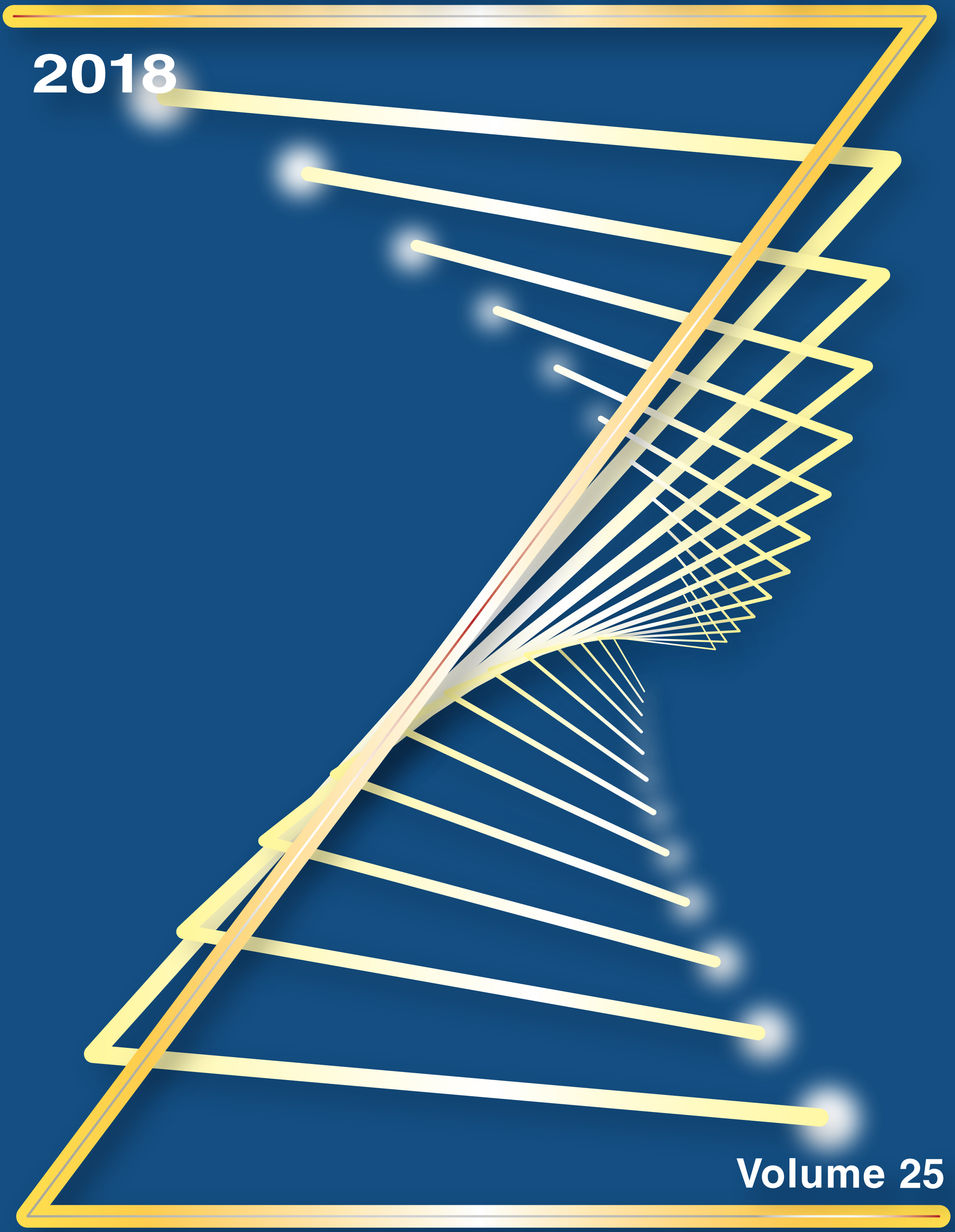
ISSN 1342-0321
IAREFM

ICR ANNUAL REPORT

2018



Volume 25

Institute for Chemical Research
Kyoto University

ICR ANNUAL REPORT 2018 (Volume 25) - ISSN 1342-0321 -

This Annual Report covers from 1 January to 31 December 2018

Editors:
Professor: UESUGI, Motonari
Professor: MIZUOCHI, Norikazu
Associate Professor: HASHIDA, Masaki
Assistant Professor: MORISAKI, Kazuhiro

Editorial Staff:
Public Relations Section: NAKAMURA, Kaori
HAMAOKA, Meri
FURUTA, Tomoyo
TANIMURA, Michiko

Published and Distributed by:
Institute for Chemical Research (*ICR*), Kyoto University

Note: *ICR* Annual Report available from the *ICR* Office,
Institute for Chemical Research, Kyoto University,
Gokasho, Uji-city, Kyoto 611-0011, Japan
Tel: +81-(0)774-38-3344
Fax: +81-(0)774-38-3014
E-mail koho@scl.kyoto-u.ac.jp
URL https://www.kuicr.kyoto-u.ac.jp/sites/icr/

Uji Library, Kyoto University
Tel: +81-(0)774-38-3010
Fax: +81-(0)774-38-4370
E-mail ujibunkan@mail2.adm.kyoto-u.ac.jp
URL http://lib.kuicr.kyoto-u.ac.jp/index.htm

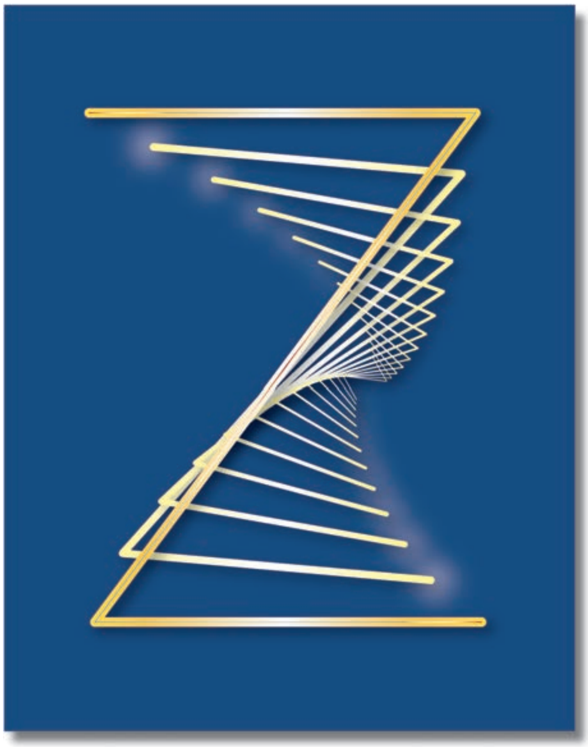
Printed by
Nakanishi Printing Co., Ltd.
Ogawa Higashi-iru, Shimodachiuri, Kamigyo-ku, Kyoto-city 602-8048, Japan
TEL: +81-(0)75-441-3155 FAX: +81-(0)75-417-2050

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 2018



Institute for Chemical Research
Kyoto University
Volume 25

Preface

Institute for Chemical Research (ICR) was founded in 1926 as the first research institute of Kyoto University with the founding vision to “Excel in the Investigation of Basic Principles of Chemistry and Their Applications.” ICR is a successor to the Specialized Center for Chemical Research established at the College of Science of Kyoto Imperial University in 1915 for the study of a special medicinal substance called “Salvarsan,” that is arsphenamine. Ever since, ICR has continuously carried out outstanding research and flourished as a large-scale organization with five research divisions and three research centers: Division of Synthetic Chemistry, Division of Materials Chemistry, Division of Biochemistry, Division of Environmental Chemistry, Division of Multidisciplinary Chemistry, Advanced Research Center for Beam Science, International Research Center for Elements Science (IRCELS), and Bioinformatics Center. Currently, almost 120 faculty members, 210 graduate students, and 60 researchers are engaged in research activities in 30 laboratories directed by full-time professors and 5 laboratories supervised by visiting professors.

Research at ICR encompasses a wide range of scientific disciplines, including physics, biology, and informatics besides chemistry. Graduate schools to which our laboratories are affiliated as a “cooperative lab” cover a broad range of fields such as science, engineering, agriculture, pharmaceutical sciences, medicine, and informatics. These laboratories are spearheading cutting-edge research and yielding groundbreaking results in their special fields. Some of the research achievements last year are as follows: *1) The First Synthesis of an Isolable Tin-containing Benzene Derivative as a Potential Intermediate; 2) Spin-orbit-torque Memory Operation of Synthetic Antiferromagnets toward Ultrahigh-density Magnetic Recording; 3) Photorefractive Effect in Organic-Inorganic Hybrid Perovskites and Its Applications; 4) Successful Application of DNP-NMR to Structural Analysis of Organic Thin Films; 5) Fabrication of High-Quality, High-Performance Tin Halide Perovskite Film for Solar Cells; 6) New Mechanism of Plasmon-induced Hole Transfer at Nano-heterointerface, 7) Development of Robust Sensor Chips for Analyzing Lignin-peptide Interactions; 8) Marine Viruses Driving the Daily Mortality Cycle of Cyanobacteria*. Some other topics were also presented in the 118th ICR Annual Symposium on November 30, 2018.

The legacy of our founding philosophy continues today and describes the essence of our research activities. With the founding vision in mind, we have entrusted our scientists with the responsibility of choosing research topics within advanced chemistry-related fields. Thus, ICR members are actively involved in interdisciplinary research projects with bottom-up paradigms in order to create new knowledge and contribute to the future of materials-related fields. One of our major challenges is to design and create smart materials from the viewpoint of not only academic interest but also green innovation and establishment of a sustainable society through “zero loss” in the production/transportation/usage of materials/energy. Toward the future, we have been collaborating with the Research Institute for Sustainable Humanosphere and the Institute of Advanced Energy since 2015 as part of the MEXT-supported joint research program. For the MEXT project of Integrated Research Consortium on Chemical Sciences (2016–2021), ICR (most importantly, IRCELS) has been making a significant contribution as one of the four core research institutions from Japanese national universities. We have also been collaborating with both domestic and overseas universities and research institutions (with 70 official international collaboration agreements) and functioning as a Joint Usage/Research Center supported by MEXT since 2010. On the basis of highly evaluated global activity in chemistry-oriented fields as well as interdisciplinary fields, ICR was newly certified as an International Joint Usage/Research Center by MEXT. In order to foster and secure young researchers through these activities, we also have original programs of unparalleled research and graduate education, including an in-house annual grant system named “ICR Grant for Promoting Integrated Research.” These collaborative achievements ensure that ICR serves as a global research core in chemistry-oriented fields.

We hope this Annual Report will serve to update you on the progress of our research activities and globalization. Finally, we appreciate your continued encouragement and support.

January 2019

Y. Tsuji

TSUJII, Yoshinobu
Director

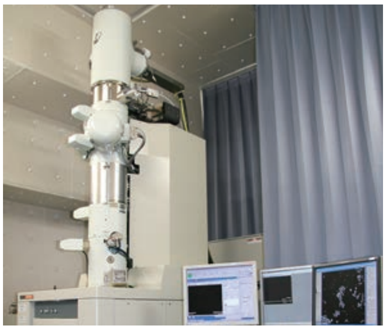
ICR News 2018

International Joint Usage/Research Center: Global Frontier/Interdisciplinary Research Core for Deepening Investigation and Promoting Collaboration in Chemistry-oriented Fields

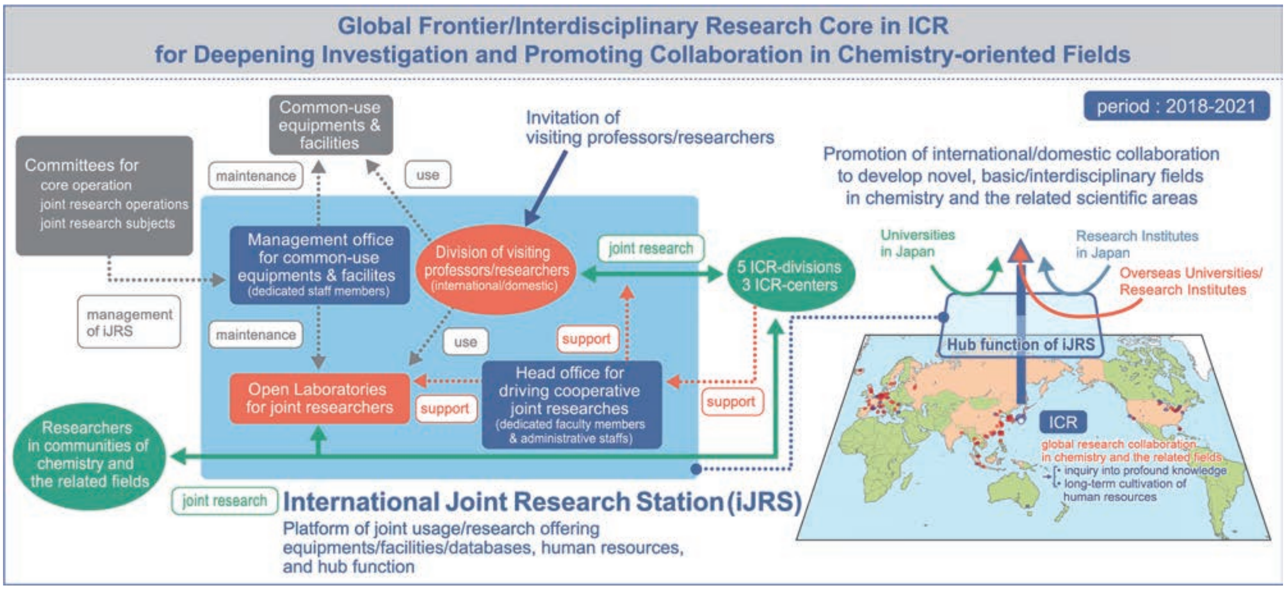
■ Prof TERANISHI, Toshiharu (Head of International Joint Research Station)

Since the fiscal year 2010, the Institute for Chemical Research (ICR) has been proactively collaborating with domestic/overseas universities and research institutes as a Joint Usage/Research Center (JURC) approved by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. In 2018, MEXT favorably evaluated the international activities of ICR-JURC to approve ICR as the international JURC (iJURC), proclaiming "the Global Frontier and Interdisciplinary Research Core in ICR for Deepening Investigation and Promoting Collaboration in Chemistry-oriented Fields". Around 100 joint research subjects including around 50 international subjects will be adopted next year (Research Project Categories: Field-specific (pre-planned) Research, Proposal-based Research, Promotion of Collaborative and Multidisciplinary Research, and Facilities and Equipment Use). Several frontier instruments, including Dynamic Nuclear Polarization Nuclear Magnetic Resonance Spectrometer, have been newly equipped and utilized in the joint research, and a management office for those common-use instruments has been also organized. ICR-iJURC will conduct advanced joint research in chemistry-related fields, with the emphasis being placed on promoting international joint usage/research, enhancing international academic network, and training young researchers with an international perspective.


Dynamic Nuclear Polarization-enhanced NMR (DNP-NMR) Systems


High Functionality Electron Microscopes


Supercomputer System



Specially Appointed Prof KANEHISA, Minoru Received the 2018 Clarivate Citation Laureates

Specially Appointed Professor Minoru Kanehisa was listed on a list of Clarivate Citation Laureates 2018 for his contributions to bioinformatics, specifically for his development of the Kyoto Encyclopedia of Genes and Genomes (KEGG). This year, Clarivate Analytics named 17 world-class researchers as Citation Laureates. This designation celebrates researchers whose work is deemed to be, ‘of Novel stature’, as attested by exceptionally high citation records within the Web of Science.

Citation Laureate 2018
Physiology or Medicine
Minoru Kanehisa

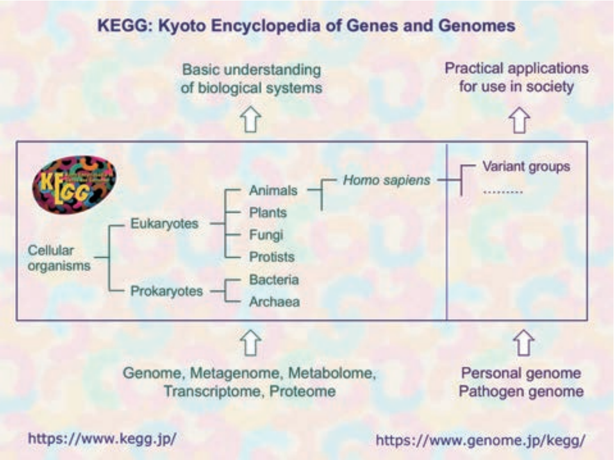
Web of Science
Clarivate

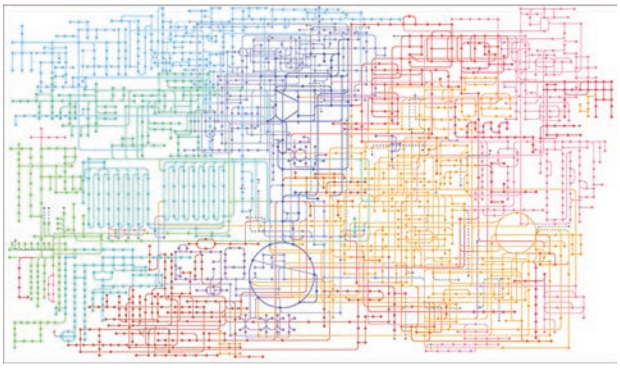
Photo Courtesy of KURIYAMA, Jin, PRAP Japan, Inc.

■ Specially Appointed Prof KANEHISA, Minoru

KEGG

KEGG (https://www.kegg.jp/ or https://www.genome.jp/kegg/) is a database resource for biological interpretation of genome sequences and other molecular datasets in life sciences. I started KEGG in 1995 under the Human Genome Project in Japan, foreseeing the need for a reference resource that would enable computational reconstruction of the biological systems, including the cell, the organism and the ecosystem, from the genome information. In the traditional view, the genome is a blueprint of life containing all necessary information that would make up a biological system. In my view, however, the genome specifies only the molecular building blocks, while the cell, the basic unit of life, contains information about how they interact and react to form a system. It must be emphasized that what we inherit is not just the genome, but the entire cell, and there is a cellular continuity of the germ line leading to the origin of life. From this perspective, cellular functions and other high-level biological features are accumulated from experimental observations reported in published literature and represented in KEGG in terms of molecular interaction/reaction networks. By integrating the molecular networks (wiring diagrams) and the genes in the genomes (building blocks) for all available cellular organisms, KEGG has become a reference resource for deciphering the genome. Currently, my main interest is to make KEGG more useful in practical applications by integrating knowledge of diseases, drugs and related human gene variants in terms of perturbed molecular networks.





The 15th International Symposium on Inorganic Ring Systems (IRIS-15)

■ Prof TOKITOH, Norihiro

The 15th International Symposium on Inorganic Ring Systems (IRIS 15, 24–29 June 2018) was held at Uji Obaku Plaza, Institute for Chemical Research (ICR), Kyoto University in conjunction with the Institute for Chemical Research International Symposium 2018 (ICRIS-2018). The conference was held under the auspices of ICR, and co-hosted by ICR Joint Usage/Research Center, the Chemical Society of Japan, Society of Synthetic Organic Chemistry Japan, Kinka Chemical Society Japan and the Society of Silicon Chemistry Japan, under the support of Kyoto University Foundation, Tokuyama Science Foundation and Kyoto Convention & Visitors Bureau.

This conference occurs every three years and is the premier international showcase for Main Group Chemistry, including Organometallic Chemistry and Inorganic Materials Chemistry. This was the first IRIS meeting to be hosted in Japan. Fortunately, 205 scientists including world-leading professors, postdoctoral fellows, and research students from around the world participated. The conference program contained 5 plenary and 15 invited lectures by internationally renowned scientists, as well as 52 short communications and 82 poster presentations. The plenary lectures were presented by Prof. Manfred Scheer (Universität Regensburg, Germany), Prof. Cameron Jones (Monash University, Australia), Prof. David Scheschkewitz (Universität des Saarlandes, Germany), Prof. Axel Schulz (Universität Rostock, Germany) and Prof. Soichiro Kyushin (Gunma University, Japan) at the KIHADA hall. For selected outstanding oral communications and posters presented by students, excellent prizes were awarded. The prizes were kindly sponsored by the Chemical Society of Japan and the Royal Society of Chemistry. In addition, it was our great pleasure and honor to celebrate the 90th birthday of Prof. Robert West, the giant legend in silicon chemistry, and we have enjoyed his chemistry as the Special Keynote Lecture. Various issues related to the synthesis, structure, theoretical chemistry and reaction mechanism of novel inorganic ring systems were actively discussed during the conference.

Symposium Photo taken on June 28.

Celebration of the 90th birthday of Prof West (left).

Lectures and Oral Presentations

Poster Session

Kyoto University Chemistry Talent-Spot Event 2018 Manila

■ Prof UESUGI, Motonari

ICR hosted a student recruitment event named “Kyoto University Chemistry Talent-Spot Event 2018 Manila” on January 21, 2018 at Manila Hotel in Manila, Philippines. The goal of this event is to recruit outstanding students to ICR as Japanese government-sponsored foreign students.

Eleven principal investigators from ICR visited Manila to interview thirty shortlisted candidates having potential for a MEXT scholarship. The actual event included eleven short tutorial lectures on a wide range of topics in chemistry and face-to-face interviews with the candidates. During our visit to Manila, we were invited to University of Santo Tomas (UST) to attend the MOU signing ceremony between ICR and UST. We also had a chance to visit the University of the Philippines Diliman to deliver tutorial lectures to its chemistry students.

In March 2018, top six students from the interview were invited to ICR for a one-week research experience program. On their last day at ICR, each gave a presentation on their research work they had been engaged in during the stay. Three out of the six applied for a MEXT scholarship, and two of them has successfully acquired the scholarship.


Tutorial Session


Student Interview Session


MOU Signing Ceremony at UST

A Sample of Acrylonitrile Butadiene Rubber (NBR), Synthesized with the Aid of the “Monovinylacetylene Method” and Conserved at ICR, Was Certified as the Chemical Heritage by the Chemical Society of Japan

■ Prof WATANABE, Hiroshi

At the Institute for Chemical Research (ICR) in 1942, Professor Junji Furukawa of Kyoto University synthesized acrylonitrile butadiene rubber (NBR) in the pilot plant scale (200 kg/day) for the first time in Japan. One of the starting materials, butadiene, was synthesized with the epoch-making “monovinylacetylene method” developed by Professor Furukawa before the second world war, and the pilot plant at ICR was later relocated to the Niihama factory of Sumitomo Chemical Co., Ltd. thereby serving as the firm basis for industrial production of NBR in Japan.

A NBR sample from the above pilot plant was donated by Professor Furukawa to ICR in 1982, and has been carefully conserved at ICR since then. The Chemical Society of Japan appreciated the historical importance of this NBR sample to have certified it as the Chemical Heritage as of March 21, 2018.


The certificate presentation ceremony on 21 March 2018; (left to right) Yasuhiro Takaki (Director of Nature and Science Museum, Tokyo University of Agriculture and Technology), Hisashi Yamamoto (President of the Chemical Society of Japan), Norihiro Tokitoh (Director of ICR) at the ceremony.


日本化学会化学遺産
認定証
京都大学化学研究所 殿

Certificate of Chemical Heritage


NBR sample certified as Chemical Heritage (black sheet) and documents of explanation

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
- 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

Prof
TOKITOH, Norihiro
(D Sc)

Assoc Prof
MIZUHATA, Yoshiyuki
(D Sc)

Assist Prof
YUKIMOTO, Mariko
(D Sc)

Techn
HIRANO, Toshiko

PD
GUO, Jing-Dong
(Ph D)

Students

FUJIMORI, Shiori (D3)
SUGAHARA, Tomohiro (D3)
YANAGISAWA, Tatsuya (D2)
OMATSU, Yamato (D1)
IWAI, Kento (D1)
HONJO, Kazuma (M2)
JUN-I, Yuta (M2)
OSHIRO, Taku (M2)
TSUJI, Shingo (M2)
JO, Minwoo (M1)

Guest Scholars

SCHMER, Alexander	Universität Bonn, Germany, 1 May–30 June
VOLK, Niklas	Universität Bonn, Germany, 1 June–31 July

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

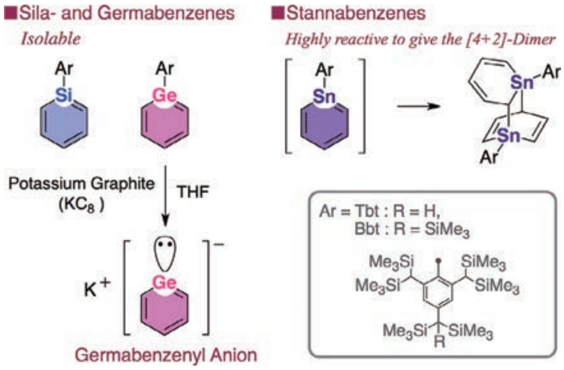
Steric Protection
Kinetic Stabilization
Low-coordinated Species
Heteroatom
Transition Metal Complexes

Selected Publications

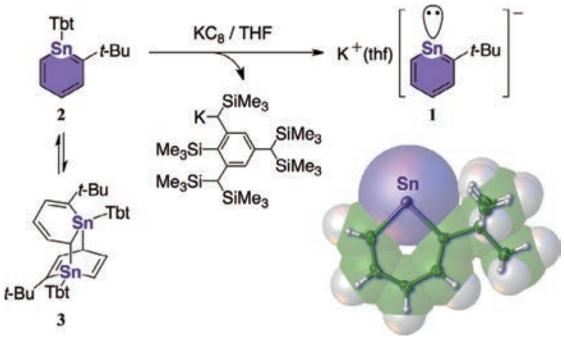
Sugahara, T.; Guo, J.-D.; Sasamori, T.; Nagase, S.; Tokitoh, N., Regioselective Cyclotrimerization of Terminal Alkynes Using a Digermyne, *Angew. Chem. Int. Ed.*, **57,** 3499-3503 (2018).
Fujimori, S.; Mizuhata, Y.; Tokitoh, N., Ru-Complexes of an Anionic Germabenzenyl Ligand, *Chem. Commun.*, **54,** 8044-8047 (2018).
Sugahara, T.; Sasamori, T.; Tokitoh, N., 2,5-Digermaselenophenes: Germanium Analogues of Selenophenes, *J. Am. Chem. Soc.*, **140,** 11206-11209 (2018).
Mizuhata, Y.; Fujimori, S.; Noda, N.; Kanesato, S.; Tokitoh, N., Generation of Stannabenzenes and Their Monomer-Dimer Equilibration, *Dalton Trans.*, **47,** 14436-14444 (2018).
Fujimori, S.; Mizuhata, Y.; Tokitoh, N., Stannabenzenylpotassium: The First Isolable Tin-containing Benzene Derivative, *Chem. Eur. J.*, **24,** 17039-17045 (2018).

Stannabenzenyl Anion: Heavy Phenyl Anion

"Heavy benzenes" in which the carbon atom(s) of the benzene ring is replaced by high-period group 14 element(s), *that is*, "heavy element" (silicon, germanium, tin, and lead), have attracted much attention from the interest of its aromaticity experimentally and theoretically. However, these compounds are extremely high-reactive species, *e.g.*, silabenzene ($HSiC_5H_5$) in which one of the skeletal carbon atom of the benzene ring is replaced by a silicon atom, is known to decompose by self-oligomerization reaction even at very low temperature of –200 °C. We have already succeeded in the synthesis and isolation of sila- and germabenzenes as stable compounds even at room temperature by taking advantage of kinetic stabilization afforded by a very bulky substituent, Tbt group, to prevent the self-oligomerization. These compounds are found to have "aromaticity" and unique electronic state. In addition, recently, we successfully synthesized the germabenzenyl anion as an isolable compound by the reaction of the corresponding isolated neutral germabenzene having a Tbt group on the germanium atom with potassium graphite (KC_8). However, in the tin case, stannabenzenes having a Tbt or Bbt group on the tin atom are extremely reactive and lead to the formation of the [4+2] dimer of stannabenzene.

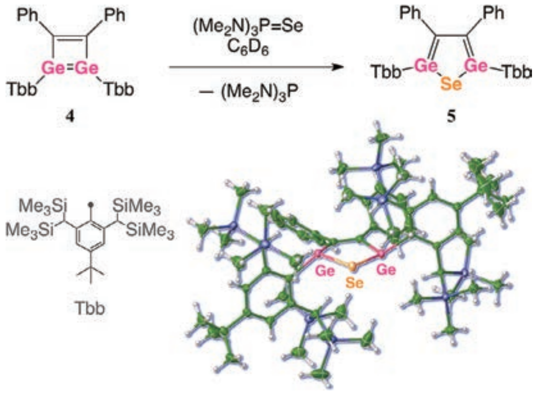


In this study, utilizing the successful method of synthesis of the germabenzenyl anion, we have reported the isolation and characterization of stannabenzenyl anion **1**. For the synthesis and isolation of a stable stannabenzene, we have introduced an additional substituent (*t*-butyl group) on the carbon atom adjacent to the tin atom. As the result of introducing *t*-butyl group, the equilibrium mixture of stannabenzene **2** and the corresponding dimer **3** could be obtained. We reasoned that the equilibrium mixture of the monomeric stannabenzene **2** and its dimer **3** would be a suitable precursor to gain the corresponding stannabenzenyl anion. The reaction of the equilibrium mixture with 2.1 equivalents of potassium graphite (KC_8) in THF successfully gave the first stable tin-containing phenyl anion derivative, stannabenzenylpotassium K^+(thf)·**1**$^-$. The properties revealed by X-ray crystallographic analysis, NMR, UV/Vis spectroscopy, and theoretical calculations showed the monomeric nature of **1** reflecting intermolecular electronic repulsion around the stannabenzenyl anion. It should be noted that this new stabilization strategy utilizing electronic repulsion is a promising method for isolating highly reactive species and that the stannabenzenyl anion is a potential intermediate for new organostannyl species.



Germanium Analogues of Selenophenes

We have reported the synthesis of 2,5-digermaselenophene **5** as purple crystals by the reaction of 1,2-digermacyclobutadiene **4**, which was obtained by the reaction of the stable digermyne TbbGe≡GeTbb with diphenylacetylene, with an equimolar amount of $(Me_2N)_3P{=}Se$ in C_6D_6 at room temperature. X-Ray crystallographic analysis revealed that 2,5-digermaselenophene **5** exhibits a nonplanar structure with a *trans*-pyramidalized geometry of the five-membered $[SeGe_2C_2]$ ring. The UV/vis spectrum of **5** in hexane showed a strong absorption at λ_{max} = 536 nm (ε 7800), which was assigned to the HOMO−LUMO transition based on TDDFT calculations (533.6 nm; $f = 0.2164$). Such an absorption at longer wavelength suggests that 2,5-digermaselenophenes could serve as promising building blocks for optoelectronic materials. Further investigation on the electrochemical properties of such digermaselenophenes is currently in progress.



Division of Synthetic Chemistry
– Structural Organic Chemistry –

http://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


PD
KIM, Kyusun
(D Eng)


PD
ZHANG, Sheng
(Ph D)


PD
IDE, Yuki
(D Sc)


PD
KIZAKI, Kazuro
(D Eng)

Researcher (pt)

ADACHI, Ayumi

Students

HASEGAWA, Shota (M2)
OKAMOTO, Shu (M1)
LI, Hui (RS)
ZHENG, Chuyu (RS)
LI, Jiayue (RS)
KAMIYA, Sota (UG)
FUSHINO, Teppei (UG)

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

Selected Publications

Hashikawa, Y.; Yasui, H.; Kurotobi, K.; Murata, Y., Synthesis and Properties of Open-Cage Fullerene C_{60} Derivatives: Impact of the Extended π-Conjugation, *Mater. Chem. Front.*, **2,** 206-213 (2018).

Zhu, G.-Z.; Liu, Y.; Hashikawa, Y.; Zhang, Q.-F.; Murata, Y.; Wang, L.-S., Probing the Interaction between the Encapsulated Water Molecule and the Fullerene Cages in $H_2O@C_{60}^-$ and $H_2O@C_{59}N^-$, *Chem. Sci.*, **9,** 5666-5671 (2018).

Hasegawa, S.; Hashikawa, Y.; Kato, T.; Murata, Y., Construction of a Metal-Free Electron Spin System by Encapsulation of an NO Molecule Inside an Open-Cage Fullerene C_{60} Derivative, *Angew. Chem. Int. Ed.*, **57,** 12804-12808 (2018).

Strelnikov, D. V.; Jasik, J.; Gerlich, D.; Murata, M.; Murata, Y.; Komatsu, K.; Kappes, M. M.; Roithova, J., Near- and Mid-IR Gas-Phase Absorption Spectra of $H_2@C_{60}^+$–He, *J. Phys. Chem. A*, **122,** 8162-8166 (2018).

Synthesis and Properties of Open-Cage Fullerene C_{60} Derivatives: Impact of the Extended π-Conjugation

We have developed the method for the synthesis of open-cage fullerene C_{60} derivatives with extended π-conjugation bearing thienyl groups (Figure 1). By applying this method to the unsymmetrical diketo derivative, the symmetric form can be obtained without changing the molecular formula. To investigate the structure-property relationship for the asymmetric and symmetric forms, we conducted the electrochemical and photophysical measurements. The UV-Vis absorption edge was shifted by 210 nm from asymmetric to symmetric forms due to the narrower HOMO-LUMO gap, which is also demonstrated by electrochemical analyses. From the theoretical calculations, the major contribution of the longest wavelength absorption for the symmetric form is assignable to unusual intramolecular charge transfer transitions whereas π-π* transition is dominant for the asymmetric form.

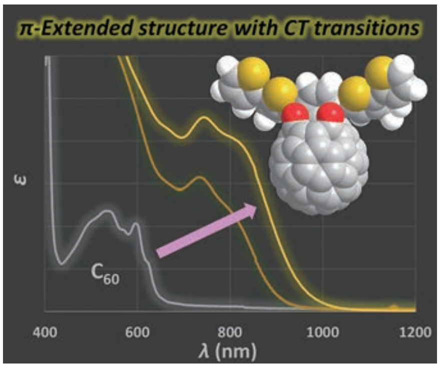


Figure 1. Bathochromic shift with intense absorption of open-cage C_{60} derivatives by effective π-extension.

Probing the Interaction between the Encapsulated Water Molecule and the Fullerene Cages in $H_2O@C_{60}^-$ and $H_2O@C_{59}N^-$

We report a high-resolution photoelectron imaging study of cryogenically-cooled $H_2O@C_{60}^-$ and $H_2O@C_{59}N^-$ endohedral fullerene anions. The electron affinity (EA) of $H_2O@C_{60}$ is measured to be 2.6923 ± 0.0008 eV, which is 0.0088 eV higher than the EA of C_{60}, while the EA of $H_2O@C_{59}N$ is measured to be 3.0058 eV ± 0.0007 eV, which is 0.0092 eV lower than the EA of $C_{59}N$ (Figure 2). The opposite shifts are found to be due to the different electrostatic interactions between the encapsulated water molecule and the fullerene cages in the two systems. There is a net coulombic attraction between the guest and host in $H_2O@C_{60}^-$, but a repulsive interaction in $H_2O@C_{59}N^-$. We have also observed low-frequency features in the photoelectron spectra tentatively attributed to the hindered rotational excitations of the encapsulated H_2O molecule, providing further insights into the guest–host interactions in $H_2O@C_{60}^-$ and $H_2O@C_{59}N^-$.

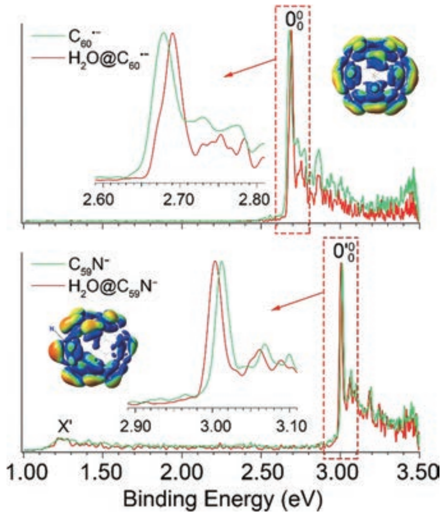


Figure 2. Photoelectron spectra of C_{60}^-, $H_2O@C_{60}^-$, $C_{59}N^-$, and $H_2O@C_{59}N^-$.

Construction of a Metal-Free Electron Spin System by Encapsulation of an NO Molecule inside an Open-Cage Fullerene C_{60} Derivative

A reactive radical species, nitric oxide (NO), was encapsulated as a unimolecular form inside an open-cage fullerene derivative under high-pressure conditions in solid state (Figure 3). Surprisingly, the molecular complex showed sharp ^1H NMR signals in spite of the existence of the paramagnetic species inside the carbon cage. Owing to the paramagnetic shifts, the escape rate of the NO was determined experimentally and compared with the DFT calculations. After constructing a stopper on the rim of the opening to prevent such escape, the NO was found to stay inside the cage even at 50°C. The ESR measurements of the powdery sample showed paramagnetic properties at low temperature. The single crystal X-ray structure analysis clearly demonstrated the existence of the encapsulated NO molecule, suggesting rapid rotation inside the cage. The ^1H NMR chemical shifts of the sharp signals displayed large temperature dependence owing to the paramagnetic effects.

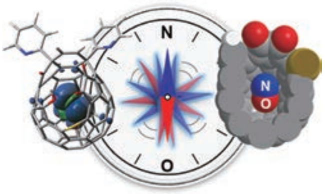


Figure 3. Spin density map and the cross sectional image of NO@open-C_{60}.

Division of Synthetic Chemistry
– Synthetic Organic Chemistry –

http://www.fos.kuicr.kyoto-u.ac.jp/EnglishTop/English.top.html


Prof
KAWABATA, Takeo
(D Pharm Sc)


Assist Prof
UEDA, Yoshihiro
(D Pharm Sc)


Assist Prof
MORISAKI, Kazuhiro
(D Pharm Sc)


Techn Staff
FUJIHASHI, Akiko


PD
YELLA, Ramesh
(Ph D)


PD
CHANDA, Tanmoy
(Ph D)

Students

GONDOH, Naruhiro (D2)
SHIBAYAMA, Hiromitsu (D2)
MATAYOSHI, Aki (D2)
CHEN, Gong (D1)
XING, Yongning (D1)
NINOMIYA, Ryo (D1)
TAKASHIMA, Megumi (M2)
YAMAMOTO, Satoru (M2)
HASHIMOTO, Hisashi (M2)
FUJIMOTO, Takumi (M2)
MURAI, Takuya (M2)
WANG, Shuo (M2)
IKEDA, Ryohei (M2)
SUGA, Akihisa (M2)
WATANABE, Yuji (M1)
GOTOH, Kengo (M1)
SATO, Yuki (M1)
NABETA, Tomoki (M1)
TOMIGAHARA, Takayuki (UG)
EMI, Ryota (UG)

Scope of Research

The research interests of this laboratory include the development of advanced molecular transformation, total synthesis of biologically active products, and molecular recognition. Programs are active in the following areas: 1) asymmetric alkylation of carbonyl compounds based on "memory of chirality", 2) organocatalysis for fine organic syntheses, 3) synthesis of unusual amino acids and nitrogen heterocycles, 4) regioselective functionalization of carbohydrates, and 5) the structural and functional investigation of heterochiral oligomers.

KEYWORDS
Site-Selective Functionalization
Molecular Recognition
Organocatalysis
Dynamic Chirality
Unusual Amino Acid

Selected Publications

Kawabata, T.; Moriyama, K.; Kawakami, S.; Tsubaki, K., Powdered KOH in DMSO: An Efficient Base for Asymmetric Cyclization via Memory of Chirality at Ambient Temperature, *J. Am. Chem. Soc.*, **130,** 4153-4157 (2008).

Kawabata, T.; Jiang, C.; Hayashi, K.; Tsubaki, K.; Yoshimura, T.; Majumdar, S.; Sasamori, T.; Tokitoh, N., Axially Chiral Binaphthyl Surrogates with an Inner N-H-N Hydrogen Bond, *J. Am. Chem. Soc.*, **131,** 54-55 (2009).

Yoshida, K.; Furuta, T.; Kawabata, T., Organocatalytic Chemoselective Monoacylation of 1, *n*-Linear Diol, *Angew. Chem. Int. Ed.*, **50,** 4888-4892 (2011).

Hamada, S.; Furuta, T.; Wada, Y.; Kawabata, T., Chemoselective Oxidation by Electronically Tuned Nitroxyl Radical Catalysts, *Angew. Chem. Int. Ed.*, **52,** 8093-8097 (2013).

Tomohara, K.; Yoshimura, T.; Hyakutake, R.; Yang, P.; Kawabata, T., Asymmetric α-Arylation of Amino Acid Derivatives by Clayden Rearrangement of Ester Enolates via Momory of Chirality, *J. Am. Chem. Soc.*, **135,** 13294-13297 (2013).

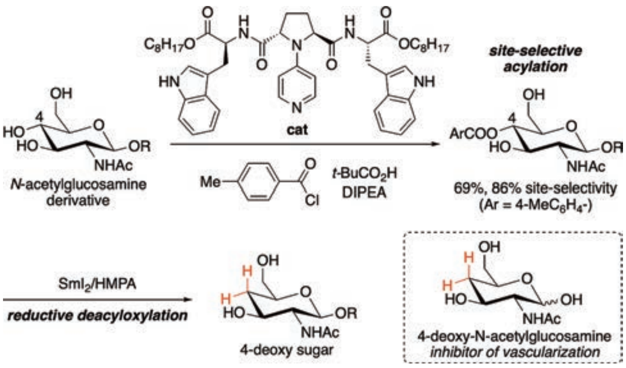
Yoshimura, T.; Tomohara, K.; Kawabata, T., Asymmetric Induction via Short-Lived Chiral Enolates with Chiral C-O Axis, *J. Am. Chem. Soc.*, **135,** 7102-7105 (2013).

Takeuchi, H.; Mishiro, K.; Ueda, Y.; Fujimori, Y.; Furuta, T.; Kawabata, T., Total Synthesis of Ellagitannins via Regioselective Sequential Functionalization of Unprotected Glucose, *Angew. Chem. Int. Ed.*, **54,** 6177-6180 (2015).

Ueda, Y.; Furuta, T.; Kawabata, T., Final-Stage Site-Selective Acylation for the Total Syntheses of Multifidosides A-C, *Angew. Chem. Int. Ed.*, **54,** 11966-11970 (2015).

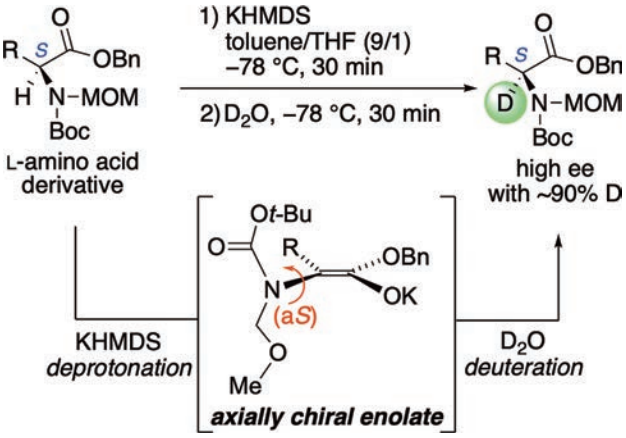
Synthesis of 4-Deoxy Pyranosides via Catalyst-Controlled Site-Selective Acylation Followed by SmI_2-Mediated Deacyloxylation

Deoxysugars have attracted increasing attention because of their biological importance. Their preparation usually required multi-step protection/deprotection sequences, starting from naturally abundant sugars because of the lack of the direct and site-selective manipulation of one of the multiple hydroxy groups of sugar derivatives. We have developed the catalyst which promotes site-selective acylation of the secondary C(4)-OH of glucopyranosides in the presence of the intrinsically more reactive primary C(6)-OH. The site-selectivity was controlled by the catalyst independent from intrinsic reactivity of the substrates; *i.e.*, *catalyst-controlled site-selectivity*. We report here concise synthesis of 4-deoxy pyranosides by reductive deacyloxylation of the 4-*O*-toluoylpyranoses obtained by catalyst-controlled site-selective introduction of the toluoyl group into pyranosides. A representative example of the present protocol includes the synthesis of a 4-deoxy-*N*-acetylglucosamine derivative, possessing inhibitory activity of vascularization, from naturally abundant glucosamine.



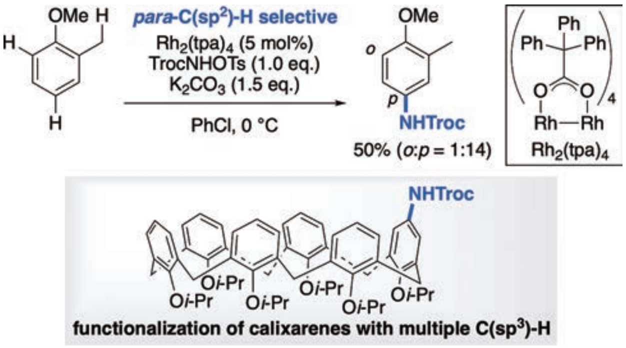
Direct Asymmetric Synthesis of α-Deuterated Amino Acid Derivatives via Memory of Chirality

α-Deuterated amino acids have been receiving increasing interests because they play critical roles in mechanistic studies of enzymatic actions and the studies on metabolism of medicinally important compounds. While various methods have been reported for their asymmetric synthesis, there have been no methods reported, in which the parent α-amino acids are employed as the sole source of chirality for the asymmetric induction. In the course of our study on asymmetric synthesis via memory of chirality (MOC), we found that optically active α-deuterated amino acids could be obtained directly from naturally abundant readily available parent amino acids. Treatment of *N*-MOM-*N*-Boc-substituted L-amino acid derivatives with potassium hexamethyldisilazide (KHMDS) at –78°C for 30 min, followed by addition of D_2O as a D source gave α-deuterated L-amino acid derivatives in retention of the configuration and in high ee with ~90% D incorporation. The asymmetric α-deuteration was expected to proceed via axially chiral enolates with a*S* configuration.



Intermolecular Chemo- and Regioselective C-H Amination of Alkoxyarenes Promoted by Dirhodium Nitrenoids

Arylamine motifs are privileged structural units for the development of functional materials and bioactive molecules. One of the most straightforward methods for their synthesis would involve $C(sp^2)$-H amination of the parent aromatics. We report here intermolecular $C(sp^2)$-H amination mediated by dirhodium nitrenoids. The reaction proceeded with oxygen-substituted arenes in a chemo- and regioselective manner. The aromatic $C(sp^2)$-H amination took place at the para position of the oxygen substituent, even in the presence of otherwise more reactive benzylic $C(sp^3)$-H bonds. The present method was successfully applied to the direct functionalization of calixarene derivative with multiple reactive $C(sp^3)$-H bonds.



Division of Synthetic Chemistry
– Advanced Inorganic Synthesis –

http://www.scl.kyoto-u.ac.jp/~teranisi/index_E.html


Prof
TERANISHI, Toshiharu
(D Eng)


Assoc Prof
SAKAMOTO, Masanori
(D Eng)


Assist Prof
SATO, Ryota
(D Sc)


Program-Specific Assist Prof
SARUYAMA, Masaki
(D Sc)


Program-Specific Assist Prof
TRINH, Thang Thuy
(Ph D)


PD
KAWAWAKI, Tokuhisa
(D Eng)


PD
EGUCHI, Daichi
(D Sc)


PD
TAKAHATA, Ryo
(D Sc)


PD
LIU, Ming-Han
(Ph D)


PD
XUE, Songlin
(D Sc)

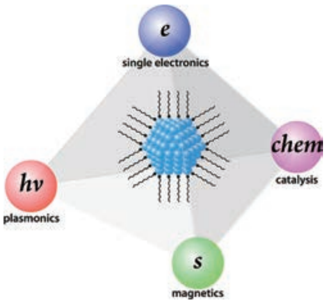

PD
LIAN, Zichao
(D Sc)

Students

KIM, Sungwon (D3)
MATSUMOTO, Kenshi (D3)
ZHANG, Jie (D2)
OKAMOTO, Yasuo (D1)
LI, Zhanzhao (D1)
SHAKUDO, Hikaru (M2)
WATANABE, Yuki (M2)
KANEKO, Ryota (M1)
GAO, Jingying (RS)

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

Selected Publications

Saruyama, M.; Kim, S.; Nishino, T.; Sakamoto, M.; Haruta, M.; Kurata, H.; Akiyama, S.; Yamada, T.; Domen, K.; Teranishi, T., Phase-Segregated $NiP_x@FeP_yO_z$ Core@Shell Nanoparticles: Ready-to-Use Nanocatalysts for Electro- and Photo-Catalytic Water Oxidation through in-situ Activation by Structural Transformation and Spontaneous Ligand Removal, *Chem. Sci.*, **9,** 4830-4836 (2018).

Lian, Z.; Sakamoto, M.; Matsunaga, H.; Vequizo, J. J. M.; Yamakata, A.; Haruta, M.; Kurata, H.; Teranishi, T., Near Infrared Light Induced Plasmonic Hot Hole Transfer at a Nano-Heterointerface, *Nat. Commun.*, **9,** 2314 (2018).

Eguchi, D.; Sakamoto, M.; Teranishi, T., Ligand Effect on the Catalytic Activity of Gold Clusters in the Electrochemical Hydrogen Evolution Reaction, *Chem. Sci.*, **9,** 261-265 (2018).

Near Infrared Light Induced Plasmonic Hot Hole Transfer at a Nano-Heterointerface

Localized surface plasmon resonance (LSPR)-induced photoenergy conversion is among the great challenges causing a paradigm shift in both scientific fields and industry regarding solar-energy utilization. Although plasmonic materials have superior light-harvesting abilities, the low conversion efficiency caused by ultrafast relaxation of the hot carrier and charge recombination is a major drawback. Furthermore, the unclear behavior of hot holes becomes an obstacle for the comprehensive understanding of LSPR-induced carrier transfer.

Herein, we elucidate the LSPR-induced behavior of hot holes in plasmonic CuS NCs and CdS/CuS HNCs using time-resolved infrared (TR-IR) spectroscopy. We discover that a multi-step carrier transfer (plasmon-induced transit carrier transfer: PITCT) realized efficient hole transfer from the CuS phase to the CdS phase. Surprisingly, the PITCT of CdS/CuS HNCs achieves high quantum yields (19%) and long-lived charge separation (9.2 μs). Because ultrafast charge recombination is a major drawback of all plasmonic energy conversion systems, the PITCT mechanism proposes here should change the conventional consensus regarding LSPR-induced energy conversion.

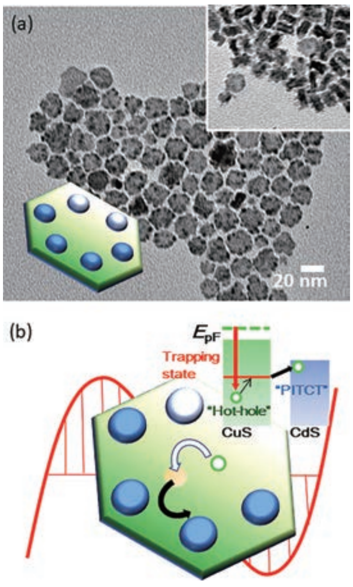


Figure 1. (a) TEM images of CdS/CuS HNCs. (b) Schematic illustration of PITCT (plasmon-induced transit carrier transfer) mechanims.

Phase-Segregated NiP$_x$@FeP$_y$O$_z$ Core@Shell Nanoparticles: Ready-to-Use Nanocatalysts for Electro- and Photo-Catalytic Water Oxidation

Production of H_2 and O_2 by efficient and sustainable electrolysis of water is important for the technology of noble clean energy such as solar-driven fuel generating system. In the water splitting reaction, the oxygen evolution reaction (OER) is considered to be bottle-neck because OER typically requires 4 electrons for O-O bond formation, which is a kinetically slow process. A high overpotential is required for OER in spite of using low abundance and high cost novel metals, such as Ir or Ru, which inhibit the water electrolysis device from the global scalability.

For the purpose of the creation of earth abundant and efficient electrocatalyst for OER, we synthesized nickel phosphide (NiP$_x$)@iron phosphate (FeP$_y$O$_z$) core@shell nanoparticles (NPs). NiP$_x$ -seed-mediated growth method allowed FeP$_y$O$_z$ to grow onto the NiP$_x$ NPs selectively (Figure 2a). NiP$_x$@FeP$_y$O$_z$ core@shell NP has crystalline NiP$_x$ core with sphere-with-rod morphology, and amorphous FeP$_y$O$_z$ shell. NiP$_x$@FeP$_y$O$_z$ NPs loaded carbon catalyst exhibited low overpotential of 0.28 V at 10 mA cm^{-2} in 0.1 M KOH solution. Furthermore, photoelectrochemical measurements showed that the photocurrent of BiVO$_4$ was greatly enhanced by simple deposition of NiP$_x$@FeP$_y$O$_z$ NPs on BiVO$_4$ electrode (Figure 2b). This NiP$_x$@FeP$_y$O$_z$ NPs can be used as ready-to-use OER catalyst without any post treatments such as annealing, because an in-situ transformation into Ni-Fe hydroxide active species. This feature is a considerable advantage of our catalytic NPs in the fabrication of large scale electro- and photocatalyst systems.

