC AOYAMA, Takashi I

Structural and Functional Analysis of the Surface Polysaccharides of Outer Membrane Vesicles Released by Bacteria
CORSARO, Maria Michela, Department of Chemical Sciences, University of Naples Federico II
Host in iJURC KURIHARA, Tatsuo I F

Molecular Mechanisms for the Inactivation of a Growth Hormone in Rice
HE, Zuhua, Chinese Academy of Sciences, CAS Center for Excellence in Molecular Plant Sciences, Institute of Plant Physiology and Ecology
Host in iJURC YAMAGUCHI, Shinjiro I

Phase Separation in Mixture of Nematic Liquid Crystal and Solvent
SHIMADA, Ryoko, Department of Mathematical and Physical Sciences, Japan Women's University
Host in iJURC SATO, Takeshi F

Chromatin, Epigenetic and Proteolytic Regulation of RNA Processing in Plant Morphogenesis
RUBIO, Vicente, Plant Molecular Genetics Dept, National Center of Biotechnology (CNB-CSIC)
Host in iJURC TSUGE, Tomohiko I

Site-Selective Protein Acetylation and Phosphorylation by Small Molecule
ZHOU, Lu, School of Pharmacy, Fudan University
Host in iJURC UESUGI, Motonari I

Developments of Highly Efficient and High Color Purity Organic Electroluminescent Devices Based on Thermally Activated Delayed Fluorescent Materials Exhibiting Ultrafast Reverse Intersystem Crossing Process
DUAN, Lian, Department of Chemistry, Tsinghua University
Host in iJURC KAJI, Hironori I

Fabrication of Nanotopographical Polymer Surfaces for Bactericidal Properties-IV
ENDOH, Maya K., Department of Material Science and Chemical Engineering, Stony Brook University
Host in iJURC TAKENAKA, Mikihito I F

Synthesis of Polyether Nanocomposite Solid Polymer Electrolytes for Lithium Ion Batteries
FERRIER, Robert C., Chemical Engineering and Materials Science, Michigan State University
Host in iJURC TSUJII, Yoshinobu I

Development and Characterization of Metal Oxide Nanocrystalline Films for Solar Water Splitting
TACHIBANA, Yasuhiro, School of Engineering, RMIT University
Host in iJURC TERANISHI, Toshiharu I

Interdisciplinary Approach to Nanostructured Materials for Applications
BUCHER, Jean-Pierre, Institut de Physique et Chimie des Matériaux (IPCMS), Université de Strasbourg
Host in iJURC TERANISHI, Toshiharu I

Search for Four-Wave-Mixing in the Vacuum - Unveiling Dark Components in the Universe -
HOMMA, Kensuke, Physics, Hiroshima University
Host in iJURC WAKASUGI, Masanori I

Tin-Perovskite Thin Film Crystallization on New Hole-Transporting Materials
ABATE, Antonio, Novel Materials and Interfaces for Photovoltaic Solar Cells, Helmholtz-Zentrum Berlin, Germany
Host in iJURC WAKAMIYA, Atsushi I

Biochemical Characterization of Aldehyde Dehydrogenases Involved in the Biosynthesis of Plant Volatile Benzenoids
KOEDUKA, Takao, Graduate School of Sciences and Technology for Innovation, Yamaguchi University
Host in iJURC TSUGE, Tomohiko

Electronic and Spintronic Properties of Multilayer System Including $NiCo_2O_4$ and Fe_3O_4
NAGAHAMA, Taro, Solid State Chemistry Laboratory, Faculty of Engineering, Hokkaido University
Host in iJURC ONO, Teruo

Structural Optimization of Amyloid Photooxygenation Catalysts for the Treatment of Alzheimer’s Disease
KANAI, Motomu, Graduate School of Pharmaceutical Sciences, The University of Tokyo
Host in iJURC KAJI, Hironori

Analysis of the Physiological Functions of Extracellular Vesicles Produced by Intestinal Bacteria and Their Application
KURATA, Atsushi, Faculty of Agriculture, Kindai University
Host in iJURC KURIHARA, Tatsuo

Structural Analysis of Water in Polymer Brush Layer Using Attenuated Total Reflection Near-Infrared Spectroscopy
GENMEI, Makoto, Graduate School of Innovative Life Science, Toyama University
Host in iJURC OHNO, Kohji

Manipulation of Three Dimensional Structure of Polymer Monoliths by 3D Printer
MURASE, Hiroki, Department of Textile and Clothing, Faculty of Home Economics, Kyoritsu Women’s University
Host in iJURC TSUJII, Yoshinobu

Giant Magnetic Resistance on Single-Electron Transistor
MAJIMA, Yutaka, Laboratory for Materials and Structures, Tokyo Institute of Technology
Host in iJURC TERANISHI, Toshiharu

Functional Analysis of Non-Canonical Strigolactones as Plant Hormones and Root-Derived Signals
SETO, Yoshiya, School of Agriculture, Meiji University
Host in iJURC YAMAGUCHI, Shinjiro

Preparation of Multi-Stimuli-Responsive Polymer via Controlled Radical Polymerization
YUSA, Shin’ichi, Graduate School of Engineering, University of Hyogo
Host in iJURC YAMAGO, Shigeru

Study of the Generation and Sustainment of High Energy Density Plasmas due to the Interaction between High Power Laser and Structured Medium
KISHIMOTO, Yasuaki, Graduate School of Energy Science, Kyoto University
Host in iJURC WAKASUGI, Masanori

SUBJECTS FOCUSING OF JOINT USAGE OF iJURC/ ICR FACILITIES

Tackling the Electronic Instability of Charge-Density Waves by Electron Energy-Loss Spectroscopy
CHU, Ming-Wen, Center for Condensed Matter Sciences, National Taiwan University
Host in iJURC KURATA, Hiroki I

Micro- and Nano-Structural Characterization by Advanced Transmission Electron Microscopy of Novel Functional Materials
CHAIRUANGSRI, Torranin, Industrial Chemistry, Chiang Mai University
Host in iJURC KURATA, Hiroki I

High-Pressure Synthesis of Transition Metal Oxides with Novel Physical Properties.
JI, Kunlang, Centre for Science at Extreme Conditions and School of Chemistry, University of Edinburgh
Host in iJURC SHIMAKAWA, Yuichi I

Synthesis and Characterization of Novel Group 16 Element Compouds
MINOURA, Mao, Department of Chemistry, College of Science, Rikkyo University
Host in iJURC MIZUHATA, Yoshiyuki I F

Analyzing Chemical Properties and Origins of Dissolved Organic Matter in Lakes and Soils by FT-ICR-MS
KIDA, Morimaru, Graduate School of Agricultural Science, Kobe University
Host in iJURC NAKAMURA, Masaharu I

Preparation of High-Efficiency Spin-Injection Materials Using Optimization of Magnetism and Crystal Structure
TANAKA, Masaaki, Department of Physical Science and Engineering, Nagoya Institute of Technology
Host in iJURC ONO, Teruo

Development of a Highly Efficient $CsPbBr_3$ Scintillator
SAITO, Hikaru, Institute for Materials Chemistry and Engineering, Kyushu University
Host in iJURC KURATA, Hiroki

High Accuracy Measurement of Hydrogen and Helium Behavior in Plasma Facing Materials for Nuclear Fusion Devices
MIYAMOTO, Mitsutaka, Interdisciplinary Faculty of Science and Engineering, Shimane University
Host in iJURC KURATA, Hiroki

Synthesis and Structural Characterization of Lewis Base Adducts of Tetrylenes
MATSUO, Tsukasa, Faculty of Science and Engineering, Kindai University
Host in iJURC MIZUHATA, Yoshiyuki

Synthesis and Structures of Cationic Aromatics Bearing Chalconenopyrylium units
NAGAHORA, Noriyoshi, Department of Chemistry, Faculty of Science, Fukuoka University
Host in iJURC MIZUHATA, Yoshiyuki

Theoretical Design of Low-Dimensional Silicon Material Embedded in a Flat Twodimensional Sheet and Exploration for Operating Principles
TAKAHASHI, Masae, Graduate School of Agricultural Science, Tohoku University
Host in iJURC MIZUHATA, Yoshiyuki F

SUBJECTS ENCOURAGING JOINT PROGRAM

Determine the Three-Dimensional Structure of ^{13}C Labeled α-Synuclein(61-95) in the Langmuir-Blodgett Film and Supported Phospholipid Bilayer by MAIRS2
WANG, Chengshan, Chemistry, Middle Tennessee State University
Host in iJURC HASEGAWA, Takeshi I

The 16th International Workshop for East Asian Young Rheologists
INOUE, Tadashi, Department of Macromolecular Science, Osaka University
Host in iJURC MATSUMIYA, Yumi I

iJURC Publications (Selected Examples)

(until 31 May 2022)

Fused-Nonacyclic Multi-Resonance Delayed Fluorescence Emitter Based on Ladder-Thiaborin Exhibiting Narrowband Sky-Blue Emission with Accelerated Reverse Intersystem Crossing

Nagata, M.; Min, H.; Watanabe, E.; Fukumoto, H.; Mizuhata, Y.; Tokitoh, N.; Agou, T.; Yasuda, T., *Angew. Chem. Int. Ed.*, **60,** 20280-20285 (2021).

Abstract

Developing organic luminophores with unique capability of strong narrowband emission is both crucial and challenging for the further advancement of organic light-emitting diodes (OLEDs). Herein, a nanographitic fused-nonacyclic π-system (**BSBS-N1**), which was strategically embedded with multiple boron, nitrogen, and sulfur atoms, was developed as a new multi-resonance thermally activated delayed fluorescence (MR-TADF) emitter. Narrowband sky-blue emission with a peak at 478 nm, full width at half maximum of 24 nm, and photoluminescence quantum yield of 89 % was obtained with **BSBS-N1**. Additionally, the spin-orbit coupling was enhanced by incorporating two sulfur atoms, thereby facilitating the spin-flipping process between the excited triplet and singlet states. OLEDs based on **BSBS-N1** as a sky-blue MR-TADF emitter achieved a high maximum external electroluminescence quantum efficiency of 21.0 %, with improved efficiency roll-off.

Determinants of Crystal Structure Transformation of Ionic Nanocrystals in Cation Exchange Reactions

Li, Z.; Saruyama, M.; Asaka, T.; Tatetsu, Y.; Teranishi, T., *Science*, **373,** 332-337 (2021).

Abstract

Changes in the crystal system of an ionic nanocrystal during a cation exchange reaction are unusual yet remain to be systematically investigated. In this study, chemical synthesis and computational modeling demonstrated that the height of hexagonal-prism roxbyite ($Cu_{1.8}S$) nanocrystals with a distorted hexagonal close-packed sulfide anion (S^{2-}) sublattice determines the final crystal phase of the cation-exchanged products with Co^{2+} [wurtzite cobalt sulfide (CoS) with hexagonal close-packed S^{2-} and/or cobalt pentlandite (Co_9S_8) with cubic close-packed S^{2-}]. Thermodynamic instability of exposed planes drives reconstruction of anion frameworks under mild reaction conditions. Other incoming cations (Mn^{2+}, Zn^{2+}, and Ni^{2+}) modulate crystal structure transformation during cation exchange reactions by various means, such as volume, thermodynamic stability, and coordination environment.

1,3-Diradicals Embedded in Curved Paraphenylene Units: Singlet versus Triplet State and In-Plane Aromaticity

Miyazawa, Y.; Wang, Z.; Matsumoto, M.; Hatano, S.; Antol, I.; Kayahara, E.; Yamago, S.; Abe, M., *Angew. J. Am. Chem. Soc.*, **143,** 7426-7439 (2021).

Abstract

Curved π-conjugated molecules and open-shell structures have attracted much attention from the perspective of fundamental chemistry, as well as materials science. In this study, the chemistry of 1,3-diradicals (**DR**s) embedded in curved cycloparaphenylene (**CPP**s) structures, **DR**-(n+3)**CPP**s (n = 0–5), was investigated to understand the effects of the curvature and system size on the spin–spin interactions and singlet versus triplet state, as well as their unique characteristics such as in-plane aromaticity. A triplet ground state was predicted for the larger 1,3-diradicals, such as the seven- and eight-paraphenylene-unit-containing diradicals **DR-7CPP** (n = 4) and **DR-8CPP** (n = 5), by quantum chemical calculations. The smaller-sized diradicals **DR**-(n+3)**CPP**s (n = 0–3) were found to possess singlet ground states. Thus, the ground-state spin multiplicity is controlled by the size of the paraphenylene cycle. The size effect on the ground-state spin multiplicity was confirmed by the experimental generation of **DR-6CPP** in the photochemical denitrogenation of its azo-containing precursor (**AZ-6CPP**). Intriguingly, a unique type of in-plane aromaticity emerged in the smaller-sized singlet states such as S-**DR-4CPP** (n = 1), as proven by nucleus-independent chemical shift calculations (NICS) and an analysis of the anisotropy of the induced current density (ACID), which demonstrate that homoconjugation between the 1,3-diradical moiety arises because of the curved and distorted bonding system.