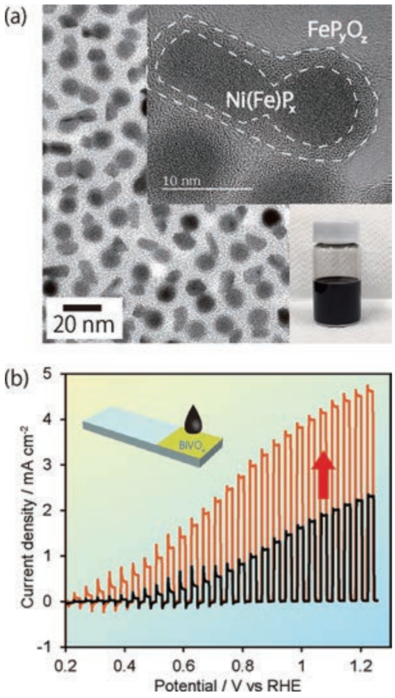


Figure 2. (a) TEM images of NiP$_x$@FeP$_y$O$_z$ core@shell NPs and the picture of their hexane solution. (b) Photo current measurement of water oxidation using (black) bare and (orange) NiP$_x$@FeP$_y$O$_z$ core@shell NPs deposited BiVO$_4$ photoanodes in 0.125 M $K_2B_4O_7$ electrolyte.

Division of Materials Chemistry
– Chemistry of Polymer Materials –

http://www.cpm.kuicr.kyoto-u.ac.jp/index_en.html


Prof
TSUJII, Yoshinobu
(D Eng)


Assoc Prof
OHNO, Kohji
(D Eng)


Assist Prof
SAKAKIBARA, Keita
(D Agr)


PD
EGUCHI, Hiroshi
(D Eng)

Assist Techn Staff
KINOSE, Yuji

Researchers (pt)
MORIKI, Yoshihito
NAKAJIMA, Yuki
NAKAMICHI, Kimiyo
SEO, Haruna
YANADA, Mizuho

Proj Res
MATSUKAWA, Kimihiro (D Eng)*

*Res of Kyoto Inst Technol

Students
SHIMIZU, Yoshihiko (D3)
HARAYAMA, Seiya (M2)
MURAJI, Koichi (M2)
NIWA, Ryota (M2)
ISHIDA, Hisayuki (M1)
OHNO, Haruhisa (M1)
TAKEDA, Yusuke (M1)
HAN, Yutong (RS)
DAI, Jingxian (RS)
OKUBO, Ryo (UG)
TORIBUCHI, Taito (UG)
YOSHIKAWA, Shuhei (UG)

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
Biointerface
Living Radical Polymerization
Hybrid Materials

Selected Publications
Tsujii, Y.; Nomura, Y.; Okayasu, K.; Gao, W.; Ohno, K.; Fukuda, T., AFM Studies on Microtribology of Concentrated Polymer Brushes in Solvents, *J. Phys.: Conf. Ser.*, **184,** 012031 (2009).

Arita, T.; Kayama, Y.; Ohno, K.; Tsujii, Y.; Fukuda, T., High-Pressure Atom Transfer Radical Polymerization of Methyl Methacrylate for Well-Defined Ultrahigh Molecular-Weight Polymers, *Polymer*, **49,** 2426-2429 (2008).

Tsujii, Y.; Ohno, K.; Yamamoto, S.; Goto, A.; Fukuda, T., Structure and Properties of High-Density Polymer Brushes Prepared by Surface-Initiated Living Radical Polymerization, *Adv. Polym. Sci.*, **197,** 1-45 (2006).

Ohno, K.; Morinaga, T.; Takeno, S.; Tsujii, Y.; Fukuda, T., Suspension of Silica Particles Grafted with Concentrated Polymer Brush: Effects of Graft Chain Length on Brush Layer Thickness and Colloidal Crystallization, *Macromolecules*, **40,** 9143-9150 (2007).

Ohno, K.; Morinaga, T.; Koh, K.; Tsujii, Y.; Fukuda, T., Synthesis of Monodisperse Silica Particles Coated with Well-Defined, High-Density Polymer Brushes by Surface-Initiated Atom Transfer Radical Polymerization, *Macromolecules*, **38,** 2137-2147 (2005).

Lubrication Properties of Concentrated Polymer Brushes Revealed by Optical Interferometry Method

Fabrication of polymer brushes onto materials is one of attractive methods to modify their surface properties. Especially, polymer brushes with high graft density, which are called as concentrated polymer brushes (CPBs), exhibits various unique features. For example, we have reported the excellent tribological properties of CPBs in their swollen state such as an extremely low friction characteristic, and its potentials as novel tribomaterials so far. In order to obtain further insights into the lubrication and wear mechanisms of CPBs, detailed observations of the contact point under sliding condition should be needed. Herein, we have investigated the tribological properties of CPBs by means of the simultaneous measurements of the film thickness of lubrication layer and friction coefficient, which were determined *in situ* by optical interferometry and tribological sliding test, respectively. The experimental setup of ball-on-disc sliding test is illustrated in Figure 1a. A Newton's ring formed at a contact point of a glass lens and a CPB-fabricated silicon substrate was recorded with a digital microscope, and the gap profile between two surfaces was calculated from this interferogram (Figure 1b and 1c). This experiment was carried out at the sliding speed from 2.8 to 100 mm/s, and as a result hydrodynamically formed lubrication layer was observed at the all of the test conditions. Interestingly, the thickness of this lubrication layer depends on the dry thickness of the CPBs fabricated on the substrate, which suggested that CPBs plays a critical role to realize an extremely low lubrication surface. Detailed lubrication mechanisms are currently being investigated by using other analytical methods such as an atomic force microscopy and a rheological measurement.

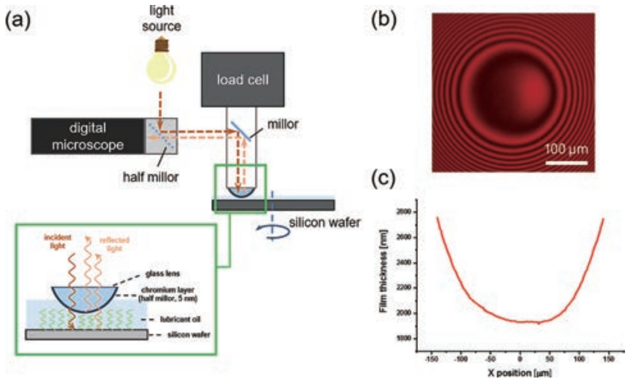


Figure 1. (a) Schematic diagram of an experimental set-up. (b) A photo image of the Newton's ring formed at the contact point. (c) A gap profile between a lens and a CPB-fabricated silicon substrate.

Versatile Preparation of Surface-Skinless Particles of Epoxy Resin-Based Monoliths Using a Well-Defined Diblock Copolymer Surfactant

Epoxy resin-based monoliths, possessing bicontinuous structure that consists of a porous channel and a resin skeleton, have a broad range of applications such as chromatography; however, the preparation of spherical particles has been limited so far. This is the first report on a versatile and facile preparation method for surface-skinless monolithic particles with micrometer diameters by polymerization-induced phase separation in an oil-in-oil emulsion system (Figure 2). The key to success was the addition of a well-defined block copolymer surfactant, compatible for both the dispersed and continuous phases in suspension polymerization. In essence, the volume ratio and length of the block copolymers were crucial to controlling the stability of emulsion and the suppression of the unwanted skin layer on the surface of the produced particles. The surface-skinless monolithic particles could be further applied to flow-through particles, which are promising for chromatography and preparative applications. The present work thus represents a new direction for versatile and large-scale preparation of monolithic particles, including silicates and polyacrylates, with several surface properties.

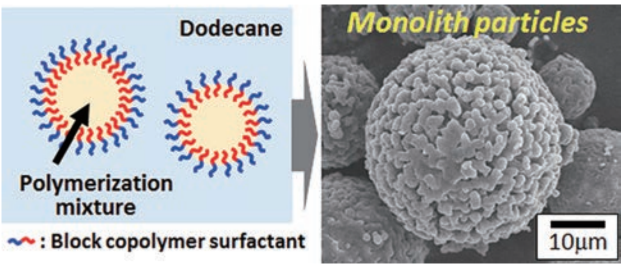


Figure 2. Preparation of epoxy resin-based monolithic particles.

Division of Materials Chemistry
– Polymer Controlled Synthesis –

http://os.kuicr.kyoto-u.ac.jp/index.html


Prof
YAMAGO, Shigeru
(D Sc)


Assoc Prof
TOSAKA, Masatoshi
(D Eng)


Assist Prof
KAYAHARA, Eiichi
(D Eng)


Assist Prof
HASHIMOTO, Sigma
(D Eng)


PD
LI, Wenjuan
(Ph D)

Program-Specific Res

FUJITA, Takehiro

Students

LU, Yangtian (D3)
SUN, Liansheng (D3)
KONO, Taro (D3)
KOBAYASHI, Go (D3)
FAN, Weijia (D3)
PARK, Beomsu (D3)
LI, Xiaopei (D1)
SHIGEKI, Erika (M2)
NAKANO, Masaya (M2)
YAMAMOTO, Koji (M2)
LIN, Yiming (M2)
IMAMURA, Yuji (M1)
JIANG, Yuhan (M1)
ONOZUKA, Kota (M1)
MATSUO, Shuntaro (M1)
HE, Yu Zhong (RS)
LIN, Hsuan-Yu (RS)
UCHIDA, Yukihiro (UG)
ONCHI, Koshiro (UG)
KUMAGAWA, Daiki (UG)
FUTOI, Kazutaka (UG)

Guest Res Assoc

BALL, Melissa Lynne (Ph D) Colombia University, U.S.A., 19 November–18 December

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

Selected Publications

Fan, W.; Tosaka, M.; Yamago, S.; Cunningham, M. F., Living Ab Initio Emulsion Polymerization of Methyl Methacrylate in Water Using a Water Soluble Organotellurium Chain Transfer Agent under Thermal and Photochemical Conditions, *Angew. Chem. Int. Ed.*, **57,** 962-966 (2018).

Kayahara, E.; Hayashi, T.; Takeuchi, K.; Ozawa, F.; Ashida, K.; Ogoshi, S.; Yamago, S., Strain-Induced Double Carbon-Carbon Bond Activations of Cycloparaphenylenes (CPPs) by a Platinum Complex and Its Application for the Synthesis of Cyclic Diketones, *Angew. Chem. Int. Ed.*, **57,** 11418-11421 (2018).

Topics

Synthesis of Structurally Controlled Hyperbranched Polymers Using a Monomer Having Hierarchical Reactivity

Hyperbranched polymers (HBPs) have attracted significant attention because of their characteristic topological structure associated with their unique physical properties compared with those of the corresponding linear polymers. Dendrimers are the most structurally controlled HBPs. However, the necessity of a stepwise synthesis have significantly limited their applications in materials science. Several methods have been developed to synthesize HBPs by a one-step procedure, as exemplified by the use of AB_2 monomers and AB' inimers under condensation and self-condensing vinyl polymerization conditions. However, none of these methods provides structurally controlled HBPs over the three-dimensional (3D) structure, i.e., molecular weight, dispersity, number of branching points, branching density, and chain-end functionalities, except under special conditions. We introduced a monomer design concept involving two functional groups with hierarchical reactivity and demonstrated the controlled synthesis of dendritic HBPs over the 3D structure by the copolymerization of the designed monomer and acrylates under living radical polymerization conditions.

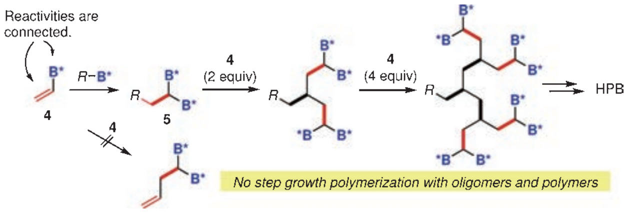


Figure 1. Scheme for the synthesis of structurally controlled hyperbranched polymer.

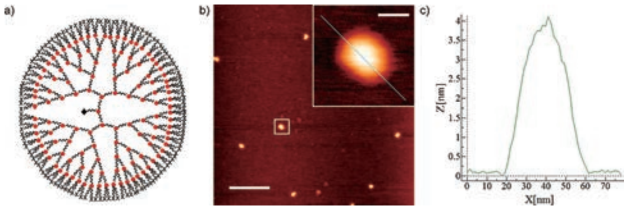


Figure 2. Structure and AFM image of the dendritic hyperbranched polymer.

Strain-Induced Double Carbon–Carbon Bond Activations of Cycloparaphenylenes by a Platinum Complex: Application to the Synthesis of Cyclic Diketones

The carbon–carbon (C−C) bond activation of [n]cycloparaphenylenes ([n]CPPs) by a transition-metal complex was achieved. The Pt^0 complex $Pt(PPh_3)_4$ regioselectively cleaves two C−C σ bonds of [5]CPP and [6]CPP to give cyclic dinuclear platinum complexes in high yields. Theoretical calculations revealed that the relief of ring strain drives the reaction. The cyclic complex was further transformed into a cyclic diketone by using a CO insertion reaction. The mechanism of the formation of the dinuclear platinum(0) complexes was elucidated with DFT calculations, which suggested a stepwise pathway. Both steps of forming the mononuclear platinum complex and the cyclic dinuclear complex were found to be highly exothermic and have low activation energies. The DFT studies also explained regioselectivity of the reaction. The activation of the more strained [5]CPP was significantly faster compared with that of less strained [6]CPP. Consistent with the proposed strain-induced process, larger CPPs, such as [7]CPP and [8]CPP, did not show reactivity.

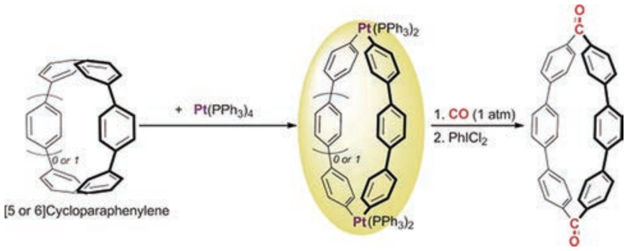


Figure 3. Carbon–Carbon Bond Activations of Cycloparaphenylenes by a Platinum Complex.

Division of Materials Chemistry
– Inorganic Photonics Materials –

http://mizuochilab.kuicr.kyoto-u.ac.jp/indexE.html


Prof
MIZUOCHI, Norikazu
(D Sc)


Assist Prof
MORISHITA, Hiroki
(D Eng)


Assist Prof
FUJIWARA, Masanori
(D Sc)


Program-Specific Res
HERBSCHLEB, Ernst David
(Ph D)


Program-Specific Res
OHKI, Izuru
(D Bioscience)


Res (pt)
HAYASHI, Kan
(D Sc)

Students

ASHIDA, Takaki (M2)
ISHIMOTO, Shintaro (M2)
NISHIKAWA, Tetsuri (M1)
WATANABE, Akira (M1)
YAMASHITA, Syungo (M1)
NAKAMURA, Masaya (UG)
MORITA, Kouki (UG)

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
Quantum Sensing
Quantum Materials
Quantum Information Science
NV Center

Selected Publications

Doi, Y.; Fukui, T.; Kato, H.; Makino, T.; Yamasaki, S.; Tashima, T.; Morishita, H.; Miwa, S.; Jelezko, F.; Suzuki, Y.; Mizuochi, N., Pure Negatively Charged State of NV Center in n-Type Diamond, *Phys. Rev. B*, **93,** [081203(R)-1]-[081203(R)-6] (2016).

Fukui, T.; Doi, Y.; Miyazaki, T.; Miyamoto, R.; Kato, H.; Matsumoto, T.; Makino, T.; Yamasaki, S.; Morimoto, R.; Tokuda, N.; Hatano, M.; Sakagawa, Y.; Morishita, H.; Tashima, T.; Miwa, S.; Suzuki, Y.; Mizuochi, N., Perfect Selective Alignment of Nitrogen-Vacancy Center in Diamond, *Appl. Phys. Express*, **7,** [55201-1]-[55201-4] (2014).

Mizuochi, N.; Makino, T.; Kato, H.; Takeuchi, D.; Ogura, M.; Okushi, H.; Nothaft, M.; Neumann, P.; Gali, A.; Jelezko, F.; Wrachtrup, J.; Yamasaki, S., Electrically Driven Single Photon Source at Room Temperature in Diamond, *Nature Photonics*, **6,** 299-303 (2012).

Zhu, X.; Saito, S.; Kemp, A.; Kakuyanagi, K.; Karimoto, S.; Nakano, H.; Munro, W. J.; Tokura, Y.; Everitt, M. S.; Nemoto, K.; Kasu, M.; Mizuochi, N.; Semba, K., Coherent Coupling of a Superconducting Flux-Qubit to an Electron Spin Ensemble in Diamond, *Nature*, **478,** 221-224 (2011).

Neumann, P.; Mizuochi, N.; Rempp, F.; Hemmer, P.; Watanabe, H.; Yamasaki, S.; Jacques, V.; Gaebel, T.; Jelezko, F.; Wrachtrup, J., Multipartite Entanglement among Single Spins in Diamond, *Science*, **320,** 1326-1329 (2008).

Optimization of Temperature Sensitivity Using the Optically Detected Magnetic Resonance Spectrum of a Nitrogen-vacancy Center Ensemble

Temperature sensing with nitrogen-vacancy (NV) centers using quantum techniques is very promising and further development is expected. Recently, the optically detected magnetic resonance (ODMR) spectrum of a high-density ensemble of the NV centers was reproduced with noise parameters [inhomogeneous magnetic field, inhomogeneous strain (electric field) distribution, and homogeneous broadening] of the NV center ensemble. In this study, we use ODMR to estimate the noise parameters of the NV centers in several diamonds. These parameters strongly depend on the spin concentration. This knowledge is then applied to theoretically predict the temperature sensitivity. Using the diffraction-limited volume of 0.1 µm^3, which is the typical limit in confocal microscopy, the optimal sensitivity is estimated to be around 0.76 mK/$\sqrt{\text{Hz}}$ with an NV center concentration of 5.0×10^{17}/cm^3 as shown in Figure 1. This sensitivity is much higher than previously reported sensitivities, demonstrating the excellent potential of temperature sensing with NV centers.

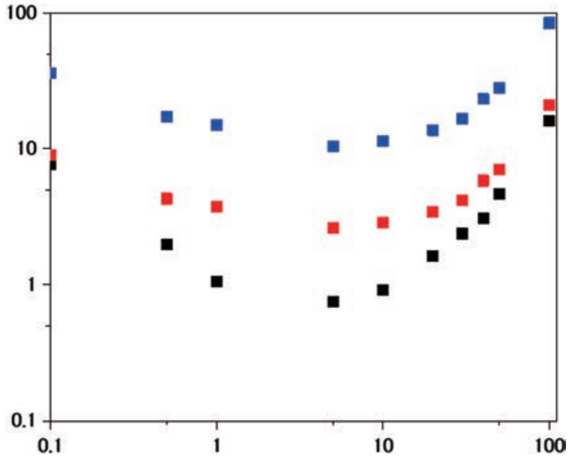


Figure 1. Numerically estimated sensitivity with respect to the NV concentration with a low microwave power ODMR. Black squares are the sensitivity of the approach using the sharp dip without an applied magnetic field. Red squares are the sensitivity using the peak structure observed in the normal ODMR under an external magnetic field exactly applied along the [001] direction. Blue squares show the results using the peak structure observed in the normal ODMR with an arbitrary direction of the magnetic field and the ODMR signal of only one of four NV axes is measured.

Engineering of Fermi Level by *nin* Diamond Junction for Control of Charge States of NV Centers

Charge-state control of NV centers in diamond is very important toward its application, because the NV centers undergo stochastic charge-state transitions between the negative charge state (NV$^-$) and the neutral charge state (NV^0) of the NV center upon illumination. In this letter, engineering of the Fermi level by a *nin* diamond junction was demonstrated for control of the charge state of the NV centers in the intrinsic (*i*) layer region as shown in Figure 2. By changing the size (*d*) of the *i*-layer region between the phosphorus-doped *n*-type layer regions (*nin*) from 2 µm to 10 µm, we realized the gradual change of the NV$^-$ charge-state population in the *i*-layer region from 60% to 80% under 532 nm excitation, which can be attributed to the band bending in the *i*-layer region as shown in Figure 3. Also, we quantitatively simulated the changes of the Fermi level in the *i*-layer region depending on *d* with various concentrations of impurities in the *i*-layer region.

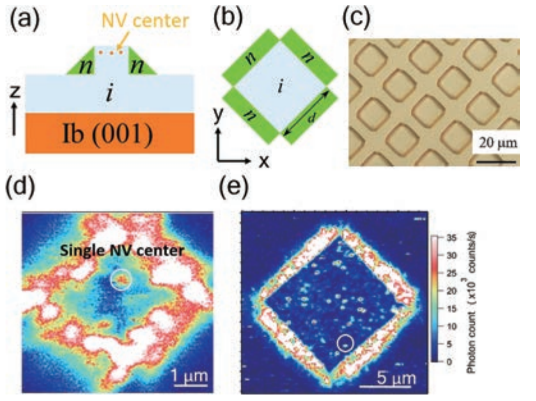


Figure 2. (a) Schematic illustration of the *nin* diamond junction in the *xy*-plane and in the (b) *z*-plane. (c) Optical microscope image of the *nin* diamond. (d) Scanning confocal microscope images of the mesa structures of *d* = 2 µm and (e) *d* = 10 µm.

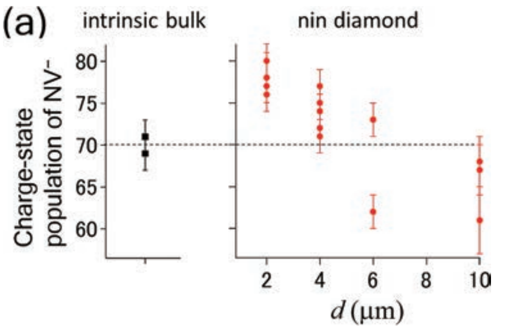


Figure 3. The dependence of the charge-state population of NV$^-$ on *d*. As reference, on the left, the estimate for the population in intrinsic bulk diamond is shown.

Division of Materials Chemistry
– Nanospintronics –

http://www.scl.kyoto-u.ac.jp/~onoweb/


Prof
ONO, Teruo
(D Sc)


Assoc Prof
MORIYAMA, Takahiro
(Ph D)


Assist Prof
SHIOTA, Yoichi
(D Eng)


PD
KIM, Duck-Ho
(Ph D)


PD
FUJIMOTO, Junji
(D Sc)

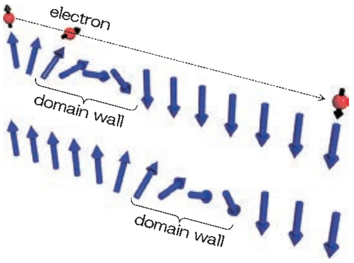
Students

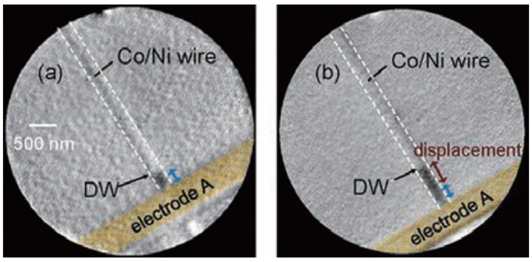
HAM, Wooseung (D3)
MIZUNO, Hayato (D3)
ANDO, Fuyuki (D2)
OKUNO, Takaya (D2)
ODA, Kento (D2)
NISHIMURA, Tomoe (D2)
ISHIBASHI, Mio (D1)
HIRATA, Yushou (D1)
LI, Tian (D1)
IINO, Tatsuya (M2)
IKEBUCHI, Tetsuya (M2)
KASUKAWA, Shuhei (M2)
IWAKI, Hiroyuki (M1)
FUNADA, Shinsaku (M1)

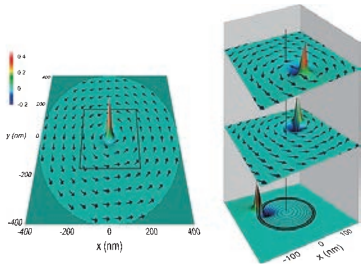
Scope of Research

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







Selected Publications

Moriyama, T.; Zhou, W.; Seki, T.; Takanashi, K.; Ono, T., Spin-Orbit-Torque Memory Operation of Synthetic Antiferromagnets, *Phys. Rev. Lett.*, **121,** 167202 (2018).
Moriyama, T.; Oda, K.; Ohkochi, T.; Kimata, M.; Ono, T., Spin Torque Control of Antiferromagnetic Moments in NiO, *Sci. Rep.*, **8,** 14167 (2018).
Kim, S.; Ueda, K.; Go, G.; Jang, P.; Lee, K.; Belabbes, A.; Manchon, A.; Suzuki, M.; Kotani, Y.; Nakamura, T.; Nakamura, K.; Koyama, T.; Chiba, D.; Yamada, T. K.; Kim, D.; Moriyama, T.; Kim, K.; Ono, T., Correlation of the Dzyaloshinskii-Moriya Interaction with Heisenberg Exchange and Orbital Asphericity, *Nat. Commun.*, **9,** 1648 (2018).
Yamada, T. K.; Suzuki, M.; Pradipto, A.; Koyama, T.; Kim, S.; Kim, K.; Ono, S.; Taniguchi, T.; Mizuno, H.; Ando, F.; Oda, K.; Kakizakai, H.; Moriyama, T.; Nakamura, K.; Chiba, D.; Ono, T., Microscopic Investigation into the Electric Field Effect on Proximity-Induced Magnetism in Pt, *Phys. Rev. Lett.*, **120,** 157203 (2018).
Baltz, V.; Manchon, A.; Tsoi, M.; Moriyama, T.; Ono, T., Antiferromagnetic Spintronics, *Rev. of Mod. Phys.*, **90,** 015005 (2018).

Antiferromagnetic Memory That Cannot Be Written by a Magnetic Field but by a Flow of Electron Spins

Conventional magnetic data storages, such as Hard disk drives (HDDs) and Magnetic random access memory (MRAM), traditionally use ferromagnets to record the information by flipping the macroscopic magnetic moments. However, as shown in Figure 1(a), a dipole field (or stray field) from the ferromagnets ultimately invokes the bit interference and prevents the information bit from packing closely. Antiferromagnets are another class of magnetic materials which have microscopic magnetic moments but they are coupled in opposite directions. Therefore, antiferromagnets have no net magnetic moment and do not produce any stray field or respond to an external magnetic field. By making use of these properties of antiferromagnets, one could make an extremely dense magnetic memory, which can be an important breakthrough for information storages. In this work, we showed the demonstration of a sequential antiferromagnetic memory operation with a spin-orbit-torque write, by the spin Hall effect, and a resistive read in the CoGd synthetic antiferromagnetic bits, in which we reveal the distinct differences in the spin-orbit-torque- and field-induced switching mechanisms of the antiferromagnetic moment. As shown in Figures (b)(c), the memory states (the Hall resistances) are altered by spin-orbit-torque but are not influenced by the external field. We, therefore, succeeded in demonstrating the antiferromagnetic memory that cannot be written by a magnetic field but by a flow of electron spins.

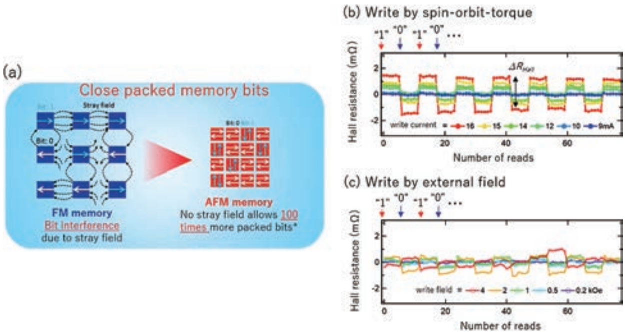


Figure 1. (a) Comparison between ferromagnetic bits and antiferromagnetic bits in terms of memory bit density. (b) After each write (“0”, “1”) by a spin-orbit-torque, the memory states were read by the Hall resistance. (c) After each write (“0”, “1”) by an external field, the memory states were read by the Hall resistance.

Modulation of the Magnetic Domain Size Induced by an Electric Field

The electric field (EF) control of magnetism has intensively investigated because of its potential importance for the reduction of power consumption in magnetic storage devices. In the past few years, we have been focusing on the electric field modulation of the magnetic anisotropy and the Curie temperature in magnetic thin films. However, the microscopic mechanism of why those magnetic properties change with an electric field was not clear in spite of several theoretical suggestions. In this work, we particularly focused on the configuration of the magnetic domains upon the application of the electric field (see Figure 2(a) for the detail measurement setup). With the electric field of ±10 V, we observed the significant change in the domain size (Figure 2(b)). Detail analyses on the modification of the magnetic domain size revealed that it is the exchange interaction that is modulated with the electric field and is changing about 50% with ±10 V. Our results suggest that the EF control of the magnetism is mainly driven by the modification of the exchange interaction which is a fundamental measure determining the magnetic interaction between microscopic spins.

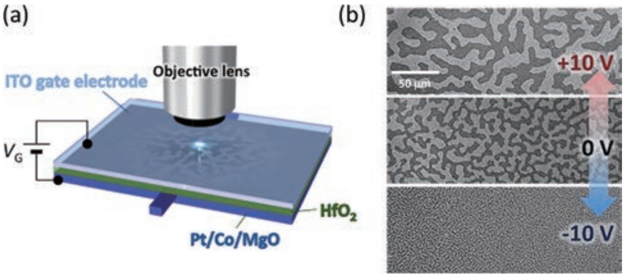


Figure 2. (a) Schematic illustration of the experimental setup (b) Modulation of the magnetic domain size with the electric field of ±10 V.

Division of Biochemistry
– Biofunctional Design-Chemistry –

http://www.scl.kyoto-u.ac.jp/~bfdc/index.html


Prof
FUTAKI, Shiroh
(D Pharm Sc)


Senior Lect
IMANISHI, Miki
(D Pharm Sc)


Assist Prof
KAWANO, Kenichi
(D Pharm Sc)

Students

AKISHIBA, Misao (D3)
SHINODA, Kouki (D3)
MASUDA, Toshihiro (D2)
ARAFILES, Jan Vincent V. (D2)
SAKAMOTO, Kentarou (D1)
HAYASHI, Syuhei (M2)
OGUSHI, Masaya (M2)
SAKAI, Takayuki (M2)
TAMEMOTO, Naoki (M2)
HSU, Wei-Yuan (M1)
NISHIMURA, Motoki (M1)
NOMURA, Yohei (M1)
SHINGA, Kenta (M1)
SUGIMOTO, Misaki (M1)
IWATA, Takahiro (UG)
KUROKI, Kakeru (UG)
NAGANO, Yuki (UG)

Scope of Research

The ultimate goal of our research is the regulation of cellular functions using 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 binding modes of zinc finger proteins and TALEs, and design of artificial transcription factors with various DNA binding specificities, 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

Selected Publications

Akishiba, M.; Takeuchi, T.; Kawaguchi, Y.; Sakamoto, K.; Yu, H. H.; Nakase, I.; Takatani-Nakase, T.; Madani, F.; Graslund, A.; Futaki, S., Cytosolic Antibody Delivery by Lipid-Sensitive Endosomolytic Peptide, *Nat. Chem.*, **9,** 751-761 (2017).

Murayama, T.; Masuda, T.; Afonin, S.; Kawano, K.; Takatani-Nakase, T.; Ida, H.; Takahashi, Y.; Fukuma, T.; Ulrich, A. S.; Futaki, S., Loosening of Lipid Packing Promotes Oligoarginine Entry into Cells, *Angew. Chem. Int. Ed. Engl.*, **56,** 7644-7647 (2017).

Azuma, Y.; Imai, H.; Kawaguchi, Y.; Nakase, I.; Kimura, H.; Futaki, S., Modular Redesign of a Cationic Lytic Peptide to Promote the Endosomal Escape of Biomacromolecules, *Angew. Chem. Int. Ed. Engl.*, **57,** 12771-12774 (2018).

Shinoda, K.; Tsuji, S.; Futaki, S.; Imanishi, M., Nested PUF Proteins: Extending Target RNA Elements for Gene Regulation, *Chembiochem*, **19,** 171-176 (2018).

Imanishi, M.; Tsuji, S.; Suda, A.; Futaki, S., Detection of N6-methyladenosine Based on the Methyl-sensitivity of MazF RNA Endonuclease, *Chem. Commun.*, **53,** 12930-12933 (2017).

Importance of Net Hydrophobicity in Cellular Uptake of All-hydrocarbon Stapled Peptides

All-hydrocarbon stapled peptides are a promising class of protein-protein interaction regulators, targetable to intracellular molecules of therapeutic potentials with high binding affinity and specificity. Cell permeation efficacy of these peptides is a critical determinant to obtain their bioactivity. However, the factors stimulating their cellular uptake remain open to dispute. Using six types of known all-hydrocarbon stapled peptides, we evaluated the effect of staple (or cross-link) formation on their cellular uptake. We found that cellular uptake of unstapled peptides (i.e., bearing olefinic non-natural amino acids for staple formation by olefin metathesis (Figure 1)) was higher than those of the corresponding stapled peptides. Additionally, insertion of these olefinic non-natural amino acids into peptide sequences *per se* was suggested to significantly increase the cellular uptake of peptides. Judged from retention times in high performance liquid chromatography, overall hydrophobicity of all the unstapled peptides was higher than stapled peptides, followed by the original peptides. There was no tight correlation between the helical content and cellular uptake of these peptides. Therefore, as long as cell permeation abilities of the peptides concern, increase in overall hydrophobicity by the introduction of non-natural amino acids should be the key driver to promote cellular uptake, rather than structure stabilization by staple formation. Involvement of micropinocytosis, a form of fluid-phase endocytosis, was confirmed for the cellular uptake of all the six peptides.

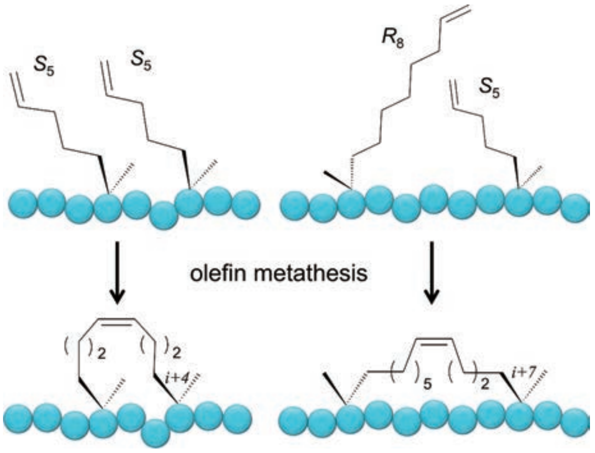


Figure 1. Strategy for stabilizing helical structure of peptides through ring-closing using olefin metathesis.

Development of a Simple Strategy to Detect Activities of N^6-methyladenosine Regulatory Enzymes

RNA methylation at the N6 position on adenine (m6A) is most prevalent internal RNA modification, which is mainly found at the RRACH sequence (R: G or A, H: U, A or C). The modification, which has been reported to regulate various physiological processes, is dynamic and reversible. It has been shown that FTO and ALKBH5 demethylate m6A and that METTL3 and METTL14 catalyze the methylation. To characterize these demethylases or methyltransferases and to find their inhibitors, it is required to develop new methods to easily detect their enzymatic activities. Here, we propose a convenient method to detect enzymatic activities of these demethylases and methyltransferases without using any specific apparatus or radioisotopes.

MazF is a bacterial toxin that plays an important role in growth regulation. MazF works as an endoribonuclease that specifically cleaves RNA at the 5'-end of ACA sequence. We found that MazF cleaved a single-stranded RNA fragment containing GGACA but not GG(m6A)CA by a conventional gel electrophoresis and a high-throughput FRET analysis (Figure 2). After being reacted with FTO or ALKBH5, the oligo RNA including an m6A was cleaved by MazF. The cleavage was inhibited by addition of known inhibitors of FTO or ALKBH5. In addition, the oligo RNA including a GGACA sequence was not cleaved by MazF after being reacted with the METTL3/METTL4 complex. These results indicate that the activities of both RNA demethylases and methylatransferases can be detected by this new method. Though the sequence is limited to "ACA", this method is easy to assay the enzymatic activities of RNA methylation/demethylation at the N6 position on adenine.

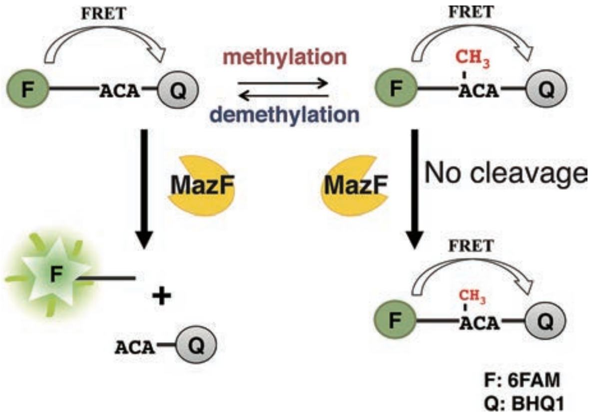


Figure 2. High-throughput detection of N^6-methyladenosine using an ACA-sequence specific MazF endoribonuclease.

Division of Biochemistry
– Chemistry of Molecular Biocatalysts –

http://www.scl.kyoto-u.ac.jp/~bunta/index-j.html

Prof
YAMAGUCHI, Shinjiro
(D Agr)

Assist Prof
WATANABE, Bunta
(D Agr)

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

Selected Publications

Watanabe, B.; Kirikae, H.; Koeduka, T.; Takeuchi, Y.; Asai, T.; Naito, Y.; Tokuoka, H.; Horoiwa, S.; Nakagawa, Y.; Shimizu, B.; Mizutani, M.; Hiratake, J., Synthesis and Inhibitory Activity of Mechanism-Based 4-Coumaroyl-CoA Ligase Inhibitors, *Bioorg. Med. Chem.*, **26,** 2466-2474 (2018).

Kuroha, T.; Nagai, K.; Gamuyao, R.; Wang, D. R.; Furuta, T.; Nakamori, M.; Kitaoka, T.; Adachi, K.; Minami, A.; Mori, Y.; Mashiguchi, K.; Seto, Y.; Yamaguchi, S.; Kojima, M.; Sakakibara, H.; Wu, J.; Ebana, K.; Mitsuda, N.; Ohme-Takagi, M.; Yanagisawa, S.; Yamasaki, M.; Yokoyama, R.; Nishitani, K.; Mochizuki, T.; Tamiya, G.; McCouch, S. R.; Ashikari, M., Ethylene-gibberellin Signaling Underlies Adaptation of Rice to Periodic Flooding, *Science*, **361,** 181-186 (2018).

Yao, J.; Mashiguchi, K.; Scaffidi, A.; Akatsu, T.; Melville, K. T.; Morita, R.; Morimoto, Y.; Smith, S. M.; Seto, Y.; Flematti, G. R.; Yamaguchi, S.; Waters, M. T., An Allelic Series at the *KARRIKIN INSENSITIVE 2* Locus of *Arabidopsis thaliana* Decouples Ligand Hydrolysis and Receptor Degradation from Downstream Signaling, *Plant J*., **96,** 75-89 (2018).

Fujikura, U.; Jing, R.; Hanada, A.; Takebayashi, Y.; Sakakibara, H.; Yamaguchi, S.; Kappel, C.; Lenhard, M., Variation in Splicing Efficiency Underlies Morphological Evolution in Capsella, *Dev. Cell*, **44,** 192-203 (2018).

Determination of a Key Residue of γ-Glutamyl Transpeptidase for Substrate Recognition

γ-Glutamyl transpeptidase (GGT) plays a central role in homeostasis of antioxidant tripeptide glutathione, and has been implicated in a vast array of physiological disorders. In this study, we synthesized a series of mechanism-based GGT inhibitors to probe electrostatic interactions between the acceptor site residues of GGT and substrates. Our chemical, enzymological, and molecular biological approaches revealed that 3-hydroxyphenylacetic acid is an excellent mimic of the cysteinylglycine moiety of glutathione, and Lys562 of human GGT strongly recognizes their negative charge on the carboxy group (Figure 1). We demonstrated that this interaction considerably enhances the human GGT specificity of our inhibitor named GGsTop. GGsTop exhibited no inhibitory activity at 10 mM on a representative member of glutamine-dependent amidotransferases essential for a wide range of biosynthetic pathway, and showed no cytotoxicity toward human fibroblasts and hepatic stellate cells up to 1 mM.

Substrate-Analog Fructosyl Peptide Oxidase Inhibitors

Fructosyl peptide oxidase (FPOX) is widely used in the area of diabetes diagnosis today. In this study, we designed and synthesized its substrate-analog inhibitors in order to unveil the substrate recognition mechanism of FPOX by X-ray diffraction analysis of enzyme-inhibitor co-crystals. Kinetic study revealed that our substrate analogs act as competitive inhibitors with K_i values ranging from 11.1 to 782 µM (Figure 2). Co-crystallization of the enzyme with our inhibitors in order to determine the three-dimensional structure of FPOX is now in progress.

Molecular Mechanism of Myocardin-Related Transcription Factor A Inhibitors

Myocardin-related transcription factor A (MRTF-A) plays a pivotal role in epidermal-msenchymal transition. Inhibition of its nuclear transport is regarded as one of the attractive therapeutic targets since MRTF-A is closely associated with cancer and tissue fibrosis. In this study, we revealed that CCG-1423, originally developed as a Rho inhibitor, binds to the nuclear localization signal of MRTF-A and inhibits its nuclear transport mediated by importin-α/β1 (Figure 3). We also demonstrated that CCG-1423 inhibits migration of melanoma cells triggered by MRTF-A activation, and the potency is affected by the stereochemistry of CCG-1423. The difference is elucidated by the binding manner of each stereoisomer to MRTF-A that speculated by a molecular modeling approach.

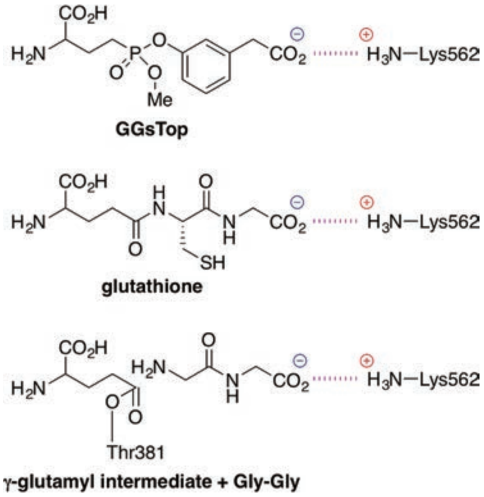


Figure 1. Proposed binding mode of GGsTop, glutathione, and acceptor substrate (Gly-Gly) to Lys562.

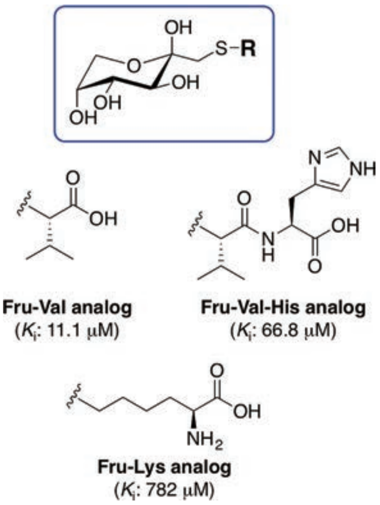


Figure 2. Chemical structures and inhibitory activity of FPOX inhibitors.

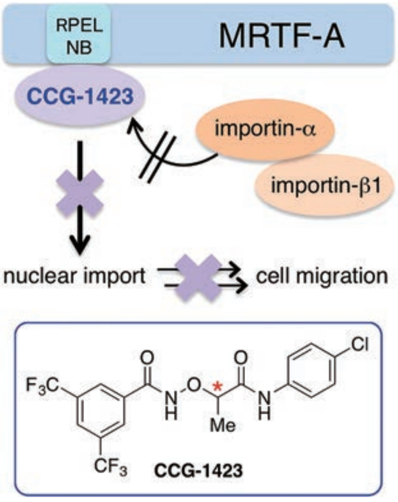


Figure 3. Molecular mechanism of MRTF-A inhibitor CCG-1423.

Division of Biochemistry
– Molecular Biology –

http://www.scl.kyoto-u.ac.jp/~molbio/index.html

Prof
AOYAMA, Takashi
(D Sc)

Assoc Prof
TSUGE, Tomohiko
(D Sc)

Assist Prof
FUJIWARA-KATO, Mariko
(D Agr)

Techn staff
YASUDA, Keiko

PD
FUJIWARA, Takashi
(D Agr)

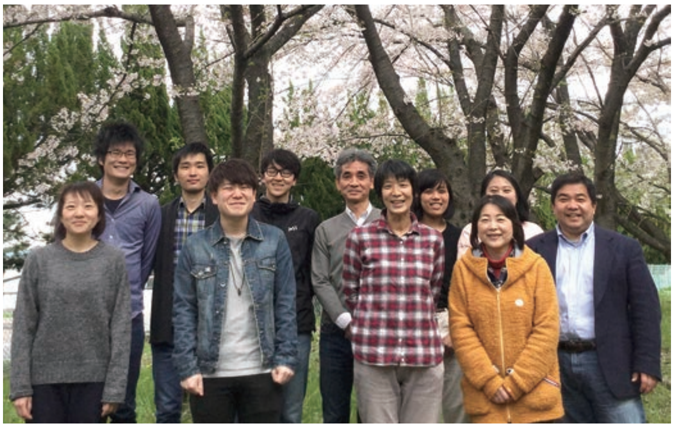
Students

ZHANG, Xiao-Juan (D3)
SHIMAMURA, Ryota (D3)
WATARI, Machiko (D3)
KURODA, Ryo (D2)
KISHIMOTO, Taichi (M2)
YAMADA, Koh (M1)

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
RNA
Signal Transduction
COP9 Signalosome



Selected Publications

Wu, Z.; Zhu, D.; Lin, X.; Miao, J.; Gu, L.; Deng, X.; Yang, Q.; Zhu, D.; Cao, X.; Tsuge, T.; Dean, C.; Aoyama, T.; Gu, H.; Qu, L.-J., RNA Binding Proteins RZ-1B and RZ-1C Play Critical Roles in Regulating Pre-mRNA Splicing and Gene Expression during Development in *Arabidopsis*, *Plant Cell*, **28,** 55-73 (2016).

Lin, Q.; Ohashi, Y.; Kato, M.; Tsuge, T.; Gu, H.; Qu, L.-J.; Aoyama, T., GLABRA2 Directly Suppresses Basic Helix-loop-helix Transcription Factor Genes with Diverse Functions in Root Hair Development, *Plant Cell*, **27,** 2894-2906 (2015).

Wada, Y.; Kusano, H.; Tsuge, T.; Aoyama, T., Phosphatidylinositol Phosphate 5-kinase Genes Respond to Phosphate Deficiency for Root Hair Elongation in *Arabidopsis thaliana*, *Plant J.*, **81,** 426-437 (2015).

Hayashi, K.; Nakamura, S.; Fukunaga, S.; Nishimura, T.; Jenness, M. K.; Murphy, A. S.; Motose, H.; Nozaki, H.; Furutani, M.; Aoyama, T., Auxin Transport Sites are Visualized *in Planta* Using Fluorescent Auxin Analogs, *Proc. Natl. Acad. Sci. USA*, **111,** 11557-11562 (2014).

Kato, M.; Aoyama, T.; Maeshima, M., The Ca^{2+}-binding Protein PCaP2 Located on the Plasma Membrane is Involved in Root Hair Development as a Possible Signal Transducer, *Plant J.*, **74,** 690-700 (2013).

Functional Differentiation of Phosphatidylinositol 4-Phosphate 5-Kinases in Higher Plants

Phosphatidylinositol 4,5-bisphosphate [PIP(4,5)P_2] acts as a signaling molecule and is involved in the regulation of a wide variety of intracellular events. PIP(4,5)P_2 modulates the functions of a variety of actin regulatory proteins and regulators of membrane traffic machinery from and to the plasma membrane by directly interacting with its effector proteins. In addition, PtdIns(4,5)P_2 signaling pathways are frequently connected to those of small GTPases belonging to the Rho and Arf families in their upstream and downstream cascades.

PtdIns(4,5)P_2 is expected to play a pivotal regulatory role in the polarized expansion of plant cells. Indeed, PtdIns(4,5)P_2 localizes to the apical plasma membrane and cytoplasmic space of not only root hairs but also pollen tubes. We are studying on signaling functions of PtdIns(4,5)P_2 and its producing enzymes, Phosphatidylinositol 4-phosphate 5-kinases (PIP5Ks), in the model plant *Arabidopsis thaliana*. *A. thaliana* encodes two type-A and nine type-B Phosphatidylinositol 4-phosphate 5-kinases (PIP5Ks), of which type-B PIP5Ks have a plant-specific structure with the MORN motif for membrane localization (Figure 1). We performed evolutionary analysis of type-B PIP5Ks using their amino-acid sequences available in public databases, and found that four clades of type-B PIP5Ks (I, II, III and IV, containing *Arabidopsis* PIP5K1-3, PIP5K4-6, PIP5K7-8, and PIP5K9, respectively) are conserved in angiosperms (Figure 2), suggesting that each clade is in charge of some essential function in plant development or survival in angiosperms. To elucidate biological functions of the each clade, we performed genetic analysis of *Arabidopsis thaliana* type-B PIP5K genes (*PIP5K1* to *9*). Although each single mutant of their genes resulted in only a mild phenotype in plant development if any, some of multiple mutants showed severe defects.

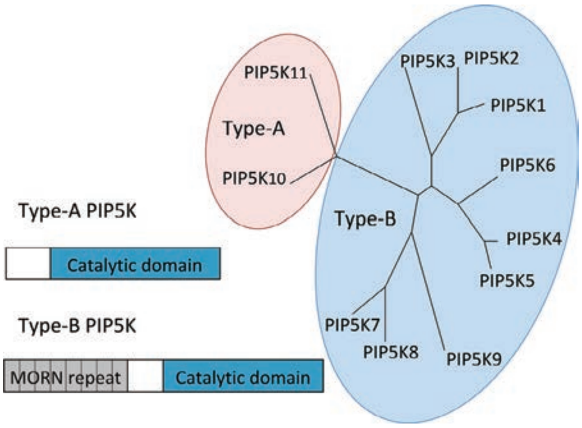


Figure 1. PIP5Ks Encoded in *A. thaliana*.
Domain structures and a phylogenic tree of *A. thaliana* type-A and type-B PIP5Ks are shown.

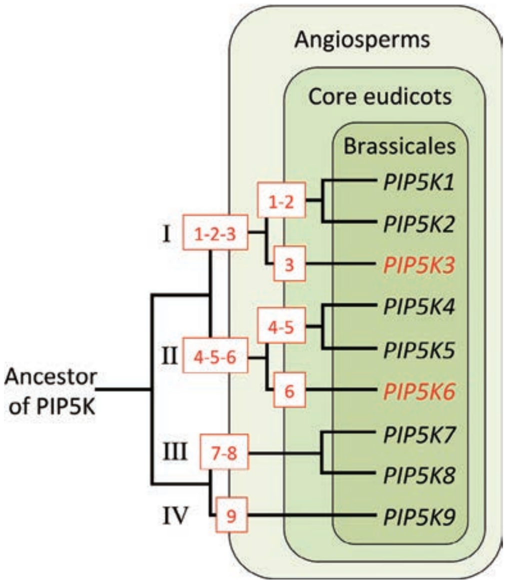


Figure 2. Schematic Phylogenic Tree of Angiosperm Type-B PIP5Ks.
A phylogenic tree of angiosperm type-B PIP5Ks is schematically shown. Four clades (I, II, III, and IV) are conserved in angiosperms.

To elucidate biological functions of clade-I PIP5Ks, we performed genetic analysis of *A. thaliana* type-B PIP5K genes using their multiple mutants. Seedlings of the *pip5k1pip5k2* double mutant showed a severe dwarfism (Figure 3), and their mature plants were infertile because of abnormal flower development. However, the dwarfism was not enhanced in *pip5k1pip5k2pip5k3* triple mutant seedlings. Root hair elongation was affected in both the *pip5k2* and *pip5k3* mutants, and the effect was enhanced in the *pip5k2pip5k3* double mutant. These results indicate that *PIP5K1* and *PIP5K2*, but not *PIP5K3*, redundantly have an essential function in plant growth and that *PIP5K2* and *PIP5K3* have a redundant function in root hair elongation.

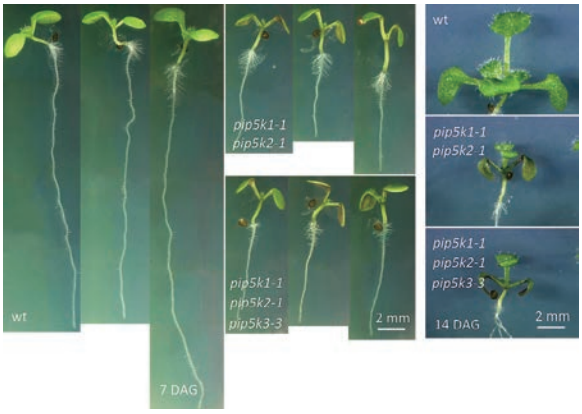


Figure 3. Phenotypes of *pip5k1*, *pip5k2*, and *pip5k3* Multiple Mutant Seedlings.
Seedlings of the wild type (wt), *pip5k1pip5k2* double, and *pip5k1pip5k2pip5k3* triple mutants 7 and 14 days after germination (DAG) are shown.

Division of Biochemistry

– Chemical Biology –

http://www.scl.kyoto-u.ac.jp/~uesugi/


Prof
UESUGI, Motonari
(D Pharm Sc)


Assoc Prof
SATO, Shinichi
(D Eng)


Senior Lect
PERRON, Amelie
(Ph D)


Assist Prof
TAKEMOTO, Yasushi
(D Eng)


Program-Specific Assist Prof
ABO, Masahiro
(D Pharm Sc)


PD
TAKASHIMA, Ippei
(D Pharm Sc)


PD
MAO, Di
(D Med Sc)


PD
TAKEMOTO, Misao
(D Eng)

Researcher (pt)

NAKAYAMA, Ayumi

Students

PUNZALAN, Louvy Lynn Calvelo (D3)
YATSUZUKA, Kenji (D3)
MENDOZA, Aileen de-Leon (D3)
JUNG, Yejin (D3)
NODA, Naotaka (D1)
HAKARIYA, Hayase (D1)
VU, Hue Thi (D1)
PINEDA ARISTA, Karla Mariel (M1)
ADO, Genyir (RS)
JIN, Shuyu (RS)

Guest Res Assoc

KRUNGCHANUCHAT, Saowalak Chiang Mai University, Thailand, 1 September 2018–28 February 2019

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 to open new avenues for small-molecule applications in a range of fields, including future concepts in drug discovery and use of small molecules for cell therapy.

KEYWORDS

Cell Therapy
Chemical Library
Chemical Biology
Chemical Genetics
Small Molecules

Selected Publications

Perron, A.; Nishikawa, Y.; Iwata, J.; Shimojo, H.; Takaya, J.; Kobayashi, K.; Imayoshi, I.; Mbenza, N. M.; Takenoya, M.; Kageyama, R.; Kodama, Y.; Uesugi, M., Small-molecule Screening Yields a Compound That Inhibits the Cancer-associated Transcription Factor Hes1 via the PHB2 Chaperone, *J. Biol. Chem.*, **293,** 8285-8294 (2018).

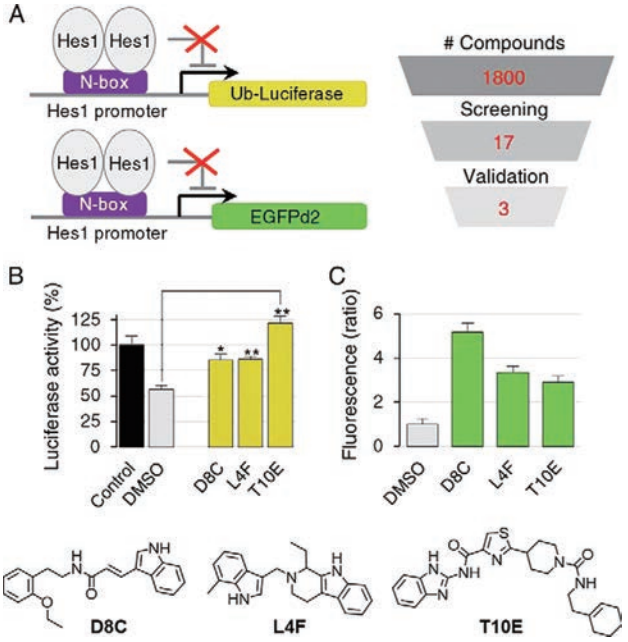
Mao, D.; Ando, S.; Sato, S.; Qin, Y.; Hirata, N.; Katsuda, Y.; Kawase, E.; Kuo, T. F.; Minami, I.; Shiba, Y.; Ueda, K.; Nakatsuji, N.; Uesugi, M., A Synthetic Hybrid Molecule for Selective Removal of Human Pluripotent Stem Cells from Cell Mixtures, *Angew. Chem. Int. Ed.*, **56,** 1765-1770 (2017).

Asano, L.; Watanabe, M.; Ryoden, Y.; Usuda, K.; Yamaguchi, T.; Khambu, B.; Takashima, M.; Sato, S.; Sakai, J.; Nagasawa, K.; Uesugi, M., Vitamin D Metabolite, 25-Hydroxyvitamin D, Regulates Lipid Metabolism by Inducing Degradation of SREBP/SCAP, *Cell Chemi. Biol.*, **24,** 207-217 (2017).

Katsuda, Y.; Sato, S.; Asano, L.; Morimura, Y.; Furuta, T.; Sugiyama, H.; Hagihara, M.; Uesugi, M., A Small Molecule That Represses Translation of G-quadruplex-containing mRNA, *J. Am. Chem. Soc.*, **138,** 9037-9040 (2016).

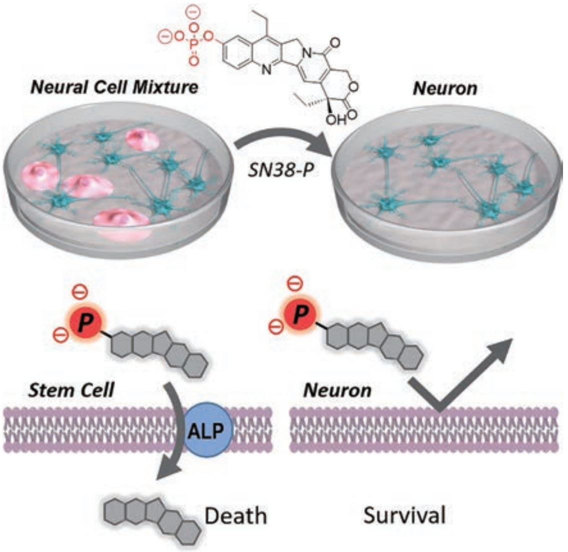
Small-molecule Screening Yields a Compound That Inhibits the Cancer-associated Transcription Factor Hes1 via the PHB2 Chaperone

The transcription factor Hes family basic helix-loop-helix transcription factor 1 (Hes1) is a downstream effector of Notch signaling and plays a crucial role in orchestrating developmental processes during the embryonic stage. However, its aberrant signaling in adulthood is linked to the pathogenesis of cancer. In the present study, we report the discovery of small organic molecules (JI051 and JI130) that impair the ability of Hes1 to repress transcription. Hes1 interacts with the transcriptional corepressor transducing-like enhancer of split 1 (TLE1) via an interaction domain comprising two tryptophan residues, prompting us to search a chemical library of 1,800 small molecules enriched for indole-like π-electron–rich pharmacophores for a compound that blocks Hes1-mediated transcriptional repression. This screening identified a lead compound whose extensive chemical modification to improve potency yielded JI051, which inhibited HEK293 cell proliferation with an EC50 of 0.3 μM. Unexpectedly, using immunomagnetic isolation and nanoscale LC-MS/MS, we found that JI051 does not bind TLE1 but instead interacts with prohibitin2 (PHB2), a cancer-associated protein chaperone. We also found that JI051 stabilizes PHB2's interaction with Hes1 outside the nucleus, inducing G2/Mcell-cyclearrest. Of note, JI051 dose-dependently reduced cell growth of the human pancreatic cancer cell line MIA PaCa-2, and JI130 treatment significantly reduced tumor volume in a murine pancreatic tumor xenograft model. These results suggest a previously unrecognized role for PHB2 in the regulation of Hes1 and may inform potential strategies for managing pancreatic cancer.



Chemical Decontamination of iPS Cell-derived Neural Cell Mixtures

This report describes the design and evaluation of phosphorylated 7-ethyl-10-hydroxycamptothecin (SN38-P), which selectively eliminates tumor-forming proliferative stem cells, including human induced pluripotent stem cells (hiPSCs) and neural stem cells, from iPSC-derived neural cell mixtures. Results of the present study demonstrate that simple phosphorylation of an anticancer drug can provide a safe, cost-effective, and chemically-defined tool for decontaminating hiPSC-derived neuron.



Division of Environmental Chemistry
– Molecular Materials Chemistry –

http://molmat.kuicr.kyoto-u.ac.jp/index-e.html


Prof
KAJI, Hironori
(D Eng)


Assist Prof
SHIZU, Katsuyuki
(D Eng)


Assist Prof
SUZUKI, Katsuaki
(D Human & Envirnmtl. Studies)


Techn Staff
OHMINE, Kyoko


Techn Staff
MAENO, Ayaka

Assist Techn Staff

YAMADA, Kyoko

Researcher

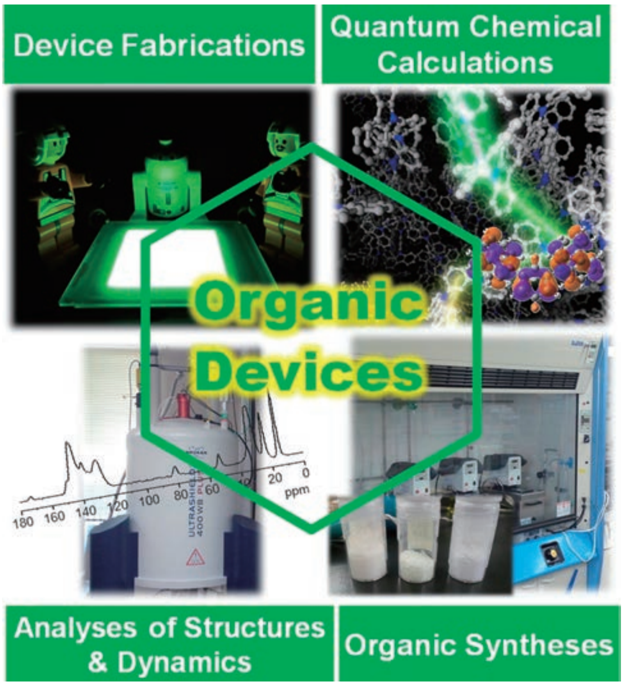
NAKAGAWA, Hiromichi (D Eng)

Students

KUBO, Shosei (D3)
WADA, Yoshimasa (D2)
WAKAYAMA, Rin (M2)
WAKISAKA, Yasuaki (M2)
SAWADA, Ayaka (M1)
MISONO, Tomoya (M1)
HU, Weizhe (RS)
MORIWAKI, Kazuki (UG)
SAKAI, Kahori (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
Organic Solar Cell
Solid-State NMR
Quantum Chemical Calculation
Amorphous Materials

Selected Publications

Kubo, S.; Kaji, H., Parameter-Free Multiscale Simulation Realising Quantitative Prediction of Hole and Electron Mobilities in Organic Amorphous System with Multiple Frontier Orbitals, *Sci. Rep.*, **8,** [5203-1]-[5203-9] (2018).

Sasabe, H.; Sato, R.; Suzuki, K.; Watanabe, Y.; Adachi, C.; Kaji, H.; Kido, J., Ultrahigh Power Efficiency Thermally Activated Delayed Fluorescent OLEDs by the Strategic Use of Electron-Transport Materials, *Adv. Optical Mater.*, **6,** [1800376-1]-[1800376-5] (2018).

Suzuki, F.; Kubo, S.; Fukushima, T.; Kaji, H., Effects of Structural and Energetic Disorders on Charge Transports in Crystal and Amorphous Organic Layers, *Sci. Rep.*, **8,** [5203-1]-[5203-9] (2018).

Wada, Y.; Kubo, S.; Kaji, H., Adamantyl Substitution Strategy for Realizing Solution-Processable Thermally Stable Deep-Blue Thermally Activated Delayed Fluorescence Materials, *Adv. Mater.*, **30,** [1705641-1]-[1705641-8] (2018).

Adamantyl Substitution Strategy for Realizing Solution-Processable Thermally Stable Deep-Blue Thermally Activated Delayed Fluorescence Materials

Highly efficient solution-processable emitters, especially deep-blue emitters, are greatly desired to develop low-cost and low-energy-consumption organic light-emitting diodes (OLEDs). A recently developed class of potentially metal-free emitters, thermally activated delayed fluorescence (TADF) materials, are promising candidates, but solution-processable TADF materials with efficient blue emissions are not well investigated. In this study, first the requirements for the design of efficient deep-blue TADF materials are clarified, on the basis of which, adamantyl-substituted TADF molecules are developed. The substitution not only endows high solubility and excellent thermal stability but also has a critical impact on the molecular orbitals, by pushing up the lowest unoccupied molecular orbital energy and triplet energy of the molecules. In the application to OLEDs, an external quantum efficiency (EQE) of 22.1% with blue emission having Commission Internationale de l'Eclairage (CIE) coordinates of (0.15, 0.19) is realized. A much deeper blue emission with CIE (0.15, 0.13) is also achieved, with an EQE of 11.2%. These efficiencies are the best yet among solution-processed TADF OLEDs of CIE y < 0.20 and y < 0.15, as far as known. This work demonstrates the validity of adamantyl substitution and paves a pathway for straightforward realization of solution-processable efficient deep-blue TADF emitters.

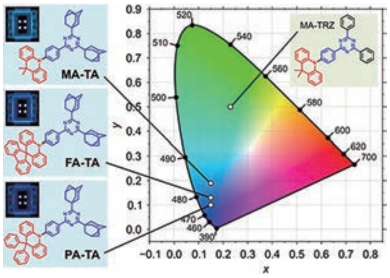


Figure 1. Molecular structures of MA-TA, FA-TA, and PA-TA, and their electroluminescence properties.

Effects of Structural and Energetic Disorders on Charge Transports in Crystal and Amorphous Organic Layers

Understanding charge transports in organic films is important for both fundamental science and practical applications. Here, contributions of off-diagonal (structural) and diagonal (energetic) disorders to charge transports were clarified using molecular-based multiscale simulation. These disorders, important for understanding charge transport in organic systems, are investigated by comparing crystal and amorphous aggregates of N,N'-diphenyl-N,N'-bis(1-naphthyl)-1,1'-biphenyl-4,4'-diamine (NPD). Although NPD has been used as a hole transport material, it also exhibits comparable electron mobility experimentally. The experimental mobility and its electric field dependence in amorphous layers were reasonably reproduced by the multiscale simulation, confirming the electron transport properties of NPD. We assumed that the structural disorder would lower mobilities; however, the mobilities were found to be independent of the degree of structural disorder. Energetic disorder markedly lowered charge mobility instead. Charge migration in crystals was dominated by maximum electronic coupling pairs, whereas small electronic coupling pairs significantly contributed to charge transport in amorphous aggregate.

Parameter-Free Multiscale Simulation Realising Quantitative Prediction of Hole and Electron Mobilities in Organic Amorphous System with Multiple Frontier Orbitals

In amorphous organic semiconducting systems, hole and electron transfer has been considered to occur based on the overlap of highest occupied molecular orbitals (HOMOs) and that of lowest unoccupied molecular orbitals (LUMOs) between two adjacent molecules, respectively. Other molecular orbitals (MOs), HOMO−1, HOMO−2, ... and LUMO+1, LUMO+2, ..., have been neglected in charge transport calculations. However, these MOs could potentially contribute to charge transport. In this study, our multiscale simulations show that carriers are effectively transported not only via HOMOs or LUMOs but also via other MOs when the MOs are close in energy. Because these multiple MOs are active in charge transports, here we call them multiple frontier orbitals. Molecules with multiple frontier orbitals are found to possess high carrier mobility. The findings in this study provide guidelines to aid design of materials with excellent charge transport properties.

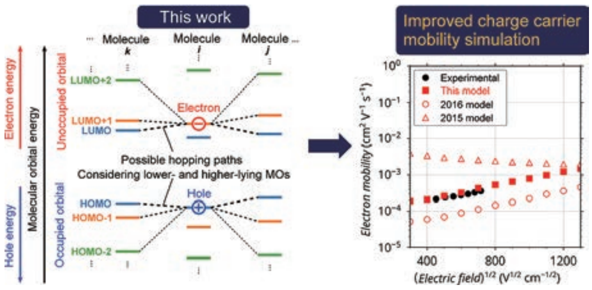


Figure 2. The charge transport simulation model for this work and electric field dependence of electron mobility.

Division of Environmental Chemistry

– Hydrospheric Environment Analytical Chemistry –

https://inter3.kuicr.kyoto-u.ac.jp/scope_E.html

Prof
SOHRIN, Yoshiki
(D Sc)

Assoc Prof
UMETANI, Shigeo
(D Sc)

Assist Prof
TAKANO, Shotaro
(D Sc)

Assist Prof
ZHENG, Linjie
(D Sc)

Techn Staff
IWASE, Misato

Students

TSUJISAKA, Makoto (D2)
TANAKA, Yuriko (M2)
FUJIWARA, Yuta (M1)
TSUCHIYA, Mao (M1)
CHAN, Cheuk-Yin (RS)

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

Selected Publications

Yang, L.; Nadeau, K.; Meija, J.; Grinberg, P.; Pagliano, E.; Ardini, F.; Grotti, M.; Schlosser, C.; Streu, P.; Achterberg, E. P.; Sohrin, Y.; Minami, T.; Zheng, L.; Wu, J.; Chen, G.; Ellwood, M. J.; Turetta, C.; Aguilar-Islas, A.; Rember, R.; Sarthou, G.; Tonnard, M.; Planquette, H.; Matoušek, T.; Crum, S.; Mester, Z., Inter-Laboratory Study for the Certification of Trace Elements in Seawater Certified Reference Materials NASS-7 and CASS-6, *Anal. Bioanal. Chem.*, **410,** 4469-4479 (2018).

Yang, S.-C.; Zhang, J.; Sohrin, Y.; Ho, T.-Y., Cadmium Cycling in the Water Column of the Kuroshio-Oyashio Extension Region: Insights from Dissolved and Particulate Isotopic Composition, *Geochim. Cosmochim. Acta*, **233,** 66-80 (2018).

Sieber, M.; Conway, T. M.; De Souza, G. F.; Obata, H.; Takano, S.; Sohrin, Y.; Vance, D., Physical and Biogeochemical Controls on the Distribution of Dissolved Cadmium and Its Isotopes in the Southwest Pacific Ocean, *Chem. Geol.* (2018) (in press).

Zheng, L.; Minami, T.; Takano, S.; Minami, H.; Sohrin, Y., Distribution and Stoichiometry of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in Seawater Around the Juan de Fuca Ridge, *J. Oceanogr.*, **75,** 669-685 (2017).

Takano, S.; Tanimizu, M.; Hirata, T.; Shin, K. T.; Fukami, Y.; Suzuki, K.; Sohrin, Y., A Simple and Rapid Method for Isotopic Analysis of Nickel, Copper, and Zinc in Seawater Using Chelating Extraction and Anion Exchange, *Anal. Chim. Acta*, **967,** 1-11 (2017).

Inter-laboratory Study for the Certification of Trace Elements in Seawater Certified Reference Materials NASS-7 and CASS-6

Certification of trace metals in seawater certified reference materials (CRMs) NASS-7 and CASS-6 is described (Yang et al., 2018a). At the National Research Council Canada (NRC), column separation was performed to remove the seawater matrix prior to the determination of Cd, Cr, Cu, Fe, Pb, Mn, Mo, Ni, U, V, and Zn, whereas As was directly measured in 10-fold diluted seawater samples, and B was directly measured in 200-fold diluted seawater samples. High-resolution inductively coupled plasma mass spectrometry (HRICPMS) was used for elemental analyses, with double isotope dilution for the accurate determination of B, Cd, Cr, Cu, Fe, Pb, Mo, Ni, U, and Zn in seawater NASS-7 and CASS-6, and standard addition calibration for As, Co, Mn, and V. In addition, all analytes were measured using standard addition calibration with triple quadrupole (QQQ)-ICPMS to provide a second set of data at NRC. Expert laboratories worldwide were invited to contribute data to the certification of trace metals in NASS-7 and CASS-6. Various analytical methods were employed by participants including column separation, co-precipitation, and simple dilution coupled to ICPMS detection or flow injection analysis coupled to chemiluminescence detection, with use of double isotope dilution calibration, matrix matching external calibration, and standard addition calibration. Results presented in this study show that majority of laboratories have demonstrated their measurement capabilities for the accurate determination of trace metals in seawater. As a result of this comparison, certified/reference values and associated uncertainties were assigned for 14 elements in seawater CRMs NASS-7 and CASS-6, suitable for the validation of methods used for seawater analysis. This subject was an international collaborative study with Dr. Zoltán Mester at NRC.

Cadmium Cycling in the Water Column of the Kuroshio-Oyashio Extension Region: Insights from Dissolved and Particulate Isotopic Composition

We measured dissolved and particulate Cd isotopic composition in the water column of a meridional transect across the Kuroshio-Oyashio Extension region in a Japanese GEOTRACES cruise to investigate the relative influence of physical and biogeochemical processes on Cd cycling in the Northwestern Pacific Ocean (Yang et al., 2018b). Located at 30–50°N along 165°E, the transect across the extension region possesses dramatic hydrographic contrast. Cold surface water and a relatively narrow and shallow thermocline characterizes the Oyashio Extension region in contrast to a relatively warm and highly stratified surface water and thermocline in the Kuroshio Extension region. The contrasting hydrographic distinction at the study site provides us with an ideal platform to investigate the spatial variations of Cd isotope fractionation systems in the ocean. Particulate samples demonstrated biologically preferential uptake of light Cd isotopes, and the fractionation effect varied dramatically in the surface water of the two regions, with relatively large fractionation factors in the Oyashio region. Based on the relationship of dissolved Cd concentrations and isotopic composition, we found that a closed system fractionation model can reasonably explain the relationship in the Kuroshio region. However, using dissolved Cd isotopic data, either a closed system or steady-state open system fractionation model may explain the relationship in the surface water of the Oyashio region. Particulate $\delta^{114/110}$Cd data further support that the surface water of the Oyashio region matches a steady-state open system model more closely. Contrary to the surface water, the distribution of potential density exhibits comparable patterns with Cd elemental and isotopic composition in the thermocline and deep water in the two extension regions, showing that physical processes are the dominant forcing controlling Cd cycling in the deep waters. The results demonstrate that Cd isotope fractionation can match either a closed or open system Rayleigh fractionation model, depending on the relative contribution of physical and biogeochemical processes on its cycling. This subject was an international collaborative study with Dr. Tung-Yuan Ho at Academia Sinica, Taiwan.

Yang, L. *et al*., Inter-Laboratory Study for the Certification of Trace Elements in Seawater Certified Reference Materials NASS-7 and CASS-6, *Anal. Bioanal. Chem.*, **410,** 4469-4479 (2018).

Yang, S.-C.; Zhang, J.; Sohrin, Y.; Ho, T.-Y., Cadmium Cycling in the Water Column of the Kuroshio-Oyashio Extension Region: Insights from Dissolved and Particulate Isotopic Composition, *Geochim. Cosmochim. Acta*, **233,** 66-80 (2018).

Figure 1. Dr. Tung-Yuan Ho at Lake Shinji.

Division of Environmental Chemistry
– Chemistry for Functionalized Surfaces –

http://www.scl.kyoto-u.ac.jp/~yoeki/


Prof
HASEGAWA, Takeshi
(D Sc)


Assist Prof
SHIMOAKA, Takafumi
(D Sc)


Assist Prof
SHIOYA, Nobutaka
(D Sc)

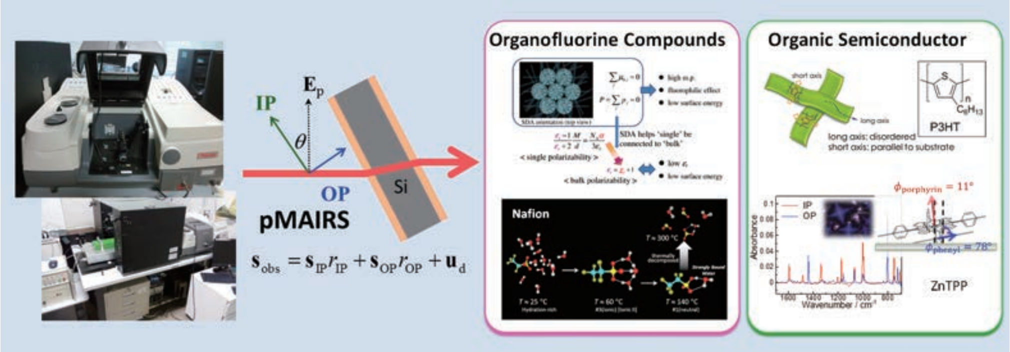
Students

TOMITA, Kazutaka (M2)
FUKUMI, Aki (M1)
FUJIWARA, Ryoi (M1)

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 Semiconductor
pMAIRS and MAIRS2



Selected Publications

Shioya, N.; Hada, M.; Shimoaka, T.; Murdey, R.; Eda, K.; Hasegawa, T., Impact of Kinetically Restricted Structure on Thermal Conversion of Zinc Tetraphenylporphyrin Thin Films to the Triclinic and Monoclinic Phases, *J. Phys. Chem. C*, **122,** 4540-4545 (2018).

Tomita, K.; Shioya, N.; Kise, R.; Shimoaka, T.; Yoshida, H.; Koganezawa, T.; Eda, K.; Hasegawa, T., Structure Control of a Zinc Tetraphenylporphyrin Thin Film by Vapor Annealing Using Fluorine Containing Solvent, *Thin Solid Films*, **665,** 85-90 (2018).

Shimoaka, T.; Ukai, H.; Kurishima, K.; Takei, K.; Yamada, N.; Hasegawa, T., Molecular Aggregation of Perfluoroalkyl Groups Can Win the Hydrogen Bonding between Amides, *J. Phys. Chem. C*, **122,** 22018-22023 (2018).

Isozaki, K.; Shimoaka, T.; Oshiro, S.; Yamaguchi, A.; Pincella, F.; Ueno, R.; Hasegawa, T.; Watanabe, T.; Takaya, H.; Nakamura, M., Robust Surface Plasmon Resonance Chips for Repetitive and Accurate Analysis of Lignin–Peptide Interactions, *ACS Omega*, **3,** 7483-7493 (2018).

Matsubara, T.; Yasumori, H.; Ito, K.; Shimoaka, T.; Hasegawa, T.; Sato, T., Amyloid-β Fibrils Assembled on Ganglioside-Enriched Membranes Contain Both Parallel β-Sheets and Turns, *J. Biol. Chem.*, **293,** 14146-14154 (2018).

Tokunaga, A.; Mutoh, K.; Hasegawa, T.; Abe, J., Reversible Valence Photoisomerization between Closed-Shell Quinoidal and Open-Shell Biradical Form, *J. Phys. Chem. Lett.*, **9,** 1833-1837 (2018).

Impact of Kinetically Restricted Structure on Thermal Conversion of Zinc Tetraphenylporphyrin Thin Films to the Triclinic and Monoclinic Phases

The powerful combination of p-polarized multiple-angle incidence resolution spectroscopy (pMAIRS) and grazing incidence X-ray diffraction (GIXD) is applied to the structural characterization of zinc tetraphenylporphyrin (ZnTPP) in vapor-deposited films as a function of the deposition rate. The deposition rate is revealed to have an impact on the initial film structure and its conversion by thermal annealing. The pMAIRS spectra reveal that a fast deposition rate yields a kinetically restricted amorphous film of ZnTPP having a “face-on orientation,” which is readily discriminated from another “randomly oriented” amorphous film generated at a slow deposition rate. In addition, the GIXD patterns reveal that the film grown at a slow deposition rate involves a minor component of triclinic crystallites. The different initial film structure significantly influences the thermal conversion of ZnTPP films. The randomly oriented amorphous aggregates with the triclinic crystallite seeds are converted to the thermodynamically stable phase (monoclinic) via the metastable triclinic phase. The kinetically restricted structure, on the other hand, is followed by a simple thermal conversion: the molecules are directly converted to the monoclinic one rather than the triclinic one.

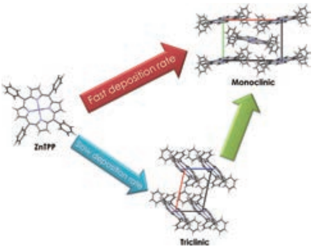


Figure 1. Schematic summary of the different two thermal conversions of ZnTPP thin films grown at fast and slow deposition rates.

Structure Control of a Zinc Tetraphenylporphyrin Thin Film by Vapor Annealing Using Fluorine Containing Solvent

The solvent vapor annealing (SVA) technique is one of the useful post processing techniques of a thin film, which is an alternative technique of the thermal annealing one. SVA has a great advantage that the molecular rearrangement in the film is made moderately by employing an appropriate solvent without the sample heating. The moderate processing is expected to yield a benefit that the molecular coalescence would be suppressed, which would readily keep the continuous surface topography of the film during the annealing, and another benefit that a metastable structure would be obtained. To make the best use of the SVA-specific characteristics, in the present study, a material having a metastable structure is chosen. The sample is ZnTPP that yields a metastable triclinic crystal structure, which can easily be converted to a monoclinic crystal structure by thermal annealing. A triclinic-structure film of ZnTPP by the combination of a wet process and the thermal annealing has thus never been reported. By choosing a fluorine-containing solvent, which has a low affinity to ZnTPP, a triclinic-structure film has first been obtained by a wet process while the surface continuity is protected.

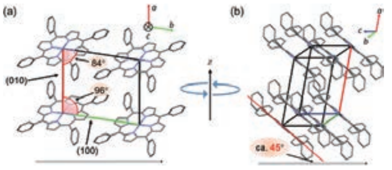


Figure 2. The schematics of molecular orientation of the triclinic crystallite from the two viewpoints.

Molecular Aggregation of Perfluoroalkyl Groups Can Win the Hydrogen Bonding between Amides

Hydrogen bonding is, in general, recognized to have a much stronger molecular interactive force than the dipole–dipole interaction that is one of the van der Waals forces. The molecular interaction between perfluoroalkyl (Rf) chains is driven by a two-dimensional dipole–dipole interaction network because of a large dipole moment along the C–F bond and a helical conformation about the Rf chain axis, which generates the Rf-specific tight and closed molecular packing. The polarization of a molecular aggregate on a macroscopic scale comprehensively explains the Rf compound-specific properties represented by the high melting point. This cooperative interaction in the two-dimensional network gives us an impression that the dipole–dipole interaction can win the H-bonding in a molecular aggregate. In the present study, amphiphilic compounds having an Rf group and an amide group are prepared, and the molecular aggregation factor is investigated by means of surface chemistry and vibrational spectroscopic techniques. In fact, we show that the dipole–dipole interaction becomes the dominant factor of the molecular aggregation of the amide-containing compound.

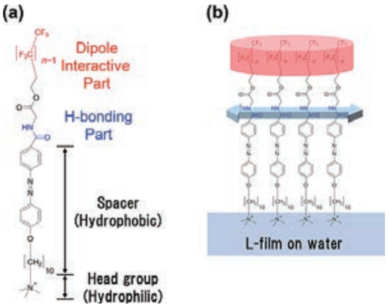


Figure 3. (a) Chemical structure of the amphiphilic compounds having an Rf group and an amide group, and (b) schematic image of a molecular aggregation of molecules on water.

Division of Environmental Chemistry
– Molecular Microbial Science –

http://www.scl.kyoto-u.ac.jp/~mmsicr/mmstojp/Top_en.html

Prof
KURIHARA, Tatsuo
(D Eng)

Assist Prof
KAWAMOTO, Jun
(D Agr)

Assist Prof
OGAWA, Takuya
(D Agr)

Assist Res Staff

KITAYAMA, Kaori

Students

KAWAI, Soichiro (D3)
CHEN, Chen (D3)
TOYOTAKE, Yosuke (D3)
MARUOKA, Naruyuki (D2)
YOKOYAMA, Fumiaki (D2)
YUSUF, Yustina (D2)
KAMASAKA, Kohei (M2)
SHIGEEDA, Takumi (M2)
LIU, Yuing (M2)
SUWANAWAT, Nittikarn (M2)
KUBOSHIMA, Misaki (M1)
KUREBAYASHI, Toshiki (M1)
HIROSE, Kazuki (M1)
YONEDA, Yuki (M1)
CHEN, Mengyi (M1)

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
Bacterial Cold-adaptaion Mechanism
Polyunsaturated Fatty Acid
Phospholipid Acyltransferase
Membrane Vesicle

Selected Publications

Ogawa, T.; Tanaka, A.; Kawamoto, J.; Kurihara, T., Purification and Characterization of 1-Acyl-*sn*-glycerol-3-phosphate Acyltransferase with a Substrate Preference for Polyunsaturated Fatty Acyl Donors from the Eicosapentaenoic Acid-producing Bacterium *Shewanella livingstonensis* Ac10, *J. Biochem.*, **164,** 33-39 (2018).

Toyotake, Y.; Cho, H. N.; Kawamoto, J.; Kurihara, T., A Novel 1-Acyl-*sn*-glycerol-3-phosphate *O*-Acyltransferase Homolog for the Synthesis of Membrane Phospholipids with a Branched-Chain Fatty Acyl Group in *Shewanella livingstonensis* Ac10, *Biochem. Biophys. Res. Commun.*, **500,** 704-709 (2018).

Tokunaga, T.; Watanabe, B.; Sato, S.; Kawamoto, J.; Kurihara, T., Synthesis and Functional Assessment of a Novel Fatty Acid Probe, ω-Ethynyl Eicosapentaenoic Acid Analog, to Analyze the in Vivo Behavior of Eicosapentaenoic Acid, *Bioconjugate Chem.*, **28,** 2077-2085 (2017).

Yokoyama, F.; Kawamoto, J.; Imai, T.; Kurihara, T., Characterization of Extracellular Membrane Vesicles of an Antarctic Bacterium, *Shewanella livingstonensis* Ac10, and Their Enhanced Production by Alteration of Phospholipid Composition, *Extremophiles*, **21,** 723-731 (2017).

Sato, S.; Kawamoto, J.; Sato, S. B.; Watanabe, B.; Hiratake, J.; Esaki, N.; Kurihara, T., Occurrence of a Bacterial Membrane Microdomain at the Cell Division Site Enriched in Phospholipids with Polyunsaturated Hydrocarbon Chains, *J. Biol. Chem.*, **287,** 24113-24121 (2012).

Elucidation of a Selective Protein-secretion Mechanism via Extracellular Membrane Vesicle of a Psychotropic Bacterium, *Shewanella* sp. HM13

Shewanella sp. HM13, a cold-adapted bacterium isolated from fish intestine, can produce larger amounts of extracellular membrane vesicles (EMVs) than the related strains, and the EMVs harbor a functionally unknown protein, P49, as a major single cargo. To elucidate the molecular mechanism of the P49-selective cargo loading to the EMVs, whole genome sequence of this strain was determined, and we found that a gene coding for P49 is located in a gene cluster composed of genes coding for homologs of subunits of type II secretion machinery (T2SS) of Gram-negative bacterium, proteins involved in bacterial surface lipoglycan, and functionally unknown proteins. When the genes coding for homologs of T2SS-like translocon were disrupted, P49 was accumulated in the cell and the post-vesicle fraction (PVF) of the culture supernatant. On the other hand, P49 localized to the EMVs disappeared in these mutants. Deletion mutants of each of lipoglycan-synthesis related genes in the gene cluster showed accumulation of P49 at the PVF and marked decrease in the amount of P49 both in the EMVs and cell fraction, suggesting that defects of these genes affect the cell surface structure and enhance secretion of P49 to the PVF without the cargo loading to EMVs. These results also suggest that T2SS-like machinery coded by P49-containing gene cluster translocates P49 to the outer membrane, and P49 interacts with the EMVs or the precursors on the outer membrane surface.

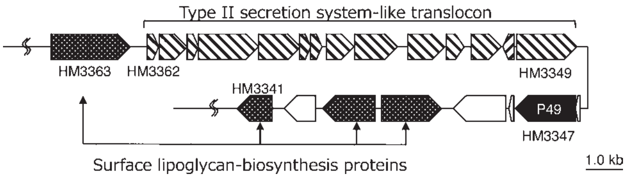


Figure 1. Genetic map of P49-containing gene cluster of *Shewanella* sp. HM13.

In vivo Characterization of a Novel Lysophosphatidic Acid Acyltransferase Homolog of *Escherichia coli*

Lysophosphatidic acid acyltransferase (LPAAT) introduces fatty acyl groups into the *sn*-2 position of membrane phospholipids. Multiple LPAAT homologs occur in some bacteria, and they are proposed to generate the membrane diversity by introducing different fatty acyl groups. *Shewanella livingstonensis* Ac10 isolated from Antarctic seawater has five LPAAT homologs (SlPlsC1 to SlPlsC5). SlPlsC1 and SlPlsC4 play an essential role in the synthesis of phospholipids containing an eicosapentaenoyl group and branched-chain fatty acyl groups, respectively. On the other hand, it has long been believed that *Escherichia coli* has one essential LPAAT homolog named PlsC. However, we demonstrated that *E. coli* possesses a physiologically functional SlPlsC4 ortholog named YihG, showing 39.1% sequence identity to SlPlsC4. YihG is also conserved in some γ-proteobacteria such as *Salmonella typhimurium* and *Vibrio cholerae*. Overexpression of YihG in *E. coli* JC201 carrying a temperature-sensitive mutation in *plsC* allowed its growth at non-permissive temperature. ESI-MS/MS and GC-MS analyses revealed that YihG introduces a *cis*-vaccenoyl group ($18:1^{\Delta 11}$) at the *sn*-2 position of phospholipids. A soft agar assay and microscopic observation showed enhanced swimming motility of the *yihG*-deleted mutant cells compared with the wild-type cells. These results suggested that *E. coli* YihG modulates the swimming motility by introducing the specific fatty acyl group into membrane phospholipids.

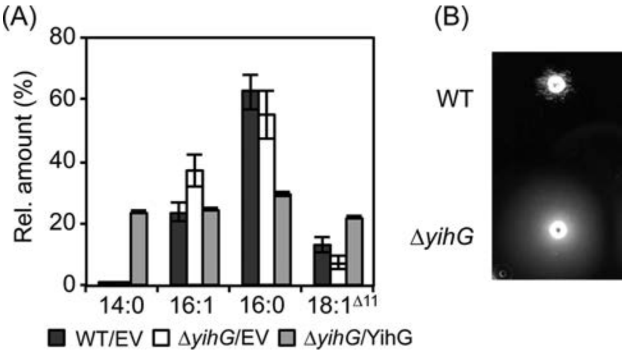


Figure 2. (A) Composition of fatty acyl groups at the *sn*-2 position of phospholipids from the wild-type strain harboring the empty vector (dark gray) and the *yihG*-deleted mutant harboring the empty vector (white) or YihG expression vector (light gray). Phospholipids were extracted and hydrolyzed by phospholipase A2, and resulting fatty acids were extracted and analyzed by GC-MS. (B) Motilities of the wild-type and *yihG*-deleted mutant cells on a 0.2% soft-agar plate. The cells were incubated at 37°C for 12 h.

Division of Multidisciplinary Chemistry
– Polymer Materials Science –

http://www.scl.kyoto-u.ac.jp/~polymat/index.html

Prof
TAKENAKA, Mikihito
(D Eng)

Assist Prof
OGAWA, Hiroki
(D Eng)

Students

KISHIMOTO, Mizuki (D1)
WATANABE, Yuki (D1)
OMOSU, Takuya (M2)
NISHIMURA, Yu (M2)
FUWA, Takuto (M2)
MATSUNAGA, Tsubasa (M2)
IKEDA, Yuta (M1)
HIKAMI, Yuichi (M1)
OKUDA, Ryo (UG)
ODA, Tappei (UG)
MITANI, Kenta (UG)

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

Selected Publications

Kishimoto, M.; Mita, K.; Jang, J.; Takahashi, N.; Ogawa, H.; Nishida, K.; Kanaya, T.; Takenaka, M., A Study on the Isothermal Crystallization of Poly(3-methylbutene-1), *Polym. J.*, **51,** 173-182 (2019).

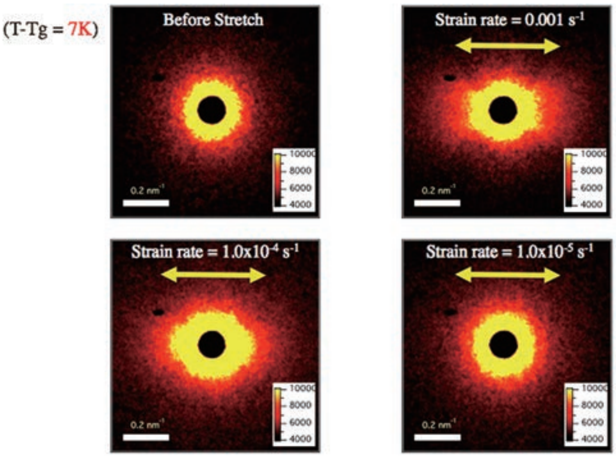
Hattori, G.; Takenaka, M.; Sawamoto, M.; Terashima, T., Nanostructured Materials via the Pendant Self-Assembly of Amphiphilic Crystalline Random Copolymers, *J. Am. Chem. Soc.*, **27,** 8376-8379 (2018).

Ogawa, H.; Takenaka, M.; Miyazaki, T.; Kanaya, T., Order-order Transition Processes of Thin-Film Symmetric and Asymmetric PS-*b*-P2VP during Spin Coating, *Macromolecules*, **51,** 10040-10051 (2018).

Strain-Induced Enhancement of Density Fluctuations in Glassy Polymers

Polymer glass cannot deform isothermally because, by definition, micro-Brownian motion will be limited in the glass state. However, plastic flow in polymer glass can easily occur under conditions of stress. Here we aim at clarifying the universality of the enhancement in other glassy polymers such as polycarbonate (PC) and polystyrene (PS).

Figure 1 shows two-dimensional (2D) SAXS patterns of PC sample before stretching. The scattering pattern before stretching was isotropic. We stretched PC to the strain $\varepsilon = 0.12$ at temperature $T = 412$K with strain rates $\dot{\varepsilon} = 1.00 \times 10^{-3}$ to 1.00×10^{-5} s^{-1}. At 1.00×10^{-3} and 1.00×10^{-4} s^{-1}, the scattering patterns become anisotropic, thereby exhibiting the so-called abnormal butterfly pattern. On the other hand, at 1.00×10^{-5} s^{-1}, the enhancement of the scattering patterns along the stretch direction is not observed. These results suggest that the density fluctuations are not enhanced by the stretch at 1.00×10^{-5} s^{-1} and that the critical strain rate $\dot{\varepsilon}_c$ of the strain-induced enhancement of density fluctuations exists between 1.00×10^{-4} and 1.00×10^{-5} s^{-1} at 412K. We also found the strain-induced enhancement of density fluctuations occurs in PS. $\dot{\varepsilon}_c$ increases with temperature. A similar tendency can be observed in PMMA and PS. These results indicate that the strain-induced enhancement of density fluctuations is a universal feature in glassy polymers.



Density fluctuations are induced at higher strain rate.

Figure 1. 2D-SAXS images of stretched PC at 412K and ε = 0.12.

Order-order Transition Processes of Thin-film Symmetric and Asymmetric PS-*b*-P2VP during Spin Coating

Order-order transitions during spin-coating processes in symmetric and asymmetric poly(styrene-block-2-vinylpyridine) (PS-*b*-P2VP) were investigated by using grazing incidence small-angle X-ray scattering (GISAXS). When the composition was symmetric (e.g., the copolymer P2VP volume fraction, f_{P2VP}, was 0.50), we found that loose-packed nano-cylindrical structures formed after the transition from micelles to a body-centered cubic (BCC) lattice structure during evaporation. After the BCC (110) plane aligned perpendicular to the substrate, microdomains coalesced into a cylindrical structure. This coalescence was caused by the convection effect of the solvent, and vitrification of PS and P2VP further prohibited transitions from the cylindrical structure, although generally, the equilibrium morphology in the bulk state is lamellae. For an asymmetric composition with $f_{\mathrm{P2VP}} = 0.70$, lamellar structures formed perpendicular to the substrate. During evaporation, the micelles transformed to hexagonal close-packed (HCP) structures, and then BCC structures appeared. The microdomains of the BCC structures merged parallel and perpendicular to the film surface before evaporation was complete, and hence, the lamellar structures were formed. Furthermore, well-packed hexagonal-packed nano-cylindrical structures with long-range order perpendicular to the substrate were formed in the PS-*b*-P2VP thin film with an $f_{\mathrm{P2VP}} = 0.30$ and corresponded to the equilibrium morphology in the bulk state. During evaporation, the micelle structures directly transitioned to nano-cylindrical structures. The micelles grew perpendicular to the film surface before evaporation was complete.

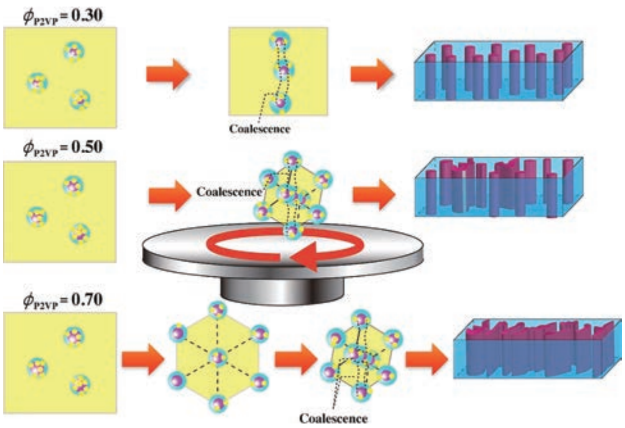


Figure 2. Cross-sectional views of the transition processes in toluene solvent during spin-coating of PS-*b*-P2VP block copolymer at $f_{\mathrm{P2VP}} = 0.30$, 0.50 and 0.70, respectively.

Division of Multidisciplinary Chemistry

– Molecular Rheology –

http://rheology.minority.jp/en/

Prof
WATANABE, Hiroshi
(D Sc)

Assoc Prof
MATSUMIYA, Yumi
(D Eng)

Students

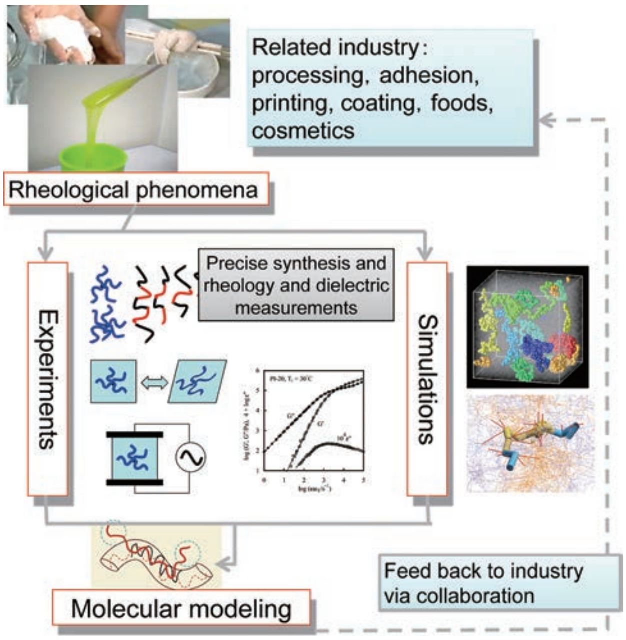
SOMA, Kae (M2)
OKAJIMA, Hiroyuki (M1)
FUKATA, Fumiya (M1)
NAGAIWA, Ryosuke (UG)
TABUKI, Kohei (UG)

Guest Scholar

KWON, Youngdon (Ph D) Sungkyunkwan University, Korea, R., 11 September 2018–31 January 2019

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 Softmatter

Selected Publications

Mongcopa, K. I. S.; Tyagi, M.; Mailoa, J. P.; Samsonidze, G.; Kozinsky, B.; Mullin, S. A.; Gribble, D. A.; Watanabe, H.; Balsara, N. P., Relationship between Segmental Dynamics Measured by Quasi-Elastic Neutron Scattering and Conductivity in Polymer Electrolytes, *ACS Macro Lett.*, **7,** 504-508 (2018).

Wu, S.; Cao, X.; Zhang, Z.; Chen, Q.; Matsumiya, Y.; Watanabe, H., Molecular Design of Highly Stretchable Ionomers, *Macromolecules*, **51,** 4735-4746 (2018).

Watanabe, H.; Matsumiya, Y.; Kwon, Y., Iscoelastic and Dielectric Relaxation of Reptating Type-A Chains Affected by Reversible Head-to-Head Association and Dissociation, *Macromolecules*, **51,** 6476-6496 (2018).

Matsumiya, Y.; Watanabe, H.; Masubuchi, Y.; Huang, Q.; Hassager, O., Nonlinear Elongational Rheology of Non-Entangled Polystyrene and Poly(p-tert-butylstyrene) Melts, *Macromolecules*, **51,** 9710-9729 (2018).

Nonlinear Elongational Rheology of Non-Entangled Polystyrene and Poly(*p-tert*-butylstyrene) Melts

Nonlinear rheological behavior under uniaxial elongation was examined for unentangled melts of polystyrene (PS27; M = 27k) and poly(*p-tert*-butyl styrene) (PtBS53; M = 53k) having nearly the same number of Kuhn segments *per* chain, n_K = 30 and 35 for PS27 and PtBS53, respectively. For both materials, the steady-state elongational viscosity η_E exhibited strain-rate-hardening and then strain-rate-softening on an increase of the Weissenberg number $Wi \geq 0.3$ ($Wi = \dot{\varepsilon}\tau_1^{\mathrm{eq}}$, with τ_1^{eq} and $\dot{\varepsilon}$ being the longest relaxation time in the linear viscoelastic regime and the Hencky strain rate, respectively). For the unentangled melts, the hardening and softening were free from any entanglement nonlinearity, so that the hardening was unequivocally related to the finite extensible nonlinear elasticity (FENE) of the chain, and the softening, to suppression of the FENE effect due to reduction of the segmental friction ζ occurring for the highly stretched and oriented chain. Thus, the ζ-reduction, speculatively discussed for entangled melts so far, was experimentally confirmed, to the first time, for unentangled melts. Quantitatively, the hardening at intermediate Wi was stronger and the softening at higher Wi was weaker for PtBS53 than for PS27 despite the similarity of their n_K values, which suggested that the magnitude of ζ-reduction depends on the chemical structure of the chains. For estimation of this magnitude, the well-established FENE bead-spring model (FENE-PM model) was modified for the ζ-reduction in an empirical way with an *assumption* that ζ at a given time is fully determined by the chain stretch/orientation and thus by the elongational stress σ_E at that time. This modified model was able to mimic the steady state η_E data excellently, and the ζ-reduction utilized in the modification was weaker for PtBS53 than for PS27k to confirm the dependence of the ζ-reduction on the chemical structure of the chain. Nevertheless, the same modified model failed to accurately describe the transient stress growth and relaxation data on start-up and cessation of fast flow (at $Wi \geq 4$), despite its success in description of the transient stress data for slow flow as well as the steady-state η_E data in the entire range of Wi. Specifically, changes of ζ in the unentangled melts with time during the relaxation for large Wi were delayed compared to the model calculation. This result suggests that ζ is determined not only by the chain stretch/orientation (*i.e.*, by σ_E) at respective times but also by the transient changes of the stretch/orientation (by $\dot{\sigma}_E$), with those changes vanishing in the steady state thereby allowing the model to describe the η_E data. The origin of the change of ζ with the transient changes of the stretch/orientation is discussed in relation to the local motion of the chain necessary for adjusting its friction to the changes of the stretch/orientation environment.