Colossal Barocaloric Effect by Large Latent Heat Produced by First-Order Intersite-Charge-Transfer Transition

Kosugi, Y.; Goto, M.; Tan, Z.; Fujita, A.; Saito, T.; Kamiyama, T.; Chen, W.; Chuang, Y.; Sheu, H.; Kan, D.; Shimakawa, Y., *Adv. Funct. Mater.*, **31,** 2009476 (2021).

Abstract

Materials which show novel thermal properties can be used to make highly efficient and environmentally friendly energy systems for thermal energy storage and refrigeration through caloric effects. An *A*-site-ordered quadruple perovskite-structure oxide, $NdCu_3Fe_4O_{12}$, is found to release significant latent heat, 25.5 kJ kg^{-1} (157 J cc^{-1}), at the intersite-charge-transfer transition temperature near room temperature. The transition is first-order and accompanied by an unusual magnetic ordering and a large negative-thermal-expansion-like volume change, and thus, it causes a large entropy change (84.2 J K^{-1} kg^{-1}). The observed entropy change is comparable to the largest changes reported in inorganic solid materials, and more importantly, it is utilized through a colossal barocaloric effect. The adiabatic temperature change by applying 5.1 kbar pressure is estimated to reach 13.7 K, which means efficient refrigeration can be realized through this effect.

Tracing the Incorporation of the “Ninth Sulfur” into the Nitrogenase Cofactor Precursor with Selenite and Tellurite

Tanifuji, K.; Jasniewski, A. J.; Villarreal, D.; Stiebritz, M. T.; Lee, C. C.; Wilcoxen, J.; Okhi, Y.; Chatterjee, R.; Bogacz, I.; Yano, J.; Kern, J.; Hedman, B.; Hodgson, K. O.; Britt, R. D.; Hu, Y.; Ribbe, M. W., *Nat. Chem.*, **13,** 1228-1234 (2021). Springer Nature

Abstract

Molybdenum nitrogenase catalyses the reduction of N_2 to NH_3 at its cofactor, an [(R-homocitrate)$MoFe_7S_9C$] cluster synthesized via the formation of a [Fe_8S_9C] L-cluster prior to the insertion of molybdenum and homocitrate. We have previously identified a [Fe_8S_8C] L*-cluster, which is homologous to the core structure of the L-cluster but lacks the ‘ninth sulfur’ in the belt region. However, direct evidence and mechanistic details of the L*- to L-cluster conversion upon ‘ninth sulfur’ insertion remain elusive. Here we trace the ‘ninth sulfur’ insertion using SeO_3^{2-} and TeO_3^{2-} as ‘labelled’ SO_3^{2-}. Biochemical, electron paramagnetic resonance and X-ray absorption spectroscopy/extended X-ray absorption fine structure studies suggest a role of the ‘ninth sulfur’ in cluster transfer during cofactor biosynthesis while revealing the incorporation of Se^{2-}- and Te^{2-}-like species into the L-cluster. Density functional theory calculations further point to a plausible mechanism involving in situ reduction of SO_3^{2-} to S^{2-}, thereby suggesting the utility of this reaction to label the catalytically important belt region for mechanistic investigations of nitrogenase.

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
GONG, Jian Ping
(D Sc)

Laboratory of Chemistry of Polymer Materials

Professor, Institute for Chemical Reaction Design and Discovery, Hokkaido University
(Kita 21 Nishi 10, Kita-ku, Sapporo, Hokkaido 001-0021)

Lecture at *ICR*
Chemistry and Physics of Soft and Wet Matters

Vis Prof
NOMURA, Nobuhiko
(D Eng)

Laboratory of Molecular Microbial Science

Professor, Faculty of Life and Environmental Sciences, University of Tsukuba
(1-1-1 Tennodai, Tsukuba, Ibaraki 305-8577)

Lecture at *ICR*
Bacterial Community Formation and Generation of Sociality

Vis Prof
SUDA, Toshimi
(D Sc)

Laboratory of Particle Beam Science

Professor, Research Center for Electron Photon Science (ELPH), Tohoku University
(Mikamine 1-2-1, Taihaku-ku, Sendai, Miyagi 982-0826)

Lecture at *ICR*
The Size of Proton

Vis Prof
MATSUDA, Hideo
(Ph D)

Laboratory of Mathematical Bioinformatics

Professor, Department of Bioinformatic Engineering, Graduate School of Information Science and Technology, Osaka University
(1-5, Yamadaoka, Suita, Osaka 565-0871)

Lecture at *ICR*
Single-Cell Trajectory and Imaging Analyses of Mouse Inflammatory Response

Vis Assoc Prof
KONDO, Mio
(D Sc)

Laboratory of Advanced Inorganic Synthesis

Associate Professor, Department of Applied Chemistry, Graduate School of Engineering, Osaka University
(2-1 Yamadaoka, Suita, Osaka 565-0871)

Lecture at *ICR*
Construction of Small-Molecule Conversion Catalysts Based on Functional Integration Strategy

Vis Assoc Prof
SETO, Yoshiya
(D Agr)

Laboratory of Chemistry of Molecular Biocatalysts

Associate Professor, Laboratory of Plant Chemical Regulation, School of Agriculture, Meiji University
(1-1-1 Higashi-mita, Tama-ku, Kawasaki, Kanagawa 214-8571)

Lecture at *ICR*
Strigolactone-Mediated Interactions between Organisms

Vis Assoc Prof
INOKUMA, Yasuhide
(D Sc)

Laboratory of Molecular Aggregation Analysis

Associate Professor, Institute for Chemical Reaction Design and Discovery, Hokkaido University
(Kita 13 Nishi 8, Kita-ku, Sapporo, Hokkaido 060-8628)

Lecture at *ICR*
Structural Organic Chemistry Developed by Molecular Ropes ~ Creation of New Molecules Based on Flexible Ideas ~

Vis Assoc Prof
SUZUKI, Kosuke
(D Eng)

Laboratory of Organometallic Chemistry

Associate Professor, Catalytic Chemistry Laboraotry, The University of Tokyo
(Hongo, Bunkyoku, Tokyo 113-8656)

Lecture at *ICR*
Precise Liquid-Phase Synthesis and Catalytic Activity of Metal-Oxide Nanoclusters

Prof Em / Specially Appointed Prof
TOKITOH, Norihiro (D Sc)

Prof Em / Specially Appointed Prof
KANEHISA, Minoru (D Sc)

PERSONAL

Retirement

Professor KURATA, Hiroki
Advanced Research Center for Beam Science
– Electron Microscopy and Crystal Chemistry –

On March 31, 2023, Dr. Hiroki Kurata retired from Kyoto University and was honored with the title of Professor Emeritus of Kyoto University.

He was born in Ehime Prefecture on February 9, 1958. In 1980, he graduated from Faculty of Engineering, Nagoya Institute of Technology. He entered the Graduate School of Science, Kyoto University in 1981. He was appointed to Research Associate at the Institute for Chemical Research (ICR), Kyoto University in 1986, and was promoted to Assistant Professor in 1987. He received the doctoral degree from Kyoto University under the supervision of Professor Natsu Uyeda in 1988. In 1991-1992, he made a research stay at Laboratoire de Physique des Solides, Centre National de la Recherche Scientifique, as a visiting researcher. He moved to Japan Atomic Energy Research Institute in 1996, and promoted to Senior Researcher in 1997, and to Principal Researcher in 2000. In 2002, he moved to Professor Seiji Isoda's lab at ICR, Kyoto University, as Associate Professor, and was promoted to Professor in 2012.

Throughout his academic career, Dr. Kurata devoted himself to crystal chemistry, focusing on research on local structural analysis and electronic state analysis of solids using many types of transmission electron microscopes. Using a high-voltage transmission electron microscope, he succeeded in two-dimensional visualization of elemental distribution with sub-nanometer spatial resolution, and experimentally clarified the relativistic effect on the inelastic scattering cross section of fast electrons.

He also developed a cold-field emission electron gun equipped with a tungsten nano-tip. This newly developed electron gun was installed in a spherical aberration corrected scanning transmission electron microscope, enabling atomic resolution structural observation and electronic state analysis. Using this microscope, he has worked on the visualization of light elements in crystals, which was difficult in the past, and succeeded in visualizing carbon atomic columns in organic molecular crystals for the first time in the world. Furthermore, by directly observing the oxygen atoms at the heterointerfaces of transition metal oxides, he has contributed to the development of a precise structure analysis method for interfaces with an accuracy of several picometers, opening up a new way for local structural analysis. Using the energy-loss near-edge structures obtained by electron energy-loss spectroscopy, he also investigated the directionality of chemical bonds of specific atoms, which are directly observed at the atomic resolution level, and clarified the local electronic structures related to structure distortions around specific atoms.

He extended his study to high energy resolution electron energy-loss spectroscopy by installing an atomic resolution analytical electron microscope equipped with a monochromator in the electron gun. He realized the visualization of the near-field electromagnetic field associated with the surface plasmon excitations in metal nanoparticles, and the two-dimensional real-space distribution of holes, which is key to manifesting the physical properties of high-temperature superconductors.

Throughout his carrier, his scientific achievements have been published as 188 original papers, 27 reviews and 5 books. His achievements were highly recognized internationally and he gave invited talk at many international conferences. His contribution to scientific communities is also to be noted. He was a member of organizing committee of the 8th Asia-Pacific Microscopy Conference (2004), the 12th International Congress of Microscopy (2006) and the 12th Frontiers of Electron Microscopy in Materials Science (2009). He has also served as a member of the board of directors of the Japanese Society of Microscopy (2001–2005) and as an Executive Editor of *Microscopy* (2011–2019) and as an Editor-in-Chief of *Kenbikyo* issued by the Japanese Society of Microscopy (2011–2013).

For his achievements, he was awarded Achievement Award for Excellent Paper from the Japanese Society of Electron Microscopy (1998), the Seto Prize from Japanese Society of Microscopy (2003), Best Material Paper Award from the Microscopy Society of America (2008), Achievement Award for Excellent Paper from the Laser Society of Japan (2017) and an Honorary Member of the Microscopy Society of Thailand (2020).

Dr. Kurata's contribution to Kyoto University and the ICR thorough his scientific, educational and administrative activities is hereby greatly acknowledged.

Awards

TOKITOH, Norihiro

CSJ Award

"Elucidation of the Inherent Potential of Heavier Main Group Elements Based on the Creation of Unexplored Molecules"

The Chemical Society of Japan

24 March 2022

HIROSE, Takashi

The Young Scientists' Award, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology

"Studies on Photophysical Functions and Mechanical Properties of Helical Molecules"

The Ministry of Education, Culture, Sports, Science and Technology (MEXT)

20 April 2022

UEDA, Yoshihiro

Asian Core Program Advanced Research Network Lectureship Award

The 15th International Conference on Cutting-Edge Organic Chemistry in Asia (ICCEOCA-15)

"Seven-Step Stereodivergent Total Syntheses of Punicafolin and Macaranganin"

Asian Core Program Advanced Research Network

27 July 2022

TERANISHI, Toshiharu

The Japanese Photochemistry Association Special Lectureship Award

"Development of Visible-to-Near Infrared Plasmonic Nanomaterials by Element Substitution"

The Japanese Photochemistry Association

14 September 2022

TAKEKUMA, Haruka

Young Scientist Incentive Award

"Design and Synthesis of Pseudo-Money Metallic Ordered Alloy Nanoparticles with Visible LSPR"

Plasmonic Photochemistry Society of Japan

18 March 2022

MATSUMOTO, Kenshi

Oral Presentation Award for Young Scientist

The 73rd Divisional Meeting of Division of Colloid and Surface Chemistry

"Diffusion Path Dependence Leading to the Formation of Unprecedented Z3-Type Fe(Pd,In)$_3$ Nanoparticles"

Division of Colloid and Surface Chemistry

06 October 2022

MORIOKA, Naoya

Best Short Presentation Award

The 5th International Forum on Quantum Metrology and Sensing

"Room-Temperature Electrical Detection of Nuclear Spins in Silicon Carbide"

Q-LEAP Quantum Metrology and Sensing

29 November 2022

HERBSCHLEB, Ernst David

The 17th Young Scientist Award of the Physical Society of Japan

"Research on the Spin Coherence and the Quantum Sensing Technique in Solid-State Systems"

The Physical Society of Japan

26 October 2022

Short Presentation Award

The 5th International Forum on Quantum Metrology and Sensing

"Enhancing Sensitivity with Entanglement in Coupled Nitrogen Vacancy Centres"

Q-LEAP Quantum Metrology and Sensing

29 November 2022

FU, Haining

Best Presentation Award

The 4th Annual Meeting of the Quantum Life Science Society

"Temperature Sensing with Germanium-Vacancy (GeV) Nanodiamond Synthesized by Detonation Method"

Quantum Life Science Society

27 May 2022

ONO, Teruo

The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology

"Pioneering Research on Magnetization Control of Nano-Magnets"