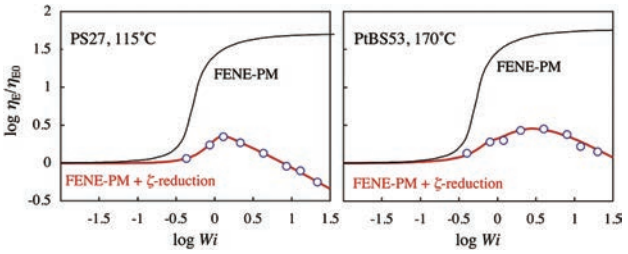


Figure 1. Steady state elongational viscosity η_E of PS27 at 115°C (left) and PtBS53 at 170°C (right). The η_E data are normalized by $\eta_{E0} = 3\eta_0$ (η_0 = zero-shear viscosity) and plotted against the Weissenberg number $Wi = \dot{\varepsilon}\tau_1^{\mathrm{eq}}$, with τ_1^{eq} being the longest relaxation time in the LVE regime measured after cessation of elongational flow. The small red circle and red curve indicate the η_E/η_{E0} ratio calculated from FENE-PM model modified for anisotropic and isotropic ζ-reduction, respectively. Black curve shows the FENE-PM calculation without ζ-reduction.

Division of Multidisciplinary Chemistry
– Molecular Aggregation Analysis –

http://www.scl.kyoto-u.ac.jp/~wakamiya/english/index.html

Prof
WAKAMIYA, Atsushi
(D Eng)

Assist Prof
MURDEY, Richard
(Ph D)

PD
LIU, Jiewei
(Ph D)

PD
TRUONG, Minh Anh
(D Eng)

PD
LEE, Hayoon
(Ph D)

Researchers (pt)

ISHIKURA, Yasuhisa
SHIMAZAKI, Ai
MIKI, Masako (D Eng)
KATO, Naoya
KAWANISHI, Yasuyoshi
YABUMOTO, Toshihiko

Assist Techn Staffs

IWASAKI, Yasuko
PARK, Kwan-Hyun
MATSUSHIGE, Yuko

Students

OZAKI, Masashi (D3)
NAKAMURA, Tomoya (D3)
YAKUMARU, Shinya (M2)

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

Selected Publications

Lin, H.-A.; Mitoma, N.; Meng, L.; Segawa, Y.; Wakamiya, A.; Itami, K., Hole-Transporting Materials Based on Thiophene-Fused Arenes from Sulfur-Mediated Thienannulations, *Mater. Chem. Front.*, **2,** 275-280 (2018).

Yang, F.; Lim, H. E.; Wang, F.; Ozaki, M.; Shimazaki, A.; Liu, J.; Mohamed, N. B.; Shinokita, K.; Miyauchi, Y.; Wakamiya, A.; Murata, Y.; Matsuda, K., Roles of Polymer Layer in Enhanced Photovoltaic Performance of Perovskite Solar Cells via Interface Engineering, *Adv. Mater. Interfaces*, **5,** 1701256 (2018).

Murdey, R.; Katoh, K.; Yamashita, M.; Sato, N., Thermally Activated Electrical Conductivity of Thin Films of Bis(phthalocyaninato)terbium(III) Double Decker Complex, *Thin Solid Films*, **646,** 17-20 (2018).

Shimogawa, H.; Murata, Y.; Wakamiya, A., NIR-Absorbing Dye Based on BF2-Bridged Azafulvene Dimer as a Strong Electron-Accepting Unit, *Org. Lett.*, **20,** 5135-5138 (2018).

Liu, J.; Ozaki, M.; Yakumaru, S.; Handa, T.; Nishikubo, R.; Kanemitsu, Y.; Saeki, A.; Murata, Y.; Murdey, R.; Wakamiya, A., Lead-Free Solar Cells Based on Tin Halide Perovskite Films with High Coverage and Improved Aggregation, *Angew. Chem. Int. Ed.*, **57,** 13221-13225 (2018).

Yang, D.-T.; Nakamura, T.; He, Z.; Wang, X.; Wakamiya, A.; Peng, T.; Wang, S., Doping Polycyclic Arenes with Nitrogen−Boron−Nitrogen (NBN) Units, *Org. Lett.*, **20,** 6741-6745 (2018).

NIR-Absorbing Dye Using BF_2-Bridged Azafulvene Dimer Unit

Dyes that absorb near infrared (NIR) light have been investigated intensively in the context of a variety of applications, including photovoltaics, photodetectors, heat absorbers, and medical applications. In many applications, the photostability and resistance to oxidation of these NIR dyes are very important. NIR dyes usually have narrow HOMO–LUMO gaps on account of the destabilized HOMO level, and are thus easily oxidized by atmospheric oxygen. A strong electron-accepting unit having low-lying LUMO levels should, therefore, be expected to lead to NIR dyes with improved air- and photo-stability.

We designed and synthesized a twofold BF_2-bridged azafulvene dimer as a strongly electron-accepting building block. As a model D–A–D dye composed of this electron-acceptor unit, compound 1 was synthesized by combined with electron-donor triarylamine units. In cyclic voltammometry in CH_2Cl_2, D–A–D dye showed two reversible reduction waves at $E_{1/2}$ = –0.78 and –0.98 V (vs. Fc/Fc^+) and two reversible oxidation waves at $E_{1/2}$ = +0.21 and +0.54 V. The first reduction potential appears at a substantially more positive potential than those of typical n-type materials such as fullerene C_{60} ($E_{1/2}$ = –0.98 V) or perylene diimide ($E_{1/2}$ = –0.97 V), demonstrating the significant electron-accepting ability of the BF_2-bridged azafulvene dimer building unit.

In the UV/vis/NIR absorption spectra in CH_2Cl_2, D–A–D dye exhibits an intense NIR absorption at λ_{abs} = 922 nm tailing up to λ_{edge} = 1150 nm, reflecting the narrow HOMO–LUMO gap, while relatively little absorption in the visible region (400-700 nm) was observed. This is the ideal photophysical property for a selective NIR absorber. The photostability test in both degassed and non-degassed toluene solution showed that in sharp contrast to a commercially available naphthalocyanine (Napht) NIR dye, the absorption of which (λ_{abs} = 865 nm) diminished to 27% in degassed toluene and to 6% in non-degassed toluene, the absorption of D–A–D dye remained unchanged (97%) even after irradiation for 50 h, clearly demonstrating the high photostability of our D–A–D dye and its resistance to oxidation by atmospheric oxygen.

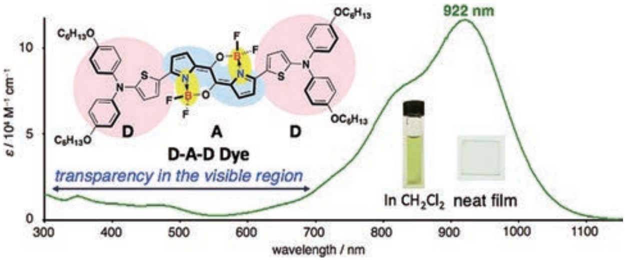


Figure 1. Absorption properties of D–A–D dye containing BF_2-bridged azafulvene dimer as a strong electron-accepting unit.

Fabrication Method for Tin-based Perovskite Films to Give Good PCEs

Metal halide perovskite solar cells (PSCs) have gained tremendous attention in the past few years. However, the toxicity of lead (Pb), commonly used in high efficiency PSCs, remains a serious problem that hampers the wide application of this ‘magic’ material. Sn-based perovskites replacing Pb^{2+} with tin (II) (Sn^{2+}) are expected to be promising candidates for lead-free perovskites. Unfortunately, power conversion efficiencies (PCEs) obtained from Sn-based PSCs are much lower than that of their Pb counterparts, and the highest PCE achieved for a Sn-based PSC to date is still below 10%. One issue is the fact that rapid oxidation of Sn^{2+} to Sn^{4+} in ambient atmosphere dopes the perovskite layer into high conductivity, resulting in severe electric shorting. Another issue also predominates when the perovskite film is fabricated with uneven thickness or pinholes, a common occurrence for Sn-based PSC. Despite the clear need to improve device performance, only a limited number of groups are investigating Sn-based PSC at present. The difficulty in fabricating high-quality Sn perovskite films is a significant impediment.

Aimed at increasing the power conversion efficiency of lead-free perovskite solar cells, we developed two simple methods to improve tin halide perovskite film structure. First, a hot antisolvent treatment (HAT) was found to increase the film coverage and prevent electric shunting in the photovoltaic device. Second, we discovered that annealing under a low partial pressure of dimethyl sulfoxide vapor increased the average crystallite size. As a result of the combined treatments, the topographical and electrical qualities of the perovskite films can substantively be improved, facilitating the fabrication of Sn-based perovskite solar cell devices with power conversion efficiencies of over 7%.

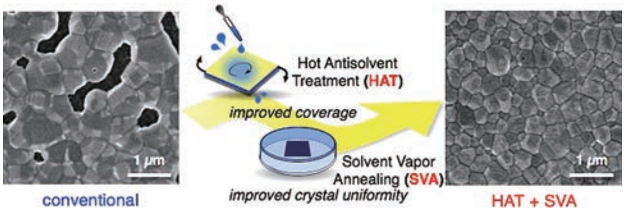


Figure 2. Top view SEM images comparing $FA_{0.75}MA_{0.25}SnI_3$ perovskite films fabricated by the conventional method (left) and with the combined HAT+SVA process (right).

Advanced Research Center for Beam Science
– Particle Beam Science –

http://wwwal.kuicr.kyoto-u.ac.jp/www/index-e.htmlx

Assoc Prof
IWASHITA, Yoshihisa
(D Sc)

Techn Staff
TONGU, Hiromu

Researcher (pt)

KATAYAMA, Ryo (D Sc)

Lect (pt)

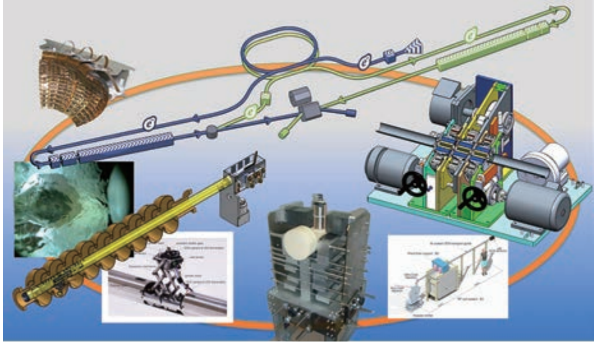
HIROTA, Katsuya (D Sc) Osaka University

Students

DENG, Weichao (M2)
YAMAZAKI, Yuki (M2)
YAKO, Tomoki (M1)
TAKEUCHI, Yusuke (M2)
ABE, Masashi (M1)

Scope of Research

We are studying particle beam science which includes particle beam generation, acceleration and manipulation for fundamental sciences as well as for practical applications, such as new materials and cancer therapy. We also concentrate on electromagnetics design such as Neutron Optics, including neutron beam focusing to highly enhance their efficiency for advanced measurements. We are the first in the world to demonstrate active neutron acceleration in order to seek the neutron Electric Dipole Moment. In addition, we contribute to advanced fault detection techniques for the International Linear Collider project superconducting accelerating cavities.



KEYWORDS

Beam Physics
Accelerator Physics
Neutron Optics
Phase Rotation
International Linear Collider

Selected Publications

Iwashita, Y.; Miyawaki, E.; Takeuchi, Y.; Tongu, H., Compact H^+ ECR Ion Source with Pulse Gas Valve, *AIP Conf. Proc.*, **2011-1,** [030011-1]-[030011-3] (2018).

Iwashita, Y.; Fuwa, Y.; Ishida, T.; Kino, K., Magnified Neutron Imaging with Modulating Permanent Magnet Sextupole Lens, *Proc. Int. Conf. Neutron Optics (NOP2017)*, **22,** [011008-1]-[011008-7] (2018).

Fuwa, Y.; Iwashita, Y., Performance Evaluation of a Klystron Beam Focusing System with Anisotropic Ferrite Magnet, *Prog. Theor. Exp. Phys.*, **2017-2,** [023G01-1]-[023G01-14] (2017).

Imajo, S.; Mishima, K.; Kitaguchi, M.; Iwashita, Y.; Yamada, N. L.; Hino, M.; Oda, T.; Ino, T.; Shimizu, H. M.; Yamashita, S.; Katayama, R., Pulsed Ultra-cold Neutron Production Using a Doppler Shifter at J-PARC, *Prog. Theor. Exp. Phys.*, **2016-1,** [013C02-1]-[013C02-22] (2016).

Fuwa, Y.; Iwashita, Y.; Tongu, H.; Inoue, S.; Hashida, M.; Sakabe, S.; Okamura, M.; Yamazaki, A., RF Synchronized Short Pulse Laser Ion Source, *Rev. Sci. Instrum.*, **87-2,** [02A911-1]-[02A911-4] (2016).

Kubo, T.; Iwashita, Y.; Saeki, T., Radio-frequency Electromagnetic Field and Vortex Penetration in Multilayered Superconductors, *Appl. Phys. Lett.*, **104,** 032603 (2014).

Evaluation of Superconducting Characteristic on the Multilayer Thin-Film Structure That Consists of NbN and Insulator Layer on Pure Nb Substrate

In recent years, it has been pointed out that the maximum accelerating gradient of a superconducting RF cavity can be pushed up by coating the inner surface of the cavity with a multilayer thin-film struture that consists of alternating insulating and superconducting layers. In this structure, the principal parameter that limits the performance of the cavity is the critical magnetic field or effective H_{C1} at which vortices start penetrating into the superconductor layer, and it is predicted to depend on the combination of the thicknesses of the layers. Hereafter, such multilayer structures on pure bulk Nb in superconducting state is referred to as S-I-S (Superconductor-Insulator-Superconductor) structure. The effective H_{C1} of a superconducting material can be evaluated by applying an AC magnetic field to the material with a small coil and detecting the induced third-harmonic signal at the coil. Hereafter, this method is called third harmonic voltage method.

For the third harmonic voltage method, an AC magnetic field at the angular frequency of 5 kHz is generated by a coil close to the superconducting sample and the third harmonic voltage $v_3(t) = V_3 \sin(3\omega t)$ induced in the coil is simultaneously measured, where ω is the angular frequency of a sinusoidal drive current, $I_0 \sin(\omega t)$ represents the current flowing through the coil, and V_3 is the amplitude of $v_3(t)$. If the temperature of a sample in the superconducting state is being raised while the amplitude of AC magnetic field H_0 is fixed, V_3 suddenly rises when H_0 exceeds the effective H_{C1} of the sample at a certain temperature. In the measurement performed at Kyoto University, H_0 is controlled by drive current I_0, and the temperature dependence of the effective H_{C1} is evaluated from the temperatures at moments when V_3/I_0 suddenly rises.

We have tested a multilayer sample that consist of NbN and SiO_2 coated on pure bulk Nb. The pure bulk Nb substrate of the sample is pretreated with the standard electropolishing recipe for bulk Nb cavity. The multilayer sample is prepared using DC magnetron sputtering technique (ULVAC, Inc.). This sample is a thin-film structure of 200-nm-thick NbN and 30-nm-thick SiO_2.

The temperature dependence of the measured effective H_{C1} of the sample is depicted in Figure 1. The horizontal and vertical axes represent the temperature and the measured effective H_{C1}, respectively. The measured values of H_{C1} of pure bulk Nb sample and the effective H_{C1} of NbN(200 nm)/SiO_2(30 nm)/Nb sample are represented by the open circles and black triangles, respectively. In general, the temperature dependence of H_{C1} satisfies the following equation:

$$F(T) = F(0) \times \left(1-\left(T/T_c\right)^2\right).$$

The red curve is the theoretical curve obtained from the function of $F(T)$ assuming $F(0)$ = 180 mT and T_c = 9.2 K, which is used for calibration. The green dashed curve is obtained by fitting data points of the sample in the region T <9.2 K to the function of $F(T)$. On the other hand, the blue one dot chain line is obtained by fitting data points of the sample in the region T >9.2 to the function $F(T)$ at which T_c was fixed at 13.8 K, a value obtained from the measurement result of the critical temperature of NbN film. At temperatures below around 9.2 K, S-I-S structure is formed because both pure bulk Nb and NbN film are in superconducting state. Thus, the effective H_{C1} of the whole NbN/SiO_2/Nb structure in the superconducting state is expressed by the green dashed curve. On the other hand, for temperatures greater than around 9.2 K, S-I-S structure does not hold. Thus, the blue one dot chain line corresponds to the effective H_{C1} of only NbN film. As a result of fitting, $F(0)$ and T_c are estimated as $(210 \pm 7) \times 10^{-3}$ and 9.21 ± 0.02 K, respectively for the green dashed curve, whereas $F(0)$ is determined as $(3.3 \pm 0.5) \times 10^{-3}$ for the blue one dot chain line. It is thus confirmed that $F(0)$ of NbN(200 nm)/SiO_2(30 nm)/Nb in the region of T <9.2 K is improved by 17 % compared to that of pure bulk Nb. The measurement result clearly showed that the effective H_{C1} of pure bulk Nb improved by using the multi-layer film coating of S-I-S structure.

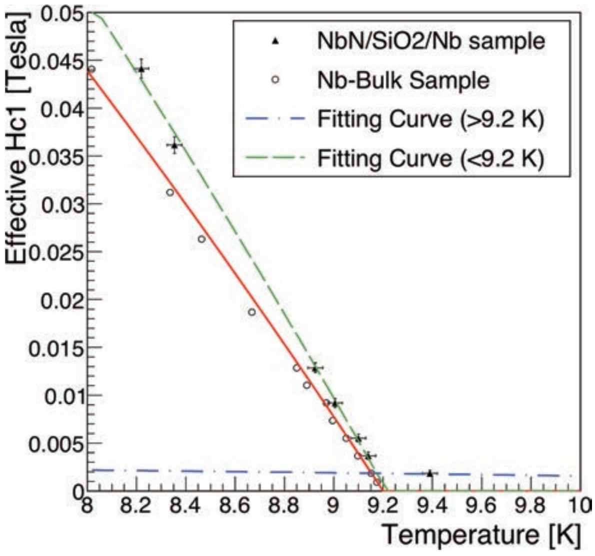


Figure 1. Comparison of measured effective H_{C1} between NbN(200 nm)/SiO_2(30 nm)/Nb and pure bulk Nb samples. The red curve represents $0.18 \times \left(1-\left(T/9.2\right)^2\right)$., which is used for calibration. The green broken line and the blue chain line are obtained by fitting data points of sample.

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

http://laser.kuicr.kyoto-u.ac.jp/e-index.html


Prof
SAKABE, Shuji
(D Eng)


Assoc Prof
HASHIDA, Masaki
(D Eng)


Assist Prof
INOUE, Shunsuke
(D Sc)


PD
KOJIMA, Sadaoki
(D Sc)


Proj Res*
NAKAMIYA, Yoshihide
(D Sc)

Students

MORI, Kazuaki (D3)
FURUKAWA, Yuki (D1)
NISHIURA, Yosuke (M2)
NISHINO, Shogo (M2)
YOSHIDA, Masahiro (M2)
HOSOKAWA, Chikai (M1)
YAMANAKA, Takashi (M1)

*Postdoctoral Research Assistant of Extreme Light Infrastructure-Nuclear Physics (ELI-NP) / Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering (IFIN-HH)

Guest Res Assoc

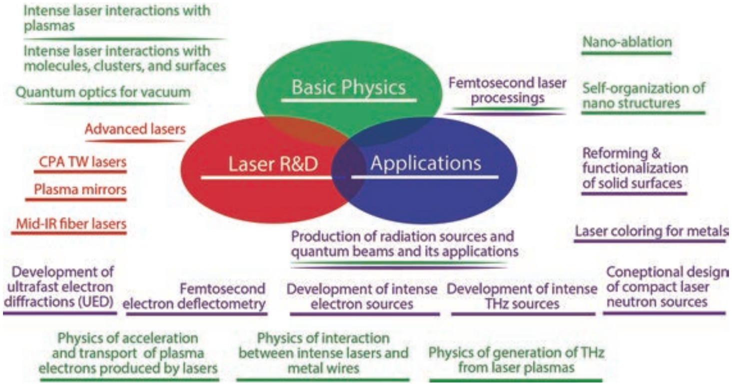
NATHAN, Goodfriend (Ph D) HiLASE, Czech R., 18 September–16 December

Scope of Research

The interaction of femtosecond laser pulses with matter involves interesting physics not seen with nanosecond laser pulses. Through investigations of the interaction physics, the potential of intense femtosecond lasers for new applications is being developed (e.g., laser-produced radiation and laser processing). Ultra-intense lasers can produce intense radiations (e.g., electrons, ions, and THz), which are promising as next-generation radiation sources. Ultra-short lasers can process any matter without thermal dissociation. Femtosecond laser processing is also the next-generation of laser processing. Our laboratory is equipped with an ultra-intense femtosecond laser named T6, to study the physics of intense laser–matter interactions and its applications.

KEYWORDS

Intense Laser Science
Laser Plasma Radiations (Electrons, Ions, and THz)
Ultrafast Electron Diffraction (UED)
Laser Nano-ablation Physics
Femtosecond Laser Processing



Selected Publications

Inoue, S.; Nakamiya, Y.; Teramoto, K.; Hashida, M.; Sakabe, S., Highly Intensified Emission of Laser-accelerated Electrons from a Foil Target through an Additional Rear Laser Plasma, *Phyiscal Review Accelerators and Beams*, **21,** 41302 (2018).

Teramoto, K.; Tokita, S.; Terao, T.; Inoue, S.; Yasuhara, R.; Nagashima, T.; Kojima, S.; Kawanaka, J.; Mori, K.; Hashida, M.; Sakabe, S., Half-Cycle Terahertz Surface Waves with MV/cm Field Strengths Generated on Metal Wires, *Appl. Phys. Lett.*, **113,** 51101 (2018).

Teramoto, K.; Inoue, S.; Tokita, S.; Yasuhara, R.; Nakamiya, Y.; Nagashima, T.; Mori, K.; Hashida, M.; Sakabe, S., Induction of Subterahertz Surface Waves on a Metal Wire by Intense Laser Interaction with a Foil, *Phys. Rev. E*, **97,** 23204 (2018).

Arikawa, Y.; Kato, Y.; Abe, Y.; Matsubara, S.; Kishimoto, H.; Nakajima, N.; Morace1, A.; Yogo, A.; Nishimura, H.; Nakai, M.; Fujioka, S.; Azechi, H.; Mima, K.; Inoue, S.; Nakamiya, Y.; Teramoto, K.; Hashida, M.; Sakabe, S., Efficient and Repetitive Neutron Generation by Double-laser-pulse Driven Photonuclear Reaction, *Plasma and Fusion Research*, **13,** 2404009 (2018).

Irizawa, A.; Suga, S.; Nagashima, T.; Higashiya, A.; Hashida, M.; Sakabe, S., Laser-induced Fine Structures on Silicon Exposed to THz-FEL, *Appl. Phys. Lett.*, **111,** 251602 (2017).

Topics

Ablation Suppression of Titanium Surface with Two Color Double-pulse Beam of Femtosecond Laser

An experiment of an ablation rate on a titanium surface irradiated by a double-pulse beam with two-color laser was demonstrated in time delays of $\Delta t = 0–700$ ps. The double pulse beam consists of 800 nm with 150 fs pulse and 400 nm with > 150 fs pulse. The fundamental-pulse fluence F_{800} is kept below ablation threshold ($F_{800\ th} = 0.108$ J/cm^2) while the second harmonic pulse fluence F_{400} are kept above the ablation threshold ($F_{400\ th} = 0.090$ J/cm^2). The ablation rate of titanium is clearly suppressed to 2.39 nm per pair at delay times of $\Delta t = 200$ ps. This ablation rate corresponds to one-third of 7.3 nm/pulse for only first pulse beam, while it corresponds to about one-half for one-color double pulse irradiation. We found that the ablation suppression with two-color double pulse beam was more enhanced than that for one-color double pulse beam. The shorting optical penetration length of the first pulse possibly related to suppression of the ablation rate.

Dot Coloring for Metal Surface by Femtosecond Laser Irradiation

Dot colorings to blue and brown have been demonstrated on the metal surface irradiated by the beam consisting of two-color femtosecond laser pulses with an appropriate time interval. Surface observation using an Electron Probe Micro Analyzer (EPMA) suggests that the dot coloring area is colored due to the formation of a uniform oxide layer on the irradiated area. The appropriate time interval for coloring is consistent with the time scale at which suppression of ablation by the double pulse irradiation is observed.

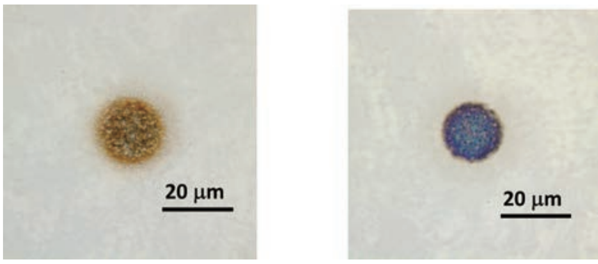


Figure 1. Double pulse irradiation (left) Brown, (right) Blue.

Highly Intensified Emission of Laser-accelerated Electrons from a Plasma-solid Hybrid Cathode

Intense ultrashort electron pulses are driven by the interaction of intense short laser pulses with solid targets. Ultrashort electron pulses are accelerated in the intense laser produced plasma. Laser-accelerated fast electrons have many possible applications, because of their higher absorptance of the laser pulse. For some applications, such as using fast electrons as probe pulses with high temporal resolution, it is desirable for a greater number of electrons to be emitted from the laser plasma. However, most laser-accelerated electrons cannot escape from the laser plasma because they are trapped by a strong quasi-static electric field, called the sheath field, produced around the steep density gradient boundary between the solid/plasma and the vacuum. Only a small fraction of electrons accelerated by intense short-pulse laser radiation escapes from the laser plasma, and most of the electrons expend their energy heating the target or producing other types of radiation. We demonstrate the intensification of electrons escaping from an intense laser plasma by using double femtosecond laser pulses. An intense pulse from a chirped pulse amplification laser (CPA1) for driving fast electrons is used to irradiate a foil target, the rear of which is pre-irradiated with another laser pulse (CPA2). Pre-irradiation with CPA2 controls the electron density distributions in the target to suppress sheath field growth and expand the target plasma into which the fast electrons are released. The number of escaping electrons increases greatly when the target is irradiated with CPA2 540 ps prior to CPA1. The number of escaping electrons with an energy of 380 keV released into vacuum is 7 times that for single-pulse irradiation. These results are supported by two-dimensional (2D) particle-in-cell (PIC) simulations of plasma produced by CPA2 and analytical evaluation considering the expansion of the plasma. These results show that over 10% of the accelerated electrons will be converted to escaping electrons by controlling the expanding plasma. These results show that the intense laser-irradiated foil could be used as a plasma-attached cathode, with great potential for high-brightness electron guns.

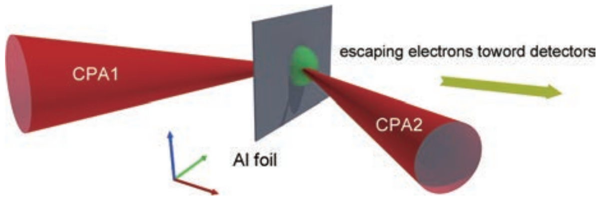


Figure 2. Schematic of the experimental setup. Two laser pulses (CPA1 and CPA2) are focused on the Al target (thickness: 11 µm).

Advanced Research Center for Beam Science
– Electron Microscopy and Crystal Chemistry –

http://eels.kuicr.kyoto-u.ac.jp/Root/English

Prof
KURATA, Hiroki
(D Sc)

Assist Prof
NEMOTO, Takashi
(D Sc)

Assist Prof
HARUTA, Mitsutaka
(D Sc)

Program-Specific Res*
OGAWA, Tetsuya
(D Sc)

Program-Specific Res*
KIYOMURA, Tsutomu

*Nanotechnology Platform

Researcher (pt)

FUJIYOSHI, Yoshifumi

Students

YAMAGUCHI, Atsushi (D3)
LAI, Ming Wei (D3)
NII, Aoi (M2)
SHIRASAWA, Yuri (M2)
SHINYA, Tomoki (M1)
TOBA, Tomohito (M1)
IWASHIMIZU, Chisaki (M1)

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　Spectrum Imaging　Template Matching　Nonrigid Registration　Atomic-Resolution Anisotropic Spectroscopy

Selected Publications

Aso, R.; Kan, D.; Shimakawa, Y.; Kurata, H., Atomic Level Observation of Octahedral Distortions at the Perovskite Oxide Heterointerface, *Sci. Rep.*, **3,** [2214-1]-[2214-6] (2013).

Saito, H.; Kurata, H., Formation of a Hybrid Plasmonic Waveguide Mode Probed by Dispersion Measurement, *J. Appl. Phys.*, **117,** [133107-1]-[133107-7] (2015).

Haruta, M.; Hosaka, Y.; Ichikawa, N.; Saito, T.; Shimakawa, Y.; Kurata, H., Determination of Elemental Ratio in an Atomic Column by Electron Energy-Loss Spectroscopy, *ACS Nano*, **10,** 6680-6684 (2016).

Haruta, M.; Fujiyoshi, Y.; Nemoto, T.; Ishizuka, A.; Ishizuka, K.; Kurata, H., Atomic-Resolution Two-Dimensional Mapping of Holes in the Cuprate Superconductor $La_{2-x}Sr_xCuO_{4\pm\delta}$, *Phys. Rev. B*, **97,** [205139-1]-[205139-5] (2018).

Yamaguchi, A.; Haruta, M.; Nemoto, T.; Kurata, H., Probing Directionality of Local Electronic Structure by Momentum-Selected STEM-EELS, *Appl. Phys. Lett.*, **113,** [053101-1]-[053101-4] (2018).

Atomic-Resolution Two-Dimensional Mapping of Holes in the Cuprate Superconductor $La_{2-x}Sr_xCuO_{4\pm\delta}$

One of the key factors in understanding high-T_c cuprate superconductors is the spatial distribution of holes in the sample. Since electron-energy-loss spectroscopy (EELS) can directly measure the unoccupied 2*p* states of the oxygen, EELS combined with scanning transmission electron microscopy (STEM-EELS) has the ability to resolve different oxygen states with atomic resolution. However, since cuprate superconductors are extremely sensitive to electron irradiation, it has not been possible to characterize them with atomic resolution. Here, we succeeded in atomic-resolution two-dimensional mapping of holes in the high-T_c superconductor of hole-doped type $La_{2-x}Sr_xCuO_{4\pm\delta}$ by overcoming the problem of irradiation damage using an advanced integration technique.

STEM-EELS was carried out at room temperature on a JEM-ARM200F. In order to achieve atomic-resolution imaging without specimen damage, a low probe current (21 pA) and a short dwell time of 5 ms were used with a scan step of 0.651 nm/pixel and a relatively wide energy dispersion of 0.25 eV/pixel. Spectrum imaging (SI) is a technique that collects the spacial distribution of EELS data. SI data were acquired from a 32.55 × 130.2 nm^2 (50 × 200 pixel^2) region. The total acquisition time for a single SI data was 66 s and the total dose was 2.4×10^3 C/cm^2. Although the individual single spectrum was very noisy, if the many crystallographically equivalent positions could be integrated, we might be able to realize atomic-resolution spectroscopy under the present conditions. However, the atomic-scale HAADF-STEM image obtained in the SI mode is distorted due to sample drift during the long acquisition time. Therefore, we devised the following procedure. First, we obtained many SI data with atomic resolution from a wide single-crystal region using a low-current condition. Next, we obtained a nondistorted HAADF image with the same scan step using a fast dwell time (the template image of the unit cell). Then, we selected many crystallographically equivalent regions from a target HAADF-STEM image by judging the correlation with the template image (template matching) and applied rigid and nonrigid registration of these equivalent regions to fit the template image by using the SMARTALIGN software package (HREM Research) and finally applied them to the corresponding SI data. Upon repeating this procedure over many SI data, the S/N ratio improved dramatically, maintaining spatial resolution without causing irradiation damage. The total accumulation numbers of the spectra were 12008, 14348, and 4712 for the $x = 0.15$, 0.3, and 0.4 samples, respectively.

Figure 1(a) shows O *K*-edge spectra of $La_{2-x}Sr_xCuO_{4\pm\delta}$ averaged over the whole unit. The prepeak (528.5 eV) that appears for doped samples corresponds to holes in the oxygen 2*p* state. Figures 1(b) and 1(c) show the spectra for the center of the apical and purely planar oxygen sites [labeled planar1 in Figure 2(a)], respectively. Figure 2 shows the results obtained by template matching and nonrigid registration. Figures 2(c)–2(e) show atomic-resolution hole maps obtained using hole-peak signals (1.5 eV window) of the O *K* edge. In the case of $x = 0.15$, the hole map exhibits an anisotropic distribution, where only the planar oxygen sites are displayed brightly. Planar 2 oxygen columns appear darker than planar 1 oxygen columns. If, as in the planar 1 oxygen columns, the hole state ($2p_x$) in planar oxygen is perpendicular to the electron beam (parallel to the direction of momentum transfer upon inelastic scattering), the prepeak intensity must be higher than that ($2p_y$) at the CuO column. We have demonstrated the anisotropic chemical bond related to the difference between p_x and p_y orbitals was observed with atomic resolution. The present approach enables atomic-resolution anisotropic spectroscopy.

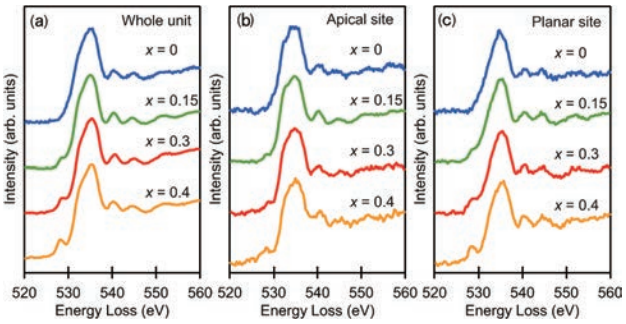


Figure 1. O *K*-edge spectra of $La_{2-x}Sr_xCuO_{4\pm\delta}$. (a) Atomic-resolution spectra averaged over the whole unit, and (b) apical and (c) planar oxygen site spectra after nonrigid alignment.

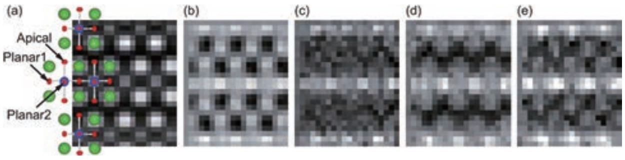


Figure 2. Atomic-resolution hole mapping. (a) Template HAADF image of $La_{2-x}Sr_xCuO_{4\pm\delta}$ observed along the [100] zone axis of the tetragonal phase. La (Sr), Cu, and O atoms correspond to green, blue, and red, respectively. (b) Atomic-resolution oxygen mapping of $La_{1.85}Sr_{0.15}CuO_{4\pm\delta}$. Atomic-resolution hole mapping of (c) $x = 0.15$, (d) $x = 0.3$, and (e) $x = 0.4$.

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

http://www.scl.kyoto-u.ac.jp/~fujii/indexE.html

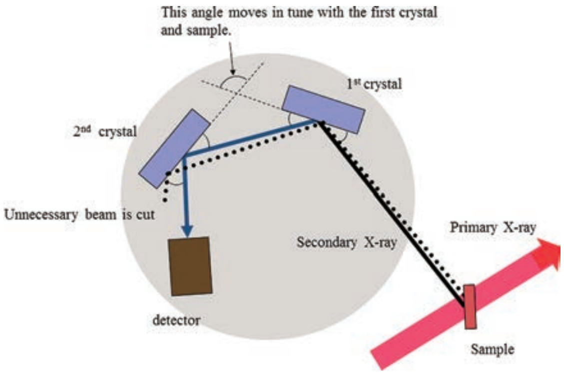
Assoc Prof
ITO, Yoshiaki
(Ph D)

Assist Prof
FUJII, Tomomi
(D Sc)

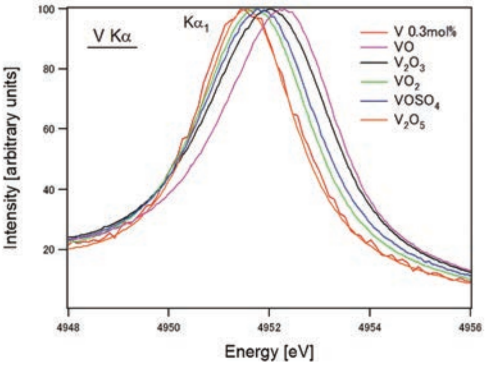
Scope of Research

Our laboratory analyzes the electronic state of atomic or molecular structure in materials, which are obtained from diffraction and spectra observed by X-ray irradiation, respectively, to elucidate the relationships between the structure and the physical properties. Our main themes are (1) high-resolution experimental and theoretical studies on the natural linewidth of elements in materials, (2) the development of the spectrometer in the measurements of the diagram lines in soft X-rays region, and (3) structural determination of novel protein molecules and their complexes.

KEYWORDS
High Resolution X-ray Crystal Spectrometer
Natural Linewidth
Chemical Shift
Structural Biology
Protein Crystallography



Oxidation state on V and Mn $K\alpha_1$ x-ray emission spectra



Selected Publications

Ito, Y.; Tochio, A.; Vlaicu, H.; Yamashita, M.; Fukushima, S.; Polasik, M.; Slabkowska, K.; Syrocki, L.; Szymanska, E.; Rzadkiewicz, J.; Indelicato, P.; Marques, J. P.; Martins, M. C.; Santos, J. P.; Parente, F., Structure of High-resolution $K\beta_{1,3}$ X-Ray Emission Spectra for the Elements from Ca to Ge, *Phys. Rev.*, **A97,** [052505-1]-[052505-10] (2018).

Menesguen, Y.; Lepy, M.-C.; Honicke, P.; Muller, M.; Unterumsberger, R.; Beckoff, B.; Hoszowska, J.; Dousse, J.-Cl.; Blachucki, W.; Ito, Y.; Yamashita, M.; Fukushima, S., Experimental Determination of X-Ray Atomic Fundamental Parameters of Nickel, *Metrologia*, **55,** 56 (2018).

Tanikawa, T.; Ito, Y.; Fukushima, S.; Yamashita, M.; Sugiyama, A.; Mizoguchi, T.; Okamoto, T.; Hirano, Y., Calcium Is Cycled Tightly in *Cryptomeria Japonica* Stands on Soils with Low Acid Buffering Capacity, *For. Ecol. Manage.*, **399,** 64-73 (2017).

Ito, Y.; Tochio, T.; Ohashi, H.; Yamashita, M.; Fukushima, S.; Polasik, M.; Slabkowska, K.; Syrocki, L.; Szymanska, E.; Rzadkiewicz, J.; Indelicato, P.; Marques, J. P.; Martins, M. C.; Santos, J. P.; Parente, F., $K\alpha_{1,2}$ X-ray Linewidths, Asymmetry Indecies, and [*KM*] Shake Probabilities in Elements Ca to Ge and Comparison with Theory for Ca, Ti, and Ge, *Phys. Rev.*, **A94,** [42506-1]-[42506-11] (2016).

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).

Fujii, T.; Yamauchi, T.; Ishiyama, M.; Gogami, Y.; Oikawa, T.; Hata, Y., Crystallographic Studies of Aspartate Racemase from *Lactobacillus sakei* NBRC 15893, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **71,** 1012-1016 (2015).

The Spin Doublets, FWHM, and Shake Probabilities in 3d $K\beta_{1,3}$ Spectra

The content described below is another result of our research on the spin doublets and the asymmetry of the $K\beta_{1,3}$ x-ray emission spectra in the 3*d* transition metals that has been unknown in the history of about 100 years in Atomic Physics.

The $K\beta_{1,3}$ x-ray emission spectra include *Kβ*’ and *Kβ*” satellites on the low- and high-energy side of the $K\beta_{1,3}$ peak position, respectively, as explained in the case of copper. These satellites have also been investigated until now both experimentally and theoretically for all 3*d* transition metals. Shake-up from the 3*d* shell was also shown to account reasonably well for the measured $K\beta_{1,3}$ line shape, although a complete quantitative fitting has not been reported and possible contributions from other shells were not investigated. The low-energy satellite group, denoted by *Kβ*’, received special attention, and several other sources such as exchange interaction and plasmon oscillations were suggested as its origin. It has been assumed that the line shape can be fully accounted for by satellites resulting from 3*l* spectator holes in addition to the nominal single-electron diagram transitions.

We have investigated the $K\beta_{1,3}$ x-ray spectra of the elements from Ca to Ge using a high-resolution antiparallel double-crystal x-ray spectrometer (Figure 1). Each $K\beta_{1,3}$ natural line width has been corrected using the instrumental function of this type of x-ray spectrometer, and the spin doublet energies have been obtained from the peak position values in $K\beta_{1,3}$ x-ray spectra (Figure 2). Moreover, it has been found that the contribution of satellite lines are considered to be [*KM*] shake processes (Figure 3).

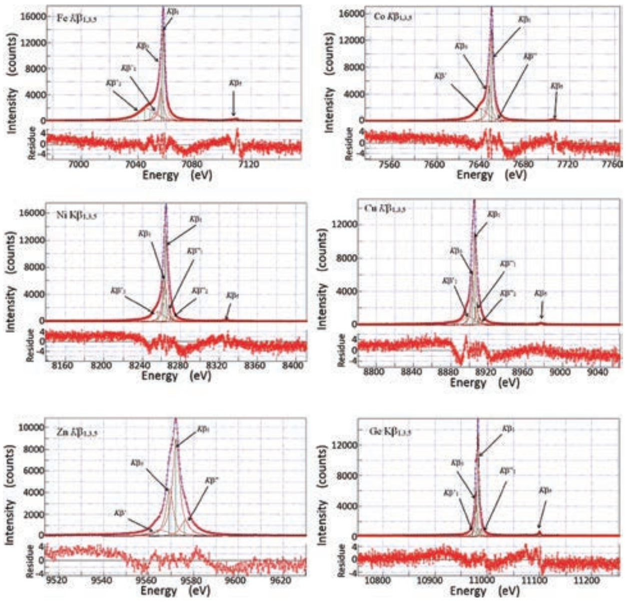


Figure 1. The observed $K\beta_{1,3}$ spectra in elements Fe to Ge are shown with the fitting Lorentzian function (Phys Rev A97, 052505). These spectra were measured using the antiparallel double-crystal x-ray spectrometer described in detail in Phys Rev A94,042506. In this figure, the *Kβ*” line is a satellite line resulting from a 3*d* spectator hole.

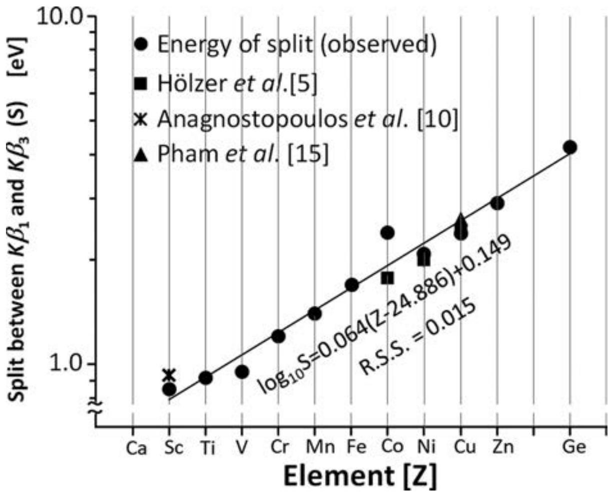


Figure 2. The spin doublet energies of $K\beta_1$ and $K\beta_3$ lines for elements Sc to Ge. The least-squares fitting was executed using data in the present work.

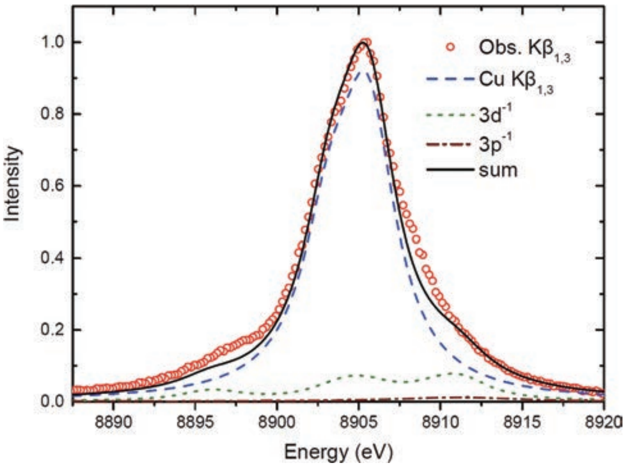


Figure 3. Comparison of the high-resolution experimental spectra with the predicted $K\beta_{1,3}$ spectra of Cu including the contributions of the $K\beta_{1,3}$ diagram lines and the satellite lines for [1s3p] and [1s3*d*] hole states.

International Research Center for Elements Science
– Synthetic Organotransformation –

http://es.kuicr.kyoto-u.ac.jp/index_en.html

Prof
NAKAMURA, Masaharu
(D Sc)

Assoc Prof
TAKAYA, Hikaru
(D Eng)

Assist Prof
ISOZAKI, Katsuhiro
(D Eng)

Assist Prof
IWAMOTO, Takahiro
(D Eng)

PD
PINCELLA, Francesca
(Ph D)

PD
GELDSETZER, Jan
(Ph D)

Researchers (pt)

MATSUDA, Hiroshi
AGATA, Ryosuke
NAKAMURA, Yuki

Students

HOSOKAWA, Atsushi (M2)
SYANOH, Takafumi (M2)
IWAKAMI, Mako (M1)
LU, Siming (M1)
KAWASAKI, Hiroto (M1)
JEON, Jaeyoung (RS)
WANG, Jun (RS)
JIANG, Jiayi (RS)
ZHANG, Yaqi (RS)
ABE, Ayaka (UG)
NAKATANI, Yuuya (UG)
NOMURA, Satsuki (UG)

Guest Res Assoc

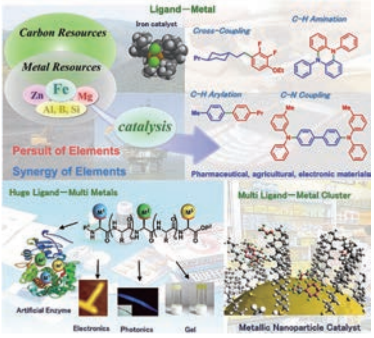
DOKSANSKA, Barbora Lucie	University of St Andrews, U.K., 13 June–6 August
TAILOR, Sanita	University of Bristol, U.K., 19 June–21 August

Guest Scholar

HAJRA, Alakananda (D Eng)	Visva-Bharati University, India, 1 July–14 August

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 smart materials based on synergistic effect of various metals on artificial peptides (3) development of smart metallic nanoparticle catalysts based on supramolecular approaches (4) understanding of reaction mechanism of these catalytic reactions with the help of quantum chemical methods and synchrotron X-ray absorption spectroscopy.



KEYWORDS

Selective Organic Reaction
Metallic Nanoparticle Catalyst
Iron Catalyst
Solution-Phase XAS Analysis
Metalated Peptide Catalyst

Selected Publications

Sugimoto, K.; Takaya, H.; Maekawa, M.; Kuroda-Sowa, T., Controlled Self-Assembly of a 2-D Sheet Coordination Polymer and Monomer Containing an Eight-Membered Cu_4I_4 Crown Motif, *Cryst. Growth. Des.*, **18,** 571-575 (2018).

Hirano, M.; Sano, K.; Kanazawa, Y.; Komine, N.; Maeno, Z.; Mitsudome, T.; Takaya, H., Mechanistic Insights on Pd/Cu-Catalyzed Dehydrogenative Coupling of Dimethyl Phthalate, *ACS Catal.*, **8,** 5827-5841 (2018).

Isozaki, K.; Shimoaka, T.; Oshiro, S.; Yamaguchi, A.; Pincella, F.; Ueno, R.; Hasegawa, T.; Watanabe, T.; Takaya, H.; Nakamura, M., Robust Surface Plasmon Resonance Chips for Repetitive and Accurate Analysis of Lignin–Peptide Interactions, *ACS Omega*, **3,** 7483-7493 (2018).

Topics

Iron-Catalyzed Cross-Coupling Reactions

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 recent representative examples, we developed the first example of iron-catalyzed enantioselective cross-coupling reaction of alkyl halides, which enable facile access to optically active products from readily available racemic halides (Figure 1a). By using DFT and AFIR calculations, we revealed that the reaction proceeds via a novel $Fe^{I–II–III}$ mechanism (Figure 1b).

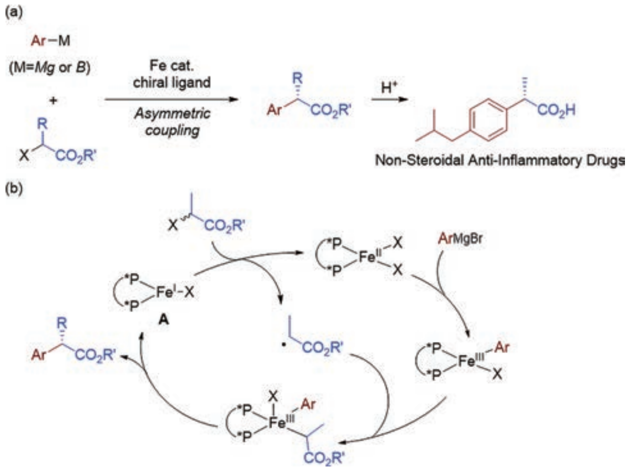


Figure 1. (a) Enantioconvergent coupling of alkyl halides and (b) its mechanism by theoretical calculation.

Moreover, we developed diastereoselective iron-catalyzed cross-coupling reaction of various glycosyl halides with aryl metal reagents for the efficient synthesis of aryl C-glycosides, which are of significant pharmaceutical interest due to their biological activities and resistance toward metabolic degradation (Figure 2).

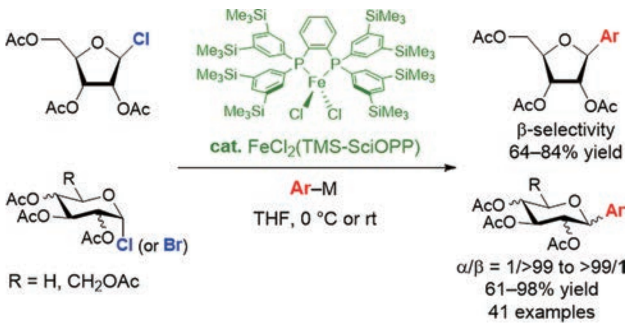


Figure 2. Synthesis of Aryl C-Glycosides via Iron-Catalyzed Cross Coupling of Halosugars.

Novel Transition-Metal Catalyst Bound with Functional Amino Acid or Peptide

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

Supramolecular Approach for Creating Enhanced Catalysis of Metallic Nanoparticles

This project focuses on the development of highly active and selective metallic nanoparticle and cluster catalysts. To achieve this purpose, four key methodologies have been developed: 1) creation of reaction field with advanced self-assembly, 2) design of selective molecular transformation with multi-points intermolecular interaction, 3) size selective synthesis of metallic nanoparticles and clusters, and 4) utilization of plasmonic resonance with light.

International Research Center for Elements Science
– Advanced Solid State Chemistry –

http://www.scl.kyoto-u.ac.jp/~shimakgr/indexE.html


Prof
SHIMAKAWA, Yuichi
(D Sc)


Assoc Prof
KAN, Daisuke
(D Sc)


Program-Specific Assist Prof
SAITO, Takashi
(D Sc)


Techn Staff
ICHIKAWA, Noriya
(D Eng)


PD (JSPS)
AMANO PATINO,
Midori Estefani
(Ph D)


PD (JSPS)
HEO, Yooun
(Ph D)


PD
GOTO, Masato
(D Sc)


PD
GUO, Haichuan
(D Sc)

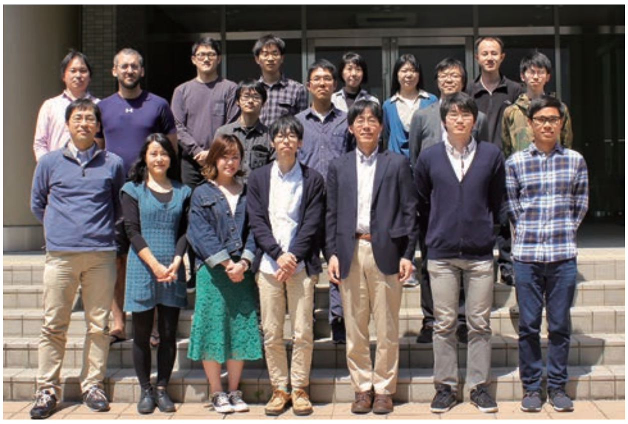
Students

- KOEDTRUAD, Anucha (D2)
- TAN, Zhenhong (D1)
- NIWA, Yasuyuki (M2)
- KOBAYASHI, Kento (M2)
- SANTO, Junya (M2)
- MATSUMOTO, Sho (M2)
- UEBAYASHI, Nao (M1)
- KOSUGI, Yoshihisa (M1)
- SUGANO, Satoshi (M1)

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

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.