The Ministry of Education, Culture, Sports, Science and Technology (MEXT)

20 April 2022

HISATOMI, Ryusuke

The 38th Inoue Research Award for Young Scientists

"Heterodyne Spectroscopy of Magnon-Induced Brillouin Light Scattering in Ferromagnetic Insulator"

Inoue Foundation for Science

4 February 2022

NARITA, Hideki

The 52nd JSAP Presentation Award

"Superconducting Diode Effect in Superconductor / Ferromagnet Multilayers"

The Japan Society of Applied Physics

20 September 2022

ICR Award for Young Scientists

"Field-Free Superconducting Diode Effect in Noncentrosymmetric Superconductor/Ferromagnet Multilayers"

Institute for Chemical Research, Kyoto University

9 December 2022

FUTAKI, Shiroh

The Akabori Memorial Award 2022

“Peptides that Affect Membrane Structure and Permeability”

The Japanese Peptide Society

27 October 2022

OTONARI, Kenko

Best Presentation Award for Master’s Thesis

“Design of a Ligand-Responsive Sequence-Specific RNA Demethylase”

Graduate School of Pharmaceutical Sciences, Kyoto University

24 March 2022

KURIYAMA, Masashi

Excellent Stone Award

The 59th Japanese Peptide Symposium

“Identification of Biomolecules that Contribute to the Activity of the Cytosolic Delivery Peptide L17E”

The Japanese Peptide Society

28 October 2022

NAKAGAWA, Yuna

Best Presentation Award

The 68th Annual Meeting, The Japanese Biochemistry Society, Kinki Branch

“Intracellular Delivery of Extracellular Vesicles by Macropinocytosis-Inducing Peptides”

The Japanese Biochemistry Society, Kinki Branch

30 May 2022

TANAKA, Kamui

Best Presentation Award

The 68th Annual Meeting, The Japanese Biochemistry Society, Kinki Branch

“Inhibitor Screening and Mechanism of RNA Demethylase, FTO”

The Japanese Biochemistry Society, Kinki Branch

30 May 2022

Best Presentation Award

The 95th Annual Meeting, The Japanese Biochemistry Society

“Anaylsis of the Contribution of Ascorbic Acid to RNA Demethylase, FTO”

The Japanese Biochemistry Society

11 November 2022

YOSHIE, Shunsuke

Best Presentation Award

The 72nd Annual Meeting, The Pharmaceutical Society of Japan, Kansai Branch

“Search of Macropinocytosis-Related Genes”

The Pharmaceutical Society of Japan, Kansai Branch

8 October 2022

TAKANO, Shotaro

Young Scientist Award

The 115th Meeting of Discussion Group for Plasma Spectrochemistry

“Development of Precise Isotopic Analysis of Trace Metals and Its Application to Oceanochemistry and Geochemistry”

Discussion Group for PLASMA Spectrochemistry

20 May 2022

OKA, Takayuki

2022 Young Scientist Presentation Award

The Annual Meeting of the Spectroscopical Society of Japan

“Polymorphism in Organic Semiconductor Thin Films Revealed by Infrared Spectroscopy”

The Spectroscopical Society of Japan

14 October 2022

Student Poster Award

The 51st Japan Conference on Crystal Growth

“Influence of Alkyl Chain Length on the Polymorphism in Organic Semiconductor Thin Films”

The Japanese Association for Crystal Growth

14 December 2022

TSUDZUKI, Taiku

Young Scientist Award

The 95th Annual Meeting of the Japanese Biochemical Society

“Function of Surface Polysaccharide Synthesis Enzymes Involved in the Cargo Transport to Extracellular Membrane Vesicles”

The Japanese Biochemical Society

11 November 2022

KANEMITSU, Yoshihiko
WAKAMIYA, Atsushi

The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology

“Study on Efficient Photovoltaics Using Printable Semiconductor Materials”

The Ministry of Education, Culture, Sports, Science and Technology (MEXT)

20 April 2022

NAKAMURA, Tomoya

NIPPON SHOKUBAI Award in Synthetic Organic Chemistry

“Development of Monolayer Electron-Collecting Materials for Efficient Lead-Free Perovskite Solar Cells”

The Society of Synthetic Organic Chemistry, Japan (SSOCJ)

13 December 2022

TRUONG, Minh Anh

FUJIFILM Wako Pure Chemical Award in Synthetic Organic Chemistry

“Development of Multipodal Monolayer Materials for Efficient Perovskite Solar Cells”

The Society of Synthetic Organic Chemistry, Japan (SSOCJ)

16 February 2022

HU, Shuaifeng

Student Award

The 33rd International Photovoltaic Science and Engineering Conference (PVSEC-33)

“Interfacial Modifications for Efficient Tin–Lead Perovskite Solar Cells”

The Japan Photovoltaic Society (JSES)

17 November 2022

FUNASAKI, Tsukasa

Innovative PV Encouragement Award

The 18th Next Generation Photovoltaic Power Generation System Symposium (The 1st Symposium of The Japan Photovltaic Society)

“Development of Cyclooctatetraindole Based Tetrapodal Hole Collecting Monolayer Materials”

The Japan Photovoltaic Society (JSES)

30 August 2022

IWASHIMIZU, Chisaki

ICR Award for Graduate Students

“Electron Orbital Mapping of $SrTiO_3$ Using Electron Energy-Loss Spectroscopy”

Institute for Chemical Research, Kyoto University

9 December 2022

SHIMAKAWA, Yuichi

Yazaki Memorial Foundation for Science and Technology Award

“Exploring Novel Functional Properties in Cation-Ordered Transition-Metal Oxides”

Yazaki Memorial Foundation for Science and Technology

10 March 2022

Fellow of the Royal Society of Chemistry

“Inorganic Chemistry and Materials Sciences”

The Royal Society of Chemistry

26 April 2022

TANIFUJI, Kazuki

JSCC Research Encouragement Award

The 72nd Conference of Japan Society of Coordination Chemistry

“Studies on Biosynthesis and Catalysis of Metal-Sulfur Clusters”

Japan Society of Coordination Chemistry

28 September 2022

KANEMITSU, Yoshihiko

Outstanding Referee

American Physical Society

25 February 2022

YUMOTO, Go

ICR Award for Young Scientists

“Rapidly Expanding Spin-Polarized Exciton Halo in a Two-Dimensional Halide Perovskite at Room Temperature”

Institute for Chemical Research, Kyoto University

9 December 2022

CHO, Kenichi

The 52nd JSAP Young Scientist Presentation Award

“Exciton-Phonon Couplings in Single Lead-Halide Perovskite Nanocrystals”

The Japan Society of Applied Physics

20 September 2022

AKUTSU, Tatsuya

Japanese Society for Bioinformatics Prize 2022

“Mathematical and Pioneering Studies on Inference and Control of Biological Networks”

Japanese Society for Bioinformatics

15 September 2022

NAKAGAWA, Kotaro

ICR Award for Graduate Students

“Size-Controlled Quantum Dots Reveal the Impact of Intraband Transitions on High-Order Harmonic Generation in Solids”

Institute for Chemical Research, Kyoto University

9 December 2022

NGUYEN, Duc Anh

ICR Award for Graduate Students

“SPARSE: A Sparse Hypergraph Neural Network for Learning Multiple Types of Latent Combinations to Accurately Predict Drug-Drug Interactions”

Institute for Chemical Research, Kyoto University

9 December 2022

OKAZAKI, Yusuke

The 24th Yoshimura Award

“Microbial Ecology Opened up through Deep Freshwater Ecosystems”

The Japanese Society of Limnology

18 September 2022

Paper Awards

HUANG, Yu Min

Paper Award

“Low Current Driven Vertical Domain Wall Motion Memory with an Artificial Ferromagnet”

The Magnetics Society of Japan

7 September 2022

KOBAYASHI, Yuta

Paper Award

“Estimation of Magnetic Domain Size in Chiral Antiferromagnet Mn_3Ir by the Anomalous Hall Measurements”

The Magnetics Society of Japan

7 September 2022

Poster Awards

UCHIDA, Daichi

Poster Award

The 32nd Symposium on Physical Organic Chemistry

"Synthesis of Dichloromethyldihalogermanes Using a Novel Cleavage Reaction of a Germylene Bearing TbtCH_2 Group and Their Reduction"

The Society of Physical Organic Chemistry

22 Septemer 2022

ZHANG, Zheng

Poster Prize on the 32nd Symposium on Physical Organic Chemistry

The 32nd Symposium on Physical Organic Chemistry

"Synthesis and Emission Properties of Helicene Derivatives with 1,2,5-Thiadiazole Moieties at Both Ends"

The Society of Physical Organic Chemistry

22 Septemer 2022

ZHU, Lingkai

Poster Award

The 73rd Divisional Meeting of Division of Colloid and Surface Chemistry

"One-Pot Synthesis of Ag Colloidal Crystals"

Division of Colloid and Surface Chemistry

21 Septemer 2022

MIYAJI, Kousuke

Poster Award for Young Scientist

"Size Dependence of Luminescence in Sulfur Nanoparticles"

The Society of Nano Science and Technology

22 May 2022

HIRATA, Saya

Materials Horizons Poster Prize

Design, Synthesis and Application of Next-Generation Organic Semiconductors Symposium

"Generation and In-Plane Aromaticity of Diradical Dianion of a Cycloparaphenylene-Diketone"

Imperial College London

16 Septemer 2022

KAWAGUCHI, Yoshimasa

Excellent Poster Presentation Award

The 59th Japanese Peptide Symposium

"Development of Melittin Derivatives for Intracellular Delivery of Biomacromolecules"

The Japanese Peptide Society

28 October 2022

SAKO, Nobuaki

Japan Excellent Poster Award

The 45th Fluorine Conference of Japan

“Relationship between Molecular Aggregation Structure and Surface Property of Perfluoropolyether-Based Self-Assembled Monolayer”

The Society of Fluorine Chemistry

07 November 2022

KAZAMA, Hiroki

Poster Award

2022 Young Scientists Symposium of The Japanese Society of Microscopy

“Coupling of Surface Plasmon of Ag Nanorods and Exciton under Various Conditions”

The Japanese Society of Microscopy

12 October 2022

Obituary

Professor Emeritus
Dr. TAKANAMI, Mituru (1929–2022)

Dr. Mituru Takanami, Professor Emeritus of Kyoto University, passed away on September 25, 2022, at the age of 93.

Dr. Takanami was born in Toyama on 15th of September, 1929. He graduated from Department of Zoology, Faculty of Science, Kyoto University in 1952, and continued his studies as a graduate student at the same department under the supervision of Professor Kenji Nakamura. In 1953, he was appointed as an instructor of Faculty of Science, Kyoto University, and later reassigned to a chief researcher of the National Institute of Animal Health in the Ministry of Agriculture and Forestry. In 1961, he was granted a doctoral degree from Kyoto University for his biochemical study of ribonucleoproteins. In 1962, he promoted to an Associate Professor of Hiroshima University Research Institute for Radiation Biology and Medicine. On a leave of absence from 1963 to 1966, he worked at Brookhaven National Laboratory and University of California Space Science Laboratory, where he gained further experience on the biosynthesis of ribonucleic acids and proteins in collaboration with Professors Geoferry L. Zubay and Thomas H. Jukes.

In 1967, he moved to the Institute for Chemical Research, Kyoto University as a full Professor to direct the Laboratory of Molecular Biology. In 1981, he established the Research Facility for Nucleic Acids, through which recombinant DNA techniques and DNA sequencing methods were developed and dispersed in Japan and Asian countries. From April 1988 to March 1990, he was appointed as Director of the Institute for Chemical Research. At Graduate School of Science, Kyoto University, he gave lectures on advanced molecular genetics and supervised the dissertation works of graduate students. He retired from Kyoto University in March 1993 and was honored with the title of Professor Emeritus.

Dr. Takanami conducted extensive research in the field of molecular biology. He performed outstanding achievements consistently in elucidating molecular mechanisms for the transmission and expression of genetic information. In particular, he obtained prominent results in studies on the starting reaction of protein biosynthesis, transcriptional initiation, and the essential structure of bacterial promoters and replicons. In the course of these studies, he discovered novel restriction enzymes, and determined the total genome sequence of the bacteriophage *fd* to pioneer the field of genome sciences. He also elucidated functional structures of fundamentally important genomic regions, including the replication origin of the *Escherichia coli* chromosome, the oncogenic DNA fragment of Adenovirus type 12, the kanamycin resistance transposable element Tn*903*, and the coding region of the insecticidal fragment in the *Bacillus thuringiensis* crystal protein.

Dr. Takanami devoted himself to organizing the Molecular Biology Society of Japan and officiated as President of the Society for two years from April 1987. After the retirement from Kyoto University, while serving as School Principal of Bio-college Kyoto for four years from April 1993, he involved himself in the establishment of Kazusa DNA Research Institute, where he supervised cutting-edge projects on DNA studies, including the genome project of cyanobacterium *Synechocystis* sp. PCC6803, as the founding Director from October 1994 to August 1997. He was also an editor of the international journal Molecular and General Genetics, and the editor-in-chief of DNA Research, a pioneering international journal for DNA studies. Through dissemination of recombinant DNA techniques, he contributed intensively to the development of Japanese bioindustry. He assisted a wide variety of companies, including those of chemical, pharmaceutical and food, in their foray into the life science field based on molecular biology.