Selected Publications

Denis Romero, F.; Xiong, P.; Amano Patino, M.; Saito, T.; Kayser, P.; Attfield, J. P.; Shimakawa, Y., Suppression of Sequential Charge Transitions in $Ca_{0.5}Bi_{0.5}FeO_3$ via B-Site Cobalt Substitution, *Chem. Mater.*, **30,** 5493-5499 (2018).

Tan, Z.; Saito, T.; Denis Romero, F.; Amano Patino, M.; Goto, M.; Chen, W.-T.; Chuang, Y.-C.; Sheu, H.-S.; Shimakawa, Y., Hexagonal Perovskite $Ba_4Fe_3NiO_{12}$ Containing Tetravalent Fe and Ni Ions, *Inorg. Chem.*, **57,** 10410-10415 (2018).

Kan, D.; Aso, R.; Sato, R.; Haruta, M.; Kurata, H.; Shimakawa, Y., Tuning Magnetic Anisotropy by Interfacially Engineering the Oxygen Coordination Environment in a Transition-metal Oxide, *Nat. Mater.*, **15,** 432-437 (2016).

Chen, W.-T.; Mizumaki, M.; Seki, H.; Senn, M.; Saito, T.; Kan, D.; Attfield, J. P.; Shimakawa, Y., A Half-metallic A- and B-site-ordered Quadruple Perovskite Oxide $CaCu_3Fe_2Re_2O_{12}$ with Large Magnetization and a High Transition Temperature, *Nat. Comm.*, **5,** [3909-1]-[3909-7] (2014).

Matsumoto, K.; Haruta, M.; Kawai, M.; Sakaiguchi, A.; Ichikawa, N.; Kurata, H.; Shimakawa, Y., Selective Reduction of Layers at Low Temperature in Artificial Superlattice Thin Films, *Sci. Rep.*, **1,** [27-1]-[27-4] (2011).

Hexagonal Perovskite $Ba_4Fe_3NiO_{12}$ Containing Tetravelent Fe and Ni Ions

Some 3d-transition-metal ions in oxides can show unusually high valence states, in addition to the conventional valence states. It has been reported that both unusually high valence Fe^{4+} and Ni^{4+} are stabilized in hexagonal-type perovskite structure oxides, whose chemical formula is ABO_3. Fe^{4+} in $BaFeO_3$ (BFO) is stabilized with the 6H hexagonal perovskite structure, while unusually high valence Ni^{4+} is stabilized in the 2H hexagonal perovskite $BaNiO_3$ (BNO).

In this study, we synthesized $Ba(Fe_xNi_{1-x})O_3$ with end members of $BaNiO_3$ (x = 0) and $BaFeO_3$ (x = 1), and investigated their crystal structures and magnetic properties. We successfully synthesized by a high-pressure and high-temperature technique a new single phase, $Ba_4Fe_3NiO_{12}$ (x = 0.75), that adopts the 12R perovskite structure with the space group $R\bar{3}m$. Mössbauer spectroscopy results and structure analysis using synchrotron and neutron powder diffraction data revealed that Fe^{3+} occupies the corner-sharing octahedral site while the unusually high valence Fe^{4+} and Ni^{4+} occupy the face-sharing octahedral sites in the trimers, giving a charge formula of $Ba_4Fe^{3+}Fe^{4+}{}_2Ni^{4+}O_{11.5}$. At temperatures below about 200 K, this compound shows a ferromagnetic-like behavior with small magnetization. Ni^{4+} is suggested to have a low-spin electron configuration and not contribute to the magnetic properties of the compound, and thus, the observed weak ferromagnetism of this compound seems to originate from ferrimagnetic coupling between Fe^{3+} and Fe^{4+} spins.

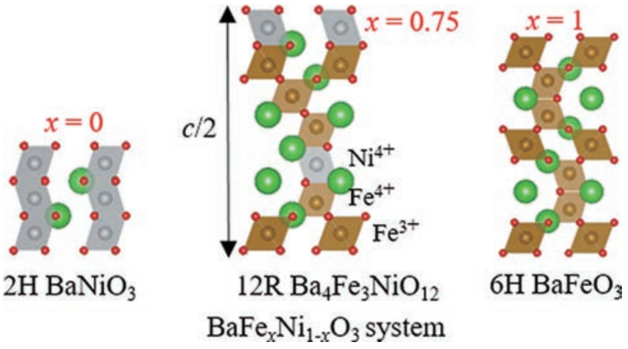


Figure 1. Crystal structures of 2H $BaNiO_3$ (left), 12R $Ba_4Fe_3NiO_{12}$ (middle) and 6H $BaFeO_3$ (right).

Nanoscale Oxygen Ion Dynamics in $SrFeO_{2.5+\delta}$ Epitaxial Thin Films

A variety of functional properties in transition metal oxides are often underpinned by oxygen vacancies. While the oxygen vacancy concentration and arrangements are well-known to have strong influence on physical properties of oxides, the oxygen dynamics in oxides—including oxygen ion incorporation and movements during redox reactions—remain elusive. Oxygen deficient iron-based perovskite-structured oxides $SrFeO_{2.5+\delta}$ ($0 \leqq \delta \leqq 0.5$) exhibit electrical transport properties that are closely associated with the oxygen off-stoichiometry. This conducting property in $SrFeO_{2.5+\delta}$ thus allows one to evaluate oxygen dynamics involving local redox reactions. In this study, by using combinations of X-ray diffraction (XRD) and conducting AFM (c-AFM), we characterize structures and local conduction properties associated with redox reactions in $SrFeO_{2.5+\delta}$ epitaxial thin films and evaluate nanoscale oxygen dynamics. Our c-AFM observations reveal that brownmillerite-to-perovskite structural changes due to air-annealing and oxidizing the film enhances conduction only in the terraces near the outer step edges. This indicates that the oxidation proceeds by preferential incorporation of oxygen in the local regions of the terraces and by diffusion of the incorporated oxygen into the film. We also show that the local conduction in the film can be controlled by electric-field-induced redox reactions. Our results highlight the significance of nanoscale oxygen dynamics and associated redox reactions in $SrFeO_{2.5}$ films.

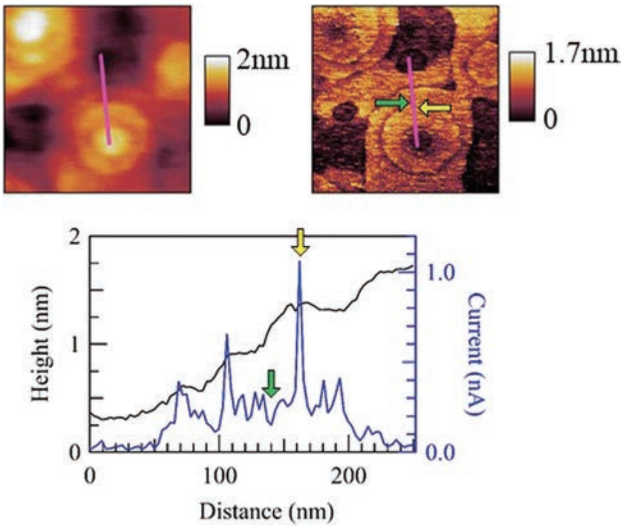


Figure 2. High-resolution topography and c-AFM images of the $SrFeO_{2.5+\delta}$ film. In the bottom, cross-section profiles along the pink lines in the topography and conduction images are plotted.

International Research Center for Elements Science
– Organometallic Chemistry –

http://om.kuicr.kyoto-u.ac.jp

Prof
OZAWA, Fumiyuki
(D Eng)

Assist Prof
WAKIOKA, Masayuki
(D Eng)

Students

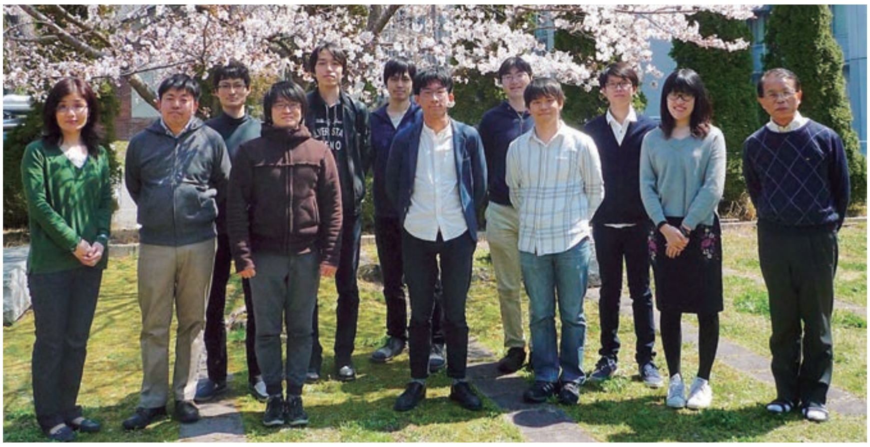
YAMASAKI, Akito (M2)	MAEDA, Junya (M1)
TORII, Naohiro (M2)	HAMADA, Yusuke (UG)
ISHIZUKA, Risa (M1)	MAKINO, Saiki (UG)

Scope of Research

This laboratory aims to establish new synthetic methodologies and new functional materials by designing well-defined catalysts based on transition metal chemistry. New concepts and ideas of molecular-based catalysts are accumulated by mechanistic investigations using experimental methods such as spectroscopy and kinetic techniques, as well as theoretical methods. The research subjects include: 1) development of novel organotransition metal systems for catalysis based on precise ligand design, and 2) preparation of π-conjugated polymers using direct arylation.

KEYWORDS

Transition Metal Complex
Homogeneous Catalyst
Reaction Mechanism
Low-coordinate Phosphorus Ligand
π-Conjugated Polymer



Selected Publications

Wakioka, M.; Yamashita, N.; Mori, H.; Nishihara, Y.; Ozawa, F., Synthesis of a 1,2-Dithienylethene-Containing Donor-Acceptor Polymer via Palladium-Catalyzed Direct Arylation Polymerization (DArP), *Molecules*, **23,** 981 (2018).

Wakioka, M.; Ozawa, F., Highly Efficient Catalysts for Direct Arylation Polymerization (DArP), *Asian J. Org. Chem.*, **7,** 1206-1216 (2018).

Taguchi, H.; Tanigawa, I.; Takeuchi, K.; Ozawa, F., On the Geometrical Stability of Square Planar Platinum(0) Complexes That Bear a PNP-Pincer-Type Phosphaalkene Ligand (Eind2-BPEP), *Chem. Eur. J.*, **24,** 17055-17061 (2018).

Synthesis of Benzothiadiazole-Containing Donor-Acceptor Polymers via Palladium-Catalyzed Direct Arylation Polymerization (DArP)

We found that the combined use of $P(2\text{-}MeOC_6H_4)_3$ (**L1**) and TMEDA as ligands effectively prevented defect formation in palladium-catalyzed direct arylation polymerization (DArP) to give donor-acceptor polymers (DA polymers) with benzothiadiazole units. The reactions of benzothiadiazole derivatives (**1-Br**) and 2,2'-bithiophene (**2-H**) formed a notable amount of insoluble materials via branching and cross-linking when only **L1** was used as the ligand. In contrast, in the presence of **L1** and TMEDA, the formation of insoluble materials was completely suppressed, and the polymers with well-controlled structures and high molecular weight were obtained. The resulting polymers exhibited device performance of polymer solar cells comparable to Migita–Stille cross-coupling polymerization products.

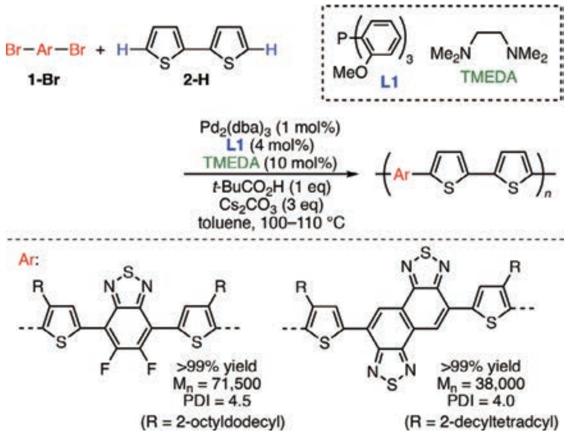


Figure 1. DArP synthesis of benzothiadiazole-containing DA Polymers.

Synthesis of a 1,2-Dithienylethene-Containing Donor-Acceptor Polymer via Palladium-Catalyzed Direct Arylation Polymerization (DArP)

We found that the mixed-ligand catalyst using $P(2\text{-}MeOC_6H_4)_3$ (**L1**) and TMEDA is effective in synthesizing DA polymers containing 1,2-dithienylethene (DTE) units via DArP. The reaction of dibromoisoindigo and 1,2-dithienylethene in the presence of the mixed-ligand catalyst affords polymer **P1** with high molecular weight (M_n = 15,700). The resulting polymer has a well-controlled structure and exhibits good charge transfer characteristics in an organic field-effect transistor (OFET), compared to the polymer produced by Migita–Stille cross-coupling polymerization. The DArP product displays an ideal linear relationship in the current–voltage curve, whereas the Migita–Kosugi–Stille product shows a V_G-dependent change in the charge mobility.

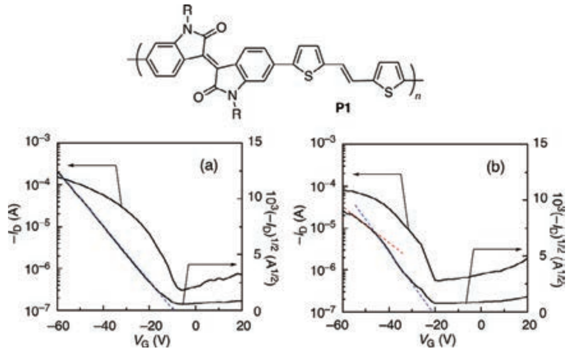


Figure 2. Charge transfer characteristics of the OFETs using **P1** prepared by DArP (a) and Migita–Stille coupling polymerization (b) (V_D = −60 V).

Square Planar Pt(0) Phosphaalkene Complexes

The four-coordinate Pt(0) complex $[Pt(PPh_3)(Eind_2\text{-}BPEP)]$ (**1**) bearing a pyridine-based PNP-pincer type phosphaalkene ligand ($Eind_2$-BPEP) adopts a highly planar structure around the Pt; this coordination geometry is very uncommon for formal d^{10} metals. In this study, a series of L with different electronic properties [DMAP (**2**), 3,5-lutidine (**3**), PMe_3 (**4**), *t*BuNC (**5**), CO (**6**)] were introduced in place of PPh_3, and their effects on the coordination geometry and spectroscopic properties were examined. X-ray diffraction analysis revealed that all complexes adopted a square-planar configuration. In contrast, DFT calculations indicated that the geometrical stability towards distortion around Pt varied with the ligand. The complexes with pyridine-based ligands had rigid planar structures, whereas those with π-accepting ligands, such as CO, were relatively flexible towards distortion. The electronic effects of the ligands were reflected in the spectroscopic properties of the complexes, which showed a large color change in the near-infrared region.

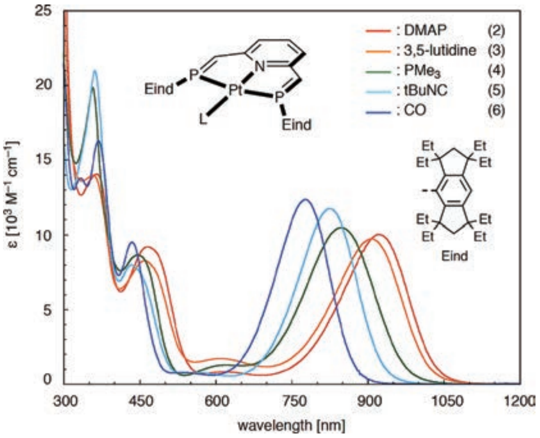


Figure 3. UV-vis-NIR spectra of $[Pt(L)(Eind_2\text{-}BPEP)]$ complexes in THF at room temperature.

International Research Center for Elements Science
– Nanophotonics –

http://www.scl.kyoto-u.ac.jp/~opt-nano/index-e.html


Prof
KANEMITSU, Yoshihiko
(D Eng)


Assoc Prof
HIRORI, Hideki
(D Sc)


Assist Prof
TAHARA, Hirokazu
(D Sc)


PD
LE, Phuong Quang
(D Eng)


PD
AHAREN, Tomoko
(Ph D)


Program-Specific Res
YUMOTO, Go
(D Sc)

Students

YAMADA, Takumi (D3)
HANDA, Taketo (D2)
SANARI, Yasuyuki (D1)
NAKAHARA, Satoshi (M2)
OHARA, Keiichi (M1)
MASADA, Sojiro (M1)

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, and 3) photophysics of solar cell materials.

KEYWORDS
Femtosecond Laser Spectroscopy
Semiconductor Nanoparticles
Perovskites
Single Photon Spectroscopy
Solar Cells

Selected Publications

Yamada, T.; Aharen, T.; Kanemitsu, Y., Near-band-edge Optical Responses of $CH_3NH_3PbCl_3$ Single Crystals: Photon Recycling of Excitonic Luminescence, *Phys. Rev. Lett.*, **120,** [057404-1]-[057404-6] (2018).

Tahara, H.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Quantum Coherence of Multiple Excitons Governs Absorption Cross-sections of PbS/CdS Core/Shell Nanocrystals, *Nat. Commun.*, **9,** [3179-1]-[3179-8] (2018).

Tahara, H.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Harmonic Quantum Coherence of Multiple Excitons in PbS/CdS Core-shell Nanocrystals, *Phys. Rev. Lett.*, **119,** [247401-1]-[247401-6] (2017).

Yamada, Y.; Yamada, T.; Le, P. Q.; Maruyama, N.; Nishimura, H.; Wakamiya, A.; Murata, Y.; Kanemitsu, Y., Dynamic Optical Properties of $CH_3NH_3PbI_3$ Single Crystals as Revealed by One- and Two-Photon Excited Photoluminescence Measurements, *J. Am. Chem. Soc.*, **137,** 10456-10459 (2015).

Yamada, Y.; Nakamura, T.; Endo, M.; Wakamiya, A.; Kanemitsu, Y., Photocarrier Recombination Dynamics in Perovskite $CH_3NH_3PbI_3$ for Solar Cell Applications, *J. Am. Chem. Soc.*, **136,** 11610-11613 (2014).

Influence of Exciton-exciton Interactions on Optical Gain of Lead Halide Perovskite Nanocrystals

Recently, low threshold optical amplification has been observed in all-inorganic lead halide perovskite $CsPbX_3$ (X = Cl, Br, I) nanocrystals (NCs), which exhibits their excellent potential for an optical gain material. In the nonlinear optical response region, multiple excitons are generated in NCs and the many-body interactions affect the optical gain. Therefore, understanding of exciton-exciton interactions is important for optimal laser design. In this study, we performed femtosecond transient absorption spectroscopy on $CsPbI_3$ NCs and observed fast spectral changes originating from exciton-exciton interactions. We revealed the exciton-exciton interaction between a hot exciton generated by the pump pulse and an exciton at the band edge depends on the hot exciton state. Furthermore, we found optical gain depends on the hot exciton state due to such a hot-exciton-state-dependent interaction.

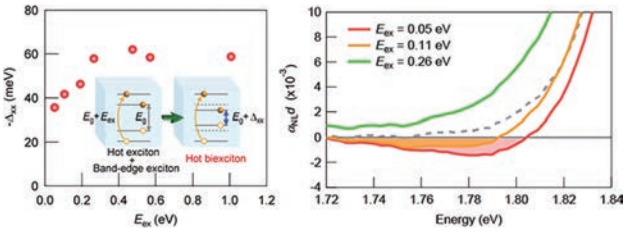


Figure 1. Pump excess energy dependence of the exciton-exciton interaction strength and nonlinear absorption spectra of $CsPbI_3$ NCs.

Trion Formation Mechanism in Lead Halide Perovskite Nanocrystals

Lead halide perovskite nanocrystals (NCs) are promising candidates for application to efficient light emitting devices. In the perovskite NCs, we have reported that charged excitons, so-called trions, contribute to carrier dynamics and play a key role in non-radiative decay processes. Therefore, revealing trion formation mechanism is important for improving the photoluminescence efficiency. Here, we performed transient absorption spectroscopy on both pristine $CsPbBr_3$ NCs and those surface-treated by sodium thiocyanate (NaSCN). By comparing the transient absorption signals in $CsPbBr_3$ NCs with and without the surface treatment, we revealed surface trap states strongly contribute to trion formation under weak excitation conditions. We also found that biexciton Auger recombination becomes the dominant process in trion formation as we increase the excitation intensity.

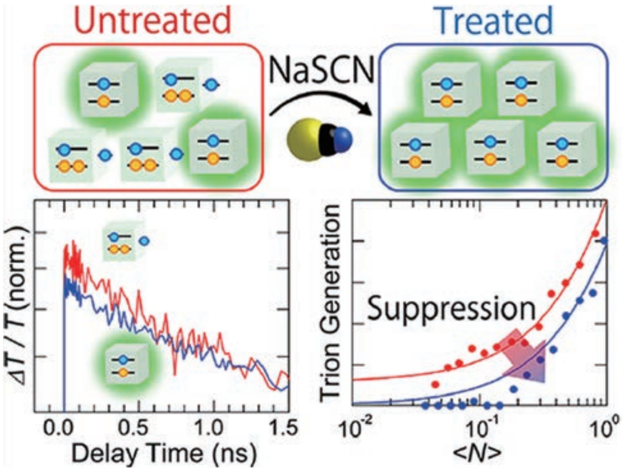


Figure 2. Transient absorption dynamics and estimated excitation intensity dependence of trion generation amplitudes in both pristine and surface-treated $CsPbBr_3$ NCs.

Optical Phase Shifter Based on Lead Halide Perovskite Single Crystals

Having large absorption coefficients and high photoluminescence efficiencies, lead halide perovskites are one of the most promising materials for optoelectronic applications such as solar cells and light emitting diodes. In order to reveal the unique nonlinear optical properties of lead halide perovskites, we investigated a high-quality lead bromide perovskite ($CH_3NH_3PbBr_3$) single crystal. We utilized a laser interferometric technique to measure the photo-induced refractive index changes with high accuracy. We observed long-lived refractive phase shift and revealed the mechanism of such a nonlinear optical response by performing excitation-intensity-dependent and time-resolved measurements. Moreover, we demonstrated that owing to the photorefractive properties, the perovskite single crystal works as a phase shifter of laser light to generate any desired polarization.

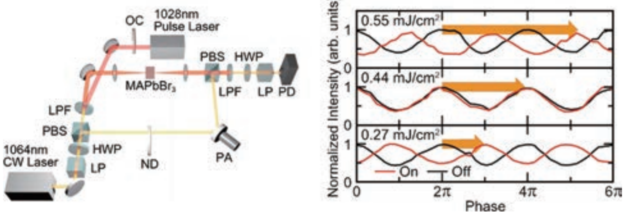


Figure 3. Schematic of interference-detection system and photocarrier-induced refractive phase shift in a $CH_3NH_3PbBr_3$ single crystal.

Bioinformatics Center
– Chemical Life Science –

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


Prof
OGATA, Hiroyuki
(D Sc)


Assist Prof
BLANC-MATHIEU, Romain
(D Sc)


Assist Prof
ENDO, Hisashi
(D Environmental Science)

Researcher (pt)

YAMAMOTO, Rumiko

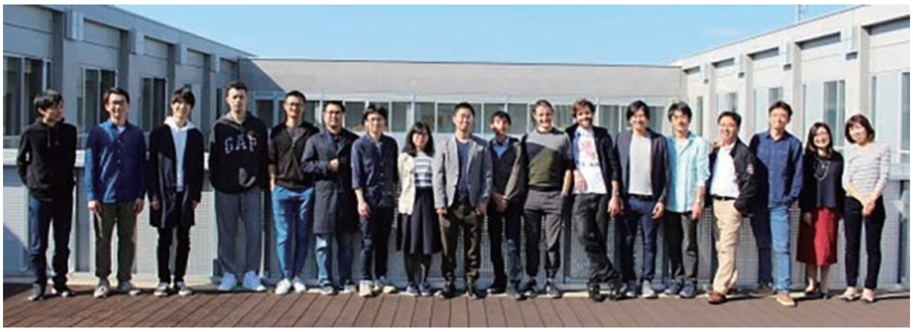
Students

YOSHIKAWA, Genki (D2)
NISHIYAMA, Hiroki (D2)
PRODINGER, Florian (D2)
LI, Yanze (M2)
KURONISHI, Megumi (M2)
ARAMAKI, Takuya (M2)
KANEKO, Hiroto (M2)
KATO, Yasutaka (M2)
YOSHIDA, Koki (M1)
JIANG, Junhuan (RS)
MENG, Lingjie (RS)
XIA, Jun (RS)
ZHANG, Ruixuan (RS)
RODRIGO, Hernandez Velazquez (UG)
FAN, Minyue (UG)

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



Selected Publications

Li, Y.; Hingamp, P.; Watai, H.; Endo, H.; Yoshida, T.; Ogata, H., Degenerate PCR Primers to Reveal the Diversity of Giant Viruses in Coastal Waters, *Viruses*, **10,** 496 (2018).

Endo, H.; Ogata, H.; Suzuki, K., Contrasting Biogeography and Diversity Patterns between Diatoms and Haptophytes in the Central Pacific Ocean, *Sci. Rep.*, **8,** 10916 (2018).

Mihara, T.; Koyano, H.; Hingamp, P.; Grimsley, N.; Goto, S.; Ogata, H., Taxon Richness of "Megaviridae" Exceeds Those of Bacteria and Archaea in the Ocean, *Microbes Environ.*, **33,** 162-171 (2018).

Yoshida, T.; Nishimura, Y.; Watai, H.; Haruki, N.; Morimoto, D.; Kaneko, H.; Honda, T.; Yamamoto, K.; Hingamp, P.; Sako, Y.; Goto, S.; Ogata, H., Locality and Diel Cycling of Viral Production Revealed by a 24 h Time Course Cross-omics Analysis in a Coastal Region of Japan, *ISME J.*, **12,** 1287-1295 (2018).

Yoshikawa, G.; Askora, A.; Blanc-Mathieu, R.; Kawasaki, T.; Li, Y.; Nakano, M.; Ogata, H.; Yamada, T., Xanthomonas Citri Jumbo Phage XacN1 Exhibits a Wide Host Range and High Complement of tRNA Genes, *Sci. Rep.*, **8,** 4486 (2018).

Nishiyama, H.; Nagai, T.; Kudo, M.; Okazaki, Y.; Azuma, Y.; Watanabe, T.; Goto, S.; Ogata, H.; Sakurai, T., Supplementation of Pancreatic Digestive Enzymes Alters the Composition of Intestinal Microbiota in Mice, *Biochem. Biophys. Res. Commun.*, **495,** 273-279 (2018).

Unraveling the Diversity and Ecological Role of Eukaryotic Viruses in the Sunlit Ocean

Viruses are abundant, diverse and essential component of marine ecosystems. They killed a large fraction of cells daily, thereby having a consequent impact on the ocean biogeochemistry and evolution of their host. While most efforts to characterize their diversity and ecology have been focused on bacterial viruses, current molecular sequence data derived from marine samples indicate that the diversity of eukaryotic viruses is vast and largely unexplored; with virtually no knowledge on the role that the various lineages fulfill in the environment.

We use omics data and associated metadata generated during the *Tara Ocean* expedition to explore the diversity and ecological role of eukaryotic viruses in the marine realm. Samples were collected in the sunlit layer of worldwide-distributed oceanic stations (Figure 1.A) and processed to generate metagenomes of bacterial-sized organisms (0.2 to 3 micron). This captures sequences of dsDNA viruses with large virion or dsDNA viruses replicated within their host cell. Samples were also processed to generate meta-transcriptomes of eukaryotic organisms (0.8 to 2000 micron). This captures transcripts of viruses actively infecting their hosts and RNA genomes. We use state of the art bioinformatics techniques to query viral genes out the several terabytes of molecular sequences generated. Next, we use marker genes to depict the diversity of eukaryotic viruses (Figure 1.B) and we compute their abundance across samples. This serves as the baseline to explore association between eukaryotic viral abundance and environmental parameters. For example, we test for association between viral abundance and export of carbon in the water column. We also look for co-abundance patterns between viral marker genes and host marker genes to detect virus-cell interactions. Results will serve as guidelines for further targeted studies aiming at characterizing viral-host systems and their role in oceans.

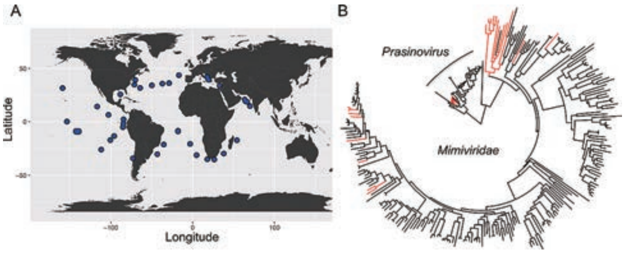


Figure 1. (A) Sampling sites of *Tara Oceans* expedition (2009-2012) used to analyze eukaryotic viruses. (B): Phylogeny of DNA polymerase B for large dsDNA viruses belonging to *Prasinovirus* and *Mimiviridae* unveils their large diversity in the sunlit ocean. Red: know viruses. Black: Viruses new to science.

Mice Intestinal Microbiota is Affected by the Administration of Pancreatic Enzymes

Pancreatic enzyme replacement therapy (PERT) is a treatment given to chronic pancreatitis patients to alleviate them of their pancreatic exocrine insufficiency (PEI) associated symptoms. Meanwhile, it has been recently inferred in a clinical study that the altered composition of intestinal microbiota is associated with the pathogenesis of the disease. Thus, in our study, we hypothesized that PERT exerts its effect not only through replenishing pancreatic digestive enzymes, but also by modifying the intestinal microbiota. To test this hypothesis, we conducted bacterial 16S rRNA gene targeted amplicon sequencing to investigate the intestinal microbiota of mice treated with either pancrelipase or tap water. The results have shown a difference in bacterial composition between these two groups of mice. Most interestingly two well-known beneficial bacteria have shown higher relative abundance in pancrelipase treated mice (Figure 2). One of them is *Akkermansia muciniphila*, which is known to benefit health through promoting intestinal barrier function. Another is *Lactobacillus reuteri*, which is a probiotic bacterium known to relieve intestinal inflammation. These results support our idea that PERT attenuates PEI-associated symptoms through the promotion of the colonization of beneficial bacteria, in addition to its already known mechanism. This project was done in collaboration with Dr. Sakurai’s group in Kindai Univerisity Hospital.

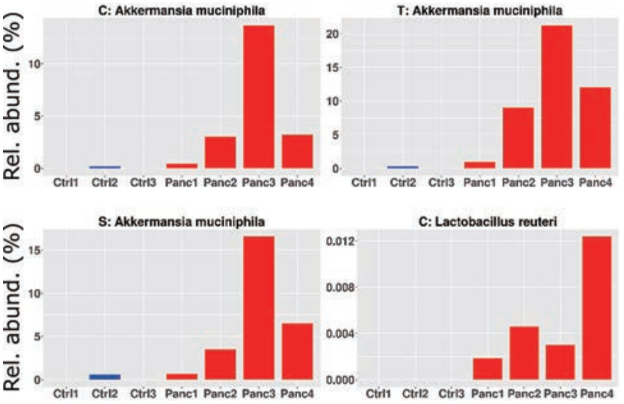


Figure 2. Relative abundance of two beneficial bacteria presenting significant difference in between pancrelipase-treated (shown in red) and tap water treated mice (shown in blue). The intestinal microbiota was observed at the cecum (C), transverse colon (T), and stool (S). Ctrl: control, Panc: Pancrelipase.

Bioinformatics Center
– Mathematical Bioinformatics –

http://www.bic.kyoto-u.ac.jp/takutsu/index.html

Prof
AKUTSU, Tatsuya
(D Eng)

Assoc Prof
TAMURA, Takeyuki
(D Inf)

Assist Prof
MORI, Tomoya
(D Inf)

SPD (JSPS)
LIN, Chun-Yu
(Ph D)

SPD (JSPS)
MÜNZNER,
Ulrike Tatjana Elisabeth
(Ph D)

Students

LIU, Pengyu (D3)
YU, Coleman (D2)
TAKAGI, Motoshige (D2)
LI, Ruiming (D1)
WANG, Feiqi (D1)
OHTOMO, Masahiro (D1)
CAO, Yu (M2)
MARUTA, Kunpei (M2)
PI, Wenya (M2)
KUMANO, Sou (M1)

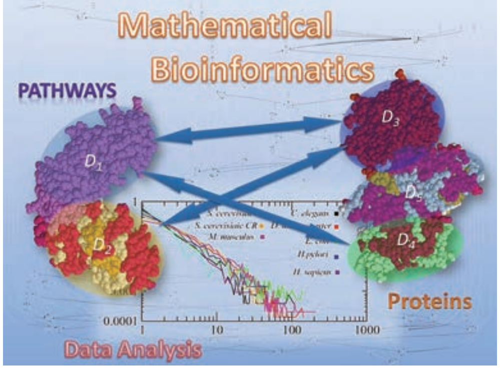
Guest Res Assoc

GUO, Wei-Feng (Ph D)	Northwestern Polytechnical University, China, P.R., 22 Novemver 2018–1 February 2019

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



Selected Publications

Akutsu, T., Algorithms for Analysis, Inference, and Control of Boolean Networks, *World Scientific* (2018).

Melkman, A. A.; Cheng, X.; Ching, W. K.; Akutsu, T., Identifying a Probabilistic Boolean Threshold Network from Samples, *IEEE Transactions on Neural Networks and Learning Systems*, **29,** 869-881 (2018).

Akutsu, T.; Jansson, J.; Li, R.; Takasu, A.; Tamura, T., New and Improved Algorithms for Unordered Tree Inclusion, *Proc. 29th Int. Symp. Algorithms and Computation*, [27-1]-[27-12] (2018).

Li, J.; Nagamochi, H.; Akutsu, T., Enumerating Substituted Benzene Isomers of Tree-like Chemical Graphs, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **15,** 633-646 (2018).

Bao, Y.; Hayashida, M.; Liu, P.; Ishitsuka, M.; Nacher, J. C.; Akutsu, T., Analysis of Critical and Redundant Vertices in Controlling Directed Complex Networks Using Feedback Vertex Sets, *J. Comput. Biol.*, **25,** 1071-1090 (2018).

Exact Identification of the Structure of a Probabilistic Boolean Threshold Network from Samples

Various kinds of mathematical models have been utilized for understanding dynamical behavior of biological systems. Among them, the Boolean network (BN) is a simple but well-studied discrete model, especially for modeling genetic regulatory networks and for neural networks. In a BN, each node takes a Boolean value, 0 or 1, at each time step, and the states of all nodes are updated synchronously according to Boolean functions assigned to nodes, where each node corresponds to a gene or neuron, and 1 and 0 mean that genes/neurons are active and inactive, respectively. The probabilistic Boolean network (PBN) is a probabilistic extension of BN in which multiple Boolean functions can be assigned to each node and one function is randomly selected at each time step according to the prescribed probability distribution. The probabilistic Boolean threshold network (PTBN) is a restriction of PBN in which every Boolean function is limited to threshold functions: $w_1x_1 + \ldots + w_nx_n \geq \theta$ (Figure 1). Note that Boolean threshold functions have been extensively studied for analyzing the ability of neurons and neural networks.

In our previous work, we studied the exact identification of the structure of a PBN from samples, which is potentially important for identifying genetic network structures in cells and/or neural network structures in brains. In this work, we extend our previous approach to the analysis of PBTN. We show that wide classes of PBTN with unit coefficients can be exactly identified from samples under reasonable constraints, which include: 1) PBTNs consisting of pairs of threshold functions with different numbers of input variables and 2) PBTNs in which any number of threshold functions can be assigned provided that all functions have the same number of input variables. We also show that the problem of deciding the equivalence of two Boolean threshold functions is solvable in pseudo-polynomial time but remains computationally hard (co-NP complete).

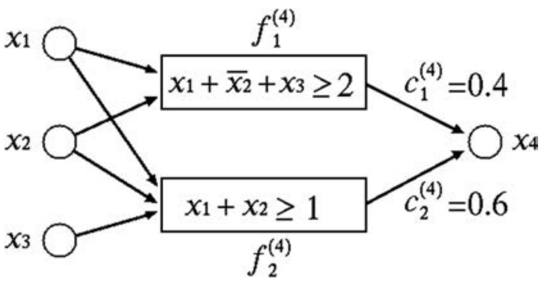


Figure 1. Part of a probabilistic Boolean threshold network. Two threshold functions are assigned to node x_4: one is selected with probability 0.4 and the other with probability 0.6.

Grid-based Computational Methods for the Design of Constraint-based Parsimonious Chemical Reaction Networks to Simulate Metabolite Production: GridProd

Constraint-based metabolic flux analysis of knockout strategies is an efficient method to simulate the production of useful metabolites in microbes. Owing to the recent development of technologies for artificial DNA synthesis, it may become important in the near future to mathematically design minimum metabolic networks to simulate metabolite production.

We developed an efficient method for computing the design of minimum metabolic networks by using constraint-based flux balance analysis to simulate the production of useful metabolites. When the growth rate of this obtained parsimonious metabolic network is maximized, higher production rates are observed for many target metabolites when compared to existing methods. The set of reactions used in this parsimonious flux distribution consists of reactions included in the original genome scale model iAF1260. Under the conditions that the growth rate is maximized and the minimum cases of flux variability analysis are considered, the developed method produced more than 90% of metabolites, while the existing methods produced less than 50%.

The source code is freely available and is implemented in MATLAB and COBRA toolbox.

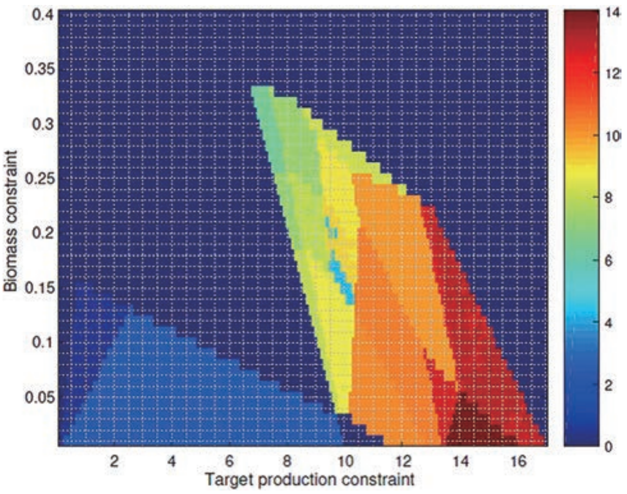


Figure 2. An example of the production rate heatmap for a target metabolite where each grid represents constraints for the ranges by the production rate and the growth rate.

Bioinformatics Center
– Bio-knowledge Engineering –

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


Prof
MAMITSUKA, Hiroshi
(D Sc)


Assist Prof
NGUYEN, Canh Hao
(D Knowledge Science)


Program-Specific Res
WIMALAWARNE, Kishan
(D Eng)

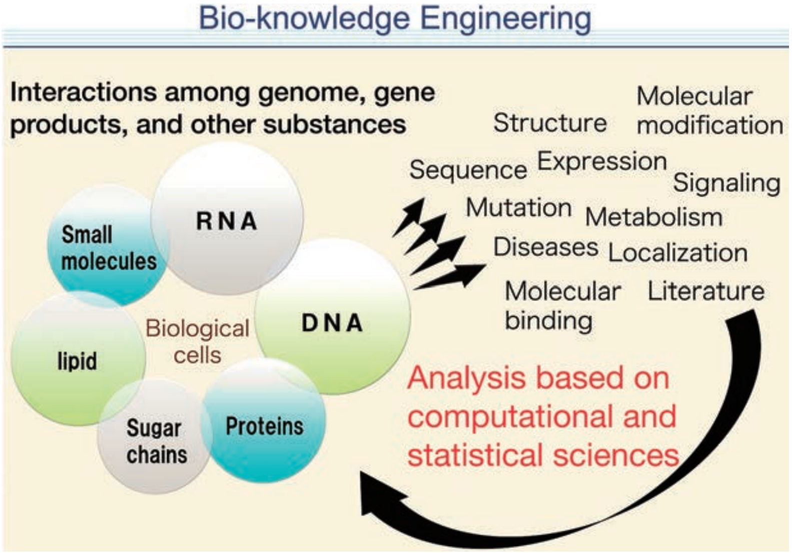

Program-Specific Res
SUN, Lu
(D Eng)

Students

NGUYEN, Dai Hai (D2)   NGUYEN, Duc Anh (D1)   TOHZAKI, Yudai (M2)

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
Computational Genomics
Data Mining
Machine Learning
Systems Biology

Selected Publications

Wimalawarne, K.; Mamitsuka, H., Efficient Convex Completion of Coupled Tensors Using Coupled Nuclear Norms, *Proceedings of the Thirty-second Conference on Neural Information Processing Systems (NIPS 2018)*, 6902-6910 (2018).

Wimalawarne, K.; Yamada, M.; Mamitsuka, H., Convex Coupled Matrix and Tensor Completion, *Neural Computation*, **30(11),** 3095-3127 (2018).

Nguyen, D. H.; Nguyen, C. H.; Mamitsuka, H., SIMPLE: Sparse Interaction Model over Peaks of MoLEcules for Fast, Interpretable Metabolite Identification from Tandem Mass Spectra, *Bioinformatics*, **34(13),** i323-i332 (2018).

Mamitsuka, H., Data Mining for Systems Biology: Methods and Protocols (2nd Edition), *Methods Mol. Biol.*, **1807,** (2018).

Karasuyama, M.; Mamitsuka, H., Factor Analysis on a Graph, *Proceedings of Machine Learning Research (Proceedings of the 21st International Conference on Artificial Intelligence and Statistics (AISTATS 2018))*, **84,** 1117-1126 (2018).

Advanced Machine Learning for Mass Spectrometry

Metabolites are small molecules, which are used in, or created by, the chemical reactions occurring in every cell of living organisms. They play lots of important roles including signaling, energy transport, building blocks of cells, etc. Identifying metabolites or interpreting their biochemical characteristics is an essential part of the metabolomics to enlarge the knowledge of biological systems. It is also a key to development of many applications and areas such as biotechnology, biomedicine or pharmaceutical sciences. Mass spectrometry is a common technique in analytical chemistry for metabolite identification. A mass spectrometer analyzes a chemical sample by fragmenting it and measuring the mass-to-charge ratios (m/z) of its fragments to obtain a mass spectrum (MS). A MS can be represented by a list of peaks, each of which corresponds to a fragment captured by the device. MS can provide more structural information about the sample and be helpful to deal with small-sized molecules such as metabolites.

There have been a number of computational methods proposed for metabolite identification from MS data. In general, they can be divided into three main categories: i) searching in spectral libraries; ii) in silico fragmentation and iii) machine learning. We focus on the machine learning approach, where the common scheme is, given a set of mass spectra, to learn a mapping from a spectrum to a molecule (Figure 1). This has two steps: 1) fingerprint prediction: predict a fingerprint with supervised ML and 2) candidate retrieval: use the predicted fingerprint to query the database. Kernel learning methods have been shown to be powerful tools in fingerprint prediction. For example, FingerID and CSI:FingerID are notable ones, which used support vector machine with kernels for pairs of MS and for pairs of corresponding fragmentation trees. However, existing methods are mainly based on individual peaks in the spectra, without explicitly considering the co-occurrence of peaks, which we call peak interactions. Also, these are computationally heavy and not desirable for the interpretation purposes.

The aim of our research is to propose and develop statistical learning models for identifying metabolites with the following main criterions: 1) High accuracy: given a query MS of a unknown metabolite, the proposed models are expected to produce a highly accurate list of candidate metabolites with most similar MS spectra; 2) Fast prediction: in order to be able to process large-scale datasets of metabolites in reality, it is desirable for the proposed model to produce good lists of candidates with fast prediction as well. Based on these, we developed a sparse interaction model, which we call SIMPLE, allowing to incorporate peak interactions for fingerprint prediction and is computationally lighter than existing kernel-based methods. As shown in Figure 2, the proposed methods achieved comparative prediction accuracy with much faster prediction (around 100 times). Furthermore, thanks to the interpretability, SIMPLE clearly revealed individual peaks and peak interactions, which contribute to enhancing the performance of fingerprint prediction.

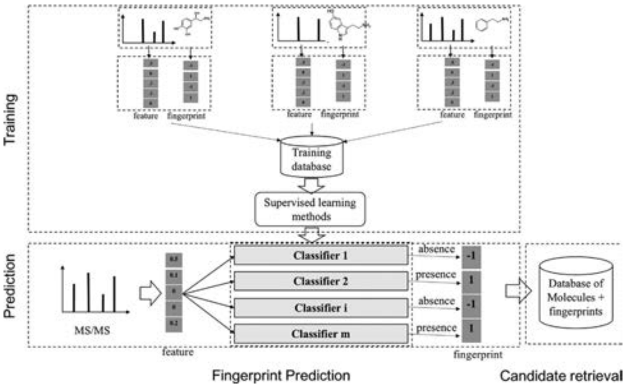
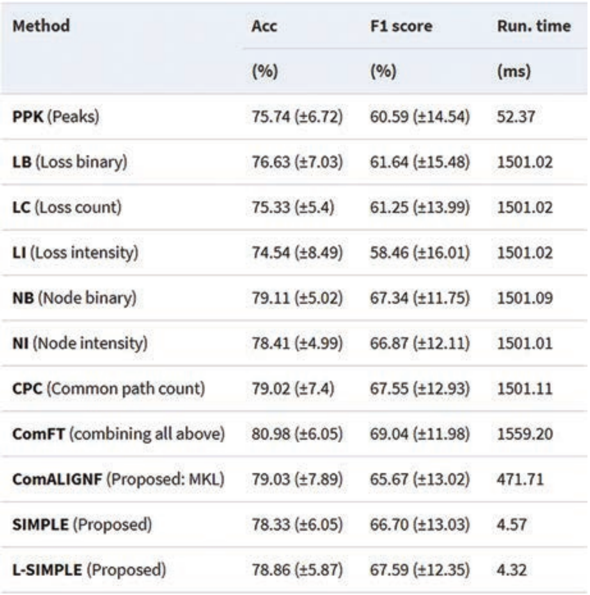


Figure 1. A general scheme to identify unknown metabolites based on molecular fingerprint vectors. There are two main steps: 1) fingerprint prediction; 2) Candidate retrieval.



Method	Acc	F1 score	Run. time
	(%)	(%)	(ms)
PPK (Peaks)	75.74 (±6.72)	60.59 (±14.54)	52.37
LB (Loss binary)	76.63 (±7.03)	61.64 (±15.48)	1501.02
LC (Loss count)	75.33 (±5.4)	61.25 (±13.99)	1501.02
LI (Loss intensity)	74.54 (±8.49)	58.46 (±16.01)	1501.02
NB (Node binary)	79.11 (±5.02)	67.34 (±11.75)	1501.09
NI (Node intensity)	78.41 (±4.99)	66.87 (±12.11)	1501.01
CPC (Common path count)	79.02 (±7.4)	67.55 (±12.93)	1501.11
ComFT (combining all above)	80.98 (±6.05)	69.04 (±11.98)	1559.20
ComALIGNF (Proposed: MKL)	79.03 (±7.89)	65.67 (±13.02)	471.71
SIMPLE (Proposed)	78.33 (±6.05)	66.70 (±13.03)	4.57
L-SIMPLE (Proposed)	78.86 (±5.87)	67.59 (±12.35)	4.32

Figure 2. Micro-average performance and prediction time of kernel-based methods and proposed methods.

HAKUBI RESEARCHERS' ACTIVITIES IN ICR

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

Research Topic

Synthesis and Exploration of Novel Charge Transition Oxide Materials for Future Multifunctional Devices

Program-Specific Assist Prof
DENIS ROMERO, Fabio
(Ph D)

Host Laboratory Laboratory of Advanced Solid State Chemistry

Host Professor SHIMAKAWA, Yuichi

Outline of Research

The wide range of electronic, magnetic, and transport properties exhibited by oxide materials has led to their widespread adoption as the basis of electronic devices and consequently contributed greatly to the exponential technological development over the past century. Continuing progress is fundamentally dependent on the discovery of new materials and the tunability of their fundamental properties. However, traditional synthetic methods are fundamentally unsuited to the preparation of a wide range of materials that could be imagined, and thus the development of new synthetic protocols is necessary to drive materials discovery forwards. My research focuses on the use of low-temperature topochemical methods and extreme conditions in order to prepare new materials with technologically useful properties for future devices.