His sincere and warm personality earned the respect of his friends, colleagues, and students. His contribution to the development of molecular biology during its early days in academic, educational, and industrial societies is gratefully acknowledged.

PUBLICATIONS
INTERNATIONAL RESEARCH COLLABORATIONS
SELECTED GRANTS
THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Jun-i, Y.; Mizuhata, Y.; Tokitoh, N., Template Synthesis of Novel Norcorrole Complexes with a Phenyl-Substituted Phosphorus Center, *Eur. J. Org. Chem.*, **2022(5),** e202101312 (2022).

Jun-i, Y.; Mizuhata, Y.; Tokitoh, N., Convergent Synthesis of *E*-Disilene by the Reduction of Diastereomerically Separable 1,2-Dichlorodisilanes, *Eur. J. Inorg. Chem.*, **2022(5),** e202100962 (2022).

Oshiro, T.; Mizuhata, Y.; Tokitoh, N., Reaction of an Overcrowded 1,2-Diaryl-1,2-Dibromodisilene with 1-Vinylcyclohepta-1,3,5-Triene: Isolation of a 2-Vinylsilacyclopropane Derivative and Its Thermal Conversion to a Silacyclopent-3-Ene Derivative, *Heterocycles*, **104,** 389-396 (2022).

Sasamori, T.; Sugahara, T.; Tokitoh, N., Amidinate Bromogermylene Resulting from Carbodiimide Insertion into Ar-GeBr Bond, *Mendeleev Commun.*, **32(1),** 63-65 (2022).

Noda, N.; Jung, Y.; Ado, G.; Mizuhata, Y.; Higuchi, M.; Ogawa, T.; Ishidate, F.; Sato, S.-I.; Kurata, H.; Tokitoh, N.; Uesugi, M., Glucose as a Protein-Condensing Cellular Solute, *ACS Chem. Biol.*, **17(3),** 567-575 (2022).

Oshiro, T.; Mizuhata, Y.; Tokitoh, N., 2-Germaazulene: Synthesis and Properties of 2-Heteraazulene Containing a Germanium Atom as a Skeletal Element, *Chem. Lett.*, **51,** 312-316 (2022).

Suzuki, W.; Takahata, R.; Chiga, Y.; Kikkawa, S.; Yamazoe, S.; Mizuhata, Y.; Tokitoh, N.; Teranishi, T., Control over Ligand-Exchange Positions of Thiolate-Protected Gold Nanoclusters Using Steric Repulsion of Protecting Ligands, *J. Am. Chem. Soc.*, **144(27),** 12310-12320 (2022).

Tsukada, H.; Hisa, T.; Shirai, T.; Oshiki, T.; Mizuhata, Y.; Tokitoh, N.; Fukumoto, H.; Agou, T., Synthesis of Perfluoroalkylene-Vinylene-Arylene Copolymers via the Mizoroki-Heck Co-Polymerization of 1,4-Divinylperfluorobutane and 1,6-Divinylperfluorohexane with Dihalogenated Arylene Monomers, *J. Fluor. Chem.*, **261-262,** 110033 (2022).

Nakamura, M.; Hyakutake, R.; Morisako, S.; Sasamori, T.; Mizuhata, Y.; Tokitoh, N.; Nakashima, K.; Fukumoto, H.; Agou, T., Boron Complexes of π-Extended Nitroxide Ligands Exhibiting Three-State Redox Processes and Near-Infrared-II (NIR-II) Absorption Properties, *Dalton Trans.*, **51,** 13675-13680 (2022).

Sugahara, T.; Hashizume, D.; Tokitoh, N.; Matsui, H.; Kishi, R.; Nakano, M.; Sasamori, T., Characterization of Resonance Structures in Aromatic Rings of Benzene and Its Heavier-Element Analogues, *Phys. Chem. Chem. Phys.*, **24,** 22557-22561 (2022).

Garcia, J. A.; Yasui, Y.; Yukimoto, M.; Mizuhata, Y.; Tokitoh, N., Synthesis of a Kinetically Stabilized 2,2-Dihydrosilene, *Chem. Lett.*, **51(9),** 898-901 (2022).

— Structural Organic Chemistry —

Huang, G.; Hasegawa, S.; Hashikawa, Y.; Ide, Y.; Hirose, T.; Murata, Y., An H_2O_2 Molecule Stabilized inside Open-Cage C_{60} Derivatives by a Hydroxy Stopper, *Chem. Eur. J.*, **28(2),** e202103836 (2022).

Miki, K.; Dan Zhang, Z.; Kaneko, K.; Kakiuchi, Y.; Kojima, K.; Enomoto, A.; Oe, M.; Nogita, K.; Murata, Y.; Harada, H.; Ohe, K., Amphiphilic γ-Cyclodextrin-Fullerene Complexes with Photodynamic Activity, *Mater. Adv.*, **3,** 312-317 (2022).

Zhang, S.; Hashikawa, Y.; Murata, Y., Cage-Opened C_{60} Isomers with Different Reactivities, *Asian J. Org. Chem.*, **11(3),** e202100676 (2022).

Nakakuki, Y.; Hirose, T.; Matsuda, K., Logical Design of Small HOMO–LUMO Gap: Tetrabenzo[*f,jk,mn,r*][7]helicene as a Small-Molecule Near-Infrared Emitter, *Org. Lett.*, **24(2),** 648-652 (2022).

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Liu, C.; Song, J.; Ogata, H.; Akutsu, T., MSNet-4mC: Learning Effective Multi-Scale Representations for Identifying DNA N4-methylcytosine Sites, *Bioinformatics*, **38(23),** 5160-5167 (2022).

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Zhu, J.; Azam, N. A.; Haraguchi, K.; Zhao, L.; Nagamochi, H.; Akutsu, T., An Inverse QSAR Method Based on Linear Regression and Integer Programming, *Front. Biosci.*, **27(6),** 1-14 (2022).

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Guo, S.; Liu, P.; Ching, W.-K.; Akutsu, T., On the Distribution of Successor States in Boolean Threshold Networks, *IEEE Trans. Neural. Netw. Learn. Syst.*, **33(9),** 4147-4159 (2022).

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Zhu, J.; Haraguchi, K.; Nagamochi, H.; Akutsu, T., Adjustive Linear Regression and Its Application to the Inverse QSAR, *The 15th International Joint Conference on Biomedical Engineering Systems and Technologies (BIOINFORMATICS)*, **3,** 144-151 (2022).

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— Bio-knowledge Engineering —

Liu, L.; Mamitsuka, H.; Zhu, S., HPODNets: Deep Graph Convolutional Networks for Predicting Human Protein-Phenotype Associations, *Bioinformatics*, **38(3),** 799-808 (2022).

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Nguyen, D. A.; Nguyen, C. H.; Petschner, P.; Mamitsuka, H., SPARSE: A Sparse Hypergraph Neural Network for Learning Multiple Types of Latent Combinations to Accurately Predict Drug-Drug Interactions, *Bioinformatics*, **38(1),** i333-i341 (2022).

Paltun, B. G.; Kaski, S.; Mamitsuka, H., DIVERSE: Bayesian Data IntegratiVE Learning for Precise Drug ResponSE Prediction, *IEEE/ACM Trans. Comput. Biol. Bioinform.*, **19(4),** 2197-2207 (2022).

HAKUBI PROJECT
— Optoelectronic Energy Recycling and Quantum Cooperative Effects in Semiconductor Nanostructures —

Cho, K.; Tahara, H.; Yamada, T.; Suzuura, H.; Tadano, T.; Sato, R.; Saruyama, M.; Hirori, H.; Teranishi, T.; Kanemitsu, Y., Exciton-Phonon and Trion-Phonon Couplings Revealed by Photoluminescence Spectroscopy of Single $CsPbBr_3$ Perovskite Nanocrystals, *Nano Lett.*, **22,** 7674-7681 (2022).

INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]
Monash University, Biomedicine Discovery Institute, Department of Biochemistry and Molecular Biology

Royal Melbourne Institute of Technology University Melbourne, School of Engineering

[Canada]
University of Manitoba, Department of Chemistry

[China, P.R.]
Chinese Academy of Sciences, Changchun Institute of Applied Chemistry

Chinese Academy of Sciences, Institute of Modern Physics

Fudan University, Department of Chemistry

Fudan University, Institute of Science and Technology for Brain-Inspired Intelligence

Fudan University, School of Computer Science

Fudan University, School of Pharmacy

Fudan University, Shanghai Key Lab of Intelligent Information Processing

Lanzhou University, School of Nuclear Science and Technology

The University of Hong Kong, Department of Methematics

Tsinghua University, Department of Chemistry

Tsinghua University, Key Lab of Organic Optoelectronics and Molecular Engineering of Ministry of Education

University of Chinese Academy of Science, School of Nuclear Science and Technology

Yanshan University, Key Laboratory of Applied Chemistry

[Croatia]
Ruđer Bošković Institute, Division of Organic Chemistry and Biochemistry

[Czech Republic]
The Czech Academy of Sciences, Institute of Hydrobiology

[Finland]
Aalto University, Department of Computer Science

[France]
Centre National de la Recherche Scientifique

French Alternative Energies and Atomic Energy Commission (CEA), Laboratoire de Physiologie Cellulaire & Végétale

University of Brest, Centre National de la Recherche Scientifique

University of Grenoble Alpes, IRIG, INRA, CNRS, CEA, Laboratoire Physiologie Cellulaire & Vegetale

University of Toulouse, Plant Science Research Laboratory

[Germany]
European Molecular Biology Laboratory

GSI Helmholtzzentrum für Schwerionenforschung

Humboldt-Universitat zu Berlin, Institute of Biology

Max Planck Institute for the Structure and Dynamics of Matter

[Hungary]
Semmelweis University, Department of Pharmacodynamics

[India]
Banaras Hindu University, Department of Geology

Indian Institute of Technology Bombay, Department of Chemistry

[Italy]
University of Campania “Luigi Vanvitelli”, Department of Experimental Medicine

University of Naples “Federico II”, Department of Chemical Sciences

[Korea, R.]
Ewha Womans University, College of Pharmacy

Institute for Basic Science, Center for Exotic Nuclear Studies

Soongsil University, Department of Chemistry, College of Natural Sciences

[Lithuania]
Kaunas University of Technology, Department of Organic Chemistry

Vilnius University Institute of Chemical Physics

[Norway]
University of Bergen, Department of Biology

[Russia]
Far Eastern Federal University, Institute of High Technologies and Advanced Materials

[Spain]
Centro Nacional de Biotecnología-CSIC

Universidad de Valencia, Instituto de Ciencia Molecular

[Sri Lanka]
University of Colombo, Department of Chemistry

[Taiwan]
Academia Sinica, Research Center for Environmental Changes

National Yang Ming Chiao Tung University, Center for Intelligent Drug Systems and Smart Bio-Devices

[Thailand]
Chiang Mai University, Faculty of Science

[The Netherlands]
University of Amsterdam, Swammerdam Institute for Life Science

[U.K.]
Imperial College London, Department of Mechanical Engineering

National Physical Laboratory

University of Surrey, Department of Physics

University of Edinburgh, Centre for Science at Extreme Conditions (CSEC) and School of Chemistry

[U.S.A.]
Carnegie Mellon University, Department of Chemistry

Los Alamos National Laboratory, Theoretical Division

Middle Tennessee State University, Department of Chemistry

Stanford University, Department of Chemistry

Stanford University, Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory

Stony Brook University, Department of Materials Science and Chemical Engineering

The Ohio State University, Department of Civil, Environmental and Geodetic Engineering

The Ohio State University, Department of Microbiology

University of California, Irvine, Department of Chemistry

University of California, Irvine, Department of Molecular Biology and Biochemistry

University of Hawaii, Department of Chemistry

University of Miami, Department of Chemistry

University of Michigan, Department of Chemical Engineering

University of Pennsylvania, Department of Materials Science and Engineering

*The list shows the institutions with which papers are co-authored.