ACTIVITIES OF JOINT USAGE/RESEARCH CENTER

JURC Cooperative Research Subjects 2018

(1 April 2018 ~ 31 March 2019)

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

Fabrication of Chiral Metal Nanocrystals and Clarification of Their Optical Property
KAWAI, Takeshi, Faculty of Engineering, Tokyo University of Science
Host in JURC KURATA, Hiroki

Probing Ultrafast Motion of Critical Surface Pushed by Multi-picosecond Relativistic Radiation Pressure
FUJIOKA, Shinsuke, Institute of Laser Engineering, Osaka University
Host in JURC INOUE, Shunsuke I

Development of Neutron Velocity Concentrator
KITAGUCHI, Masaaki, Center for Experimental Studies, Kobayashi-Maskawa Institute for the Origin of Particles and the Universe (KMI), Nagoya University
Host in JURC IWASHITA, Yoshihisa

Synthesis of Transition Metal Complexes Bearing a Low-coordinate Phosphorus Ligand and Their Application to Catalytic Reactions
MATSUO, Tsukasa, Faculty of Science and Engineering / Graduate School of Science and Engineering Research, Kindai University
Host in JURC OZAWA, Fumiyuki

Feasibility Study of Novel Cooling Devices with Perovskite Semiconductors
YAMADA, Noboru, Department of Science of Technology Innovation, Nagaoka University of Technology
Host in JURC KANEMITSU, Yoshihiko

Optical Properties of Pb Perovskite Solar Cells by Heterodyne Interference Spectroscopy
OGAWA, Yoshihiro, Joetsu University of Education
Host in JURC KANEMITSU, Yoshihiko

Development of First-row Late Transition-metal Complexes with Constrained Geometry Using Tridentate Anionic Ligands
YAMAGUCHI, Yoshitaka, Faculty of Engineering, Division of Materials Science and Chemical Engineering, Yokohama National University
Host in JURC NAKAMURA, Masaharu

Analysis of Complex Networks with Degree Correlations
TAKEMOTO, Kazuhiro, Department of Bioscience and Bioinformatics, Kyushu Institute of Technology
Host in JURC AKUTSU, Tatsuya

Novel Approaches to Prediction of Caspase Cleavage Sites
SONG, Jiangning, Monash Biomedicine Discovery Institute, Monash University
Host in JURC AKUTSU, Tatsuya I

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

Development of Prediction Method for Growth Conditions Based on Microbial Genome Information
GOTO, Susumu, Joint Support-Center for Data Science Research, Research Organization of Information and Systems
Host in JURC OGATA, Hiroyuki

Ecological Roles of Giant Viruses during the Succession after Red Tide Blooms
NAGASAKI, Keizo, Faculty of Agriculture and Marine Science, Kochi University
Host in JURC OGATA, Hiroyuki

Isolation and Genome Analysis of New Giant Viruses from Japanese Aquatic Environments
TAKEMURA, Masaharu, Faculty of Science, Tokyo University of Science
Host in JURC OGATA, Hiroyuki

Machine Learning Based Integration of Diverse Biological Data with Network
KARASUYAMA, Masayuki, Department of Computer Science, Nagoya Institute of Technology
Host in JURC MAMITSUKA, Hiroshi I

Total Synthesis of Blespirol
IMAYOSHI, Ayumi, Graduate School of Life and Environmental Sciences, Kyoto Prefectural University
Host in JURC KAWABATA, Takeo F

Synthesis of Novel Non-alternant Heterocycles toward Organic Functional Material
KUROTOBI, Kei, National Institute of Technology, Kurume College
Host in JURC MURATA, Yasujiro

Development of Small-molecule n-Type Organic Semiconductors That Can Be Processed via Precursor Approaches
SUZUKI, Mitsuharu, Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST)
Host in JURC MURATA, Yasujiro

Synthesis and Thermoelectric Performance of π-Conjugated Coordination Polymers
MURATA, Michihisa, Department of Applied Chemistry, Osaka Institute of Technology
Host in JURC MURATA, Yasujiro

Synthesis and Properties of Novel Tehinoacenes Synthesized by Addition–Elimination Reaction and Following Cyclization
SUGA, Seiji, Graduate School of Natural Science and Technology, Okayama University
Host in JURC MURATA, Yasujiro

In Vivo Detection of Temperature Change Using Optical Spectroscopic Characterization of Metal Nanoparticle
ISHIHARA, Miya, National Defense Medical College
Host in JURC TERANISHI, Toshiharu F

I : International Joint Research
F : Female PI

Structure Analysis of Monolayer Assembly with π-Conjugated Units Studied by pMAIRS
YAMAMOTO, Shunsuke, Institute of Multidisciplinary Research for Advanced Materials, Tohoku University
Host in JURC HASEGAWA, Takeshi

Relationship between Hydrogen Bonding and Rheological Properties of Polyurethanes Having Several Chemical Structures
URAKAWA, Osamu, Graduate School of Science, Osaka University
Host in JURC MATSUMIYA, Yumi

Analysis of Molecular Condensation in Temperature Gradient Field Created through Plasmonic Heating
SHIMADA, Ryoko, Department of Mathematical and Physical Sciences, Faculty of Science, Japan Women's University
Host in JURC WATANABE, Hiroshi F

Study on Improvement of Transportation Efficiency of Metal Ions through a Liquid Membrane
MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education
Host in JURC SOHRIN, Yoshiki

Hydrogen Absorption Properties for Shape Controlled Pd Nanoparticles in Wide Temperature Region
YAMAUCHI, Miho, International Institute for Carbom-Neutral Energy Research, Kyushu University
Host in JURC TERANISHI, Toshiharu F

Fabrication and Evaluation of Dye-sensitized Solar Cells Using Mixture of Flavonoid Compounds, and Their Theoretical Studies toward Improvement of the Efficiency
YOSHIDA, Kumi, Department of Complex Systems Science, Graduate School of Information Science, Nagoya University
Host in JURC WAKAMIYA, Atsushi F

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

Directional Neutron Generation via Laser-driven-photonuclear Reaction by Using a Spin Polarized Deuterium Target
ARIKAWA, Yasunobu, Institute of Laser Engineering, Osaka University
Host in JURC INOUE, Shunsuke

X-Ray Structural Studies on Reaction Mechanism of Maleylacetate Reductase
OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University
Host in JURC FUJII, Tomomi

X-ray Crystallographic Studies on Thermostability and Substrate Specificity of L-Asparaginase
KATO, Shiro, International Institute of Rare Sugar Research and Education, Kagawa University
Host in JURC FUJII, Tomomi

Fundamental Study on Micro-fabrication of Semiconductor with Controlling Laser Absorption
KUSABA, Mitsuhiro, Electronics, Information and Communication Engineering, Osaka Sangyo University
Host in JURC HASHIDA, Masaki

Advanced Functionality on Materials Induced by Intense THz Interaction
NAGASHIMA, Takeshi, Faculty of Science and Engineering, Setsunan University
Host in JURC HASHIDA, Masaki

A Study of Laser Driven High-intensity Terahertz Surface Wave
TOKITA, Shigeki, Institute of Laser Engineering, Osaka University
Host in JURC SAKABE, Shuji

Intense Deuteron Beam Generation by Ultra-intense Laser Irradiation for Development of Li-battery Diagnostics and Laser-driven Compact Neutron Source
FUJITA, Kazuhisa, The Graduate School for the Creation of New Photonics Industries
Host in JURC SAKABE, Shuji

Investigation of Accelerator Beam Component Using Permanent Magnets
TERUNUMA, Nobuhiro, Accelerator Laboratory, High Energy Accelerator Research Organization
Host in JURC IWASHITA, Yoshihisa

Fabrication Process of a Superconducting Electron Accelerating Cavity Operated by Small Electricity Power for a CEP-stabilized Free-Electron Laser
HAJIMA, Ryoichi, Quantum Beam Science Research Division, National Institutes for Quantum and Radiological Science and Technology
Host in JURC IWASHITA, Yoshihisa

Research on the High-performance Superconducting Cavity and the Cost Reduction by Noble Inner-surface Processes
SAEKI, Takayuki, Accelerator Laboratory, High Energy Accelerator Research Organization
Host in JURC IWASHITA, Yoshihisa

Study on Magnification of the Pulsed-neutron Transmission Image Using the Sextupole Magnet, Aimed at Visualization of Charge and Discharge in the Electrode Materials of Li-ion Batteries
KINO, Koichi, Research Institute for Measurement and Analytical Instrumentation, National Institute of Advanced Industrial Science and Technology
Host in JURC IWASHITA, Yoshihisa

Construction of Metal-substituted Carbenium Ion and Silyl Cation and Their Applications for Lewis Acid Catalysts
OKAZAKI, Masaaki, Graduate School of Science and Technology, Hirosaki University
Host in JURC OZAWA, Fumiyuki

Basic Study for Unveiling Crystal Structure of Carbon-, Nitrogen-based Frameworks
SAKAUSHI, Ken, Center for Green Research on Energy and Environmental Materials, National Institute for Materials Science
Host in JURC KAJI, Hironori

Investigation on Quantum Properties of Luminescent Nanomaterials Using Novel Techniques of Laser Microscopic Spectroscopy
IHARA, Toshiyuki, Advanced ICT Research Institute, National Institute of Information and Communications Technology
Host in JURC KANEMITSU, Yoshihiko

Discovery of Novel Functional Transition-metal Oxides with Ultra-high-pressure Condition
CHEN, Wei-Tin, Center for Condensed Matter Sciences, National Taiwan University
Host in JURC SHIMAKAWA, Yuichi I

Synthesis of Low-coordinated Heavier Group 14 Species Bearing Stable Redox Behavior and Elucidation of Their Structures
SASAMORI, Takahiro, Graduate School of Natural Sciences, Nagoya City University
Host in JURC TOKITOH, Norihiro

Base Metal Catalysis for Creation of Functional Materials
ILIES, Laurean, Department of Chemistry, School of Science, The University of Tokyo
Host in JURC NAKAMURA, Masaharu

Unraveling In-plane Aromaticity in Cycloparaphenylenes
MURANAKA, Atsuya, Advanced Elements Chemistry Laboratory (The Uchiyama Group), RIKEN
Host in JURC YAMAGO, Shigeru

Study of the Reaction Mechanisms of Radical Polymerization Utilizing the Reactivity of Organotellurium Compounds
NAKAMURA, Yasuyuki, Adhesive Materials Group, Research Center for Structural Materials, National Institute for Materials Science
Host in JURC YAMAGO, Shigeru

Differential Molecular Network Analysis through Statistical Machine Learning
KAYANO, Mitsunori, Research Center for Global Agromedicine, Obihiro University of Agriculture and Veterinary Medicine
Host in JURC MAMITSUKA, Hiroshi

Studies on the Reactivities between Curved Pi-conjugated Molecules and Transition Metal Complexes and Their Applications
OGOSHI, Sensuke, Graduate School of Engineering, Osaka University
Host in JURC YAMAGO, Shigeru

Organic Photovoltaic Devices Composed of Novel Organic Semiconductors
IE, Yutaka, The Institute of Scientific and Industrial Research, Osaka University
Host in JURC WAKAMIYA, Atsushi

Electronic Landscape and Optoelectronics of Non-lead Perovskite Solar Cell
SAEKI, Akinori, Graduate School of Engineering, Osaka University
Host in JURC WAKAMIYA, Atsushi

Biogeochemical Study of Bioactive Trace Metals in the Aerosols over Northern North Pacific Ocean
NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kindai University
Host in JURC SOHRIN, Yoshiki

Correlated Molecular Motion in Polymeric Liquids
SUKUMARAN, Sathish Kumar, Graduate School of Organic Materials Science, Yamagata University
Host in JURC WATANABE, Hiroshi I

The Study on Density Fluctuations of Polycarbonate by Using Time-resolved Scattering Method
NISHITSUJI, Shotaro, Graduate School of Organic Materials Science, Yamagata University
Host in JURC TAKENAKA, Mikihito

Depth-resolved Structure Analysis of Organic Thin Films by Energy Dispersive GISAXS Utilizing Tender X-rays
YAMAMOTO, Katsuhiro, Graduate School of Engineering, Nagoya Institute of Technology
Host in JURC TAKENAKA, Mikihito

Analysis of Physical Properties and Structure of Partially Fluorinated Phospholipid Bilayer
SONOYAMA, Masashi, Faculty of Science and Technology, Gunma University
Host in JURC HASEGAWA, Takeshi

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

Dynamics of the Transcription Factor ARR1 on Plant Chromosomal DNA
KIM, Jong-Myong, RIKEN Center for Sustainable Resource Science
Host in JURC AOYAMA, Takashi

Discovery and Use of Bioactive Self-Assembling Molecules
ZHOU, Lu, School of Pharmacy, Fudan University
Host in JURC UESUGI, Motonari I

Promotion of Wound Healing by a Synthetic Cell-adhesion Molecule
NISHIKAWA, Makiya, Faculty of Pharmaceutical Sciences, Tokyo University of Science
Host in JURC UESUGI, Motonari

Study of Spin-filtering Effect of the Magnetic Insulator Films with Perpendicular Magnetic Anisotropy
TANAKA, Masaaki, Department of Physical Science and Engineering, Nagoya Institute of Technology
Host in JURC ONO, Teruo

Real Time Observation of Topological Hall Effect
KIM, Kab-Jin, Department of Physics, Korea Advanced Institute of Science and Technology
Host in JURC ONO, Teruo I

Electric Field Induced Skyrmion Motion
NAKATANI, Yoshinobu, Department of Communication Engineering and Informatics, The University of Electro-Communications
Host in JURC ONO, Teruo

Studies on Spin Dynamics of TADF Molecules
IKOMA, Tadaaki, Graduate School of Science and Technology, Niigata University
Host in JURC KAJI, Hironori

Characteristics of Membrane Vesicles Produced by Intestinal Bacteria and Fermented Food-derived Bacteria and Their Biogenesis
KURATA, Atsushi, Faculty of Agriculture, Kindai University
Host in JURC KURIHARA, Tatsuo

Determination and Functional Analyses of Cyclization Enzymes in the Biosynthesis of Plant Polycyclic Aromatic Compounds
TAKANASHI, Kojiro, Institute of Mountain Science, Shinshu University
Host in JURC WATANABE, Bunta

Development of Recognition and Separation System Highly Selective for Rare Metals
YAMAZAKI, Shoko, Department of Chemistry, Nara University of Education
Host in JURC UMETANI, Shigeo F

Reptation Relaxation of Entangled Polymer Chains Undergoing Head-to-Head Association and Dissociation
KWON, Youngdon, School of Chemical Engineering, Sungkyunkwan University
Host in JURC MATSUMIYA, Yumi I

Antisense-Induced Guanine Quadruplex Formation in mRNAs
HAGIHARA, Masaki, Graduate School of Science and Technology, Hirosaki University
Host in JURC SATO, Shinichi

Development of Catalysts for Regio- and Stereoselective Oxidation
ITO, Akichika, Gifu Pharmaceutical University
Host in JURC KAWABATA, Takeo

Development of Organocatalytic Site-selective Phosphorylation and Sulfation Reactions of Carbohydrate and Its Application to Drug Delivery
NAGASAWA, Hideko, Gifu Pharmaceutical University
Host in JURC KAWABATA, Takeo F

Synergistic Effect of Surfactant for Solid Phase Extraction Using Solvent Impregnated Resin
KURAHASHI, Kensuke, Environmental and Materials Chemistry Course, Osaka Prefecture University College of Technology
Host in JURC SOHRIN, Yoshiki

Room Temperature Operation of Au_{25} Cluster Single-electron Transistor
MAJIMA, Yutaka, Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology
Host in JURC TERANISHI, Toshiharu

Vibrational Spectroscopy Study on Ozonolysis of Kalanchoe Pinnata Leaf Surface
HAMA, Tetsuya, Institute of Low Temperature Science, Hokkaido University
Host in JURC HASEGAWA, Takeshi

Creation of Organic Functional Materials Based on Macrocycles Incorporating Triphenylamine Units
IWANAGA, Tetsuo, Department of Chemistry, Faculty of Science, Okayama University of Science
Host in JURC WAKAMIYA, Atsushi

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Regulatory Network of Gene Expression for Plant Cell Morphogenesis
QU, Li-Jia, School of Life Sciences, Peking University
Host in JURC AOYAMA, Takashi I

Modulation of New Cellular Functions of Vitamin D
NAGASAWA, Kazuo, Department of Biotechnology and Life Science, Tokyo University of Agriculture and Technology
Host in JURC UESUGI, Motonari

Interface Structure and Spin Current Phenomena of Spinel Ferrite/Heavy Metal Systems
NAGAHAMA, Taro, Graduate School of Engineering, Hokkaido University
Host in JURC ONO, Teruo

Observation of Current-Driven Domain Wall Motions in the Ni Nanowire
YAMADA, Keisuke, Faculty of Engineering, Gifu University
Host in JURC ONO, Teruo

Electric Field Effect on Magnetic Domain Wall Velocity in a System with an Induced Magnetic Moment
CHIBA, Daichi, School of Engineering, The University of Tokyo
Host in JURC ONO, Teruo

Mechanism Study of Heterogeneous Catalysis on Zeolites by DNP-NMR
XU, Jun, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences
Host in JURC KAJI, Hironori I

Determination of High-order Structure of Organic Device Molecules Using Dynamic Nuclear Polarization Solid-state NMR
KOBAYASHI, Takeshi, U.S. Department of Energy, Ames National Laboratory
Host in JURC KAJI, Hironori I

Functional Study of Metal-induced Proteins in Microbial Metal Respiration
MIHARA, Hisaaki, Department of Biotechnology, College of Life Sciences, Ritsumeikan University
Host in JURC KURIHARA, Tatsuo

Studies on the Formation Mechanism of the Bound D-Amino Acids Using the Synthetic Peptides
OMORI, Taketo, Faculty of Engineering, Osaka Institute of Technology
Host in JURC KURIHARA, Tatsuo

Studies on the Biosynthesis and Physiological Functions of Human Steroidal Hormones in Plant
OHNISHI, Toshiyuki, Graduate School of Agriculture, Shizuoka University
Host in JURC WATANABE, Bunta

Studies on Mesenchymal Stem Cells Differentiation Induced by Two-Dimensional Ordered Arrays of Monodisperse Microparticles with a Polymer Brush for Regenerative Medicine
YAMAMOTO, Masaya, Graduate School of Engineering, Tohoku University
Host in JURC OHNO, Kohji

Intramolecular Photoinduced Charge Separation in D-A Cycloparaphenylenes
FUJITSUKA, Mamoru, The Institute of Scientific and Industrial Research, Osaka University
Host in JURC YAMAGO, Shigeru

Development of Novel π-Conjugated Polymers and Their Application to Organic Photovoltaics
OSAKA, Itaru, Graduate School of Engineering, Hiroshima University
Host in JURC WAKIOKA, Masayuki

Theoretical Study on Chemoselective Acylation Catalyzed by 4-Pyrrolidinopyridine Derivatives
YAMANAKA, Masahiro, Department of Chemistry, College of Science, Rikkyo University
Host in JURC KAWABATA, Takeo

Search for Four Wave-mixing in the Vacuum
HONMA, Kensuke, Graduate School of Science, Hiroshima University
Host in JURC SAKABE, Shuji I

Exploring Functional Properties Transition Metal Oxides by Electric-field-induced Electrochemical Etching
HATANO, Takafumi, Department of Crystalline Materials Science, Nagoya University
Host in JURC KAN, Daisuke

Study on Unusual Photoresponses of Upper Critical Solution Temperature of Polymer Solutions Using an Azobenzene-doped Liquid-crystalline Solvent
YAMAMOTO, Takahiro, Research Institute for Sustainable Chemistry, National Institute of Advanced Industrial Science and Technology (AIST)
Host in JURC OHNO, Kohji

Interfacial Structure Control and Photo-induced Charge Transfer Dynamics of Semiconductor Nanocrystal Based Hybrid Materials
TACHIBANA, Yasuhiro, School of Aerospace, Mechanical and Manufacturing Engineering, RMIT University
Host in JURC TERANISHI, Toshiharu I

Electrical Control and Detection of Qubit of NV Center
MAKINO, Toshiharu, Energy Technology Research Institute, National Institute of Advanced Industrial Science and Technology (AIST)
Host in JURC MIZUOCHI, Norikazu

Toward Long Spin Coherence Time of NV Center in Diamond
TOKUDA, Norio, Faculty of Electrical and Computer Engineering, Institute of Science and Engineering, Kanazawa University
Host in JURC MIZUOCHI, Norikazu

Research toward Ultra-high Sensitivity Sensor by Using Diamond
HATANO, Mutsuko, School of Engineering, Department of Electrical and Electronic Engineering, Tokyo Institute of Technology
Host in JURC MIZUOCHI, Norikazu F

Development of Functional Supramolecular Multiblock Copolymer
HAINO, Takeharu, Graduate School of Science, Hiroshima University
Host in JURC YAMAGO, Shigeru

Investigation of Relationship between Sequence Length and Segment Size of Various Kinds of Two-component Multiblock Copolymers
TAKANO, Atsushi, Graduate School of Engineering, Nagoya University
Host in JURC WATANABE, Hiroshi

SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

Nano-electron Spectroscopic Study on Hydrogen and Helium Behavior in Plasma Facing Materials for Nuclear Fusion Devices
MIYAMOTO, Mitsutaka, Interdisciplinary Faculty of Science and Engineering, Shimane University
Host in JURC KURATA, Hiroki

Elucidation of the Fluorous Interactions in the Crystal Structures of Fluorine-containing Conjugated Molecules by the Single-crystal X-Ray Structural Analysis
AGOU, Tomohiro, Department of Biomolecular Functional Engineering, College of Engineering, Ibaraki University
Host in JURC TOKITOH, Norihiro

Synthesis and Structure of Kinetically Stabilized Main Group Element Compounds Using Triptycylmethyl Groups
MINOURA, Mao, College of Science, Rikkyo University
Host in JURC TOKITOH, Norihiro

Theoretical Design of Flat and Perfect Two-dimensional π-Conjugated “Silicene” and the Search of Their Solid-state Properties
TAKAHASHI, Masae, Graduate School of Agricultural Science, Tohoku University
Host in JURC TOKITOH, Norihiro F

Analysis of Gap Plasmon Modes by Electron Energy-loss Spectroscopy
SAITO, Hikaru, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University
Host in JURC KURATA, Hiroki

Synthesis and Elucidation of Properties of Unsymmetrically-substituted Disilyne and Related π-Electron Systems
IWAMOTO, Takeaki, Graduate School of Science, Tohoku University
Host in JURC TOKITOH, Norihiro

Synthesis and Structural Characterization of Low-coordinate Compounds of Group 14 Elements
MATSUO, Tsukasa, Faculty of Science and Engineering, Kindai University
Host in JURC TOKITOH, Norihiro

Synthesis and Structures of Phosphorus-containing Aromatics Bearing an Amine Moiety
NAGAHORA, Noriyoshi, Department of Chemistry, Faculty of Science, Fukuoka University
Host in JURC TOKITOH, Norihiro

Studies of Porphyrin Hetero-dimer Formation by Using High-resolution FT-MS Spectroscopic Monitoring. Precise Analysis of Its Molecular Recognition, Oligomerization, and Dynamic Chirality
TOKUNAGA, Yuji, Graduate School of Engineering, University of Fukui
Host in JURC NAKAMURA, Masaharu

Study of the Mechanism of Steroid Hormone Production Using Imaging Mass Spectrometry
HATANO, Osamu, Department of Anatomy and Cell Biology, Nara Medical University
Host in JURC ISOZAKI, Katsuhiro

Determination of Compositions of Protected Novel Metal Clusters with Precise Mass Analysis
KOYASU, Kiichirou, Department of Chemistry, School of Science, The University of Tokyo
Host in JURC ISOZAKI, Katsuhiro

Synthesis of Metal Clusters Protected by Hydrophilic Thiolate, and Precise Separation and Evaluation by LC/MS
NEGISHI, Yuichi, Faculty of Science, Department of Applied Chemistry, Tokyo University of Science
Host in JURC ISOZAKI, Katsuhiro

SUBJECTS ENCOURAGING JOINT PROGRAM

Joint Seminar 2018 on Next Generation Materials
FUJIMOTO, Kenjiro, Department of Pure and Applied Chemistry, Faculty of Science and Technology, Tokyo University of Science
Host in JURC KAN, Daisuke I

Facile Intracellular Delivery by the Structural Alteration of Oligoarginines
CHENG, Richard, Department of Chemistry, National Taiwan University
Host in JURC FUTAKI, Shiroh I

Novel Drug-delivery System Using Albumin as a Reservoir
SAGAN, Sandrine, Laboratoire des Biomolécules, UMR7203 CNRS–University Pierre et Marie Curie –École Normale Supérieure Paris
Host in JURC FUTAKI, Shiroh I F

Functional Design for Drag Delivery into Brain
GIRALT, Ernest, Institute for Research in Biomedicine, University of Barcelona
Host in JURC FUTAKI, Shiroh I

Modification of Cell-penetrating Peptides for the Effective Delivery of Molecules into the Cells
HUDECZ, Ferenc, ELTE-Hungarian Academy of Sciences
Host in JURC FUTAKI, Shiroh I

The 14th International Workshop for East Asian Young Rheologists
INOUE, Tadashi, Graduate School of Science, Osaka University
Host in JURC WATANABE, Hiroshi I

Study on Emergent Spin-orbit Phenomena in Artificial Superlattices without Structural Inversion Symmetry
KIM, Sanghoon, Physics Department, University of Ulsan
Host in JURC ONO, Teruo I

3rd Solid-State Chemistry Forum
MIYASAKA, Hitoshi, Institute for Materials Research, Tohoku University
Host in JURC SHIMAKAWA, Yuichi

JURC Publications (Selected Examples)

(until 31 May 2018)

Directional Linearly Polarized Terahertz Emission from Argon Clusters Irradiated by Noncollinear Double-pulse Beams
Mori, K.; Hashida, M.; Nagashima, T.; Li, D.; Teramoto, K.; Nakamiya, Y.; Inoue, S.; Sakabe, S., *Appl. Phys. Lett.*, **111,** 241107 (2017).

Abstract

It has been demonstrated that the interaction between argon clusters and intense femtosecond double laser pulses with appropriate intervals in time and space provides important properties for terahertz electromagnetic wave generation, namely, high forward directivity, power enhancement, and linear polarization with a variable direction. Irradiating argon clusters with double pulses (1 and 3 mJ, 40 fs, 810 nm) in 133-ps and 40-μm intervals results in terahertz wave emission in the forward direction that is 10 times greater than that for a single pulse. The polarization direction of terahertz electromagnetic waves can be varied by changing the relative focal positions of the first and second pulses.

Critical Controllability Analysis of Directed Biological Networks Using Efficient Graph Reduction
Ishitsuka, M.; Akutsu, T.; Nacher, J. C., *Sci. Rep.*, **7,** 14361 (2017).

Abstract

Network science has recently integrated key concepts from control theory and has applied them to the analysis of the controllability of complex networks. One of the proposed frameworks uses the Minimum Dominating Set (MDS) approach, which has been successfully applied to the identification of cancer-related proteins and in analyses of large-scale undirected networks, such as proteome-wide protein interaction networks. However, many real systems are better represented by directed networks. Therefore, fast algorithms are required for the application of MDS to directed networks. Here, we propose an algorithm that utilises efficient graph reduction to identify critical control nodes in large-scale directed complex networks. The algorithm is 176-fold faster than existing methods and increases the computable network size to 65,000 nodes. We then applied the developed algorithm to metabolic pathways consisting of 70 plant species encompassing major plant lineages ranging from algae to angiosperms and to signalling pathways from *C. elegans, D. melanogaster* and *H. sapiens*. The analysis not only identified functional pathways enriched with critical control molecules but also showed that most control categories are largely conserved across evolutionary time, from green algae and early basal plants to modern angiosperm plant lineages.

Fullerene C_{70} as a Nanoflask That Reveals the Chemical Reactivity of Atomic Nitrogen
Morinaka, Y.; Zhang, R.; Sato, S.; Nikawa, H.; Kato, T.; Furukawa, K.; Yamada, M.; Maeda, Y.; Murata, M.; Wakamiya, A.; Nagase, S.; Akasaka, T.; Murata, Y., *Angew. Chem. Int. Ed.*, **56,** 6488-6491 (2017).

Abstract

To investigate the intrinsic reactivity of atomic nitrogen, which had previously been accomplished only by examining its decay in the gas phase using special equipment, a nitrogen atom was inserted into a series of molecule-encapsulating C_{60} and C_{70} fullerenes. Among the studied endofullerenes, $H_2@C_{70}$ was able to encapsulate an additional nitrogen atom within the fullerene cage under radiofrequency plasma conditions. The product was analyzed by ESR spectroscopy and mass spectrometry in solution, which revealed that the nitrogen atom with a quartet ground state does not react but weakly interact with the H_2 molecule, thus demonstrating the utility of such fullerenes as “nanoflasks”.

Vitamin D Metabolite, 25-Hydroxyvitamin D, Regulates Lipid Metabolism by Inducing Degradation of SREBP/SCAP
Asano, L.; Watanabe, M.; Ryoden, Y.; Usuda, K.; Yamaguchi, T.; Khambu, B.; Takashima, M.; Sato, S.; Sakai, J.; Nagasawa, K.; Uesugi, M., *Cell Chem. Biol.*, **24,** 207-217 (2017).

Abstract

Sterol regulatory element-binding proteins (SREBPs) are transcription factors that control lipid homeostasis. SREBP activation is regulated by a negative feedback loop in which sterols bind to SREBP cleavage-activating protein (SCAP), an escort protein essential for SREBP activation, or to insulin-induced genes (Insigs) (endoplasmic reticulum [ER] anchor proteins), sequestering the SREBP-SCAP-Insig complex in the ER. We screened a chemical library of endogenous molecules and identified 25-hydroxyvitamin D (25OHD) as an inhibitor of SREBP activation. Unlike sterols and other SREBP inhibitors, 25OHD impairs SREBP activation by inducing proteolytic processing and ubiquitin-mediated degradation of SCAP, thereby decreasing SREBP levels independently of the vitamin D receptor. Vitamin D supplementation has been proposed to reduce the risk of metabolic diseases, but the mechanisms are unknown. The present results suggest a previously unrecognized molecular mechanism of vitamin D-mediated lipid control that might be useful in the treatment of metabolic diseases.

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

Abstract

We have developed a novel diastereoselective iron-catalyzed cross-coupling reaction of various glycosyl halides with aryl metal reagents for the efficient synthesis of aryl *C*-glycosides, which are of significant pharmaceutical interest due to their biological activities and resistance toward metabolic degradation. A variety of aryl, heteroaryl, and vinyl metal reagents can be cross-coupled with glycosyl halides in high yields in the presence of a well-defined iron complex, composed of iron(II) chloride and a bulky bisphosphine ligand, TMS-SciOPP. The chemoselective nature of the reaction allows the use of synthetically versatile acetyl-protected glycosyl donors and the incorporation of various functional groups on the aryl moieties, producing a diverse array of aryl *C*-glycosides, including Canagliflozin, an inhibitor of sodium-glucose cotransporter 2 (SGLT2), and a prevailing diabetes drug. The cross-coupling reaction proceeds via generation and stereoselective trapping of glycosyl radical intermediates, representing a rare example of highly stereoselective carbon–carbon bond formation based on iron catalysis. Radical probe experiments using 3,4,6-tri-*O*-acetyl-2-*O*-allyl-α-d-glucopyranosyl bromide (**8**) and 6-bromo-1-hexene (**10**) confirm the generation and intermediacy of the corresponding glycosyl radicals. Density functional theory (DFT) calculations reveal that the observed anomeric diastereoselectivity is attributable to the relative stability of the conformers of glycosyl radical intermediates. The present cross-coupling reaction demonstrates the potential of iron-catalyzed stereo- and chemoselective carbon–carbon bond formation in the synthesis of bioactive compounds of certain structural complexity.

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
MOTOME, Yukitoshi
(D Sc)

Laboratory of Nanospintronics

Professor, The University of Tokyo
(7-3-1 Hongo, Bunkyo-ku, Tokyo
113-8656)

Lecture at *ICR*
Splitting Spins

Vis Prof
KOBAYASHI, Takeshi
(Ph D)

Laboratory of Molecular Materials Chemistry

Associate Scientist, Ames Laboratory, Iowa State University
(311 Iowa State University, Ames, IA
50011, U.S.A.)

Vis Prof
SHIMIZU, M. Hirohiko
(D Sc)

Laboratory of Particle Beam Science

Professor, Laboratory for Particle Properties, Department of Physics, Nagoya University
(Furo-cho, Chikusa-ku, Nagoya-shi, Aichi
464-8601)

Lecture at *ICR*
Systematization of Slow Neutron Beam Optics

Vis Prof
GOTO, Susumu
(D Eng)

Laboratory of Chemical Life Science

Professor, Database Center for Life Science (DBCLS), Joint Support-Center for Data Science Research (DS Center), Research Organization of Information and Systems (ROIS)
(Wakashiba, Kashiwa-shi, Chiba 277-0871)

Lecture at *ICR*
Life Science Database Integration Based on Semantic Web Technology

Vis Assoc Prof
ISHIDA, Shintaro
(D Sc)

Laboratory of Organoelement Chemistry

Associate Professor, Department of Chemistry, Graduate School of Science, Tohoku University
(6-3, Aramaki Aza-Aoba, Aoba-ku,
Sendai-shi, Miyagi 980-8578)

Lecture at *ICR*
Novel Transformation of Stable Low-coordinate Silicon Compounds

Vis Assoc Prof
ZHOU, Lu
(Ph D)

Laboratory of Chemical Biology

Associate Professor, School of Pharmacy, Fudan University
(826 Zhangheng Road, Pudong District,
Shanghai, China, P.R.)

Lecture at *ICR*
Structure-based Design of Metalloprotein and Bioactive Molecules

Vis Assoc Prof
SAKAI, Takamasa
(D Eng)

Laboratory of Molecular Rheology

Associate Professor, The University of Tokyo
(7-3-1 Hongo, Bunkyo-ku, Tokyo
113-8656)

Lecture at *ICR*
Elucidation of Correlation between Structure and Physical Property of Polymer Gel by Using Hydrogel with Well-defined Structure

Vis Assoc Prof
OKAMOTO, Yoshihiko
(D Sc)

Laboratory of Advanced Solid State Chemistry

Associate Professor, Department of Applied Physics, Graduate School of Engineering, Nagoya University
(Furo-cho, Chikusa-ku, Nagoya-shi, Aichi
464-8603)

Lecture at *ICR*
Engineering Structural and Physical Properties of Geometrically Frustrated Materials through Multiple Ions' Ordered Arrangements

Prof Em KANEHISA, Minoru (D Sc)

Appointed as Res (pt) at ICR,
1 April 2012–31 March 2019

PERSONAL

Retirement

Professor OZAWA, Fumiyuki
International Research Center for Elements Science
– Organometallic Chemistry –

On 31 March 2019, Dr. OZAWA, Fumiyuki retired from Institute for Chemical Research (ICR), Kyoto University after about 16 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Ozawa was born in Niigata Prefecture in March 1954. He graduated from Faculty of Engineering, Tokyo Metropolitan University in 1976, and went on to the graduate school at Tokyo Institute of Technology to study organometallic chemistry under the direction of the late Professor Akio Yamamoto. He was employed as Assistant Professor at Research Laboratory of Resources Utilization, Tokyo Institute of Technology in 1980, and granted the degree of Doctor of Engineering in 1984. He spent the year 1987–1988 as Visiting Associate at California Institute of Technology. In 1989, he was appointed as Associate Professor at Catalysis Research Center, Hokkaido University. He moved to Faculty of Engineering, Osaka City University in 1994, and was promoted to Professor in 1995. In 2003, he moved to International Research Center for Elements Science, which was newly established in ICR the same year. He served as the head of this center in 2009–2011 and 2015–2017. He also greatly contributed to the establishment of a series of MEXT inter-university research projects since 2005.

Throughout his academic career, Dr. Ozawa devoted himself to fundamental research on organometallic chemistry. He elucidated the mechanisms of various organometallic reactions relevant to catalytic transformations. In particular, the studies on organopalladium complexes established the basic concept of configurational constraints on organometallic reactions. He discovered the palladium-catalyzed double carbonylation. He also developed a rational design method of reactive organopalladium complexes for alkene insertion and applied it to the catalytic asymmetric Heck reaction. The insertion chemistry was extended to silyl and related complexes and applied to catalysis.

Since the late 1990's, he started the chemistry of phosphaalkene complexes, taking advantage of the research project on the Chemistry of Inter-Element Linkage. Phosphaalkenes with P=C double bonds have been prepared since the late 1970's, but they have been scarcely utilized in organometallic chemistry. He revealed remarkable reactivities of phosphaalkene complexes and demonstrated the great potential in organometallic chemistry. For example, phosphaalkene palladium complexes efficiently catalyze dehydrative condensation of active methylene compounds or anilines with allylic alcohols under mild conditions. The palladium-catalyzed allylation was known as the Tsuji-Trost reaction but required the pre-activation of allylic alcohols by conversion into allylic esters. The phosphaalkene complexes allowed eliminating the pre-activation step. This finding provided the opportunity to open up many simple catalytic allylation protocols using allylic alcohols. He also showed that phosphaalkene ligands allow isolation of transition metal complexes with unusual structures. For example, a PNP-pincer type phosphaalkene ligand forms platinum(0) complexes with a square planar configuration, the coordination geometry of which is very uncommon for formal d^{10} complexes.

His research activities also included polymer synthesis. He studied catalytic methods of synthesizing functional polymers via olefin metathesis and cross-coupling reactions. The latest example is the palladium-catalyzed direct allylation polymerization (DArP), which produces π-conjugated polymers (conductive polymers) used in optoelectronic devices. Such polymers have so far been prepared by catalytic cross-coupling polymerization using organometallic monomers, but he documented for the first time that the same polymers could be synthesized more easily by direct arylation using C-H bond activation. He developed mixed ligand catalysts for DArP and realized the precise synthesis of highly head-to-tail regioregular poly(3-hexylthiophene) and donor-acceptor type alternating copolymers with well-controlled structures.

His educational contribution to Kyoto University is also noteworthy. He has guided 34 graduate students and 28 undergraduates and sent them out to industry and academia. He also accepted many foreign postdocs and students. He has been an active member of domestic and international academic societies. In particular, he made a great contribution to organometallic chemistry as the Chair of Division of Organometallic Chemistry, Kinki Chemical Society.

Dr. Ozawa's contribution to Kyoto University and the Institute through his scientific, educational and administrative activities is hereby gratefully acknowledged.

Awards

HIROSE, Takashi

Publons Peer Review Awards 2018

“For Placing in the Top 1% of Reviewers in Chemistry during the 2017-2018 Award Year”

Publons

12 September 2018

HASHIKAWA, Yoshifumi

ICR Award for Young Scientists

“Facile Access to Azafullerenyl Cation $C_{59}N^+$ and Specific Interaction with Entrapped Molecules”

Institute for Chemical Research, Kyoto University

30 November 2018

HASEGAWA, Shota

ICR Award for Graduate Students

“Construction of a Metal-Free Electron Spin System by Encapsulation of an NO Molecule inside an Open-Cage Fullerene C_{60} Derivative”

Institute for Chemical Research, Kyoto University

30 November 2018

KAWABATA, Takeo

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

“Studies on Principles of Asymmetric Induction Based on Memory of Chirality”
Minister of Education, Culture, Sports, Science and Technology

17 April 2018

KAWAWAKI, Tokuhisa

Young Best Presentation Award

The 16th Annual Meeting of the Society of Nano Science and Technology

“Hydrogen Evolution Properties of Plasmonic Metal-Chalcogenide Heteronanoparticles”

The Society of Nano Science and Technology

11 May 2018

EGUCHI, Daichi

CSJ Presentation Award 2018

The 98th Annual Meeting of the Chemical Society of Japan

“Ligand Effect of Porphyrin-Protected Gold Clusters in the Electrochemical Hydrogen Eolution Reaction”

The Chemical Society of Japan

16 April 2018

MATSUMOTO, Kenshi

CSJ Presentation Award for Industries

The 98th Annual Meeting of the Chemical Society of Japan

“Creation of Novel Fe-Pd Ordered Alloy Nanoparticles by Introducing Third Element”

The Chemical Society of Japan

12 April 2018

OKAMOTO, Yasuo

Young Best Presentation Award

The 16th Annual Meeting of Nano Science and Technology

“Control of Geometric Anisotropy of Janus Porphyrin Coordinated Gold Clusters”

The Society of Nano Science and Technology

11 May 2018

YAMAGO, Shigeru

Inoue Harushige Prize

"Development of Highly-functional Adhesives and Dispersants with a Novel Living Radical Polymerization Method"

Inoue Harushige Prize Committee

18 July 2018

LU, Yangtian

ICR Award for Graduate Students

"Synthesis of Structurally Controlled Hyperbranched Polymers Using a Monomer Having Hierarchical Reactivity"

Institute for Chemical Research, Kyoto University

30 November 2018

MORISHITA, Hiroki

The Best Oral Presentation Award

The 31th Diamond Symposium

"Electrical Detection and Control of Nitrogen Nuclear Spins Coherence in NV Centers"

Japan New Diamond Forum

17 March 2018

FUJIMOTO, Sho

English Encouragement Presentation Award

The 65th JSAP Spring Meeting

"Spin Transport in p-Type Diamond Induced by Spin-pumping"

The Japan Society of Applied Physics

19 September 2018

MIZUNO, Hayato

ICR Award for Graduate Students

"Electric-field-induced Modulation of the Anomalous Hall Effect in a Heterostructured Itinerant Ferromagnet $SrRu0_3$"

Institute for Chemical Research, Kyoto University

30 November 2018

LI, Tian

Young Researcher Award

2018 International Conference on Solid State Devices and Materials

"Current Density Dependence of Asymmetric Magnetoresistance in Pt/Py Bilayers under Various Magnetic Field Strength"

The Chemical Society of Japan

11 September 2018

AKISHIBA, Misao

10th IPS/55th JPS Excellent Presentation Award

The 10th International Symposium / The 55th Japanese Peptide Symposium

"L17E-mediated Cytosolic Delivery and Its Mode of Action"

The Japanese Peptide Society

7 December 2018

MASUDA, Toshihiro

2018 Young Scientist Award

22nd Korean Peptide and Protein Society Symposium

"Approach to Control Cell Movement by Affecting Membrane Tension"

Korean Peptide and Protein Society

25 June 2018

YAMAGUCHI, Shinjiro

Highly Cited Researchers 2018

Clarivate Analytics

27 November 2018

TAKASHIMA, Ippei

CSJ Presentation Award 2018

The 98th Annual Meeting of the Chemical Society of Japan

"Self-assembling Molecules Functionalize Transplanted Cells"

The Chemical Society of Japan

13 April 2018

SHIZU, Katsuyuki

Lecture Award

International Congress on Pure & Applied Chemistry 2018

"Enhanced Electroluminescence from Delayed-Fluorescence Emitters by Suppressing Nonradiative Decay"

Asia Chem Corporation

19 April 2018

ZHENG, Linjie

Oceanochemistry Encouragement Prize (U30)

Research Institute of Oceanochemistry

"Development of Quantitative Method of Bioactive Trace Metals (Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb) in Seawater and its Application to the North Pacific Ocean"

Research Institute for Oceanochemistry Foundation

28 April 218

SHIOYA, Nobutaka

2018 Young Scientist Presentation Award

Annual Meeting of the Spectroscopical Society of Japan 2018

"Structural Characterization of the Face-on Phase in a Pentacene Thin Film by Using Vis and IR pMAIRS"

The Spectroscopical Society of Japan

25 May 2018

KAWAMOTO, Jun

Young Scientist Award

19th Annual Meeting of the Japanese Society for Extremophiles

"Elucidation of Cold-Adapted Mechanism of an Antarctic Bacterium"

The Japanese Society for Extremophiles

8 December 2018

KAWAI, Soichiro

Best Oral Presentation Award

65th Annual Meeting of the Japanese Biochemical Society, Kinki Branch

"Construction of a Low-Temperature Protein Expression System Using a Cold-Adapted Bacterium, *Pseudoalteromonas* sp. Sq02, as the Host"

The Japanese Biochemical Society, Kinki Branch

26 May 2018

OGAWA, Hiroki

The 9th Bridgestone Softmaterial Frontier Award

The Society of Rubber Science and Technology, Japan

"Visualization of Nanostructures in Patterned Thin Films Using GISAXS-CT"

The Society of Rubber Science and Technology, Japan

30 May 2018

WAKAMIYA, Atsushi

The 70th KCS Award in Chemical Technology

"Development of Printable Perovskite Solar Cells Using Original Precursor Materials"

KINKA Chemical Society

25 May 2018

KATAYAMA, Ryo

The Best Oral Presentation Annual Meeting Award

15th Annual Meeting of Particle Accelerator Society of Japan

"Evaluation of Superconducting Characteristics on the Multilayer Thin-Film Structure Using the Third Harmonic Voltage Method"

Particle Accelerator Society of Japan

10 August 2018

SAKABE, Shuji

Contribution Award

"Remarkable Contribution to the Operation and Management of the Laser Society of Japan"

The Laser Society of Japan

31 May 2018

NISHIURA, Yosuke

Student Presentation Award of the Physical Society of Japan Division 2

2018 Autumn Meeting of the Physical Society of Japan

"Detection of α Particles Generated by $^{7}Li(p,\alpha)^{4}He$ · $^{19}F(p,\alpha)^{16}O$ Reaction Induced by Laser Accelerated Proton by Two Step Etching of CR-39"

The Physical Society of Japan

6 October 2018

ISOZAKI, Katsuhiro

2018 Kansai Branch Award of the Society of Synthetic Organic Chemistry, Japan

"Construction of Supramolecular Reaction Fields on Metallic Nanoclusters toward Accelerated Catalytic Reactions through Intermolecular Interactions"

The Society of Synthetic Organic Chemistry, Japan

4 December 2018

WAKIOKA, Masayuki

32nd Young Scholar Lectures of CSJ

The 98th Annual Meeting of the Chemical Society of Japan

"Development of Highly Efficient Catalysts for Direct Arylation Polymerization"

The Chemical Society of Japan

22 March 2018

TAHARA, Hirokazu

ICR Award for Young Scientists

"Quantum Coherence of Multiple Excitons Governs Absorption Cross-sections of PbS/CdS Core/shell Nanocrystals"

Institute for Chemical Research, Kyoto University

30 November 2018

HANDA, Taketo

JSAP Young Scientist Presentation Award

The 78th Autumn Meeting, 2017

“Fundamental Optical Properties and Photocarrier Loss Mechanisms in Long-Term Stable Lead-Free $CH_3NH_3SnI_3$ Thin Films and Solar Cells”

The Japan Society of Applied Physics

17 March 2018

ICR Award for Graduate Students

“Radiative Recombination and Electron-phonon Coupling in Lead-free $CH_3NH_3SnI_3$ Perovskite Thin Films”

Institute for Chemical Research, Kyoto University

30 November 2018

SANARI, Yasuyuki

Student Presentation Award of the Physical Society of Japan Division 5

The Physical Society of Japan 2018 Autumn Meeting

“Zener Tunneling Induced Crystallization Growth in Phase-Change Materials Revealed by Intense Terahertz Pulses”

The Physical Society of Japan

6 October 2018

NAKAHARA, Satoshi

Student Presentation Award of the Physical Society of Japan Division 5

The Physical Society of Japan 2018 Autumn Meeting

“Trion Generation Mechanism in Lead Halide Perovskite Nanocrystals”

The Physical Society of Japan

6 October 2018

NGUYEN, Dai Hai

ICR Award for Graduate Students

“SIMPLE: Sparse Interaction Model over Peaks of MoLEcules for Fast, Interpretable Metabolite Identification from MS/MS”

Institute for Chemical Research, Kyoto University

30 November 2018

KANEHISA, Minoru

The 2018 Clarivate Citation Laureates

“For Contributions to Bioinformatics, Specifically for His Development of the Kyoto Encyclopedia of Genes and Genomes (KEGG)”

Clarivate Analytics

20 September 2018

Paper Awards

TOKITOH, Norihiro;

SASAMORI, Takahiro[1]

Award for Excellence to Authors Publishing in Bioscience, Biotechnology, and Biochemistry in 2017

"The (Oxalato)Aluminate Complex as an Antimicrobial Substance Protecting the "Shiro" of *Tricholoma Matsutake* from Soil Micro-organisms"

Japan Society for Bioscience, Biotechnology, and Agrochemistry

15 March 2018

[1] Graduate School of Natural Sciences, Nagoya City University

---

TOSAKA, Masatoshi

CERI Best Paper Award

The 28th Elastomer Symposium, The Society of Rubber Science and Technology, Japan

"Dominating Factor of Strain-induced Crystallization in Natural Rubber"

Chemicals Evaluation and Research Institute, Japan

31 May 2018

KOJIMA, Sadaoki

Best Paper Award

"Super-Ponderomotive Electron Acceleration in Blowout Plasma Heated by Multi-Picosecond Relativistic Intensity Laser Pulse"

The Laser Society of Japan

31 May 2018

TAHARA, Hirokazu

Award for the Presentation of an Excellent Paper

The 38th Annual Meeting of the Laser Society of Japan

"Multiexciton Coherence in PbS Nanocrystals Studied by Femtosecond Phase-locked Pulse-pair Spectroscopy"

The Laser Society of Japan

31 May 2018

YAMADA, Takumi

Award for the Presentation of an Excellent Paper

The 38th Annual Meeting of the Laser Society of Japan

"Space- and Time-Resolved Photoluminescence Measurement by Femtosecond Multi-Photon Excitation Microscopy: Photon Recycling in Lead-Halide Perovskites"

The Laser Society of Japan

31 May 2018

Poster Awards

SUGAHARA, Tomohiro

Best Poster Award

Meeting for Young Scientists on Organic Reactions

“Reactivity of 1,2/1,4-Digermabenzenes”

Organizing Committee of Meeting for Young Scientists on Organic Reaction

6 July 2018

Chemical Science Award

28th International Symposium on the Organic Chemistry of Sulfur

“Chalcogenation Reactions of 1,2-Digermacyclobutadiene”

Royal Society of Chemistry

31 August 2018

Chemical Communications Presentation Prize

The 45th Symposium on Main Group Element Chemistry

“Reactions of a Bromogermylene with Alkynes: Formation of Bromovinylgermylenes via Aryl-migration”

Royal Society of Chemistry

15 December 2018

IWAI, Kento

Best Poster Award

Meeting for Young Scientists on Organic Reactions

“Development of Stabilization Method for Metalylenes Utilizing Electronic Repulsion”

Organizing Committee of Meeting for Young Scientists on Organic Reaction

6 July 2018

OSHIRO, Taku

Best Poster Award

Meeting for Young Scientists on Organic Reactions

“Attempted Synthesis of 1-Metallaazulene”

Organizing Committee of Meeting for Young Scientists on Organic Reaction

6 July 2018

LIAN, Zichao

The Best Poster Award

Asian Symposium on Nanoscience & Nanotechnology 2018 (ASNANO2018)

“Observation of Near Infrared Light-Induced Plasmonic Hot Hole Transfer in CdS/CuS Heterostructured Nanocrystals”

The Society of Nano Science and Technology

13 May 2018

MATSUMOTO, Kenshi

JIM Best Poster Award

2018 Fall Annual (163th) Meeting of the Japan Institute of Metals and Materials

“Formation of Novel Fe-Pd Ordered Alloy Nanoparticles Induced by in Element”

The Japan Institute of Metals and Materials

20 September 2018

HISATOMI, Tatsuya

PMF Excellent Presentation Award

26th Polymer Materials Forum

“Ordered Structures of Ionic-polymer-brush-grafted Particles in Organic Solvents”

The Society of Polymer Science, Japan

24 May 2018

ISHIDA, Hisayuki

Excellent Poster Award for Young Scientists

2018 Autumn Meeting of the Society of Fiber Science and Technology, Japan

"Anchoring Properties of Liquid Crystals on LB film of Cellulosic Janus-Type Bottlebrush"

The Society of Fiber Science and Technology, Japan

1 November 2018

LU, Yangtian

BCSJ Award for Poster Presentation

International Symposium on Main Group Chemistry Directed towards Organic Synthesis

"One Pot Synthesis of Structure Controlled Hyper-branched Polymers by Using a Monomer with Hierarchical Reactivity"

Organization Committee of MACOS

25 August 2018

ARAFILES, Jan Vincent V.

Zhonghe Poster Prize

The 15th Chinese International Peptide Symposium

"Quantifying the Efficiency of CPP-Mediated Cytosolic Delivery of Biomacromolecules"

Hainan Zhonghe Co., Ltd., & Hainan Zhonghe Pharmaceutical Co., Ltd.

6 July 2018

JPS Excellent Poster Presentation Award

The 10th International Symposium / The 55th Japanese Peptide Symposium

"Identified Macropinocytosis-inducing Peptide and its Mode-of-Action"

The Japanese Peptide Society

7 December 2018

SAKAMOTO, Kentarou

JPS Excellent Poster Presentation Award

The 10th International Symposium / The 55th Japanese Peptide Symposium

"Improving Endosomolytic Activity of L17E"

The Japanese Peptide Society

7 December 2018

HAKARIYA, Hayase

Best Poster Award

iCeMS Retreat 2018

"Metastatic Approach for Cell Engraftment with a Self-assembling Molecule, Adhesamine 3.0"

Kyoto University iCeMS

26 June 2018

LIN, Chun-Yu

The Best Poster Award

IIBMP2018

"Pan-cancer Module Network Analysis for Identifying Dominating Networks Across Human Cancers"

IIBMP2018

21 September 2018

Obituary

Professor Emeritus

Dr. HANAI, Tetsuya (1927–2017)

Dr. Tetsuya Hanai, Professor Emeritus of Kyoto University, passed away in Uji on December 12, 2017, at the age of 90.

Dr. Hanai was born in Tokyo on May 23, 1927. In 1951, he graduated from Kyoto Imperial University with a major in Physics and joined the Institute for Chemical Research (ICR), Kyoto University, where he started his studies on the dielectric properties of colloidal materials under the supervision of Professor Rempei Gotoh. After having received his PhD (Doctor of Science) from Kyoto University in 1961, he had an opportunity to spend for three years at the Department of Colloid Science, the University of Cambridge. In 1966, Dr. Hanai was appointed to an Associate Professor of ICR and was promoted to a Full Professor in 1985 in charge of the Laboratory of Dielectrics. In 1991, he retired after forty years of service at Kyoto University to be honored with the title of Professor Emeritus of Kyoto University.

Dr. Hanai's professional career covers a wide range of colloid chemistry and dielectrics, but his research interests have focused on the dielectric properties of heterogeneous systems as well as theoretical considerations of interfacial polarization. His early work concerned the dielectric properties of emulsions, which were successfully explained by his own dielectric theory for concentrated particle suspensions. The studies have advanced our knowledge on the dielectric behavior of heterogeneous systems, and his theory has been widely accepted to be called Hanai's mixture theory. Later, with Dr. Akihiko Irimajiri, Dr. Hanai extended his studies to the field of bio-dielectrics. They proposed sophisticated models for biological cells and intracellular organelles such as the so-called double-shell and multi-stratified shell models. These models have become indispensable for characterizing biological cells in dielectric studies. Moreover, dielectric analysis was performed on various industrial membranes such as reverse osmosis and ion-exchange membranes, giving us great insight into the heterogeneous structures related to the membrane functions.

Dr. Hanai is also widely recognized for his pioneering studies on black lipid membranes. During his stay at Cambridge, in co-operation with Dr. Denis A Haydon, he developed techniques to construct the black lipid membranes and measured their electric properties. The studies contributed much to the modeling of the physicochemical properties of biological membranes. Important findings were that the capacitance of the membranes was independent of the nature and concentration of the surrounding electrolyte and that only the hydrocarbon part of the membranes contributed to the capacitance. He verified that the thickness of the hydrocarbon part estimated from the capacitance was twice the average hydrocarbon chain length of lipids.

In addition to these excellent research achievements, his activities in education and academic society are noteworthy. He gave lectures on advances in dielectric spectroscopy of colloidal systems at the Graduate School of Science, Kyoto University and supervised the dissertation work of many graduate students. He also provided lectures on selected topics as well as physical chemistry and colloid chemistry at several different universities. He has published many review articles and books that provide an easy-to-understand introduction for students and young researchers who are interested in the electric properties of heterogeneous systems including colloids, biological cells and membranes. He served as an active member of academic societies such as the Division of Colloid and Surface Chemistry in the Chemical Society Japan and the Membrane Society of Japan.

Dr. Hanai is respected by his students and loved by his colleagues for his sincere and warm personality as well as his scientific talent.

Obituary

Professor Emeritus

Dr. BANDO, Yoshichika (1934–2018)

Dr. Yoshichika Bando, Professor Emeritus of Kyoto University, passed away on February 7, 2018, at the age of 84.