SELECTED GRANTS

DIVISION OF SYNTHETIC CHEMISTRY
— Organoelement Chemistry —

Tokitoh, N.
New Main Group Element Chemistry and Materials Science Based on Heavy Aryl Anions
Grant-in-Aid for Scientific Research (S)
26 June 2019–31 March 2024

Tokitoh, N.
Synthesis of Hexasilabenzene
Grant-in-Aid for Challenging Research (Pioneering)
1 April 2020–31 March 2022

Yukimoto, M.
Creation of Tautomerizable Heavy Amides
Grant-in-Aid for Early-Career Scientists
1 April 2022–31 March 2024

— Structural Organic Chemistry —

Murata, Y.
Creation and Development of Nanoscale Laboratory
Grant-in-Aid for Scientific Research (S)
31 May 2017–31 March 2022

Hirose, T.
Creation of Asymmetric Molecular Functions Based on the Precise Molecular Arrangements of Helical pi-Conjugated Compounds
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 December 2020–31 March 2024

Hashikawa, Y.
Creation of Carbon Nanocages Targeting Single Molecule Chemistry
Grant-in-Aid for Early-Career Scientists
1 April 2020–31 March 2022

Hashikawa, Y.
Creation of Metal-Doped Spherically π-Conjugated Systems
ISHIZUE 2022 of Kyoto University
1 April 2022–31 March 2023

Hashikawa, Y.
Creation of Functional Elbow-Shaped Nanocarbon Materials
The Mazda Foundation
1 November 2022–31 March 2024

Hashikawa, Y.
Construction of Higher Order Structures Integrated by Precisely Arranged Hydroxy Groups in a 3D Manner
Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area)
1 April 2020–31 March 2022

Hashikawa, Y.
Creation of Experimental Hydration Models Based on Spherical pi-Systems
Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area)
1 April 2022–31 March 2024

Zhang, S.
Creation of Expanded and Heteroatom-Embedded New Fullerenes
Grant-in-Aid for JSPS Fellows
11 October 2019–31 March 2022

— Synthetic Organic Chemistry —

Ohmiya, H.
Development of Highly Selective Reactions Based on Organo/Metal Hybrid Catalysis
Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area)
30 June 2017–31 March 2022

Ohmiya, H.
Development of Organocatalysis Enabling Controlled Reactions by Electrons
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2019–31 March 2023

Ohmiya, H.
Organocatalytic Chemistry Pioneered by Radicals
Grant-in-Aid for Scientific Research (A)
5 April 2021–31 March 2025

Ueda, Y.
Catalytic Asymmetric Synthesis of Inherently Chiral Calixarenes and Its Application to Unique Molecular Recognition
Grant-in-Aid for Scientific Research (C)
1 April 2020–31 March 2023

Ueda, Y.
Selective Chemical Trasformation of Specific Sugars for Diversification of Glycan Mediating Membrane Dynamics
Grant-in-Aid for Transformative Research Areas (B)
23 August 2021–31 March 2024

Abbreviations and Acronyms

AMED : Japan Agency for Medical Reserach and Development
JSPS : Japan Society for the Promotion of Science
JST : Japan Science and Technology Agency
MEXT : Ministry of Education, Culture, Sports, Science and Technology
NEDO : New Energy and Industrial Technology Development Organization

Nagao, K.
Bond Formation through Non-Acidic Catalytic Generation of Carbocation
Grant-in-Aid for Early-Career Scientists
1 April 2021–31 March 2024

Nagao, K.
Catalytic Generation of Sulfur Cation Radical Species by Dynamic Exciton and Its Application to Bond Formation Reactions
Grant-in-Aid for Transformative Research Areas (A)
10 September 2021–31 March 2023

— Advanced Inorganic Synthesis —

Teranishi, T.
Nanoscale Element Replacement Science: Structural Transformation of Nanocrystalline Phases and Development of Novel Functions
Grant-in-Aid for Scientific Research (S)
26 June 2019–31 March 2024

Teranishi, T.
Synthesis of Unprecedented Ordered Alloy Nanoparticles and Development of Their Structure-Specific Properties
Grant-in-Aid for Challenging Research (Exploratory)
28 June 2019–31 March 2022

Teranishi, T.
Creation of Unprecedented Nanomaterials by Precious Arrangement of Atomic Layers and Crystal Phases
CREST (Core Research for Evolutional Science and Technology), JST
1 October 2021–31 March 2027

Sakamoto, M.
Infrared Light Responsive Photocataýst for Infrared Light to Energy Conversion
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2022

Saruyama, M.
Synthesis and Function of Diverse Three-Dimensional Inorganic Nanoparticle Superstructures
Grant-in-Aid for Challenging Research (Exploratory)
30 July 2020–31 March 2023

Sakamoto, M.
Development of Flexible and Transparent Conductive Sheet
A-STEP (Adaptable and Seamless Technology Transfer Program through Target-Driven R&D), JST
1 December 2020–31 March 2023

Sakamoto, M.
Development of Transparent Solar Cells Converting Infrared Light
FOREST (Fusion Oriented Research for Disruptive Science and Technology), JST
1 January 2021–31 March 2023

Sakamoto, M.
Infrared Light Responsive Photocatalyst for Infrared Light to Energy Conversion
Grant-in-Aid for Scientific Research (A)
5 April 2021–31 March 2026

Takahata, R.
Modeling of Defects and Exploration of Novel Materials by Using Cadmium Chalcogenide Clusters with Definite Structures
Grant-in-Aid for Early-Career Scientists
1 April 2021–31 March 2024

Saruyama, M.
Creation of Structure-Specific Reaction Sites through Self-Assembly of Nanocrystals
FOREST (Fusion Oriented Research for Disruptive Science and Technology), JST
1 April 2022–31 March 2025

Sato, R.
Scientific Principles of Visible Plasmonic Nanoalloys
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2022

Matsumoto, K.
Inter-Element Miscibility Driven Rearrangement from Disordered to Long-Range Ordered Alloy Structures
Grant-in-Aid for Early-Career Scientists
1 April 2022–31 March 2025

Trinh, T.
Evolution of New Magnetic Materials with Ultrahigh Coercivity
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2022

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

Tsujii, Y.
Development of High-Performance Sliding Parts with Concentrated Polymer Brushes (CPB) and Their Application to Devices
A-STEP (Adaptable and Seamless Technology Transfer Program through Target-Driven R&D), JST
1 December 2020–31 March 2025

Tsujii, Y.
Hierarchical Understanding and Controlling the Wear Phenomena of Ultralow-Friction Polymer Brushes
CREST (Core Research for Evolutional Science and Technology), JST
1 October 2021–31 March 2027

Tsujii, Y.
Development of Next-Generation Ship-Bottom Coating and Coating Process toward Energy Saving and Low Environmental Load
Environment Research and Technology Development Fund, ERCA (Environmental Restoration and Conservation Agency)
1 April 2022–31 March 2025

— Polymer Controlled Synthesis —

Yamago, S.
Development of New Fabrication Methods of Polymer Materials Based on the Structurally Controlled Hyperbranched Polymers
Grant-in-Aid for Scientific Research (S)
5 July 2021–31 March 2026

Yamago, S.
International Research Center for Basic Organic Device Chemistry by True Integration of Synthesis and Device
Core-to-Core Program, JSPS
1 April 2022–31 March 2026

— Inorganic Photonics Materials —

Mizuochi, N.
Research of Quantum Sensing by Advanced Control of the Quantum State of NV Center in Diamond
Grant-in-Aid for Scientific Research (A)
5 April 2021–31 March 2024

Morishita, H.
Development of NV Quantum Spintronics Fundamental Technologies for Connecting Classical and Quantum Information
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2021–31 March 2025

Morioka, N.
Study of Spin-Optical-Charge Dynamics of Defects in Silicon Carbide for Highly Efficient Electrical Spin Readout
Grant-in-Aid for Scientific Research (B)
1 April 2022–31 March 2025

Herbschleb, E. D.
Enhanced Quantum Sensing with a Nitrogen-Vacancy Centre as Gateway to the Electron Spin of Phosphorus
Grant-in-Aid for Early-Career Scientists
1 April 2022–31 March 2023

Hayashi, K.
2D Placement of Nano-Quantum Sensors on Diamond Surfaces
Grant-in-Aid for Early-Career Scientists
1 April 2021–31 March 2024

— Nanospintronics —

Ono, T.
Ferrimagnetic Spintronics and Device Application
Grant-in-Aid for Scientific Research (S)
31 August 2020–31 March 2025

Ono, T.
Developlement of 3D Magnetic Memory
CREST (Core Research for Evolutional Science and Technology), JST
1 October 2021–31 March 2027

Moriyama, T.
Spin Super Fluidity Using Antiferromagnet
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 December 2020–31 March 2024

Moriyama, T.
Antiferromagnetic THz Spintronics
Grant-in-Aid for Scientific Research (A)
5 April 2021–31 March 2024

Shiota, Y.
Polarization Control of Spin Wave Spin Current and Its Device Application
Grant-in-Aid for Scientific Research (B)
1 April 2022–31 March 2025

Hisatomi, R.
Observation of Spin Rotation Coupling toward Non-Inertial Spintronics
Grant-in-Aid for Early-Career Scientists
1 April 2020–31 March 2022

Hisatomi, R.
Optospinmechanics Using Surface Acoustic Waves
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 November 2020–31 March 2024

Narita, H.
Control of Superconductivity by Noncollinear Magnetism
Grant-in-Aid for Early-Career Scientists
1 April 2021–31 March 2024

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

Futaki, S.
Intracellular Fate of Extracellular Fine Particles and the Control System
CREST (Core Research for Evolutional Science and Technology), JST
1 October 2018–31 March 2024

Imanishi, M.
Biological Function of Non-Canonical Nucleic Acids
Grant-in-Aid for Transformative Research Areas (B)
23 August 2021–31 March 2024

Kawaguchi, Y.
Intracellular Delivery and Phase Separation Control of Antibodies Based on Coacervate
Strategic Basic Research Programs ACT-X, JST
1 April 2022–31 March 2025

Hirose, H.
Search for Peptides that Promote Internalization and Endoplasmic Release of Extracellular Vesicles
Grant-in-Aid for Scientific Research (C)
1 April 2022–31 March 2025

— Chemistry of Molecular Biocatalysts —

Yamaguchi, S.
Molecular Mechanisms for the Timing of the Production of Stem Cells in Plants
Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area)
30 June 2017–31 March 2022

Mashiguchi, K.
Analysis of the Novel Enzymes Responsible for the Non-Canonical Strigolactone Biosynthesis
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2024

— Molecular Biology —

Aoyama, T.
Roles of Phosphoinositid Signaling in Plant Cell Morphogenesis
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

Tsuge, T.
Molecular Mechanism Governing Plant Plasticity through Pre-mRNA 3’UTR Regulation
Grant-in-Aid for Scientific Research (C)
1 April 2022–31 March 2025

Kato, M.
Phosphoinositides Involved in Pollen Germination
Grant-in-Aid for Scientific Research (C)
1 April 2021–31 March 2025

— Chemical Biology —

Uesugi, M.
Designer Melanin for Analyzing and Controlling Cells
Grant-in-Aid for Challenging Research (Exploratory)
9 July 2021–31 March 2023

Uesugi, M.
Asian Chemical Biology Intiative
Core-to-Core Program, JSPS
1 April 2022–31 March 2025

Uesugi, M.
Chemical Biology of Cellular Self-Assemblies
Grant-in-Aid for Scientific Research (A)
1 April 2022–31 March 2025

Uesugi, M.
Development of Artificial Chaperones
Grant-in-Aid for Transformative Research Areas (A)
16 June 2022–31 March 2024

Uesugi, M.
Grand Design Platform and Database for the Development of Innovative Adjuvant and Vaccine Carrier
P-PROMOTE (Project for Promotion of Cancer Research and Therapeutic Evolution), AMED
20 May 2022–31 March 2024

Uesugi, M.
PD-1 Blockade Caner Immunotherapy Combined with Small Molecule Activators of T Cell Fatty Acid Oxidation
Program on R&D of New Generation Vaccine Including New Modality Application, AMED
1 July 2022–31 March 2027

Sato, S.
Understanding Cellular Function with Short RNAs and Small Molecules
Grant-in-Aid for Scientific Research (B)
1 April 2020–31 March 2023

Sato, S.
A New Oligonucleotide Therapeutics that Induces a Cooperative RNA G-Quadruplex Formation for Gene Silencing
Grant-in-Aid for Challenging Research (Pioneering)
9 July 2021–31 March 2025

Takemoto, Y.
Exploration of Radical-Sensitive Signal Peptide
Grant-in-Aid for Scientific Research (C)
1 April 2022–31 March 2025

Takemoto, Y.
Understanding and Application of Radical-Sensitive Peptide
Takeda Science Foundation
1 September 2021–31 May 2024

Abo, M.
Development of Self-Assembling Chemicals which Have Chaperone Activity in Live Cells
Grant-in-Aid for Scientific Research (C)
1 April 2021–31 March 2024

Takemoto, M.
Mechanistic Analysis for the Immune Activation of T Cells by Covalent Natural Compounds
Grant-in-Aid for Scientific Research (C)
1 April 2022–31 March 2025

DIVISION OF ENVIROMENTAL CHEMISTRY

— Molecular Materials Chemistry —

Kaji, H.
Material Design Based on Dynamic Excition and Their Applications
Grant-in-Aid for Transformative Research Areas (A)
19 November 2020–31 March 2025

Suzuki, K.
Spatiotemporal Analysis of Dynamic Exciton by Solid-State NMR
Grant-in-Aid for Transformative Research Areas (A)
19 November 2020–31 March 2025