Dr. Bando was born in Tokushima on January 15, 1934. After graduation from the Faculty of Science, Kyoto University in 1956, he continued his study as a graduate student at the Department of Chemistry, Faculty of Science in Kyoto University. After finishing the graduation course, he joined Nippon Kayaku Co., Ltd., and then entered a doctoral course of Department of Chemistry, Graduate School of Science, Kyoto University. In 1960 he was appointed an instructor of the Department of Chemistry, Faculty of Science, Kyoto University under the supervision of Professor Sukeji Kachi. He was granted a doctoral degree for his studies on the preparation and properties of ultrafine particles of metal alloys. In 1964 he was appointed an instructor of the Laboratory of Solid State Chemistry of the Institute for Chemical Research, Kyoto University under the supervision of Emeritus Professor Toshio Takada. In 1968 he was promoted to Associate Professor of the same laboratory. In 1976 Dr. Bando was appointed full Professor of Kyoto University and directed the Facility of Inorganic Synthesis of the same institute. Dr. Bando retired from Kyoto University on March 31, 1997, and was honored with the title of Professor Emeritus, Kyoto University. After retirement, he was appointed as a professor of the Faculty of Engineering, Okayama University of Science.

During years Dr. Bando's research work covered a wide range of solid state chemistry. He studied the Martensitic transformation of fine particles of metal alloys, various synthesis methods of oxides and hydroxides of transition metals, growth of single crystals by the chemical transport, and also growth of epitaxial films and artificial superlattices of oxides and chalcogenides. Basic research done by him found fruitful practical applications; e.g. production of iron oxide fine particles to be used as magnetic recording materials, cosmetics and magnetic heads made of a crystal-oriented spinel ferrite. Dr. Bando also rose into worldwide notice for his outstanding work about the epitaxial films and artificial superlattices of high-Tc cuprate superconductors.

Dr. Bando was awarded several prizes for his brilliant achievements by The Japan Society of Powder and Powder Metallurgy.

Dr. Bando delivered lectures on advanced inorganic synthesis at the Graduate School of Science at Kyoto University and supervised dissertation works of graduate students. He was invited as a visiting professor by the University of Tokyo, Nagoya University, Kobe University, and some other institutions. He served as a president of The Japan Society of Powder and Powder Metallurgy from 1996 to 1998, and as a director or a councilor of several other societies.

His sincere and warmhearted character was admired by his friends, colleagues, and students.

PUBLICATIONS
INTERNATIONAL RESEARCH COLLABORATIONS
SELECTED GRANTS
THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY
— Organoelement Chemistry —

Suzuki, Y.; Sasamori, T.; Guo, J.-D.; Tokitoh, N., A Redox-active Bis(ferrocenyl)germylene and Its Reactivity, *Chem. Eur. J.*, **24,** 364-368 (2018).

Sugahara, T.; Guo, J.-D.; Sasamori, T.; Nagase, S.; Tokitoh, N., Reversible Addition of Terminal Alkenes to Digermynes, *Chem. Commun.*, **54,** 519-522 (2018).

Hayakawa, N.; Sugahara, T.; Numata, Y.; Kawaai, H.; Yamatani, K.; Nishimura, S.; Goda, S.; Suzuki, Y.; Tanikawa, T.; Nakai, H.; Hashizume, D.; Sasamori, T.; Tokitoh, N.; Matsuo, T., 1,2-Dihalodigermenes Bearing Bulky Eind Groups: Synthesis, Characterization, and Conversion to Halogermylenoids, *Dalton Trans.*, **47,** 814-822 (2018).

Hayakawa, N.; Sadamori, K.; Mizutani, S.; Agou, T.; Sugahara, T.; Sasamori, T.; Tokitoh, N.; Hashizume, D.; Matsuo, T., Synthesis and Characterization of *N*-Heterocyclic Carbene-coordinated Silicon Compounds Bearing a Fused-Ring Bulky Eind Group, *Inorganics*, **6,** 30-41 (2018).

Arai, K.; Ueda, Y.; Morisaki, K.; Furuta, T.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Intermolecular Chemo- and Regioselective Aromatic C–H Amination of Alkoxyarenes Promoted by Rhodium Nitrenoids, *Chem. Commun.*, **54,** 2264-2267 (2018).

Sugahara, T.; Guo, J.-D.; Sasamori, T.; Nagase, S.; Tokitoh, N., Regioselective Cyclotrimerization of Terminal Alkynes Using a Digermyne, *Angew. Chem. Int. Ed.*, **57,** 3499-3503 (2018).

Agou, T.; Ikeda, S.; Sasamori, T.; Tokitoh, N., Synthesis and Structure of Lewis Base-coordinated Phosphanylalumanes Bearing P–H and Al–Br Moieties, *Eur. J. Inorg. Chem.*, **2018,** 1984-1987 (2018).

Sugahara, T.; Sasamori, T.; Tokitoh, N., Chalcogenation Reaction of Cyclic Digermenes, *Chem. Lett.*, **47,** 719-722 (2018).

Fujimori, S.; Mizuhata, Y.; Tokitoh, N., Heavy Phenyllithium and -sodium: Synthesis and Characterization of Germanium Analogues of Phenyl Anion (“Germabenzenyl Anions”), *Chem. Lett.*, **47,** 708-710 (2018).

Agou, T.; Ohata, R.; Mizuhata, Y.; Tokitoh, N.; Fukumoto, H.; Kubota, T., Synthesis of a New Highly-fluorinated *cis*-1,2-Cyclopentanediol and Its Application for Fluorinated Oligoesters, *J. Fluor. Chem.*, **210,** 78-82 (2018).

Fujimori, S.; Mizuhata, Y.; Tokitoh, N., Ru-Complexes of an Anionic Germabenzenyl Ligand, *Chem. Commun.*, **54,** 8044-8047 (2018).

Agou, T.; Wada, N.; Hosoya, T.; Fukumoto, H.; Kubota, T.; Fujisawa, K.; Mizuhata, Y.; Tokitoh, N., Syntheses and Structures of d^{10} Coinage Metal Complexes of Electron-accepting Phosphine Ligands Featuring a 3,3,4,4,5,5-Hexafluorocyclopentene Framework, *Inorg. Chem.*, **57,** 9105-9114 (2018).

Agou, T.; Aso, D.; Kataoka, S.; Tuchimochi, R.; Fukumoto, H.; Yamazaki, T.; Kawasaki-Takasuka, T.; Mizuhata, Y.; Tokitoh, N.; Kubota, T., Facile Transformation of 2*H*,3*H*-Decafluoropentane (HFC-4310mee) into (*Z*)-2*H*-Nonafluoropent-2-ene and Its Application to the Synthesis of Polyfluorinated Homoallylic Ketones by Claisen Rearrangement, *J. Fluor. Chem.*, **213,** 74-79 (2018).

Sasamori, T.; Suzuki, Y.; Sugamata, K.; Sugahara, T.; Tokitoh, N., Synthesis of Ferrocenyl-substituted Organochalcogenyldichlorogermanes, *Inorganics*, **6,** 68-76 (2018).

Sugahara, T.; Sasamori, T.; Tokitoh, N., 2,5-Digermaselenophenes: Germanium Analogues of Selenophenes, *J. Am. Chem. Soc.*, **140,** 11206-11209 (2018).

Omatsu, Y.; Mizuhata, Y.; Tokitoh, N., Synthesis of Dodecaallylhexasilacyclohexane and Its Convertibility, *Z. Anorg. Allg. Chem.*, **644,** 930-934 (2018).

Hashimoto, S.; Kayahara, E.; Mizuhata, Y.; Tokitoh, N.; Takeuchi, K.; Ozawa, F.; Yamago, S., Synthesis and Physical Properties of Polyfluorinated Cycloparaphenylenes, *Org. Lett.*, **20,** 5973-5976 (2018).

Roy, M. M. D.; Fujimori, S.; Ferguson, M. J.; McDonald, R.; Rivard, E.; Tokitoh, N., Neutral, Cationic and Hydride-substituted Siloxygermylenes, *Chem. Eur. J*, **24,** 14392-14399 (2018).

Sugahara, T.; Guo, J.-D.; Hashizume, D.; Sasamori, T.; Nagase, S.; Tokitoh, N., The Selective Formation of a 1,2-Disilabenzene from the Reaction of a Disilyne with Phenylacetylene, *Dalton Trans.*, **47,** 13318-13322 (2018).

Mizuhata, Y.; Fujimori, S.; Noda, N.; Kanesato, S.; Tokitoh, N., Generation of Stannabenzenes and Their Monomer-dimer Equilibration, *Dalton Trans.*, **47,** 14436-14444 (2018).

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

Agou, T.; Nemoto, S.; Yamada, S.; Konno, T.; Mizuhata, Y.; Tokitoh, N.; Ebina, R.; Ishii, A.; Hosoya, T.; Fukumoto, H.; Kubota, T., A Straightforward Synthesis of Polyfluorinated Furan Derivatives and Their Property, *Asian J. Org. Chem.*, **7,** 2484-2489 (2018).

Murai, T.; Xing, Y.-N.; Kuribayashi, T.; Lu, W.-J.; Guo, J.-D.; Yella, R.; Hamada, S.; Sasamori, T.; Tokitoh, N.; Kawabata, T.; Furuta, T., Synthesis and Structural Properties of Axially Chiral Binaphthothiophene Dicarboxylic Acid, *Chem. Pharm. Bull.*, **66,** 1203-1206 (2018).

— Structural Organic Chemistry —

Nakakuki, Y.; Hirose, T.; Matsuda, K., Synthesis of Helical Analogue of Kekulene: a Flexible π-Expanded Helicene with Large Helical Diameter Acting as a Soft Molecular Spring, *J. Am. Chem. Soc.*, **140,** 15461-15469 (2018).

Carné-Sánchez, A.; Craig, G. A.; Larpent, P.; Hirose, T.; Higuchi, M.; Kitagawa, S.; Matsuda, K.; Urayama, K.; Furukawa, S., Self-assembly of Metal–Organic Polyhedra into Supramolecular Polymers with Intrinsic Microporosity, *Nat. Commun.*, **9,** 2506 (2018).

Nakakuki, Y.; Hirose, T.; Sotome, H.; Miyasaka, H.; Matsuda, K., Homogeneously π-Extended Helicene as a Primary Substructure of Helically Twisted Chiral Graphenes, *J. Am. Chem. Soc.*, **140,** 4317-4326 (2018).

Hashikawa, Y.; Yasui, H.; Kurotobi, K.; Murata, Y., Synthesis and Properties of Open-Cage Fullerene C_{60} Derivatives: Impact of the Extended π-Conjugation, *Mater. Chem. Front.*, **2,** 206-213 (2018).

Yang, F.; Lim, H. E.; Wang, F.; Ozaki, M.; Shimazaki, A.; Liu, J.; Miyauchi, Y.; Wakamiya, A.; Murata, Y.; Matsuda, K., Roles of Polymer Layer in Enhanced Photovoltaic Performance of Perovskite Solar Cells via Interface Engineering, *Adv. Mater. Inter.*, **5,** [1701256-1]-[1701256-10] (2018).

Zhu, G.-Z.; Liu, Y.; Hashikawa, Y.; Zhang, Q.-F.; Murata, Y.; Wang, L.-S., Probing the Interaction between the Encapsulated Water Molecule and the Fullerene Cages in $H_2O@C_{60}^-$ and $H_2O@C_{59}N^-$, *Chem. Sci.*, **9,** 5666-5671 (2018).

Kurimoto, Y.; Mitsudo, K.; Mandai, H.; Wakamiya, A.; Murata, Y.; Mori, H.; Nishihara, Y.; Suga, S., Efficient Synthesis and Properties of [1]Benzothieno[3,2-b]thieno[2,3-d]furans and [1]Benzothieno[3,2-b]thieno[2,3-d]thiophenes, *Asian J. Org. Chem.*, **7,** 1635-1641 (2018).

Hasegawa, S.; Hashikawa, Y.; Kato, T.; Murata, Y., Construction of a Metal-Free Electron Spin System by Encapsulation of an NO Molecule Inside an Open-Cage Fullerene C_{60} Derivative, *Angew. Chem. Int. Ed.*, **57,** 12804-12808 (2018).

Liu, J.; Ozaki, M.; Yakumaru, S.; Handa, T.; Nishikubo, R.; Kanemitsu, Y.; Saeki, A.; Murata, Y.; Wakamiya, A., Lead-Free Solar Cells Based on Tin Halide Perovskite Films with High Coverage and Improved Aggregation, *Angew. Chem. Int. Ed.*, **57,** 13221-13225 (2018).

Shimogawa, H.; Murata, Y.; Wakamiya, A., NIR-Absorbing Dye Based on BF_2-Bridged Azafulvene Dimer as an Electron-Accepting Unit, *Org. Lett.*, **20,** 5135-5138 (2018).

Strelnikov, D. V.; Jasik, J.; Gerlich, D.; Murata, M.; Murata, Y.; Komatsu, K.; Kappes, M. M.; Roithova, J., Near- and Mid-IR Gas-Phase Absorption Spectra of $H_2@C_{60}^+$-He, *J. Phys. Chem. A*, **122,** 8162-8166 (2018).

Yang, F.; Liu, J.; Lim, H. E.; Ishikura, Y.; Shinokita, K.; Miyauchi, Y.; Wakamiya, A.; Murata, Y.; Matsuda, K., High Bending Durability of Efficient Flexible Perovskite Solar Cells Using Metal Oxide Electron Transport Layer, *J. Phys. Chem. C*, **122,** 17088-17095 (2018).

Hashikawa, Y.; Murata, Y., Wavelength-Dependent Efficiency of Sequential Photooxygenation: C=C Bond Cleavage on Open-Cage C_{60} Derivatives, *ChemPlusChem*, **83,** 1179-1183 (2018).

Ayoub, G.; Strukil, V.; Fabian, L.; Mottillo, C.; Bao, H.; Murata, Y.; Moores, A.; Margetic, D.; Eckert-Maksic, M.; Friscic, T., Mechanochemistry vs. Solution Growth: Striking Differences in Bench Stability of a Cimetidine Salt Based on Synthetic Method, *CrystEngComm*, **20,** 7242-7247 (2018).

Hashikawa, Y.; Hasegawa, S.; Murata, Y., A Single but Hydrogen-Bonded Water Molecule Confined in an Anisotropic Subnanospace, *Chem. Commun.*, **54,** 13686-13689 (2018).

— Synthetic Organic Chemistry —

Arai, K.; Ueda, Y.; Morisaki, K.; Furuta, T.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Intermolecular Chemo- and Regioselective Aromatic C-H Amination of Alkoxyarenes Promoted by Rhodium Nitrenoids, *Chem. Commun.*, **54,** 2264-2267 (2018).

Ohtsuki, H.; Takashima, M.; Furuta, T.; Kawabata, T., Direct Asymmetric Synthesis of a-Deuterated a-Amino Acid Derivatives from the Parent a-Amino Acid via Memory of Chirality, *Tetrahedron Lett.*, **59,** 1188-1191 (2018).

Murai, T.; Xing, Y.; Kuribayashi, T.; Lu, W.; Guo, J.; Yella, R.; Hamada, S.; Sasamori, T.; Tokitoh, N.; Kawabata, T.; Furuta, T., Synthesis and Structural Properties of Axially Chiral Binaphthothiophene Dicarboxylic Acid, *Chem. Pharm. Bull.*, **66,** 1203-1206 (2018).

— Advanced Inorganic Synthesis —

Nakahara, S.; Tahara, H.; Yumoto, G.; Kawawaki, T.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Suppression of Trion Formation in $CsPbBr_3$ Perovskite Nanocrystals by Postsynthetic Surface Modification, *J. Phys. Chem. C*, **122,** 22188-22193 (2018).

Yarita, N.; Aharen, T.; Tahara, H.; Saruyama, M.; Kawawaki, T.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Observation of Positive and Negative Trions in Organic-Inorganic Hybrid Perovskite Nanocrystals, *Phys. Rev. Mater.*, **2,** [116003-1]-[116003-8] (2018).

Lian, Z.; Sakamoto, M.; Kobayashi, Y.; Tamai, N.; Ma, J.; Sakurai, T.; Seki, S.; Nakagawa, T.; Lai, M.; Haruta, M.; Kurata, H.; Teranishi, T., Durian-Shaped CdS@ZnSe Core@mesoporous-Shell Nanocrystals for Enhanced and Sustainable Photocatalytic Hydrogen Evolution, *J. Phys. Chem. Lett.*, **9,** 2212-2217 (2018).

Tahara, H.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Quantum Coherence of Multiple Excitons Governs Absorption Cross-sections of PbS/CdS Core/Shell Nanocrystals, *Nat. Commun.*, **9,** 3179 (2018).

Yumoto, G.; Tahara, H.; Kawawaki, T.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Hot Biexciton Effect on Optical Gain in $CsPbI_3$ Perovskite Nanocrystals, *J. Phys. Chem. Lett.*, **9,** 2222-2228 (2018).

Saruyama, M.; Kim, S.; Nishino, T.; Sakamoto, M.; Haruta, M.; Kurata, H.; Akiyama, S.; Yamada, T.; Domen, K.; Teranishi, T., Phase-Segregated $NiP_x@FeP_yO_z$ Core@Shell Nanoparticles: Ready-to-Use Nanocatalysts for Electro- and Photo-Catalytic Water Oxidation through in-situ Activation by Structural Transformation and Spontaneous Ligand Removal, *Chem. Sci.*, **9,** 4830-4836 (2018).

Yoshinaga, T.; Xiong, A.; Ham, Y.; Kaung, Y.; Niishiro, R.; Akiyama, S.; Sakamoto, M.; Hisatomi, T.; Domen, K.; Teranishi, T., Boosting Photocatalytic Overall Water Splitting by Co Doping into Mn_3O_4 Nanoparticles as Oxygen Evolution Cocatalysts, *Nanoscale*, **10,** 10420-10427 (2018).

Lian, Z.; Sakamoto, M.; Matsunaga, H.; Vequizo, J. J. M.; Yamakata, A.; Haruta, M.; Kurata, H.; Teranishi, T., Near Infrared Light Induced Plasmonic Hot Hole Transfer at a Nano-Heterointerface, *Nat. Commun.*, **9,** 2314 (2018).

Okawa, S.; Hirasawa, T.; Sato, R.; Kushibiki, T.; Ishihara, M.; Teranishi, T., Numerical and Experimental Investigations of Dependence of Photoacoustic Signals from Gold Nanoparticles on the Optical Properties, *Opt. Rev.*, **25,** 365-374 (2018).

Eguchi, D.; Sakamoto, M.; Teranishi, T., Ligand Effect on the Catalytic Activity of Gold Clusters in the Electrochemical Hydrogen Evolution Reaction, *Chem. Sci.*, **9,** 261-265 (2018).

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

Nakanishi, Y.; Ishige, R.; Ogawa, H.; Sakakibara, K.; Ohno, K.; Morinaga, T.; Sato, T.; Kanaya, T.; Tsujii, Y., USAXS Analysis of Concentration-Dependent Self-Assembling of Polymer-Brush-Modified Nanoparticles in Ionic Liquid: [I] Concentrated-Brush Regime, *J. Chem. Phys.*, **148,** [124902-1]-[124902-9] (2018).

Shimizu, Y.; Sakakibara, K.; Tsujii, Y., Strain Hardening of Highly Stretchable Elastomeric Composites Reinforced with Well-Defined Nanofiber Network of Bacterial Cellulose, *J. Fiber Sci. Technol.*, **74,** 17-23 (2018).

Yoshikawa, C.; Hoshiba, T.; Sakakibara, K.; Tsujii, Y., Flocculation of Cells by Cellulose Nanofibers Modified with Concentrated Polymer Brushes, *ACS Appl. Nano Mater.*, **1,** 1450-1455 (2018).

Wang, C.-G.; Chen, C.; Sakakibara, K.; Tsujii, Y.; Goto, A., Facile Fabrication of Concentrated Polymer Brushes with Complex Patterning by Photocontrolled Organocatalyzed Living Radical Polymerization, *Angew. Chem. Int. Ed.*, **57,** 13504-13508 (2018).

Nguyen, T. D.; Sakakibara, K.; Imai, T.; Tsujii, Y.; Kohdzuma, Y.; Sugiyama, J., Shrinkage and Swelling Behavior of Archaeological Waterlogged Wood Preserved with Slightly Crosslinked Sodium Polyacrylate, *J. Wood Sci.*, **64,** 294-300 (2018).

Sakakibara, K.; Konishi, K.; Ishizuka, N.; Goto, A.; Tsujii, Y., Versatile Preparation of Surface-Skinless Particles of Epoxy Resin-Based Monoliths Using a Well-Defined Diblock Copolymer Surfactant, *Polym. Chem.*, **9,** 414-419 (2018).

Ohno, K.; Sakaue, M.; Mori, C., Magnetically Responsive Assemblies of Polymer-Brush-Decorated Nanoparticle Clusters That Exhibit Structural Color, *Langmuir*, **34,** 9532-9539 (2018).

Li, W.; Cao, F.; He, C.; Ohno, K.; Ngai, T., Measuring the Interactions between Protein-Coated Microspheres and Polymer Brushes in Aqueous Solutions, *Langmuir*, **34,** 8798-8806 (2018).

Kawata, Y.; Yamamoto, T.; Kihara, H.; Yamamura, Y.; Saito, K.; Ohno, K., Unusual Photoresponses in the Upper Critical Solution Temperature of Polymer Solutions Mediated by Changes in Intermolecular Interactions in an Azo-doped Liquid Crystalline Solvent, *Phys. Chem. Chem. Phys.*, **20,** 5850-5855 (2018).

Li, L.; Nakaji-Hirabayashi, T.; Kitano, H.; Ohno, K.; Saruwatari, Y.; Matsuoka, K., A Novel Approach for UV-Patterning with Binary Polymer Brushes, *Colloids Surf. B*, **161,** 42-50 (2018).

Hoshiba, T.; Yoshikawa, C.; Sakakibara, K., Characterization of Initial Cell Adhesion on Charged Polymer Substrates in Serum-Containing and Serum-Free Media, *Langmuir*, **34,** 4043-4051 (2018).

[Others]

Yoshikawa, C.; Sakakibara, K.; Tsujii, Y., Biocompatible Concentrated Polymer Brushes, *Kino Zairyo*, **38,** 28-39 (2018).

— Polymer Controlled Synthesis —

Nakamura, Y.; Ebeling, B.; Wolpers, A.; Monteil, V.; D'Agosto, F.; Yamago, S., Controlled Radical Polymerization of Ethylene Using Organotellurium Compounds, *Angew. Chem. Int. Ed.*, **57,** 305-309 (2018).

Fan, W.; Tosaka, M.; Yamago, S.; Cunningham, M. F., Living Ab Initio Emulsion Polymerization of Methyl Methacrylate in Water Using a Water Soluble Organotellurium Chain Transfer Agent under Thermal and Photochemical Conditions, *Angew. Chem. Int. Ed.*, **57,** 962-966 (2018).

Masumoto, Y.; Toriumi, N.; Muranaka, A.; Kayahara, E.; Yamago, S.; Uchiyama, M., Near-Infrared Fluorescence from In-Plane-Aromatic Cycloparaphenylene Dications, *J. Phys. Chem. A*, **122,** 5162-5167 (2018).

Li, W.; Tosaka, M.; Yamago, S., Synthesis of a Structurally Controlled Polyacrylonitrile Gel for Energy-Storage Devices by an Organotellurium-mediated Radical Copolymerization and Subsequent Cross-linking Reaction, *Reversible Deactivation Radical Polymerization: From Mechanisms to Materials and Applications, ACS Symposium Series, American Chemical Society: Washington, DC, Chapter 7*, 129-142 (2018).

Kayahara, E.; Cheng, Y.; Yamago, S., Short-step Synthesis of Large Cycloparaphenylenes, *Chem. Lett.*, **47,** 1108-1111 (2018).

Kayahara, E.; Hayashi, T.; Takeuchi, K.; Ozawa, F.; Ashida, K.; Ogoshi, S.; Yamago, S., Strain-Induced Double Carbon-Carbon Bond Activations of Cycloparaphenylenes (CPPs) by a Platinum Complex and Its Application for the Synthesis of Cyclic Diketones, *Angew. Chem. Int. Ed.*, **57,** 11418-11421 (2018).

Rattanakawin, P.; Fan, W.; Yamago, S.; Yoshimoto, K.; Ohshima, M., Synthesis of Photocleavable Block Copolymers for UV Induced Foaming, *J. Photopolym. Sci. Tec.*, **31,** 647-650 (2018).

Hashimoto, S.; Kayahara, E.; Mizuhata, Y.; Tokitoh, N.; Takeuchi, K.; Ozawa, F.; Yamago, S., Synthesis and Physical Properties of Polyfluorinated Cycloparaphenylenes, *Org. Lett.*, **20,** 5973-5976 (2018).

Fujitsuka, M.; Kayahara, E.; Chao, L.; Yamago, S.; Majima, T., Significant Structural Relaxations of Excited [n]Cycloparaphenylene Dications (n = 5–9), *Phys. Chem. Chem. Phys.*, **20,** 29207-29211 (2018).

Kaya, K.; Seba, M.; Fujita, T.; Yamago, S.; Yagci, Y., Visible Light-Induced Free Radical Promoted Cationic Polymerization Using Organotellurium Compounds, *Polym. Chem.*, **9,** 5639-5643 (2018).

Tosaka, M.; Oue, S.; Gros, A.; Huneau, B.; Verron, E.; Poompradub, S., Formation of Crystallites with Low Surface Energy — A Key to Understand the Crystallization of Oriented Polymer, *J. Fiber Sci. Technol.*, **74,** 133-142 (2018).

Tosaka, M.; Tashiro, K., Crystal Polymorphism and Structure Models of Poly(dimethylsiloxane), *Polymer*, **153,** 507-520 (2018).

Tosaka, M.; Shigeki, E., Triaxially Oriented Shape Memory Natural Rubber, *Polymer*, **157,** 151-155 (2018).

Osaka, N.; Minematsu, Y.; Tosaka, M., Effect of Lithium Salt on Thermal Behaviors of Poly(vinylidene fluoride)/Ionic Liquid Gels and Pore/Void Formation by Competition between Crystallization and Phase Separation, *RSC Adv.*, **8,** 40570-40580 (2018).

[Others]

Yamago, S.; Lu, Y., New Development of Hyperbranched Polymer Synthesis–Toward Compatibility between Structural Control and Practicality, *Chemistry*, **73,** 68-69 (2018) (in Japanese).

Fujita, T.; Yamago, S., Radical Polymerization Using Organotellurium Compounds, *Living Radical Polymerization: Recent Development of Synthesis and Application of Functional Polymers, S. Matsumoto, Ed., Chapter 6: CMC Publishing*, 46-55 (2018) (in Japanese).

Tosaka, M., New Concept on Crystallization of Oriented Polymer, *J. Soc. Fiber Sci. Technol., Jpn.*, **74,** [P-30]-[P-34] (2018) (in Japanese).

Tosaka, M., Commentary on Flory's Theory on Strain-induced Crystallization, *Nippon Gomu Kyokaishi*, **91,** 199-206 (2018) (in Japanese).

Yamago, S., Self-Assembly in Block Copolymers: Structural Control and Applications, *Structural Design and Application Development of Block Copolymer, M. Takenaka, Ed., Chapter 6: CMC Publishing*, 89-100 (2018) (in Japanese).

— Inorganic Photonics Materials —

Kurita, T.; Mineyuki, N.; Shimotsuma, Y.; Fujiwara, M.; Mizuochi, N.; Shimizu, M.; Miura, K., Efficient Generation of Nitrogen-Vacancy Center Inside Diamond with Shortening of Laser Pulse Duration, *Appl. Phys. Lett.*, **113,** [211102-1]-[211102-4] (2018).

Hayashi, K.; Matsuzaki, Y.; Taniguchi, T.; Shimo-Oka, T.; Nakamura, I.; Onoda, S.; Ohshima, T.; Morishita, H.; Fujiwara, M.; Saito, S.; Mizuochi, N., Optimization of Temperature Sensitivity Using the Optically Detected Magnetic-Resonance Spectrum of a Nitrogen-Vacancy Center Ensemble, *Phys. Rev. Appl.*, **10,** [034009-1]-[034009-8] (2018).

Saijo, S.; Matsuzaki, Y.; Saito, S.; Yamaguchi, T.; Hanano, I.; Watanabe, H.; Mizuochi, N.; Ishi-Hayase, J., AC Magnetic Field Sensing Using Continuous-Wave Optically Detected Magnetic Resonance of Nitrogen Vacancy Centers in Diamond, *Appl. Phys. Lett.*, **113,** [082405-1]-[082405-5] (2018).

Murai, T.; Makino, T.; Kato, H.; Shimizu, M.; Herbschleb, D. E.; Doi, Y.; Morishita, H.; Fujiwara, M.; Hatano, M.; Yamasaki, S.; Mizuochi, N., Engineering of Fermi Level by nin Diamond Junction for Control of Charge States of NV Centers, *Appl. Phys. Lett.*, **112,** [111903-1]-[111903-4] (2018).

Shimizu, M.; Makino, T.; Iwasaki, T.; Tahara, K.; Kato, H.; Mizuochi, N.; Yamasaki, S.; Hatano, M., Charge State Control of Ensemble Nitrogen Vacancy Center by n-i-n Diamond Junction, *Appl. Phys. Express*, **11,** [033004-1]-[033004-3] (2018).

— Nanospintronics —

Kan, D.; Moriyama, T.; Kobayashi, K.; Shimakawa, Y., Alternative to the Topological Interpretation of the Transverse Resistivity Anmomalies in $SrRuO_3$, *Phys. Rev. B*, **98,** 180408 (2018).

Moriyama, T.; Zhou, W.; Seki, T.; Takanashi, K.; Ono, T., Spin-Orbit-Torque Memory Operation of Synthetic Antiferromagnets, *Phys. Rev. Lett.*, **121,** 167202 (2018).

Ogi, H.; Iwagami, S.; Nagakubo, A.; Taniguchi, T.; Ono, T., Nano-Plate Biosensor Array Using Ultrafast Heat Transport through Proteins, *Sensors and Actuators B: Chemical*, **278,** 15-20 (2018).

Moriyama, T.; Oda, K.; Ohkochi, T.; Kimata, M.; Ono, T., Spin Torque Control of Antiferromagnetic Moments in NiO, *Sci. Rep.*, **8,** 14167 (2018).

Kasukawa, S.; Shiota, Y.; Moriyama, T.; Ono, T., Evaluation of Electric Field Effect on Interface Magnetic Properties by Propagating Spin Wave in Pt/Co/MgO Structures, *Japanese Journal of Applied Physics*, **57,** 080309 (2018).

Ikebuchi, T.; Moriyama, T.; Mizuno, H.; Oda, K.; Ono, T., Spin Current Transmission in Polycrystalline NiO Films, *Appl. Phys. Express*, **11,** 073003 (2018).

Hirata, Y.; Kim, D.; Okuno, T.; Nishimura, T.; Kim, D.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Kim, K.; Choe, S.; Ono, T., Correlation between Compensation Temperatures of Magnetization and Angular Momentum in GdFeCo Ferrimagnets, *Phys. Rev. B*, **97,** 220403 (2018).

Ando, F.; Yamada, T. K.; Koyama, T.; Ishibashi, M.; Shiota, Y.; Moriyama, T.; Chiba, D.; Ono, T., Microscopic Origin of Electric-field-induced Modulation of Curie Temperature in Cobalt, *Appl. Phys. Express*, **11,** 073002 (2018).

Ishibashi, M.; Yamada, T. K.; Shiota, Y.; Ando, F.; Koyama, T.; Kakizakai, H.; Mizuno, H.; Miwa, K.; Ono, S.; Moriyama, T.; Chiba, D.; Ono, T., Electric Field Effect on Exchange Interaction in Ultrathin Co Films with Ionic Liquids, *Appl. Phys. Express*, **11,** 063002 (2018).

Hirata, Y.; Kim, D.; Okuno, T.; Nishimura, T.; Futakawa, Y.; Yoshikawa, H.; Ham, W.; Kim, S.; Tsukamoto, A.; Shiota, Y.; Moriyama, T.; Kim, K.; Ono, T., Effect of Depinning Field on Determination of Angular-momentum-compensation Temperature of Ferrimagnets, *Appl. Phys. Express*, **11,** 063001 (2018).

Ikebuchi, T.; Moriyama, T.; Shiota, Y.; Ono, T., Homodyne Detection of Ferromagnetic Resonance by a Non-uniform Radio-frequency Excitation Current, *Appl. Phys. Express*, **11,** 053008 (2018).

Kim, S.; Ueda, K.; Go, G.; Jang, P.; Lee, K.; Belabbes, A.; Manchon, A.; Suzuki, M.; Kotani, Y.; Nakamura, T.; Nakamura, K.; Koyama, T.; Chiba, D.; Yamada, T. K.; Kim, D.; Moriyama, T.; Kim, K.; Ono, T., Correlation of the Dzyaloshinskii-Moriya Interaction with Heisenberg Exchange and Orbital Asphericity, *Nat. Commun.*, **9,** 1648 (2018).

Nishimura, T.; Kim, D.; Hirata, Y.; Okuno, T.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Shiota, Y.; Moriyama, T.; Ono, T., Correlation between Magnetic Properties and Depinning Field in Field-driven Domain Wall Dynamics in GdFeCo Ferrimagnets, *Appl. Phys. Lett.*, **112,** 172403 (2018).

Nishimura, T.; Kim, D.; Okuno, T.; Hirata, Y.; Futakawa, Y.; Yoshikawa, H.; Kim, S.; Tsukamoto, A.; Shiota, Y.; Moriyama, T.; Ono, T., Determination of Perpendicular Magnetic Anisotropy Based on the Magnetic Droplet Nucleation, *Japanese Journal of Applied Physics*, **57,** 050308 (2018).

Yamada, T. K.; Suzuki, M.; Pradipto, A.; Koyama, T.; Kim, S.; Kim, K.; Ono, S.; Taniguchi, T.; Mizuno, H.; Ando, F.; Oda, K.; Kakizakai, H.; Moriyama, T.; Nakamura, K.; Chiba, D.; Ono, T., Microscopic Investigation into the Electric Field Effect on Proximity-Induced Magnetism in Pt, *Phys. Rev. Lett.*, **120,** 157203 (2018).

Stigloher, J.; Taniguchi, T.; Madami, M.; Decker, M.; Körner, S. H.; Moriyama, T.; Gubbiotti, G.; Ono, T.; Back, C. H., Spin-wave Wavelength Down-conversion at Thickness Steps, *Appl. Phys. Express*, **11,** 053002 (2018).

Fujimoto, J., Transport Coefficients of Dirac Ferromagnet: Effects of Vertex Corrections, *Phys. Rev. B*, **97,** 104421 (2018).

Baltz, V.; Manchon, A.; Tsoi, M.; Moriyama, T.; Ono, T., Antiferromagnetic Spintronics, *Rev. Mod. Phys.*, **90,** 015005 (2018).

Suzuki, M.; Kim, K.; Kim, S.; Yoshikawa, H.; Tono, T.; Yamada, T. K.; Taniguchi, T.; Mizuno, H.; Oda, K.; Ishibashi, M.; Hirata, Y.; Li, T.; Tsukamoto, A.; Chiba, D.; Ono, T., Three-Dimensional Visualization of Magnetic Domain Structure with Strong Uniaxial Anisotropy via Scanning Hard X-ray Microtomography, *Appl. Phys. Express*, **11,** 036601 (2018).

DIVISION OF BIOCHEMISTRY
— Biofunctional Design-Chemistry —

Azuma, Y.; Imai, H.; Kawaguchi, Y.; Nakase, I.; Kimura, H.; Futaki, S., Modular Redesign of a Cationic Lytic Peptide to Promote the Endosomal Escape of Biomacromolecules, *Angew. Chem. Int. Ed. Engl.*, **57,** 12771-12774 (2018).

Tsuji, S.; Shinoda, K.; Futaki, S.; Imanishi, M., Sequence-Specific 5mC Detection in Live Cells Based on the TALE-Split Luciferase Complementation System, *Analyst*, **143,** 3793-3797 (2018).

Sakagami, K.; Masuda, T.; Kawano, K.; Futaki, S., Importance of Net Hydrophobicity in the Cellular Uptake of All-Hydrocarbon Stapled Peptides, *Mol. Pharm.*, **15,** 1332-1340 (2018).

Shinoda, K.; Tsuji, S.; Futaki, S.; Imanishi, M., Nested PUF Proteins: Extending Target RNA Elements for Gene Regulation, *Chembiochem*, **19,** 171-176 (2018).

— Chemistry of Molecular Biocatalysts —

Watanabe, B.; Kirikae, H.; Koeduka, T.; Takeuchi, Y.; Asai, T.; Naito, Y.; Tokuoka, H.; Horoiwa, S.; Nakagawa, Y.; Shimizu, B.; Mizutani, M.; Hiratake, J., Synthesis and Inhibitory Activity of Mechanism-Based 4-Coumaroyl-CoA Ligase Inhibitors, *Bioorg. Med. Chem.*, **26,** 2466-2474 (2018).

Nakayasu, M.; Akiyama, R.; Lee, H. J.; Osakabe, K.; Osakabe, Y.; Watanabe, B.; Sugimoto, Y.; Umemoto, N.; Saito, K.; Muranaka, T.; Mizutani, M., Generation of α-Solanine-Free Hairy Roots of Potato by CRISPR/Cas9 Mediated Genome Editing of the *St16DOX* Gene, *Plant Physiol. Biochem.*, **131,** 70-77 (2018).

Kuroha, T.; Nagai, K.; Gamuyao, R.; Wang, D. R.; Furuta, T.; Nakamori, M.; Kitaoka, T.; Adachi, K.; Minami, A.; Mori, Y.; Mashiguchi, K.; Seto, Y.; Yamaguchi, S.; Kojima, M.; Sakakibara, H.; Wu, J.; Ebana, K.; Mitsuda, N.; Ohme-Takagi, M.; Yanagisawa, S.; Yamasaki, M.; Yokoyama, R.; Nishitani, K.; Mochizuki, T.; Tamiya, G.; McCouch, S. R.; Ashikari, M., Ethylene-gibberellin Signaling Underlies Adaptation of Rice to Periodic Flooding, *Science*, **361,** 181-186 (2018).

Yao, J.; Mashiguchi, K.; Scaffidi, A.; Akatsu, T.; Melville, K. T.; Morita, R.; Morimoto, Y.; Smith, S. M.; Seto, Y.; Flematti, G. R.; Yamaguchi, S.; Waters, M. T., An Allelic Series at the *KARRIKIN INSENSITIVE 2* Locus of *Arabidopsis Thaliana* Decouples Ligand Hydrolysis and Receptor Degradation from Downstream Signaling, *Plant J.*, **96,** 75-89 (2018).

Fujikura, U.; Jing, R.; Hanada, A.; Takebayashi, Y.; Sakakibara, H.; Yamaguchi, S.; Kappel, C.; Lenhard, M., Variation in Splicing Efficiency Underlies Morphological Evolution in Capsella, *Dev. Cell*, **44,** 192-203 (2018).

Hasegawa, S.; Tsutsumi, T.; Fukushima, S.; Okabe, Y.; Saito, J.; Katayama, M.; Shindo, M.; Yamada, Y.; Shimomura, K.; Yoneyama, K.; Akiyama, K.; Aoki, K.; Ariizumi, T.; Ezura, H.; Yamaguchi, S.; Umehara, M., Low Infection of *Phelipanche aegyptiaca* in Micro-Tom Mutants Deficient in *CAROTENOID-CLEAVAGE DIOXYGENASE 8*, *Int. J. Mol. Sci.*, **19,** E2645 (2018).

Ramírez, V.; Xiong, G.; Mashiguchi, K.; Yamaguchi, S.; Pauly, M., Growth- and Stress-related Defects Associated with Wall Hypoacetylation are Strigolactone-dependent, *Plant Direct*, **2,** e00062 (2018).

Shindo, M.; Shimomura, K.; Yamaguchi, S.; Umehara, M., Upregulation of *DWARF27* is Associated with Increased Strigolactone Levels under Sulfur Deficiency in Rice, *Plant Direct*, **2,** e00050 (2018).

— Molecular Biology —

Ghelli, R.; Brunetti, P.; Napoli, N.; De Paolis, A.; Cecchetti, V.; Tsuge, T.; Serino, G.; Matsui, M.; Mele, G.; Rinaldi, G.; Palumbo, G. A.; Barozzi, F.; Costantino, P.; Cardarelli, M., A Newly Identified Flower-Specific Splice Variant of *AUXIN RESPONSE FACTOR8* Regulates Stamen Elongation and Endothecium Lignification in *Arabidopsis*, *Plant Cell*, **30,** 620-637 (2018).

Hirano, T.; Konno, H.; Takeda, S.; Dolan, L.; Kato, M.; Aoyama, T.; Higaki, T.; Takigawa-Imamura, H.; Sato, M. H., PtdIns(3,5)P_2 Mediates Root Hair Shank Hardening in *Arabidopsis*, *Nat. Plants*, **4,** 888-897 (2018).

— Chemical Biology —

Yatsuzuka, K.; Sato, S.; Pe, K. B.; Katsuda, Y.; Takashima, I.; Watanabe, M.; Uesugi, M., Live-Cell Imaging of Multiple Endogenous mRNAs Permits the Direct Observation of RNA Granule Dynamics, *Chem. Commun.*, **54,** 7151-7154 (2018).

Perron, A.; Nishikawa, Y.; Iwata, J.; Shimojo, H.; Takaya, J.; Kobayashi, K.; Imayoshi, I.; Mbenza, N. M.; Takenoya, M.; Kageyama, R.; Kodama, Y.; Uesugi, M., Small-Molecule Screening Yields a Compound That Inhibits the Cancer-Associated Transcription Factor Hes1 via the PHB2 Chaperone, *J. Biol. Chem.*, **293,** 8285-8294 (2018).

Mao, D.; Chung, X. K. W.; Andoh-Noda, T.; Qin, Y.; Sato, S.; Takemoto, Y.; Akamatsu, W.; Okano, H.; Uesugi, M., Chemical Decontamination of iPS Cell-Derived Neural Cell Mixtures, *Chem. Commun.*, **54,** 1355-1358 (2018).

Ohkanda, J.; Kusumoto, A.; Punzalan, L.; Masuda, R.; Wang, C.; Parvatkar, P.; Akase, D.; Aida, M.; Uesugi, M.; Higuchi, Y.; Kato, N., Structural Effect of Fusicoccin upon Upregulation of 14-3-3-Phospholigand Interaction and Cytotoxic Activity, *Chemistry*, **24,** 16066-16071 (2018).

Mashimo, Y.; Yoshioka, M.; Tokunaga, Y.; Fockenberg, C.; Terada, S.; Koyama, Y.; Shibata-Seki, T.; Yoshimoto, K.; Sakai, R.; Hakariya, H.; Liu, L.; Akaike, T.; Kobatake, E.; How, S. E.; Uesugi, M.; Chen, Y.; Kamei, K., Fabrication of a Multiplexed Artificial Cellular MicroEnvironment Array, *J. Vis. Exp.*, doi: 10.3791/57377 (2018).

Li, Q.; Yoshimura, H.; Komiya, M.; Tajiri, K.; Uesugi, M.; Hata, Y.; Ozawa, T., A Robust Split-Luciferase-Based Cell Fusion Screening for Discovering Myogenesis-Promoting Molecules, *Analyst*, **143,** 3472-3480 (2018).

DIVISION OF ENVIRONMENTAL CHEMISTRY
— Molecular Materials Chemistry —

Kubo, S.; Kaji, H., Parameter-Free Multiscale Simulation Realising Quantitative Prediction of Hole and Electron Mobilities in Organic Amorphous System with Multiple Frontier Orbitals, *Sci. Rep.*, **8,** [5203-1]-[5203-9] (2018).

Tani, K.; Yashima, T.; Miyanaga, K.; Hori, K.; Goto, K.; Tani, F.; Habuka, Y.; Suzuki, K.; Shizu, K.; Kaji, H., Carbazole and Benzophenone Based Twisted Donor-Acceptor Systems as Solution Processable Green Thermally Activated Delayed Fluorescence Organic Light Emitters, *Chem. Lett.*, **47,** 1236-1239 (2018).

Zu, G. Q.; Kanamori, K.; Maeno, A.; Kaji, H.; Nakanishi, K., Superflexible Multifunctional Polyvinylpolydimethylsiloxane-Based Aerogels as Efficient Absorbents, Thermal Superinsulators, and Strain Sensors, *Angew. Chem. Int. Ed.*, **57,** 9722-9727 (2018).

Sasabe, H.; Sato, R.; Suzuki, K.; Watanabe, Y.; Adachi, C.; Kaji, H.; Kido, J., Ultrahigh Power Efficiency Thermally Activated Delayed Fluorescent OLEDs by the Strategic Use of Electron-Transport Materials, *Adv. Optical Mater.*, **6,** [1800376-1]-[1800376-5] (2018).

Toda, A.; Taguchi, K.; Nozaki, K.; Fukushima, T.; Kaji, H., Superheated Melting Kinetics of Metastable Chain-Folded Polymer Crystals, *Cryst. Growth Des.*, **18,** 2602-2608 (2018).

Toda, A.; Yamamura, R.; Taguchi, K.; Fukushima, T.; Kaji, H., Kinetics of "Melting" of Sucrose Crystals, *Cryst. Growth Des.*, **18,** 3637-3643 (2018).

Zu, G. Q.; Kanamori, K.; Shimizu, T.; Zhu, Y.; Maeno, A.; Kaji, H.; Nakanishi, K.; Shen, J., Versatile Double-Cross-Linking Approach to Transparent, Machinable, Supercompressible, Highly Bendable Aerogel Thermal Superinsulators, *Chem. Mater.*, **30,** 2759-2770 (2018).

Osada, K.; Goushi, K.; Kaji, H.; Adachi, C.; Ishii, H.; Noguchi, Y., Observation of Spontaneous Orientation Polarization in Evaporated Films of Organic Light-Emitting Diode Materials, *Org. Electron.*, **58,** 313-317 (2018).

Suzuki, F.; Kubo, S.; Fukushima, T.; Kaji, H., Effects of Structural and Energetic Disorders on Charge Transports in Crystal and Amorphous Organic Layers, *Sci. Rep.*, **8,** [5203-1]-[5203-9] (2018).

Wada, Y.; Kubo, S.; Kaji, H., Adamantyl Substitution Strategy for Realizing Solution-Processable Thermally Stable Deep-Blue Thermally Activated Delayed Fluorescence Materials, *Adv. Mater.*, **30,** [1705641-1]-[1705641-8] (2018).

Zhang, D. D.; Song, X. Z.; Cai, M. H.; Kaji, H.; Duan, L., Versatile Indolocarbazole-Isomer Derivatives as Highly Emissive Emitters and Ideal Hosts for Thermally Activated Delayed Fluorescent OLEDs with Alleviated Efficiency Roll-Off, *Adv. Mater.*, **30,** [1705406-1]-[1705406-10] (2018).

Zu, G. Q.; Shimizu, T.; Kanamori, K.; Zhu, Y.; Maeno, A.; Kaji, H.; Shen, J.; Nakanishi, K., Transparent, Superflexible Doubly Cross-Linked Polyvinylpolymethylsiloxane Aerogel Superinsulators via Ambient Pressure Drying, *ACS Nano*, **12,** 521-532 (2018).

— Hydrospheric Environment Analytical Chemistry —

Yang, L.; Nadeau, K.; Meija, J.; Grinberg, P.; Pagliano, E.; Ardini, F.; Grotti, M.; Schlosser, C.; Streu, P.; Achterberg, E. P.; Sohrin, Y.; Minami, T.; Zheng, L.; Wu, J.; Chen, G.; Ellwood, M. J.; Turetta, C.; Aguilar-Islas, A.; Rember, R.; Sarthou, G.; Tonnard, M.; Planquette, H.; Matoušek, T.; Crum, S.; Mester, Z., Inter-Laboratory Study for the Certification of Trace Elements in Seawater Certified Reference Materials NASS-7 and CASS-6, *Anal. Bioanal. Chem.*, **410,** 4469-4479 (2018).

Yang, S.-C.; Zhang, J.; Sohrin, Y.; Ho, T.-Y., Cadmium Cycling in the Water Column of the Kuroshio-Oyashio Extension Region: Insights from Dissolved and Particulate Isotopic Composition, *Geochim. Cosmochim. Acta*, **233,** 66-80 (2018).

Umetani, S.; Sasaki, Y.; Sohrin, Y.; Mukai, H.; Yamazaki, S., Mutual Extraction Separation of Al, Ga, In and Zn with Trifluoroacetylcycloalkanones and β-Diketones, *Bunseki Kagaku*, **66,** 817-824 (2017) (in Japanese).

[Others]

Takano, S., Development of the Method for Precise Isotopic Analysis of Copper in Seawater, *Transactions of the Research Institute of Oceanochemistry*, **31,** 2-9 (2018) (in Japanese).

Zheng, L., Development of Quantitative Method of Bioactive Trace Metals (Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb) in Seawater and Its Application to the North Pacific Ocean, *Transactions of the Research Institute of Oceanochemistry*, **31,** 54-59 (2018) (in Japanese).

— Chemistry for Functionalized Surfaces —

Shioya, N.; Hada, M.; Shimoaka, T.; Murdey, R.; Eda, K.; Hasegawa, T., Impact of Kinetically Restricted Structure on Thermal Conversion of Zinc Tetraphenylporphyrin Thin Films to the Triclinic and Monoclinic Phases, *J. Phys. Chem. C*, **122,** 4540-4545 (2018).

Tomita, K.; Shioya, N.; Kise, R.; Shimoaka, T.; Yoshida, H.; Koganezawa, T.; Eda, K.; Hasegawa, T., Structure Control of a Zinc Tetraphenylporphyrin Thin Film by Vapor Annealing Using Fluorine Containing Solvent, *Thin Solid Films*, **665,** 85-90 (2018).

Shimoaka, T.; Ukai, H.; Kurishima, K.; Takei, K.; Yamada, N.; Hasegawa, T., Molecular Aggregation of Perfluoroalkyl Groups Can Win the Hydrogen Bonding between Amides, *J. Phys. Chem. C*, **122,** 22018-22023 (2018).

Isozaki, K.; Shimoaka, T.; Oshiro, S.; Yamaguchi, A.; Pincella, F.; Ueno, R.; Hasegawa, T.; Watanabe, T.; Takaya, H.; Nakamura, M., Robust Surface Plasmon Resonance Chips for Repetitive and Accurate Analysis of Lignin–Peptide Interactions, *ACS Omega*, **3,** 7483-7493 (2018).

Matsubara, T.; Yasumori, H.; Ito, K.; Shimoaka, T.; Hasegawa, T.; Sato, T., Amyloid-β Fibrils Assembled on Ganglioside-Enriched Membranes Contain Both Parallel β-Sheets and Turns, *J. Biol. Chem.*, **293,** 14146-14154 (2018).

Tokunaga, A.; Mutoh, K.; Hasegawa, T.; Abe, J., Reversible Valence Photoisomerization between Closed-Shell Quinoidal and Open-Shell Biradical Form, *J. Phys. Chem. Lett.*, **9,** 1833-1837 (2018).

— Molecular Microbial Science —

Ogawa, T.; Tanaka, A.; Kawamoto, J.; Kurihara, T., Purification and Characterization of 1-Acyl-*sn*-glycerol-3-phosphate Acyltransferase with a Substrate Preference for Polyunsaturated Fatty Acyl Donors from the Eicosapentaenoic Acid-producing Bacterium *Shewanella livingstonensis* Ac10, *J. Biochem.*, **164,** 33-39 (2018).

Toyotake, Y.; Cho, H. N.; Kawamoto, J.; Kurihara, T., A Novel 1-Acyl-*sn*-glycerol-3-phosphate *O*-Acyltransferase Homolog for the Synthesis of Membrane Phospholipids with a Branched-Chain Fatty Acyl Group in *Shewanella livingstonensis* Ac10, *Biochem. Biophys. Res. Commun.*, **500,** 704-709 (2018).

Suito, T.; Nagao, K.; Hatano, M.; Kohashi, K.; Tanabe, A.; Ozaki, H.; Kawamoto, J.; Kurihara, T.; Mioka, T.; Tanaka, K.; Hara, Y.; Umeda, M., Synthesis of Omega-3 Long-Chain Polyunsaturated Fatty Acid-Rich Triacylglycerols in an Endemic Goby, *Gymnogobius isaza*, from Lake Biwa, Japan, *J. Biochem.*, **164,** 127-140 (2018).