Shizu, K.
A Unified Theory of Electronic Transition Rate Constants for High Throughput Materials Screening
Grant-in-Aid for Scientific Research (C)
1 April 2022–31 March 2025

— Hydrospheric Environment Analytical Chemistry —

Sohrin, Y.
Ocean Section Diagnosis on the Basis of Stoichiometry and Stable Isotope Ratios of Trace Metals
Grant-in-Aid for Scientific Research (A)
1 April 2019–31 March 2023

Takano, S.
Isotopic Analysis for Estimating the Sources of Particulate Trace Metals in the Ocean
Grant-in-Aid for Early-Career Scientists
1 April 2020–31 March 2023

Takano, S.
Analysis of Silver Isotope Ratios in River Water
Mitsumasa Itou Memorial Research Grant, Research Institute for Oceanochemistry Foundation
1 April 2022–31 March 2023

Zheng, L.
Speciation and Sectional Distribution of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in the South Pacific and Indian Oceans
Grant-in-Aid for Early-Career Scientists
1 April 2021–31 March 2024

Zheng, L.
The Effect of UV Irradiation on the Determination of Trace Metals in the Seawater
Mitsumasa Itou Memorial Research Grant, Research Institute for Oceanochemistry Foundation
1 April 2022–31 March 2023

— Chemistry for Functionalized Surfaces —

Hasegawa, T.
Innovation in Control of Physical Properties of Polymer Thin-Film Materials by Micro-Morphology Analysis of Amorphous
Grant-in-Aid for Challenging Research (Exploratory)
9 July 2021–31 March 2024

Hasegawa, T.
Evolution of Near-Infrared Spectroscopy for Materials Structure Analysis: Development of NIR-MAIRS
Grant-in-Aid for Scientific Research (B)
1 April 2022–31 March 2026

Shioya, N.
Visualization of Monolayer Structures Specifically Formed by Functional Organic Materials at the Substrate Interface
Grant-in-Aid for Early-Career Scientists
1 April 2022–31 March 2025

— Molecular Microbial Science —

Kurihara, T.
Dissection of the Molecular Basis of Membrane Vesicle Biogenesis and Construction of an Extracellular Platform for Substance Production by Using a Hyper-Vesiculating Bacterium
Grant-in-Aid for Challenging Research (Pioneering)
30 July 2020–31 March 2023

Kurihara, T.
Molecular Basis for Generation of the Diversity of Bacterial Membrane Phospholipid Acyl Chains and Mechanisms Underlying their Physiological Functions
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

Kawamoto, J.
A Novel Platform for Functional Nanoparticle –The Synthesis Mechanism of Unique Outer-Membrane Vesicles of Bacteria and Its Application–
Grant-in-Aid for Scientific Research (C)
1 April 2020–31 March 2023

Kawamoto, J.
Development of Low-Temperature Biotechnology based on Bacterial Outer Membrane Vesicles
Asahi Glass Foundation
1 April 2022–31 March 2023

Kawamoto, J.
Elucidation of Outer-Membrane Vesicle Production of a Cold-Adapted Bacterium and its Application
Aid for Research of Sugiyama Chemical & Industrial Laboratory
1 April 2022–31 March 2023

Ogawa, T.
Exploration and Functional Elucidation of a Novel Protein Involved in the Metabolism of ω-3 Polyunsaturated Fatty Acids in Bacteria
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2022

Ogawa, T.
Study on the Metabolic Conversion of Omega-3 Polyunsaturated Fatty Acids through a Reconsideration of Beta-Oxidation Pathway
Grant-in-Aid for Scientific Research (C)
1 April 2021–31 March 2024

DIVISION OF MULTIDISCIPLINARY CHEMISTRY
— Molecular Rheology —

Matsumiya, Y.
Molecular Dynamics of Associative Polymers and Its Experimental Validation: Effect of Dissociation Equilibrium on Entanglement Relaxation Modes
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

Sato, T.
Development of Coarse-Grained Molecular Model for Predicting Dynamics of Entangled Associating Polymers
Grant-in-Aid for Early-Career Scientists
1 April 2021–31 March 2024

Sato, T.
A New Fluid Science for Non-Newtonian/Non-Uniform/Non-Equilibrium Flows
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 April 2022–31 March 2026

— Molecular Aggregation Analysis —

Wakamiya, A.
Fundamental Chemical Research for Efficirnt Lead Free Perovskite Solar Cells
Grant-in-Aid for Scientific Research (A)
5 April 2021–31 March 2024

Wakamiya, A.
Pb-Free Perovskite Solar Cells Consisting of Sn
Mirai Program, JST
1 April 2022–31 March 2027

Murdey, R.
Aging and Passivation Effects in Perovskite Solar Cells
Grant-in-Aid for Scientific Research (C)
1 April 2019–31 March 2022

Nakamura, T.
Two-Dimensionally Expanded pi-Systems for High-Performance Tin Perovskite Solar Cells
Grant-in-Aid for Early-Career Scientists
1 April 2021–31 March 2023

Truong, M. A.
Development of Charge-Transporting Materials for Efficient Tin-Based Perovskite Solar Cells
Grant-in-Aid for Research Activity Start-up
11 September 2020–31 March 2022

Truong, M. A.
Development of Multipodal Hole-Transporting Monolayer Materials for High Performance Perovskite Solar Cells
Grant-in-Aid for Early-Career Scientists
1 April 2022–31 March 2024

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE
— Particle Beam Science —

Wakasugi. M
Development of Fixed Unstable Nuclear Target for Unclear Reaction Study of Rare RI
Grant-in-Aid for Challenging Research (Pioneering)
30 July 2020–31 March 2023

Tsukada, K.
Isotope Dependences of Nuclear Charge Distributions and Neutron Radius by Electron Scattering
Grant-in-Aid for Scientific Research (A)
1 April 2020–31 March 2025

Ogawara, R.
Development of Prototype Device for Ion Extraction System with Resonant Oscillation
Grant-in-Aid for Early-Career Scientists
1 April 2020–31 March 2022

Ogawara, R.
Development of Internal Active Target for Beam Recycling Technology
Grant-in-Aid for Early-Career Scientists
1 April 2022–31 March 2024

— Laser Matter Interaction Science —

Tokita, S.
Formation of Ultrashort Femtosecond Pulses in the Mid-Infrared Range Based on Iron-Doped Chalcogenides for Problems of Nonlinear Optics of Media with a Reduced Dimension
Bilateral Joint Research Projects, JSPS
1 April 2021–31 March 2023

Tokita, S.
Development of Mid-Infrared High-Power Ultrashort Pulse Lasers and Its Application to Soft-Matter Micro-Processing
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

Tokita, S.
Development of an Industrial Femtosecond Laser
A Project of NEDO
15 January 2021–31 March 2023

Tokita, S.
The Power Laser DX Platform
Project for Promoting Public Utilization of Advanced Research Infrastructure, MEXT
1 April 2021–31 March 2026

Hashida, M.
Operando Measurements Using Advanced Beams to Study the Mechanism of Fine Structure Formation
Q-LEAP (Quantum Leap Flagship Program), MEXT
1 April 2018–31 March 2028

— Electron Microscopy and Crystal Chemistry —

Kurata, H.
Analysis of Electronic Structure by Aloof Beam EELS
Grant-in-Aid for Challenging Research (Exploratory)
28 June 2019–31 March 2022

Haruta, M.
Visualization of Electronic Orbitals by Transmission Electron Microscopy
Grant-in-Aid for Scientific Research (B)
1 April 2022–31 March 2025

Haruta, M.
High Spatical and High Energy Resolution Electronic State Mapping
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Synthetic Organotransformation —

Nakamura, M.
Application and Evaluation of Quantum Effect Control in Iron-Catalyzed Cross Coupling
Grant-in-Aid for Scientific Research (B)
1 April 2020–31 March 2023

— Advanced Solid State Chemistry —

Shimakawa, Y.
Exploring for Novel Multicaloric Materials
Grant-in-Aid for Challenging Research (Pioneering)
30 July 2020–31 March 2024

Shimakawa, Y.
Exploring for Novel Functional Oxide Materials by Advanced High-Pressure Synthesis and Evaluation of the Structure-Property Relationships
Fund for the Promotion of Joint International Research (Fostering Joint International Research (B))
7 October 2022–31 March 2028

Shimakawa, Y.
High-Pressure Synthesis of Novel Transition-Metal Oxides and Exploring Their Functional Properties
Grant-in-Aid for Scientific Research (A)
1 April 2020–31 March 2024

— Organometallic Chemistry —

Ohki, Y.
Electron Transfer Networks of Transition Metal Cluster Complexes for Catalytic Applications
CREST (Core Research for Evolutionary Science and Technology), JST
1 October 2021–31 March 2027

Ohki, Y.
Synthesis and Reactions of Mo-Fe-S Clusters Toward Understanding of the Mechanism of Nitrogenase
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

Ohki, Y.
Synthesis of Metal-Nanoclusters of Iron Group Metals
Grant-in-Aid for Challenging Research (Exploratory)
30 July 2020–31 March 2023

Ohki, Y.
Synthesis and Reactions of Bio-Inspired Molecular Metal-Hydride Compounds
Grant-in-Aid for Scientific Research on Innovative Areas (Research in a Proposed Research Area)
1 April 2021–31 March 2023

Tanifuji, T.
Structure-Function Relationships of a Fe/Mo-S-C Cluster Unique to N_2-Reducing Enzymes
Grant-in-Aid for Research Activity Start-up
30 August 2021–31 March 2023

Tanifuji, T.
CO_2/CO Reduction into Short-Chain Hydrocarbons Promoted by Cuboidal Metal-Sulfur Clusters
Grant-in-Aid for Scientific Research (C)
1 April 2022–31 March 2025

Higaki, T.
Atomically Precise Synthesis of Iron-Group Metal Nanoclusters to Probe the Origin of Superparamagnetism
Grant-in-Aid for Research Activity Start-up
31 August 2022–31 March 2024

— Nanophotonics —

Kanemitsu, Y.
Design of Next-Generation Flexible Photonic Devices Based on Metal Halide Perovskites
CREST (Core Research for Evolutionary Science and Technology), JST
1 September 2016–31 March 2022

Kanemitsu, Y.
Fusing Nanomaterials and Strong Electric Field Nonlinear Optics for New Advances in Photonics
Grant-in-Aid for Specially Promoted Research
23 April 2019–31 March 2024

Hirori, H.
Phononic Strong Coupling by THz Metamaterial and Its Applications to Material Control
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2025

BIOINFORMATICS CENTER

— Chemical Life Science —

Ogata, H.
Ecology of Giant Viruses Inhabiting the Aphotic Zone of the Sea
Grant-in-Aid for Scientific Research (A)
1 April 2022–31 March 2026

Ogata, H.
The Biosphere of Aggregated Particles Elucidating the Regulatory Mechanisms of Marine Carbon Cycles
Grant-in-Aid for Scientific Research (S)
1 April 2019–31 March 2023

Ogata, H.
Virus-Host Database
Grant-in-Aid for Publication of Scientific Research Results
1 April 2020–31 March 2025

Ogata, H.
Elucidation of the Virus-Driven Clockwork of the Marine Lower Trophic Level Ecosystem and Its Influence on Our Ocean
Grant-in-Aid for Scientific Research (S)
1 April 2021–31 March 2026

Ogata, H.
Study on the Molecular and Ecological Mechanisms of the Demise of Red Tides through Viral Infection
Grant-in-Aid for Scientific Research (A)
1 April 2022–31 March 2027

Endo, H.
Viral Infection and Its Control Mechanisms of Marine Plankton Communities as Revealed by Dissolved Ribosomal RNA
Grant-in-Aid for Scientific Research (B)
1 April 2022–31 March 2026

Endo, H.
Integrative Understanding of Marine Nitrogen Fixation Based on Global Observations from Tropics to Polar Regions
Grant-in-Aid for Scientific Research (B)
1 April 2022–31 March 2025

Okazaki, Y.
Who is the Host of Uncultivated Viruses? Linking Viral and Bacterial Genomes in the Environment
Grant-in-Aid for Early-Career Scientists
1 April 2022–31 March 2025

Okazaki, Y.
Challenging Dry Questions in Environmental Microbiology and Virology from Wet
Kyoto University 125th Anniversary Fund Kusunoki 125
1 April 2022–31 March 2025

Okazaki, Y.
Unveiling the Organic Matter Dynamics Functioning in Lake Hypolimnion
Grant-in-Aid for Scientific Research (A)
1 April 2022–31 March 2026

Okazaki, Y.
Microbial Nitrogen Pump: Bacterial Semi-Labile Dissolved Organic Nitrogen as a Nutrient Transport Pathway in Aquatic Systems
Grant-in-Aid for Scientific Research (B)
1 April 2021–31 March 2024

Okazaki, Y.
Elucidating the Molecular Heterogeneity of Dissolved Organic Matter that Governs Its Long-Term Persistence
Grant-in-Aid for Scientific Research (B)
1 April 2022–31 March 2025

Hikida, H.
Development of Novel Gene Engineering Technology Utilizing Giant Viruses
Strategic Basic Research Programs ACT-X, JST
1 October 2022–31 March 2025

Hikida, H.
Diversity of Giant Virus Infection Strategy
Grant-in-Aid for Early-Career Scientists
1 April 2022–31 March 2025

— Mathematical Bioinformatics —

Akutsu, T.
Analysis and Applications of Discrete Preimage Problems
Grant-in-Aid for Scientific Research (A)
1 April 2018–31 March 2022

Akutsu, T.
Advanced Studies and Developments on Discrete Preimage Problems
Grant-in-Aid for Scientific Research (A)
1 April 2022–31 March 2027

Akutsu, T.
Analysis and Control of Steady States of Multiple Biological Networks
Grant-in-Aid for Challenging Research (Exploratory)
30 June 2022–31 March 2025

Tamura, T.
Algorithms for Metabolic Network Design for Producing Useful Substances
Grant-in-Aid for Scientific Research (B)
1 April 2020–31 March 2025

— Bio-knowledge Engineering —

Mamitsuka, H.
Efficient Estimation of Data Structure from Multiple Tensors
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

Mamitsuka, H.
Integrative Diverse-Data Structure Estimation
Grant-in-Aid for Scientific Research (B)
1 April 2022–31 March 2025

Nguyen, H.
Machine Learning for Structure-Rich Data-Scarce Domains
Grant-in-Aid for Scientific Research (C)
1 April 2022–31 March 2025

Nguyen, H.
Machine Learning on Large Graphs
Grant-in-Aid for Scientific Research (C)
1 April 2018–31 March 2022

Petschner, P.
Developing Machine Learning Based Bioinformatics to Decipher Hidden Biology of Depression Symptoms
Grant-in-Aid for JSPS Fellows
13 November 2020–31 March 2023

THESES

GARCIA, Julius, Adrie Aguirre
D Sc, Kyoto University
“Synthetic Studies towards Unexplored Multiple Bonds to Silicon Utilizing Kinetic Stabilization”
Supervisor: Assoc Prof MIZUHATA,Yoshiyuki
26 September 2022

HUANG, Yu Min
D Sc, Kyoto University
“Three-Dimensional Domain Wall Motion Memory with Artificial Ferromagnet”
Supervisor: Prof ONO, Teruo
18 January 2022

IKEBUCHI, Tetsuya
D Sc, Kyoto University
“Study of Spin Conversion Efficieny and Spin Current Propagation in Crystalline Materials”
Supervisor: Prof ONO, Teruo
18 January 2022

JUNG, Yejin
D Med Sc, Kyoto University
“Discovery of Non-Cysteine-Targeting Covalent Inhibitors by Activity-Based Proteomic Screening with a Cysteine-Reactive Probe”
Supervisor: Prof UESUGI, Motonari
23 May 2022

JUN-I, Yuta
D Sc, Kyoto University
“Studies on the Effects of the Introduction of Heavy Group 14 and 15 Elements on Conjugated Systems”
Supervisor: Prof TOKITOH, Norihiro
23 March 2022

KISHIMOTO, Mizuki
D Eng, Kyoto University
“Effect of Stress Field on Self-Assembly in Crystalline Polyolefins”
Supervisor: Prof TAKENAKA, Mikihito
23 March 2022

KUZE, Keita
M Sc, Kyoto University
“Developments of Internal Active Target for Beam Recycle in Heavi-Ion Storage Ring”
Supervisor: Prof WAKASUGI, Masanori
23 March 2022

LI, Han
Ph D, Kyoto University
“Development of Plasmonic Copper chalcogenides for Efficient Solar Energy Conversion”
Supervisor: Prof TERANISHI, Toshiharu
26 September 2022

MENDOZA, Aileen de Leon
D Med, Kyoto University
“Controlled Lipid β-Oxidation and Carnitine Biosynthesis by a Vitamin D Metabolite”
Supervisor: Prof UESUGI, Motonari
24 November 2022

NODA, Naotaka
D Med, Kyoto University
“Glucose as a Protein-Condensing Cellular Solute”
Supervisor: Prof UESUGI, Motonari
23 May 2022

OSHIRO, Taku
D Sc, Kyoto University
“Synthetic Studies on Heteraazulenes Containing a Heavy Group 14 Element as a Skeletal Element”
Supervisor: Prof TOKITOH, Norihiro
23 March 2022

PRODINGER, Florian
D Sc, Kyoto University
“Novel Metabarcoding Method Reveals Pronounced Seasonality and High Turnover Rate of Imitervirales in Coastal Communities”
Supervisor: Prof OGATA, Hiroyuki
23 May 2022

SAKAI, Takayuki
D Pharm Sc, Kyoto University
“Evelopment of Methods for Cell Surface Integration of Membrane-Associated Peptides”
Supervisor: Prof FUTAKI,Shiroh
24 March 2022

SHIMAMURA, Ryota
D Sc, Kyoto University
“Cell Biology of ζ Class Phospholipase D in Arabidopsis”
Supervisor: Prof AOYAMA, Takashi
24 January 2022

TOMITA, Kazutaka
D Sc, Kyoto University
“Control of Supramolecular Structures of Porphyrin Derivatives in Thin Films”
Supervisor: Prof HASEGAWA, Takeshi
24 March 2022

WANG, Feiqi
D Inf, Kyoto University
“Design of Computational Models for Analyzing Graph-Structured Biological Data”
Supervisor: Prof AKUTSU, Tatsuya
24 March 2022

WATARI, Machiko
D Sc, Kyoto University
“Functional Differentiation among the Arabidopsis Phosphatidylinositol 4-Phosphate 5-Kinase Genes *PIP5K1*, *PIP5K2* and *PIP5K3*”
Supervisor: Prof AOYAMA, Takashi
25 July 2022

YAMAGUCHI, Atsushi
D Sc, Kyoto University
“Research on Local Direction Dependence and Core-Hole Effect of Near-Edge Fine Structures”
Supervisor: Prof KURATA, Hiroki
26 September 2022

ZHANG, Xiaojuan
D Sc, Kyoto University
“Functional Analyses of Arabidopsis Cleavage Factor I”
Supervisor: Prof AOYAMA, Takashi
23 May 2022

THE 122ND ICR ANNUAL SYMPOSIUM

SEMINARS MEETINGS AND SYMPOSIA

THE 122ND ICR ANNUAL SYMPOSIUM

(9 December 2022)

ORAL PRESENTATION

TANIFUJI, Kazuki (Organometallic Chemistry)
"Investigations into Biosynthesis of Nitrogenase Cofactor via Semi-Synthetic Approach"

ISOZAKI, Katsuhiro (Synthetic Organotransformation)
"Catalytic Transformations Enabled by Gold Nanoclusters Bearing Supramolecular Reaction Field"

SHIOYA, Nobutaka (Chemistry for Functionalized Surfaces)
"Polymorphism in Organic Semiconductor Thin Films: From Monolayer to Bulk"

IMANISHI, Miki (Biofunctional Design-Chemistry)
"Detection and Manipulation of RNA Modifications"

NAGAO, Kazunori (Synthetic Organic Chemistry)
"A Photoredox/Cobalt/Brønsted Acid Cooperative Catalysis Enabling Hydrofunctionalization of Aliphatic Alkenes"

— ICR Award for Young Scientists —

NARITA, Hideki (Nanospintronics)
"Field-Free Superconducting Diode Effect in Noncentrosymmetric Superconductor/Ferromagnet Multilayers"

YUMOTO, Go (Nanophotonics)
"Rapidly Expanding Spin-Polarized Exciton Halo in a Two-Dimensional Halide Perovskite at Room Temperature"

— ICR Award for Graduate Students —

NAKAGAWA, Kotaro (Nanophotonics)
"Size-Controlled Quantum Dots Reveal the Impact of Intraband Transitions on High-Order Harmonic Generation in Solids"

NGUYEN, Duc Anh (Bio-knowledge Engineering)
"SPARSE: A Sparse Hypergraph Neural Network for Learning Multiple Types of Latent Combinations to Accurately Predict Drug-Drug Interactions"

IWASHIMIZU, Chisaki (Electron Microscopy and Crystal Chemistry)
"Electron Orbital Mapping of $SrTiO_3$ Using Electron Energy-Loss Spectroscopy"

— ICR Grants for Promoting Integrated Research —

TAHARA, Hirokazu (Nanophotonics)
"Study of Cooperative Quantum Optical Properties in Nanocrystal Superlattices"

SEKIGUCHI, Fumiya (Nanophotonics)
"Exploration of Terahertz Nonreciprocal Nonlinear Phenomena in Superconductor Hosting an Artificial Superlattice"

YUMOTO, Go (Nanophotonics)
"Development of Polarization-Resolved Pump-Probe Microscopy and Study of Spatiotemporal Dynamics of Spins in Two-Dimensional Halide Perovskites"

POSTER PRESENTATIONS

LW : Laboratory Whole Presentation
LT : Laboratory Topic
GE : General Presentation

— Organoelement Chemistry —

GE NISHINO, Ryohei; MIZUHATA, Yoshiyuki; TOKITOH Norihiro
"Novel Germanium Transfer Reaction *via* the Germanium Exchange on the Germabenzenyl Ring"

— Structural Organic Chemistry —

LW "Recent Activities in Structural Organic Chemistry Laboratory"

GE ZHANG, Zheng; MURATA, Yasujiro; HIROSE, Takashi
"Synthesis and Circularly Polarized Light Emission Properties of Helicene Derivatives with 1,2,5-thiadiazole Moieties at Both Ends"

— Synthetic Organic Chemistry —

LW "Radicals Open up New Catalysts, Reactions, and Functions"

GE OTA, Kenji; NAGAO, Kazunori; HATA, Dai; MIYAMOTO, Naoya; TOKUNOH, Ryosuke; SASAKI, Yusuke; OHMIYA, Hirohisa
"Synthesis of Alkylphosphonate Oligonucleotides through Light-Driven Radical-Polar Crossover"

— Advanced Inorganic Synthesis —

LW "Introduction of Recent Researches in Advanced Inorganic Synthesis Group"

GE TAKAHATA, Ryo
"Structural Isomerization and Evolution of Au Clusters Induced by Ligand Exchange Reactions"

— Chemistry of Polymer Materials —

LW "Recent Research in Chemistry of Polymer Materials Laboratory"

GE FUJJIMOTO, Seitaro
"Synthesis of Novel Cellulose-Nanocrystal Derivatives Asymmetrically Substituted with Two Types of Graft Polymer"

— Polymer Controlled Synthesis —

LW "Research Activities in Laboratory of Polymer Controlled Synthesis"

GE WU, Jiade; TOSAKA, Masatoshi; YAMAGO, Shigeru
"Controlled Ring-Opening Copolymerization of a Novel Cyclic Carbonate Monomer with an Ortho-Nitrobenzyl Group and Photo-Degradation of the Resulting Copolymers"

— Inorganic Photonics Materials —

LW "Research Introduction of Inorganic Photonics Materials"

— Nanospintronics —

GE KOBAYASHI, Yuta
"Pulse-Width Dependence of Spin-Orbit Torque Switching in Mn_3Sn/Pt Thin Films"

— Biofunctional Design-Chemistry —

LW "Recent Research in the Laboratory of Biofunctional Design-Chemistry"

GE TANAKA, Kamui; IMANISHI Miki; FUTAKI Shiroh
"Screening of FTO Inhibitors and an Effect of L-Ascorbic Acid on FTO Activity"

— Chemistry of Molecular Biocatalysts —

LW "Introduction of Chemistry of Molecular Biocatalysts Lab"

— Molecular Biology —

LW "Research of Molecular Biology Laboratory"

— Chemical Biology —

LW "Create New World of Bioactive Synthetic Molecules"

— Molecular Materials Chemistry —

LW "Molecular Materials Chemistry"

GE KANDA, Syun; KAJI, Hironori
"Thickness-Dependent Charge Mobility Distribution in Organic Amorphous Film"

— Hydrospheric Environment Analytical Chemistry —

LW "Reveal the Ocean by Using Trace Elements and Their Isotopes"

GE IWASE, Misato; ISOBE, Kota; ZHENG, Linjie; TAKANO, Shotaro; SOHRIN, Yoshiki
"Solid-Phase Extraction of Palladium, Platinum, and Gold Using Chelating Adsorbents with Ethylenediamine Groups"

— Chemistry for Functionalized Surfaces —

GE OKA, Takayuki; SHIOYA, Nobutaka; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
"Influence of Alkyl Chain Length on the Polymorphism in Organic Semiconductor Thin Films"

GE SAKO, Nobuaki; SHIMOAKA, Takafumi; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
"Relationship between Molecular Aggregation Structure and Surface Property of Perfluoropolyether-Based Self-Assembled Monolayer"

— Molecular Microbial Science —

LW "Molecular Microbial Science Laboratory"

GE TSUDZUKI, Taiku; IMAI, Tomoya; KAWAMOTO, Jun; OGAWA, Takuya; KURIHARA, Tatsuo
"Function of Sugar-Phosphate Transferase Homologs in the Cargo Protein Transport to Bacterial Extracellular Membrane Vesicles"

— Polymer Materials Science —

GE HARA, Yuta; TAKENAKA, Mikihito; OGAWA, Hiroki; MASHITA, Ryo
"Correlation between Filler Orientation and Void Distribution under Stretching of Filler-Filled Rubber by SAXS-CT"

GE ARAKAWA, Masato; TAKENAKA, Mikihito
"Study on the Change of Density Distribution of LLDPE during Drawing Process"

—Molecular Rheology —

LW "Research Activities in Molecular Rheology Laboratory"

— Molecular Aggregation Analysis —

LW "Research in Molecular Aggregation Analysis"

GE KANEKO, Ryuji; MORISHITA, Taro; MATSUSHIGE, Yuko; TROUNG, Minh Anh; MURDEY, Richard; NAKAMURA, Tomoya; WAKAMIYA, Atsushi
"Controlling Crystal Growth of Perovskite Semiconductors Using Formamidinium Salts for Large-Scalable Process of Perovskite Solar Cells"

— Particle Beam Science —

LW "Particle Beam Science Lab."

LT "Renewal of KAKEN Electron Linac (KEL)"

— Laser Matter Interaction Science —

LW "Introduction of the Laser Matter Interaction Science Laboratory"

— Electron Microscopy and Crystal Chemistry —

LW "Research Activities in Division of Electron Microscopy and Crystal Chemistry"

GE KAZAMA, Hiroki; NEMOTO, Takashi; HARUTA, Mitsutaka; KURATA, Hiroki
"Coupling of Surface Plasmon of Ag Nanorods and Exciton of Organic Materials"

— Atomic and Molecular Structures —

LW “Introduction of Atomic and Molecular Structures Laboratory”

— Synthetic Organotransformation —

GE IMAI, Makiko; NAKAMURA, Yuki; SUZUKI, Shogo; ISOZAKI, Katsuhiro; NAKAMURA, Masaharu; MATSUMURA, Hiroyuki (Daicel); KITAYAMA, Kenji (Daicel)
“Isolation of Novel Cellulose Nanostructures by Mild Degradation Reaction of Woody Biomass”

GE WU, Dongran; MATSUDA, Hiroshi; AVENA, Ramon; AOKI, Satoshi; PINCELLA, Francesca; NAKAMURA, Masaharu
“Synthetic Study of Iron-Catalyzed Monoaminated Biaryl Compounds”

— Advanced Solid State Chemistry —

LW “Research Introduction in Advanced Solid State Chemistry Laboratory”

— Organometallic Chemistry —

LW “Recent Research Topics of Organometallic Chemistry Laboratory”

— Nanophotonics —

LW “Recent Research Topics of Nanophotonics Group”

— Chemical Life Science —

LW “Chemical Life Science”

— Mathematical Bioinformatics —

LT LIU, Chunting
“MSNet-4mC: Learning Effective Multi-Scale Representations for Identifying DNA N4-Methylcytosine Sites”

GE LI, Ruiming; LEE, Jung-Yu; YANG, Jinn-Moon; AKUTSU, Tatsuya
“Densest Subgraph-Based Methods for Protein-Protein Interaction Hot Spot Prediction”

— Bio-knowledge Engineering —

LT NGUYEN, Duc Anh; NGUYEN, Canh Hao; PETSCHNER, Peter; MAMITSUKA, Hiroshi
“Advanced Hypergraph Neural Network Models to Accurately Predict Drug-Drug Interactions”

SEMINARS

Prof AJAYAGHOSH, Ayyappanpillai
Council of Scientific & Industrial Research, National Institute for Interdisciplinary Science and Technology (CSIR-NIIST), India
“Functional Dye Based Optical Materials and Their Application”
17 October 2022

Prof AWAGA, Kunio
Department of Chemistry and IRCCS, Nagoya University, Aichi, Japan
“Interdisciplinary Research on Solid-State Science and Electrochemistry of Molecular Materials”
5 August 2022

Prof BAUMGARTNER, Thomas
York University, Canada
“(Un)usual Phosphorus-Based Concepts for Organic Materials”
13 October 2022

Dr BLANC-MATHIEU, Romain
Université Grenoble Alpes, CEA, France
“A Structural Classification for Plant Transcription Factors”
19 July 2022

Prof CAI, Pinghe
Department of Marine Chemistry and Geochemistry, Xiamen University, China
“Precise Measurements of ^{226}Ra in Marine Samples by High-Sensitivity ICP-MS”
26 September 2022

Dr CHAFFRON, Samuel
CNRS, Nantes University, France
“Community Network Models to Reveal Marine Plankton Systems Ecology”
24 October 2022

Prof DAS, Apurba K.
Indian Institute of Technology Indore, India
“Chemical Reactions Directed Evolution of Dynamic Soft Biomaterials”
3 October 2022

Dr DOBA, Takahiro
Hokkaido University, Hokkaido, Japan
“Iron-Catalyzed C-H/C-H Coupling for Synthesis of Functional Small Molecules and Polymers”
22 September 2022

Prof FIRDAUS, Mochamad Lutfi
Graduate School of Science Education, University of Bengkulu, Indonesia
“The Emerging Digital Image Colorimetry for Green, Low-Cost, and Portable Qualitative and Quantitative Analysis”
31 October 2022

AI Engineer FUCHS, Florian
Sony AI, Zurich, Switzerland
“Outracing Champion Gran Turismo drivers with Deep Reinforcement Learning”
26 October 2022

Prof FUCHTER, Matthew J.
Department of Chemistry, Imperial College London, U.K.
“Maximising Dissymmetry and Handling Directionality in Chiral Materials”
8 September 2022

Dr GAIA, Morgan
Genoscope, CEA, Every, France
“The Viral Eukaryogenesis Hypothesis in the Tree of Life”
22 June 2022

Ms GAUDIN, Marinna
CNRS, Nantes University, France
“Towards Omics-Based Distribution Modeling of Marine Plankton Associations at Global Scale”
19 October 2022

Dr GUIDI, Lionel
CNRS, Sorbonne University, France
“The Biological Carbon Pump from Genes to the Ecosystem”
23 June 2022

Prof HU, Bin
Department of Materials Science and Engineering, University of Tennessee, Tennessee, U.S.A.
“Spin-Orbital Coupling Effects in Organic Molecules and 2D-Superlattice Perovskites”
5 August 2022

Prof JIA, Li
The University of Akron, U.S.A.
“Metal-Catalyzed Carbonylative Polymerizations - A Quest for Sustainable Commodity Plastics”
5 July 2022

Mr KATO, Yasutaka
STJ Advisors Group Limited, Aichi, Japan
“Work & Private Life ~3 Years Post Graduation from Ogata Lab.”
11 March 2022

Assist Prof KIM, Hyunwoo
POSTECH, Korea
“Radical-Polar Crossover Strategy in Organic Electrosynthesis”
22 November 2022

Prof KIM, Sekwon
Korea Advanced Institute of Science & Technology, Daejeon, Korea
“Spin Superfluidity ”
6 January 2022

Prof KLIPP, Edda
Humboldt University of Berlin, Berlin, Germany
“Mathematical Modeling of Signaling Networks in Time and Space”
12 April 2022

Prof MEYER, Karsten
Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany
“From the Norbornyl Cation Story to Basic Coordination Chemistry at Iron and Uranium-Mediated Electrocatalytic Water Splitting”
20 September 2022

Dr MIZUMAKI, Masaichiro
Japan Synchrotron Radiation Research Institute, Hyogo, Japan
“Application of Bayesian Estimation to Synchrotron Radiation Measurement Data”
12 October 2022

Dr MOTOTAKE, Yoh-ichi
The Institute of Statistical Mathematics, Tokyo, Japan
“Material Pattern Informatics Using Topological Data Analysis”
12 October 2022

Prof PAINELLI, Anna
Department of Chemistry, Life Sciences and Environmental Sustainability, University of Parma, Parma, Italy
“Thermally Activated Delayed Fluorescence (TADF): Understanding a Complex Photophysical Phenomenon in Condensed Phase”
4 November 2022

Prof PASZKOWSKI, Uta
Department of Plant Sciences, University of Cambridge, U.K.
“Molecular Genetics of Arbuscular Mycorrhizal Symbiosis in Cereals”
19 July 2022

Prof PRATT, Derek
Department of Chemistry and Biomolecular Science, University of Ottawa, Canada
“Mechanisms of Free Radical Oxidation and Their Inhibition: from Hydrocarbons to Living Organisms”
14 October 2022

Ms PRONDZINSKY, Paula
Tokyo Institute of Technology, Tokyo, Japan
“Adaptations of Methanogenic Archaea to Different Temperature Environments”
7 April 2022

Dr SALCHER, Michaela Maria
The Czech Academy of Sciences, Czech Republic
“Tackling the “Uncultivated Microbial Majority” of Freshwater Lakes by High-Throughput Isolation”
3 October 2022

Prof SASAMORI, Takahiro
University of Tsukuba, Ibaraki, Japan
“Introduction of Single Crystal X-ray Diffraction Analysis -Key Points of Measurement and Evaluating the Results-”
19 December 2022

Assoc. Prof SONG, Jiangning
Monash University, Australia
“Artificial Intelligence to Explore Multi-Modality Molecular Data and Accelerate Biomedical Knowledge Discovery”
14 July 2022

Prof STREUBEL, Rainer
Institute for Inorganic Chemistry, University of Bonn, Bonn, Germany
“Insights into Phosphinidenoid Complex Chemistry”
12 September 2022

Prof STUDER, Armido
WWU Münster, Germany
“NHC Radical Catalysis”
25 November 2022

Prof ULRICH, Gilles
Centre National de la Recherche Scientifique (CNRS), France
“Luminescent Borate Complexes and Their Emissive Ligands”
27 September 2022

Assist Prof WICKENS, Zachary K.
University of Wisconsin-Madison, U.S.A.
“Selective Synthesis via Light and Electricity”
21 November 2022

Prof WIRTH, Thomas
Cardiff University, U.K.
“Intensification and Electrification of Flow Chemistry”
3 October 2022

Prof XU, Hao
Brandeis University, U.S.A.
“Searching for New Reactivity: Iron-Catalyzed Selective Nitrogen Atom Transfer”
14 October 2022

Prof ZHAO, Yunde
Section of Cell and Developmental Biology, University of California San Diego, U.S.A.
“Development of Gene Editing Technologies for Auxin Research and Crop Improvement”
11 November 2022

MEETINGS AND SYMPOSIA

IUPAC Global Women's Breakfast 2022 – Kyoto University and OIST
Organized by PINCELLA, Francesca
16 Feb 2022 (Online)

The 42nd Anniversary Meeting of Prof. Masayoshi Ishibashi, Research Institute of Oceanochemistry Foundation
Organized by SOHRIN, Yoshiki
23 April, 2022 (Kyoto, Japan)

SCRIT Collabolation Annual Meeting in Kyoto
Organized by WAKASUGI, Masanori
6 May 2022 (Kyoto, Japan)

International Colloquium on Magnetic Films and Surfaces
Organized by ONO, Teruo
10 July 2022 (Okinawa, Japan)

The 2nd International Workshop on Advanced Intelligent Modeling Technologies for Smart Cities
Organized by AKUTSU, Tatsuya; CAI, Hongmin; CHENG, Xiaoqing
9 August 2022 (Online)

CSN Satellite Workshop 2022
Organized by TSUGE, Tomohiko
28 August 2022 (Toscana, Italy)

Databases for Medical and Pharmaceutical Sciences (Workshop in IIBMP 2022)
Organized by AKUTSU, Tastuya
13 September 2022 (Osaka, Japan)

The 32nd Symposium on Physical Organic Chemistry
Organized by TOKITOH, Norihiro
20-22 September 2022 (Kyoto, Japan)

The 34th Symposium on Plant Lipids
Organized by AOYAMA, Takashi
20 September 2022 (Kyoto, Japan)

2022 Young Scientists Symposium of the Japanese Society of Microscopy
Organized by HARUTA, Mitsutaka
10 October 2022 (Kyoto, Japan)

The 76th Annual Autumn Meeting of the Research Institute for Oceanochemistry Foundation
Organized by SOHRIN, Yoshiki
29 October 2022 (Kyoto, Japan)

Modification of Cell Fcuntions by Engineering Membrane Lipid Metabolism
Organized by KURIHARA, Tatsuo; HEMMI, Hisashi
10 November 2022 (Nagoya, Japan)

The 6th MAIRS Workshop
Organized by HASEGAWA, Takeshi
18 November 2022 (Kyoto, Japan)

Past, Present, and Future of Asian Lacquer: Urushi from Art to Electronics
Organized by PINCELLA, Francesca; FORTE, Erika; MINEO, Keito; WU, Beiling; NAKAMURA, Masaharu
12 December 2022 (Kyoto, Japan)

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