Sato, S. B.; Sugiura, M.; Kurihara, T., Dimer-Monomer Equilibrium of Human HSP27 Is Influenced by the In-Cell Macromolecular Crowding Environment and Is Controlled by Fatty Acids and Heat, *Biochem. Biophys. Acta Proteins Proteom.*, **1866,** 692-701 (2018).

[Others]

Kurihara, T., Organization and Functionalization of Biological Membranes: From the Studies on Unsaturated Fatty Acids, *CSJ Current Rev.*, **30,** 50-55 (2018) (in Japanese).

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

— Polymer Materials Science —

Hattori, G.; Takenaka, M.; Sawamoto, M.; Terashima, T., Nanostructured Materials via the Pendant Self-Assembly of Amphiphilic Crystalline Random Copolymers, *Journal of the American Chemical Society*, **27,** 8376-8379 (2018).

Azuma, T.; Seino, Y.; Sato, H.; Kasahara, Y.; Kodera, K.; Miyagi, K.; Shiraishi, M.; Matsuki, R.; Kosaka, T.; Himi, T.; Nagahara, S.; Chandra, A.; Nakatani, R.; Hayakawa, T.; Yoshimoto, K.; Omosu, T.; Takenaka, M., Defect Dynamics in Directed Self-Assembly of Block Copolymers, *Advances in Patterning Materials and Processes XXXV*, **10586,** 105860S (2018).

Ogura, Y.; Takenaka, M.; Sawamoto, M.; Terashima, T., Fluorous Gradient Copolymers via in-Situ Transesterification of a Perfluoromethacrylate in Tandem Living Radical Polymerization: Precision Synthesis and Physical Properties, *Macromolecules*, **51,** 864-871 (2018).

Shimokita, K.; Saito, I.; Yamamoto, K.; Takenaka, M.; Yamada, L. N.; Miyazaki, T., Effect of Preferential Orientation of Lamellae in the Interfacial Region between a Block Copolymer-Based Pressure-Sensitive Adhesive and a Solid Substrate on the Peel Strength, *Langmuir*, **34,** 2856-2864 (2018).

Nakanishi, Y.; Ishige, R.; Ogawa, H.; Sakakibara, K.; Ohno, K.; Morinaga, T.; Sato, T.; Kanaya, T.; Tsujii, Y., USAXS Analysis of Concentration-Dependent Self-Assembling of Polymer-Brush-modified Nanoparticles in Ionic Liquid: [I] Concentrated-Brush Regime, *J. Chem. Phys.*, **148, [**124902-1]-[124902-9] (2018).

Miyazaki, T.; Shimokita, K.; Ogawa, H.; Yamamoto, K., System for in situ Observation of Three-Dimensional Structural Changes in Polymer Films during Uniaxial Deformation. Corrigendum, *J. Appl. Cryst.*, **48,** 1016-1022 (2018).

Ogawa, H.; Takenaka, M.; Miyazaki, T.; Kanaya, T., Order-order Transition Processes of Thin-film Symmetric and Asymmetric PS-*b*-P2VP during Spin Coating, *Macromolecules*, **51,** 10040-10051 (2018).

— Molecular Rheology —

Mongcopa, K. I. S.; Tyagi, M.; Mailoa, J. P.; Samsonidze, G.; Kozinsky, B.; Mullin, S. A.; Gribble, D. A.; Watanabe, H.; Balsara, N. P., Relationship between Segmental Dynamics Measured by Quasi-Elastic Neutron Scattering and Conductivity in Polymer Electrolytes, *ACS Macro Lett.*, **7,** 504-508 (2018).

Wu, S.; Cao, X.; Zhang, Z.; Chen, Q.; Matsumiya, Y.; Watanabe, H., Molecular Design of Highly Stretchable Ionomers, *Macromolecules*, **51,** 4735-4746 (2018).

Watanabe, H.; Matsumiya, Y.; Kwon, Y., Viscoelastic and Dielectric Relaxation of Reptating Type-A Chains Affected by Reversible Head-to-Head Association and Dissociation, *Macromolecules*, **51,** 6476-6496 (2018).

Matsumiya, Y.; Watanabe, H.; Masubuchi, Y.; Huang, Q.; Hassager, O., Nonlinear Elongational Rheology of Non-Entangled Polystyrene and Poly(p-tert-butylstyrene) Melts, *Macromolecules*, **51,** 9710-9729 (2018).

— Molecular Aggregation Analysis —

Lin, H.-A.; Mitoma, N.; Meng, L.; Segawa, Y.; Wakamiya, A.; Itami, K., Hole-Transporting Materials Based on Thiophene-Fused Arenes from Sulfur-Mediated Thienannulations, *Mater. Chem. Front.*, **2,** 275-280 (2018).

Yang, F.; Lim, H. E.; Wang, F.; Ozaki, M.; Shimazaki, A.; Liu, J.; Mohamed, N. B.; Shinokita, K.; Miyauchi, Y.; Wakamiya, A.; Murata, Y.; Matsuda, K., Roles of Polymer Layer in Enhanced Photovoltaic Performance of Perovskite Solar Cells via Interface Engineering, *Adv. Mater. Interfaces*, **5,** 1701256 (2018).

Tahara, H.; Aharen, T.; Wakamiya, A.; Kanemitsu, Y., Photorefractive Effect in Organic–Inorganic Hybrid Perovskites and Its Application to Optical Phase Shifter, *Adv. Opt. Mater.*, **6,** 1701366 (2018).

Murdey, R.; Katoh, K.; Yamashita, M.; Sato, N., Thermally Activated Electrical Conductivity of Thin Films of Bis(phthalocyaninato)terbium(III) Double Decker Complex, *Thin Solid Films*, **646,** 17-20 (2018).

Jung, M.; Lee, J.; Jung, H.; Kang, S.; Wakamiya, A.; Park, J., Highly Efficient Pyrene Blue Emitters for OLEDs Based on Substitution Position Effect, *Dyes and Pigments*, **158,** 42-49 (2018).

Handa, T.; Aharen, T.; Wakamiya, A.; Kanemitsu, Y., Radiative Recombination and Electron-Phonon Coupling in Lead-Free $CH_3NH_3SnI_3$ Perovskite Thin Films, *Phys. Rev. Mater.*, **2,** 75402 (2018).

Liu, M.; Endo, M.; Shimazaki, A.; Wakamiya, A.; Tachibana, Y., Identifying an Optimum Perovskite Solar Cell Structure by Kinetic Analysis: Planar, Mesoporous Based, or Extremely Thin Absorber Structure, *ACS Appl. Energy Mater.*, **8,** 3722-3732 (2018).

Yang, F.; Liu, J.; Lim, H.; Ishikura, Y.; Shinokita, K.; Miyauchi, Y.; Wakamiya, A.; Murata, Y.; Matsuda, K., High Bending Durability of Efficient Flexible Perovskite Solar Cells Using Metal Oxide Electron Transport Layer, *J. Phys. Chem. C*, **122,** 17088-17095 (2018).

Shimogawa, H.; Murata, Y.; Wakamiya, A., NIR-Absorbing Dye Based on BF_2-Bridged Azafulvene Dimer as a Strong Electron-Accepting Unit, *Org. Lett.*, **20,** 5135-5138 (2018).

Liu, J.; Ozaki, M.; Yakumaru, S.; Handa, T.; Nishikubo, R.; Kanemitsu, Y.; Saeki, A.; Murata, Y.; Murdey, R.; Wakamiya, A., Lead-Free Solar Cells Based on Tin Halide Perovskite Films with High Coverage and Improved Aggregation, *Angew. Chem. Int. Ed.*, **57,** 13221-13225 (2018).

Yang, D.-T.; Nakamura, T.; He, Z.; Wang, X.; Wakamiya, A.; Peng, T.; Wang, S., Doping Polycyclic Arenes with Nitrogen–Boron–Nitrogen (NBN) Units, *Org. Lett.*, **20,** 6741-6745 (2018).

Mitsudo, K.; Shigemori, K.; Mandai, H.; Wakamiya, A.; Suga, S., Synthesis and Properties of Dithieno-Fused 1,4-Azaborine Derivatives, *Org. Lett.*, **20,** 7336-7340 (2018).

Wakamiya, A., Materials Chemistry for Efficient Printable Perovskite Solar Cells, *Low Temperature and Materials Sciences (Kyoto University)*, **33,** 3-9 (2018) (in Japanese).

[Others]

Nakamura, T.; Wakamiya, A., Organic Semiconductors for Perovskite Solar Cells, *Gekkan Kagaku*, **73,** 68-69 (2018) (in Japanese).

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

— Particle Beam Science —

Iwashita, Y.; Terunuma, N., Design Study of PM Dipole for ILC Damping Ring, *IOP Conf. Series: Journal of Physics: Conf. Series*, **1067,** [022015-1]-[022015-4] (2018).

Iwashita, Y.; Miyawaki, E.; Takeuchi, Y.; Tongu, H., Compact H^+ ECR Ion Source with Pulse Gas Valve, *AIP Conf. Proc.*, **2011(1),** [030011-1]-[030011-3] (2018).

Iwashita, Y.; Fuwa, Y.; Ishida, T.; Kino, K., Magnified Neutron Imaging with Modulating Permanent Magnet Sextupole Lens, *Proc. Int. Conf. Neutron Optics (NOP2017)*, **22,** [011008-1]-[011008-7] (2018).

Katayama, R.; Mishima, K.; Yamashita, S.; Kitaguchi, M.; Yoshioka, T.; Seki, M.; Mitsuhashi, M.; Sugihara, M.; Hino, M.; Watanabe, E.; Tsuya, D.; Saito, M.; Yamada, N. L., Development of New Neutron Mirrors for Measuring the Neutron Electric Dipole Moment, *Proc. Int. Conf. Neutron Optics (NOP2017)*, **22,** [011009-1]-[011009-8] (2018).

Tsuchikawa, Y.; Abo, K.; Furuzawa, D.; Hirota, K.; Ichikawa, G.; Imajo, S.; Ito, I.; Iwashita, Y.; Kitaguchi, M.; Kiyanagi, Y.; Miwata, Y.; Sato, K.; Shimizu, H. M.; Takeshita, H.; Tsuchida, K.; Tsurita, Y.; Uritani, A.; Watanabe, K.; Yamagata, Y.; Yamazaki, A.; Yoshihashi, S., Construction of the 2nd Beamline of Nagoya University Accelerator-driven Neutron Source (NUANS), *Proc. Int. Conf. Neutron Optics (NOP2017)*, **22,** [011024-1]-[011024-4] (2018).

Mishima, K.; Awano, K.; Fuwa, Y.; Goto, F.; Haddock, C. C.; Hino, M.; Hirose, M.; Hirota, K.; Ieki, S.; Imajo, S.; Ino, T.; Iwashita, Y.; Katayama, R.; Kawahara, H.; Kitaguchi, M.; Kitahara, R.; Koga, J.; Morishita, A.; Nagae, T.; Nagakura, N.; Naganawa, N.; Oi, N.; Oide, H.; Otono, H.; Seki, Y.; Sekiba, D.; Shima, T.; Shimizu, H. M.; Snow, W. M.; Sumi, N.; Sumino, H.; Tada, S.; Taketani, K.; Tasaki, S.; Tomita, T.; Umemoto, A.; Yamada, T.; Yamashita, S.; Yokohashi, M.; Yoshioka, T., Fundamental Physics Activities with Pulsed Neutron at J-PARC(BL05), *Proc. Int. Conf. Neutron Optics (NOP2017)*, **22,** [011033-1]-[011033-9] (2018).

Imajo, S.; Iwashita, Y.; Mishima, K.; Kitaguchi, M.; Shimizu, H. M.; Ino, T.; Yamashita, S.; Hirota, K.; Goto, F.; Fuwa, Y.; Katayama, R.; NOP Collaboration, Ultracold Neutron Time Focusing Experiment with an Improved UCN Rebuncher at J-PRAC/MLF, *Proc. Int. Conf. Neutron Optics (NOP2017)*, **22,** [011038-1]-[011038-8] (2018).

[Others]

Iwashita, Y.; Hayakawa, T.; Kawamura, N.; Makimura, S.; Mishima, K.; Nomura, D.; Shimomura, K.; Yamamoto, S.; Yamazaki, T., Diversified Application of ILC, *Proc. of IPAC2018*, 502-504 (2018).

Ito, H.; Antoine, C. Z.; Four, A.; Hayano, H.; Kubo, T.; Saeki, T.; Ito, R.; Nagata, T.; Iwashita, Y.; Katayama, R.; Tongu, H.; Oikawa, H., Lower Critical Field Measurement System of Thin Film Superconductor, *Proc. of IPAC2018*, 3882-3884 (2018).

Ito, R.; Nagata, T.; Hayano, H.; Kubo, T.; Saeki, T.; Ito, T.; Iwashita, Y.; Katayama, R.; Oikawa, H., Development of Coating Technique for Superconducting Multilayered Structure, *Proc. of IPAC2018*, 4954-4956 (2018).

Kondo, Y.; Hasegawa, K.; Morishita, T.; Bae, S.; Choi, H.; Kim, B.; Ko, H. S.; Fukao, Y.; Futatsukawa, K.; Kawamura, N.; Mibe, T.; Miyake, Y.; Otani, M.; Shimomura, K.; Yamazaki, T.; Yoshida, M.; Hayashizaki, N.; Iijima, T.; Sue, Y.; Iinuma, H.; Nakazawa, Y.; Ishida, K.; Iwashita, Y.; Iwata, Y.; Kitamura, R.; Li, S.; Razuvaev, G. P.; Saito, N., Re-Acceleration of Ultra Cold Muon in J-PARC Muon Facility, *Proc. of IPAC2018*, 5041-5046 (2018).

Sawamura, M.; Hajima, R.; Saeki, T.; Iwashita, Y.; Tongu, H.; Nakamura, T.; Watanabe, N., Present Status of Superconducting Spoke Cavity Fabrication, *Proc. of the 15th Annual Meeting of Particle Accelerator Society of Japan*, 418-420 (2018) (in Japanese).

Nagata, T.; Ito, R.; Hayano, H.; Kubo, T.; Saeki, T.; Iwashita, Y.; Katayama, R.; Ito, H.; Oikawa, H., Development of Superconducting Multilayered Structure Using by Reactive Sputtering Method, *Proc. of the 15th Annual Meeting of Particle Accelerator Society of Japan*, 425-427 (2018) (in Japanese).

Ito, H.; Hayano, H.; Saeki, T.; Kubo, T.; Iwashita, Y.; Katayama, R.; Tongu, H.; Oikawa, H.; Ito, R.; Nagata, T., Lower Critical Field Measurement of Thin Film Superconductor Using Third Harmonic Method, *Proc. of the 15th Annual Meeting of Particle Accelerator Society of Japan*, 442-446 (2018) (in Japanese).

Fuwa, Y.; Iwashita, Y., High Speed Control of Cavity Input Coupling Using Quick Stub Tuner, *Proc. of the 15th Annual Meeting of Particle Accelerator Society of Japan*, 473-475 (2018) (in Japanese).

Nakazawa, Y.; Iinuma, H.; Iwashita, H.; Iwata, Y.; Otani, M.; Kawamura, N.; Mibe, T.; Yamazaki, T.; Yoshida, M.; Kitamura, R.; Yasuda, H.; Kondo, Y.; Hasegawa, K.; Morishita, T.; Saito, N.; Sue, Y.; Hayashizaki, N., Performance Test of Inter-digital H-mode Drift-tube Linac Prototype with Alternative Phase Focusing for Muon Linac, *Proc. of the 15th Annual Meeting of Particle Accelerator Society of Japan*, 904-908(2018) (in Japanese).

Takeuchi, Y.; Iwashita, Y.; Tongu, H., Development of Real-Time Mass Analysis System with Permanent Magnet for Ion Beam, *Proc. of IPAC2018*, 2236-2238 (2018).

Katayama, R.; Iwashita, Y.; Tongu, H.; Antoine, C. Z.; Four, A.; Hayano, H.; Kubo, T.; Saeki, T.; Ito, H.; Ito, R.; Nagata, T.; Oikawa, H., Evaluation of Superconducting Characteristics on the Thin-film Structure by NbN and Insulator Coatings on Pure Nb Substrate, *Proc. of IPAC2018*, 3653-3655 (2018).

Takeuchi, Y.; Tongu, H.; Iwashita, Y., Development of Real-Time Mass Analysis System with Permanent Magnet for Ion Beam, *Proc. of IPAC2018*, 2236-2238 (2018).

Katayama, R.; Iwashita, Y.; Tongu, H.; Hayano, H.; Kubo, T.; Saeki, T.; Ito, H.; Ito, R.; Nagata, T.; Oikawa, H., Evaluation of Superconducting Characteristics on the Multilayer Thin-film Structure Using the Third Harmonic Voltage Method, *Proc. of the 15th Annual Meeting of Particle Accelerator Society of Japan*, 27-30 (2018) (in Japanese).

Takeuchi, Y.; Tongu, H.; Iwashita, Y., Compact ECR H$^+$ Ion Source with Permanent Magnet, *Proc. of the 15th Annual Meeting of Particle Accelerator Society of Japan*, 404-407 (2018) (in Japanese).

Yako, T.; Iwashita, Y.; Terunuma, N.; Tongu, H.; Katayama, R.; Takeuchi, Y.; Abe, M.; Fuwa, Y., Design of Main Dipole Magnet Using Permanent Magnet for ILC Damping Ring, *Proceedings of the 15th Annual Meeting of Particle Accelerator Society of Japan*, 518-520 (2018) (in Japanese).

Abe, M.; Iwashita, Y.; Katayama, R.; Tongu, H.; Takeuchi, Y.; Yako, T.; Terunuma, N.; Fuwa, Y., Design of Correction Magnet with Permanent Magnet for Damping Ring, *Proceedings of the 15th Anuanl Meeting of Particle Acceleretor Society of Japan*, 534-536 (2018) (in Japanese).

Tongu, H.; Iwashita, Y., Development of Nondestructive Inspection Device for Superconducting Cavity, *Proceedings of the 15th Annual Meeting of Particle Accelerator Society of Japan*, 460-463 (2018) (in Japanese).

— Laser Matter Interaction Science —

Inoue, S.; Nakamiya, Y.; Teramoto, K.; Hashida, M.; Sakabe, S., Highly Intensified Emission of Laser-accelerated Electrons from a Foil Target through an Additional Rear Laser Plasma, *Phyiscal Review Accelerators and Beams*, **21,** 41302 (2018).

Teramoto, K.; Tokita, S.; Terao, T.; Inoue, S.; Yasuhara, R.; Nagashima, T.; Kojima, S.; Kawanaka, J.; Mori, K.; Hashida, M.; Sakabe, S., Half-cycle Terahertz Surface Waves with MV/cm Field Strengths Generated on Metal Wires, *Appl. Phys. Lett.*, **113,** 51101 (2018).

Teramoto, K.; Inoue, S.; Tokita, S.; Yasuhara, R.; Nakamiya, Y.; Nagashima, T.; Mori, K.; Hashida, M.; Sakabe, S., Induction of Subterahertz Surface Waves on a Metal Wire by Intense Laser Interaction with a Foil, *Phyis. Rev. E*, **97,** 23204 (2018).

Arikawa, Y.; Kato, Y.; Abe, Y.; Matsubara, S.; Kishimoto, H.; Nakajima, N.; Morace1, A.; Yogo, A.; Nishimura, H.; Nakai, M.; Fujioka, S.; Azechi, H.; Mima, K.; Inoue, S.; Nakamiya, Y.; Teramoto, K.; Hashida, M.; Sakabe, S., Efficient and Repetitive Neutron Generation by Double-laser-pulse Driven Photonuclear Reaction, *Plasma and Fusion Research*, **13,** 2404009 (2018).

— Electron Microscopy and Crystal Chemistry —

Haruta, M.; Fujiyoshi, Y.; Nemoto, T.; Ishizuka, A.; Ishizuka, K.; Kurata, H., Atomic-Resolution Two-Dimensional Mapping of Holes in the Cuprate Superconductor La$_{2-x}$Sr$_x$CuO$_{4\pm\delta}$, *Phys. Rev. B*, **97,** [205139-1]-[205139-5] (2018).

Yamaguchi, A.; Haruta, M.; Nemoto, T.; Kurata, H., Probing Directionality of Local Electronic Structure by Momentum-Selected STEM-EELS, *Appl. Phys. Lett.*, **113,** [053101-1]-[053101-4] (2018).

Fujiyoshi, Y.; Kurata, H., Surface Plasmon Resonances in a Branched Silver Nanorod, *J. Appl. Phys.*, **124,** [093103-1]-[093103-6] (2018).

Haruta, M.; Higuchi, H.; Nemoto, T.; Kurata, H., Local Quantification of Coordination Number for Perovskite-Related Oxides Using Atomic Resolution EELS Maps, *Appl. Phys. Lett.*, **113,** [083110-1]-[083110-5] (2018).

Lian, Z.; Sakamoto, M.; Kobayashi, Y.; Tamai, N.; Ma, J.; Sakurai, T.; Seki, S.; Nakagawa, T.; Lai, M.; Haruta, M.; Kurata, H.; Teranishi, T., Durian-Shaped CdS@ZnSe Core@Mesoporous-Shell Nanocrystals for Enhanced and Sustainable Photocatalytic Hydrogen Evolution, *J. Phys. Chem. Lett.*, **9,** 2212-2217 (2018).

Saruyama, M.; Kim, S.; Nishino, T.; Sakamoto, M.; Haruta, M.; Kurata, H.; Akiyama, S.; Yamada, T.; Domen, K.; Teranishi, T., Phase-Segregated NiP$_x$@FeP$_y$O$_z$ Core@Shell Nanoparticles: Ready-to-Use Nanocatalysts for Electro- and Photo-Catalytic Water Oxidation through in-situ Activation by Structural Transformation and Spontaneous Ligand Removal, *Chem. Sci.*, **9,** 4830-4836 (2018).

Lian, Z.; Sakamoto, M.; Matsunaga, H.; Vequizo, J. J. M.; Yamakata, A.; Haruta, M.; Kurata, H.; Teranishi, T., Near Infrared Light Induced Plasmonic Hot Hole Transfer at a Nano-Heterointerface, *Nat. Commun.*, **9,** [2314-1]-[2314-7] (2018).

Yoshida, K.; Toyoura, K.; Matsunaga, K.; Nakahira, A.; Kurata, H.; Ikuhara, Y. H.; Sasaki, Y., Structural Analyses of Sodium Cations Embedded within Zeolitic Nanocavities, *Microporous and Mesoporous Materials*, **259,** 195-202 (2018).

Shirai, K.; Fazio, G.; Sugimoto, T.; Selli, D.; Ferraro, L.; Watanabe, K.; Haruta, M.; Ohtani, B.; Kurata, H.; Valentin, C. D.; Matsumoto, Y., Water-Assisted Hole Trapping at the Highly Curved Surface of Nano-TiO_2 Photocatalyst, *J. Am. Chem. Soc.*, **140,** 1415-1422 (2018).

Shoji, S.; Ogawa, T.; Hashishin, T.; Tamiaki, H., Self-Assemblies of Zinc Bacteriochlorophyll-d Analogues Having Amide, Ester, and Urea Groups as Substituents at 17-Position and Observation of Lamellar Supramolecular Nanostructures, *ChemPhysChem*, **19,** 913-920 (2018).

Imura, Y.; Mori, T.; Morita-Imura, C.; Kataoka, H.; Akiyama, R.; Kurata, H.; Kawai, T., Preparation and Length Control of Water-Dispersible Ultrathin Gold and Silver Bimetallic Nanowires, *Colloids and Surfaces A*, **543,** 9-14 (2018).

— Atomic and Molecular Structures —

Ito, Y.; Tochio, A.; Vlaicu, H.; Yamashita, M.; Fukushima, S.; Polasik, M.; Slabkowska, K.; Syrocki, L.; Szymanska, E.; Rzadkiewicz, J.; Indelicato, P.; Marques, J. P.; Martins, M. C.; Santos, J. P.; Parente, F., Structure of High-resolution $K\beta_{1,3}$ X-ray Emission Spectra for the Elements from Ca to Ge, *Phys. Rev.*, **A97,** [052505-1]-[052505-10] (2018).

Menesguen, Y.; Lepy, M.-C.; Honicke, P.; Muller, M.; Unterumsberger, R.; Beckoff, B.; Hoszowska, J.; Dousse, J.-Cl.; Blachucki, W.; Ito, Y.; Yamashita, M.; Fukushima, S., Experimental Determination of X-ray Atomic Fundamental Parameters of Nickel, *Metrologia*, **55,** 56 (2018).

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Synthetic Organotransformation —

Sugimoto, K.; Takaya, H.; Maekawa, M.; Kuroda-Sowa, T., Controlled Self-Assembly of a 2-D Sheet Coordination Polymer and Monomer Containing an Eight-Membered Cu_4I_4 Crown Motif, *Cryst. Growth Des.*, **18,** 571-575 (2018).

Hirano, M.; Sano, K.; Kanazawa, Y.; Komine, N.; Maeno, Z.; Mitsudome, T.; Takaya, H., Mechanistic Insights on Pd/ Cu-Catalyzed Dehydrogenative Coupling of Dimethyl Phthalate, *ACS Catal.*, **8,** 5827-5841 (2018).

Isozaki, K.; Shimoaka, T.; Oshiro, S.; Yamaguchi, A.; Pincella, F.; Ueno, R.; Hasegawa, T.; Watanabe, T.; Takaya, H.; Nakamura, M., Robust Surface Plasmon Resonance Chips for Repetitive and Accurate Analysis of Lignin–Peptide Interactions, *ACS Omega*, **3,** 7483-7493 (2018).

— Advanced Solid State Chemistry —

Xiong, P.; Denis Romero, F.; Hosaka, Y.; Guo, H.; Saito, T.; Chen, W.-T.; Chuang, Y.-C.; Sheu, H.-S.; McNally, G.; Attfield, J. P.; Shimakawa, Y., Charge Disproportionation in $Sr_{0.5}Bi_{0.5}FeO_3$ Containing Unusually High Valence $Fe^{3.5+}$, *Inorg. Chem.*, **57,** 843-848 (2018).

Arevalo-Lopez, A. M.; Hosaka, Y.; Guo, H.; Denis Romero, F.; Saito, T.; Attfield, J. P.; Shimakawa, Y., Spin Order in the Charge Disproportionated Phases of the *A*-site Layer Ordered Triple Perovskite $LaCa_2Fe_3O_9$, *Phys. Rev. B*, **97,** 24421 (2018).

Xiong, P.; Hosaka, Y.; Saito, T.; Shimakawa, Y., High Pressure Synthesis and Physical Properties of $Sr_{0.5-x}Ca_xBi_{0.5}FeO_3$, *J. Jpn. Soc. Powder Powder Metallurgy*, **65,** 269-273 (2018).

Kan, D.; Anada, M.; Wakabayashi, Y.; Tajiri, H.; Shimakawa, Y., Oxygen Octahedral Distortions in the Compressively Strained $SrRuO_3$ Epitaxial Thin Films, *J. Appl. Phys.*, **123,** 235303 (2018).

Denis Romero, F.; Xiong, P.; Amano Patino, M.; Saito, T.; Kayser, P.; Attfield, J. P.; Shimakawa, Y., Suppression of Sequential Charge Transitions in $Ca_{0.5}Bi_{0.5}FeO_3$ via B-Site Cobalt Substitution, *Chem. Mater.*, **30,** 5493-5499 (2018).

Kan, D.; Shimakawa, Y., Defect-Induced Anomalous Transverse Resistivity in an Itinerant Ferromagnetic Oxide, *Phys. Status Solidi B*, **255,** [1800175-1]-[1800175-6] (2018).

Tan, Z.; Saito, T.; Denis Romero, F.; Amano Patino, M.; Goto, M.; Chen, W.-T.; Chuang, Y.-C.; Sheu, H.-S.; Shimakawa, Y., Hexagonal Perovskite $Ba_4Fe_3NiO_{12}$ Containing Tetravalent Fe and Ni Ions, *Inorg. Chem.*, **57,** 10410-10415 (2018).

Shimakawa, Y.; Lufaso, M.; Woodward, P. M., Negative and Positive Thermal Expansion-like Volume Changes Due to Intermetallic Charge Transfer Based on an Ionic Crystal Model of Transition-metal Oxides, *APL Materials*, **6,** 086106 (2018).

[Others]

Kan, D.; Shimakawa, Y., Atomic Level Engineering of Structual and Functional Properties of Transition Metal Oxides (Memorial Lectuer of JSPM Award), *J. Jpn. Soc. Powder Powder Metallurgy*, **65,** 255-260 (2018) (in Japanese).

— Organometallic Chemistry —

Wakioka, M.; Yamashita, N.; Mori, H.; Nishihara, Y.; Ozawa, F., Synthesis of a 1,2-Dithienylethene-Containing Donor-Acceptor Polymer via Palladium-Catalyzed Direct Arylation Polymerization (DArP), *Molecules*, **23,** 981 (2018).

Wakioka, M.; Ozawa, F., Highly Efficient Catalysts for Direct Arylation Polymerization (DArP), *Asian J. Org. Chem.*, **7,** 1206-1216 (2018).

Taguchi, H.; Tanigawa, I.; Takeuchi, K.; Ozawa, F., On the Geometrical Stability of Square Planar Platinum(0) Complexes That Bear a PNP-Pincer-Type Phosphaalkene Ligand (Eind2-BPEP), *Chem. Eur. J.*, **24,** 17055-17061 (2018).

— Nanophotonics —

Kanemitsu, Y.; Okano, M.; Le, P. Q.; Yamada, Y., Review—Light Emission from Thin Film Solar Cell Materials: An Emerging Infrared and Visible Light Emitter, *ECS J. Solid State Sci. Technol.*, **7,** R3102-R3110 (2018).

Yamada, T.; Aharen, T.; Kanemitsu, Y., Near-band-edge Optical Responses of $CH_3NH_3PbCl_3$ Single Crystals: Photon Recycling of Excitonic Luminescence, *Phys. Rev. Lett.*, **120,** [057404-1]-[057404-6] (2018).

Yamaguchi, M.; Zhu, L.; Akiyama, H.; Kanemitsu, Y.; Tampo, H.; Shibata, H.; Lee, K.-H.; Araki, K.; Kojima, N., Analysis of Future Generation Solar Cells and Materials, *Jpn. J. Appl. Phys.*, **57,** [04FS03-1]-[04FS03-6] (2018).

Tahara, H.; Aharen, T.; Wakamiya, A.; Kanemitsu, Y., Photorefractive Effect in Organic-Inorganic Hybrid Perovskites and Its Application to Optical Phase Shifter, *Adv. Opt. Mater.*, **6,** [1701366-1]-[1701366-6] (2018).

Yumoto, G.; Tahara, H.; Kawawaki, T.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Hot Biexciton Effect on Optical Gain in $CsPbI_3$ Perovskite Nanocrystals, *J. Phys. Chem. Lett.*, **9,** 2222-2228 (2018).

Uchida, K.; Otobe, T.; Mochizuki, T.; Kim, C.; Yoshita, M.; Tanaka, K.; Akiyama, H.; Pfeiffer, L. N.; West, K. W.; Hirori, H., Coherent Detection of THz-induced Sideband Emission from Excitons in the Nonperturbative Regime, *Phys. Rev. B*, **97,** [165122-1]-[165122-7] (2018).

Handa, T.; Aharen, T.; Wakamiya, A.; Kanemitsu, Y., Radiative Recombination and Electron-Phonon Coupling in Lead-free $CH_3NH_3SnI_3$ Perovskite Thin Films, *Phys. Rev. Mater.*, **2,** [075402-1]-[075402-9] (2018).

Zhu, L.; Akiyama, H.; Kanemitsu, Y., Intrinsic and Extrinsic Drops in Open-circuit Voltage and Conversion Efficiency in Solar Cells with Quantum Dots Embedded in Host Materials, *Sci. Rep.*, **8,** [11704-1]-[11704-12] (2018).

Tahara, H.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Quantum Coherence of Multiple Excitons Governs Absorption Cross-sections of PbS/CdS Core/shell Nanocrystals, *Nat. Commun.*, **9,** [3179-1]-[3179-8] (2018).

Kanemitsu, Y.; Handa, T., Photophysics of Metal Halide Perovskites: from Materials to Devices, *Jpn. J. Appl. Phys.*, **57,** [090101-1]-[090101-17] (2018).

Liu, J.; Ozaki, M.; Yakumaru, S.; Handa, T.; Nishikubo, R.; Kanemitsu, Y.; Saeki, A.; Murata, Y.; Murdey, R.; Wakamiya, A., Lead-Free Solar Cells Based on Tin Halide Perovskite Films with High Coverage and Improved Aggregation, *Angew. Chem. Int. Ed.*, **57,** 13221-13225 (2018).

Wang, Y.; Harada, T.; Le, P. Q.; Kanemitsu, Y.; Nakano, T., Helix Induction to Polyfluorenes Using Circularly Polarized Light: Chirality Amplification, Phase-Selective Induction, and Anisotropic Emission, *Macromolecules*, **51,** 6865-6877 (2018).

Nakahara, S.; Tahara, H.; Yumoto, G.; Kawawaki, T.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Suppression of Trion Formation in $CsPbBr_3$ Perovskite Nanocrystals by Postsynthetic Surface Modification, *J. Phys. Chem. C*, **122,** 22188-22193 (2018).

Nagai, M.; Tomioka, T.; Ashida, M.; Hoyano, M.; Akashi, R.; Yamada, Y.; Aharen, T., Longitudinal Optical Phonons Modified by Organic Molecular Cation Motions in Organic-inorganic Hybrid Perovskites, *Phys. Rev. Lett.*, **121,** [145506-1]-[145506-6] (2018).

Miyagawa, K.; Nagai, M.; Yamashita, G.; Ashida, M.; Kim, C.; Akiyama, H.; Kanemitsu, Y., Quantitative Monitoring of the Internal Field in the Depletion Layer of a GaAs-Based Solar Cell with Terahertz Radiation, *Appl. Phys. Lett.*, **113,** [163501-1]-[163501-4] (2018).

Sanari, Y.; Tachizaki, T.; Saito, Y.; Makino, K.; Fons, P.; Kolobov, A. V.; Tominaga, J.; Tanaka, K.; Kanemitsu, Y.; Hase, M.; Hirori, H., Zener Tunneling Breakdown in Phase-change Materials Revealed by Intense Terahertz Pulses, *Phys. Rev. Lett.*, **121,** [165702-1]-[165702-6] (2018).

Yarita, N.; Aharen, T.; Tahara, H.; Saruyama, M.; Kawawaki, T.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Observation of Positive and Negative Trions in Organic-Inorganic Hybrid Perovskite Nanocrystals, *Phys. Rev. Mater.*, **2,** [116003-1]-[116003-8] (2018).

[Others]

Tahara, H.; Handa, T.; Kanemitsu, Y., Photophysics of Organic-inorganic Hybrid Perovskite Solar Cells, *Proc. SPIE*, [1052702-1]-[1052702-10] (2018).

Handa, T.; Aharen, T.; Wakamiya, A.; Kanemitsu, Y., Photoelectronic Properties of Lead-free $CH_3NH_3SnI_3$ Perovskite Solar Cell Materials and Devices, *SPIE 10737, Organic, Hybrid, and Perovskite Photovoltaics XIX*, 107371X (2018).

BIOINFORMATICS CENTER
— Chemical Life Science —

Li, Y.; Hingamp, P.; Watai, H.; Endo, H.; Yoshida, T.; Ogata, H., Degenerate PCR Primers to Reveal the Diversity of Giant Viruses in Coastal Waters, *Viruses*, **10,** 496 (2018).

Endo, H.; Ogata, H.; Suzuki, K., Contrasting Biogeography and Diversity Patterns between Diatoms and Haptophytes in the Central Pacific Ocean, *Sci. Rep.*, **8,** 10916 (2018).

Mihara, T.; Koyano, H.; Hingamp, P.; Grimsley, N.; Goto, S.; Ogata, H., Taxon Richness of “Megaviridae” Exceeds Those of Bacteria and Archaea in the Ocean, *Microbes Environ.*, **33,** 162-171 (2018).

Yoshida, T.; Nishimura, Y.; Watai, H.; Haruki, N.; Morimoto, D.; Kaneko, H.; Honda, T.; Yamamoto, K.; Hingamp, P.; Sako, Y.; Goto, S.; Ogata, H., Locality and Diel Cycling of Viral Production Revealed by a 24 h Time Course Cross-Omics Analysis in a Coastal Region of Japan, *ISME J.*, **12,** 1287-1295 (2018).

Yoshikawa, G.; Askora, A.; Blanc-Mathieu, R.; Kawasaki, T.; Li, Y.; Nakano, M.; Ogata, H.; Yamada, T., Xanthomonas Citri Jumbo Phage XacN1 Exhibits a Wide Host Range and High Complement of tRNA Genes, *Sci. Rep.*, **8,** 4486 (2018).

Nishiyama, H.; Nagai, T.; Kudo, M.; Okazaki, Y.; Azuma, Y.; Watanabe, T.; Goto, S.; Ogata, H.; Sakurai, T., Supplementation of Pancreatic Digestive Enzymes Alters the Composition of Intestinal Microbiota in Mice, *Biochem. Biophys. Res. Commun.*, **495,** 273-279 (2018).

Ogata, H., Habitat Alterations by Viruses: Strategies by Tupanviruses and Others, *Microbes Environ.*, **33,** 117-119 (2018).

Arai, W.; Taniguchi, T.; Goto, S.; Moriya, Y.; Uehara, H.; Takemoto, K.; Ogata, H.; Takami, H., MAPLE 2.3.0: An Improved System for Evaluating the Functionomes of Genomes and Metagenomes, *Biosci. Biotechnol. Biochem.*, **9,** 1515-1517 (2018).

Carradec, Q.; Pelletier, E.; Da Silva, C.; Alberti, A.; Seeleuthner, Y.; Blanc-Mathieu, R.; Lima-Mendez, G.; Rocha, F.; Tirichine, L.; Labadie, K.; Kirilovsky, A.; Bertrand, A.; Engelen, S.; Madoui, M.-A.; Meheust, R.; Poulain, J.; Romac, S.; Richter, D.; Yoshikawa, G.; Dimier, C.; Kandels-Lewis, S.; Picheral, M.; Searson, S.; Tara Oceans Coordinators; Jaillon, O.; Aury, J.-M.; Karsenti, E.; Sullivan, M. B.; Sunagawa, S.; Bork, P.; Not, F.; Hingamp, P.; Raes, J.; Guidi, L.; Ogata, H.; de Vargas, C.; Iudicone, D.; Bowler, C.; Wincker, P., A Global Ocean Atlas of Eukaryotic Genes, *Nat. Commun.*, **9,** 373 (2018).

Seeleuthner, Y.; Mondy, S.; Lombard, V.; Carradec, Q.; Pelletier, E.; Wessner, M.; Leconte, J.; Mangot, J. F.; Poulain, J.; Labadie, K.; Logares, R.; Sunagawa, S.; de Berardinis, V.; Salanoubat, M.; Dimier, C.; Kandels-Lewis, S.; Picheral, M.; Searson, S.; Tara Oceans Coordinators; Pesant, S.; Poulton, N.; Stepanauskas, R.; Bork, P.; Bowler, C.; Hingamp, P.; Sullivan, M. B.; Iudicone, D.; Massana, R.; Aury, J. M.; Henrissat, B.; Karsenti, E.; Jaillon, O.; Sieracki, M.; de Vargas, C.; Wincker, P., Single-cell Genomics of Multiple Uncultured Stramenopiles Reveals Underestimated Functional Diversity across Oceans, *Nat. Commun.*, **9,** 310 (2018).

— Mathematical Bioinformatics —

Akutsu, T.; Jansson, J.; Li, R.; Takasu, A.; Tamura, T., New and Improved Algorithms for Unordered Tree Inclusion, *Proc. 29th Int. Symp. Algorithms and Computation*, [27-1]-[27-12] (2018).

Akutsu, T.; de la Higuera, C.; Tamura, T., A Simple Linear-time Algorithm for Computing the Centroid and Canonical Form of a Plane Graph and Its Applications, *Proc. Annual Symposium on Combinatorial Pattern Matching*, [10-1]-[10-12] (2018).

Hayashida, M.; Koyano, H.; Akutsu, T., Grammar-based Compression for Directed and Undirected Generalized Series-parallel Graphs Using Integer Linear Programming, *Proc. 11th Int. Conf. Biomedical Engineering Systems and Technologies (BIOSTEC 2018)*, **3,** 105-111 (2018).

Song, J.; Li, F.; Takemoto, K.; Haffari, G.; Akutsu, T.; Chou, K.-C.; Webb, G. I., PREvaIL, an Integrative Approach for Inferring Catalytic Residues Using Sequence, Structural, and Network Features in a Machine-learning Framework, *Journal of Theoretical Biology*, **443,** 125-137 (2018).

Wang, J.; Yang, B.; Leier, A.; Marquez-Lago, T. T.; Hayashida, M.; Rocker, A.; Zhang, Y.; Akutsu, T.; Chou, K.-C.; Strugnell, R. A.; Song, J.; Lithgow, T., Bastion6: A Bioinformatics Approach for Accurate Prediction of Type VI Secreted Effectors, *Bioinformatics*, **34,** 2546-2555 (2018).

Bao, Y.; Hayashida, M.; Liu, P.; Ishitsuka, M.; Nacher, J. C.; Akutsu, T., Analysis of Critical and Redundant Vertices in Controlling Directed Complex Networks Using Feedback Vertex Sets, *J. Comput. Biol.*, **25,** 1071-1090 (2018).

Mori, T.; Ngouv, H.; Hayashida, M.; Akutsu, T.; Nacher, J. C., ncRNA-disease Association Prediction Based on Sequence Information and Tripartite Network, *BMC Systems Biology*, **12(S1),** [37-1]-[37-11] (2018).

Nakajima, N.; Hayashida, M.; Jansson, J.; Maruyama, O.; Akutsu, T., Determining the Minimum Number of Protein-protein Interactions Required to Support Known Protein Complexes, *PLoS ONE*, **13,** [e0195545-1]-[e0195545-17] (2018).

Li, J.; Nagamochi, H.; Akutsu, T., Enumerating Substituted Benzene Isomers of Tree-Like Chemical Graphs, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **15,** 633-646 (2018).

Melkman, A. A.; Cheng, X.; Ching, W. K.; Akutsu, T., Identifying a Probabilistic Boolean Threshold Network from Samples, *IEEE Transactions on Neural Networks and Learning Systems*, **29,** 869-881 (2018).

Ruan, P.; Hayashida, M.; Akutsu, T.; Vert, J.-P., Improving Prediction of Heterodimeric Protein Complexes Using Combination with Pairwise Kernel, *BMC Bioinformatics*, **19(S1),** 73-84 (2018).

Song, J.; Li, F.; Leier, A.; Marquez-Lago, T. T.; Akutsu, T.; Haffari, G.; Chou, K.-C.; Webb, G. I.; Pike, R. N., PROSPERous: High-throughput Prediction of Substrate Cleavage Sites for 90 Proteases with Improved Accuracy, *Bioinformatics*, **34,** 684-687 (2018).

Liu, L.; Mori, T.; Zhao, Y.; Hayashida, M.; Akutsu, T., Euler String-based Compression of Tree-structured Data and Its Application to Analysis of RNAs, *Current Bioinformatics*, **13,** 25-33 (2018).

Tamura, T.; Lu, W.; Song, J.; Akutsu, T., Computing Minimum Reaction Modifications in a Boolean Metabolic Network, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **15,** 1853-1862 (2018).

Tamura, T., Grid-based Computational Methods for the Design of Constraint-based Parsimonious Chemical Reaction Networks to Simulate Metabolite Production: GridProd, *BMC Bioinformatics*, **19(1),** 325 (2018).

[Others]

Akutsu, T., Algorithms for Analysis, Inference, and Control of Boolean Networks, *World Scientific* (2018).

Akutsu, T., Algorithms for Analysis and Control of Boolean Networks, *Lecture Notes in Computer Science*, **10849,** 3-7 (2018).

— Bio-knowledge Engineering —

Wimalawarne, K.; Mamitsuka, H., Efficient Convex Completion of Coupled Tensors Using Coupled Nuclear Norms, *Proceedings of the Thirty-second Conference on Neural Information Processing Systems (NIPS 2018)*, 6902-6910 (2018).

Wimalawarne, K.; Yamada, M.; Mamitsuka, H., Convex Coupled Matrix and Tensor Completion, *Neural Computation*, **30(11),** 3095-3127 (2018).

Nguyen, D. H.; Nguyen, C. H.; Mamitsuka, H., SIMPLE: Sparse Interaction Model over Peaks of MoLEcules for Fast, Interpretable Metabolite Identification from Tandem Mass Spectra, *Bioinformatics*, **34(13),** i323-i332 (2018).

You, R.; Zhang, Z.; Xiong, Y.; Sun, F.; Mamitsuka, H.; Zhu, S., GOLabeler: Improving Sequence-Based Large-scale Protein Function Prediction by Learning to Rank, *Bioinformatics*, **34(14),** 2465-2473 (2018).

Mamitsuka, H., Data Mining for Systems Biology: Methods and Protocols (2nd Edition), *Methods Mol. Biol.*, **1807,** (2018).

Takahashi, K.; duVerle, D. A.; Yotsukura, S.; Takigawa, I.; Mamitsuka, H., SiBIC: A Tool for Generating a Network of Biclusters Captured by Maximal Frequent Itemset Mining, *Methods Mol. Biol.*, **1807,** 95-111 (2018).

Deng, J.; Yuan, Q.; Mamitsuka, H.; Zhu, S., DrugE-Rank: Predicting Drug-Target Interactions by Learning to Rank, *Methods Mol. Biol.*, **1807,** 195-202 (2018).

Peng, S.; Mamitsuka, H.; Zhu, S., MeSHLabeler and DeepMeSH: Recent Progress in Large-Scale MeSH Indexing, *Methods Mol. Biol.*, **1807,** 203-209 (2018).

Karasuyama, M.; Mamitsuka, H., Factor Analysis on a Graph, *Proceedings of Machine Learning Research (Proceedings of the 21st International Conference on Artificial Intelligence and Statistics (AISTATS 2018))*, **84,** 1117-1126 (2018).

Yamada, M.; Tang, J.; Lugo-Martinez, J.; Hodzic, E.; Shrestha, R.; Saha, A.; Ouyang, H.; Yin, D.; Mamitsuka, H.; Sahinalp, C.; Radivojac, P.; Menczer, F.; Chang, Y., Ultra High-Dimensional Nonlinear Feature Selection for Big Biological Data, *IEEE Transactions on Knowledge and Data Engineering*, **30(7),** 1352-1365 (2018).

Junning, G.; Shuwei, Y.; Mamitsuka, H.; Zhu, S., AiProAnnotator: Low-Rank Approximation with Network Side Information for High-performance, Large-scale Human Protein Abnormality Annotator, *Proceedings of the 2018 IEEE International Conference on Bioinformatics and Biomedicine (BIBM 2018)*, 13-20 (2018).

[Others]

Mamitsuka, H., Textbook of Machine Learning and Data Mining (with Bioinformatics Applications) (2018).

INTERNATIONAL RESEARCH COLLABORATIONS

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

RMIT University, School of Engineering

[Canada]
Queen’s University, Department of Chemical Engineering

Queen’s University, Department of Chemistry

[China, P.R.]
Beijing Institute of Technology of China, Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials, Materials, School of Chemistry and Chemical Engineering

Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, State Key Laboratory of Polymer Physics and Chemistry

Fudan University, Center for Computational System Biology, ISTBI

Fudan University, School of Computer Science and Shanghai Key Lab of Intelligent Information Processing

Nankai University, College of Chemistry

Peking University, School of Life Science

Shenzhen University, College of Chemistry Environmental Engineering

Sun Yat-sen University, Institute for Solar Energy Systems

The Chinese University of Hong Kong, Department of Chemistry

The University of Hong Kong, Department of Mathematics

Xi’an Jiaotong University, School of Mathematics and Statistics

[Denmark]
Technical University of Denmark, Department of Chemical and Biochemical Engineering

[France]
CEA-Saclay, Service of Accelerators, Cryogenics and Magnetism

Centre National de la Recherche Scientifique

Ecole Centrale de Nantes, Institut de Recherche en Génie Civil et Mécanique (GeM)

Laboratoire National Henri Becquerel (LNHB)

Sorbonne University, Laboratoire Kastler Brossel

Université de Lyon

Université de Nantes, Department of Computer Science

Université de Rennes, Sciences Chimiques de Rennes

[Germany]
European Molecular Biology Laboratory

University of Bonn, Institute for Inorganic Chemistry

[Israel]
Ben-Gurion University of the Negev, Department of Computer Science

[Italy]
Università di Milano Bicocca, Dipartimento di Scienza dei Materiali

[Korea, R.]
Kyung Hee University, Department of Chemical Engineering

Sungkyunkwan University, School of Chemical Engineering

The Catholic University of Korea, Department of Chemistry

[Norway]
Bergen University, Department of Biology

[Poland]
Nicolaus Copernicus University, Faculty of Chemistry

[Portugal]
Laboratoira de Instrumentacao e Fisica Experimental de Particulas

Universidade de Lisboa, Faculdade de Ciencias

Universidade Nova de Lisboa, Fauldade de Ciencias e Tecnologia

[Romania]
National Institute of Materials Physics

[Singapore]
Nanyang Technological University, Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences

[Spain]
Universidad Complutense, Departamento de Química Inorgánica, Facultad de C.C. Químicas

[Thailand]
Chulalongkorn University, Department of Chemical Technology, Faculty of Science

[Tiwan]
National Chiao Tung University, Institute of Bioinformatics and Systems Biology

[U.K.]
The University of Edinburgh, Centre for Science at Extreme Conditions and School of Chemistry

[U.S.A.]
Brown University, Department of Chemistry

Department of Electrical Engineering, Princeton University

DOE Joint Genome Institute

Harvard University, John A. Paulson School of Engineering and Applied Sciences

Lawrence Berkeley National Laboratory, Joint Center for Energy Storage Research

Lawrence Berkeley National Laboratory, Materials Science Division

National Institute of Standards and Technology Center for Neutron Research

Robert Bosch LLC, Research and Technology Center

Seeo Inc.

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

University of California, Berkeley, Department of Chemical and Biomolecular Engineering

University of Maryland, 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.
Synthesis of Heavier Group 14 Element Analogues of Phenyl Anion and Their Properties
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2019

Mizuhata, Y.
Synthesis of Novel Conjugated Molecules Utilizing Phenyl Anions as Building Blocks
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2021

— Structural Organic Chemistry —

Hirose, T.
Synthesis of π-Extended Helical Aromatic Molecules towards Creation of Novel Molecular Functions with Chirality
Grant-in-Aid for Scientific Research (C)
1 April 2018–31 March 2021

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

Murata, Y.
Spherical π-Figuration Based on Functionalization of Sub-Nano Space
Grant-in-Aid for Scientific Research on Innovative Areas
1 April 2017–31 March 2019

Hashikawa, Y.
Nanostructure Control and Creation of Novel Functions on Three-Dimensional Pi-Conjugated Molecules Using Weak Interactions
Grant-in-Aid for Early-Career Scientists
1 April 2018–31 March 2020

— Synthetic Organic Chemistry —

Kawabata, T.
Regioselective Molecular Transformation of Multifunctionalized Molecules
Grant-in-Aid for Scientific Research (S)
1 April 2014–31 March 2019

Ueda, Y.
Synthesis of Glycoside-Based Middle Molecules via Sequential Site-Selective Functionalization
Grant-in-Aid for Scientific Research on Innovative Area “Middle Molecular Strategy: Creation of Higher Bio-Functional Molecules by Integrated Synthesis”
1 April 2018–31 March 2020

Ueda, Y.
Silyl-Group-Directed Site-Selective C-H Functionalization
Grant-in-Aid for Early-Career Scientists
1 April 2018–31 March 2020

DIVISION OF MATERIALS CHEMISTRY
— Chemistry of Polymer Materials —

Tsujii, Y.
Reinforcement of Resiliency of Concentrated Polymer Brushes and Its Tribological Applications – Development of Novel “Soft and Resilient Tribology (SRT)” System
ACCEL Program by JST
1 September 2015–31 March 2019

— Polymer Controlled Synthesis —

Yamago, S.
New Organic Chemistry and Material Science of Curved π-Conjugated Molecules
Grant-in-Aid for Scientific Research (S)
1 April 2016–31 May 2020

— Inorganic Photonics Materials —

Mizuochi, N.
High Sensitive and High Resolution Quantum Nano-sensor by Diamond
Grant-in-Aid for Scientific Research (A)
1 April 2016–31 March 2019

Mizuochi, N.
Innovative Magnetic Sensor Based on Nano-electronics of Carbon Materials
CREST (Core Research for Evolutional Science and Technology), JST
1 April 2014–31 March 2019

Abbreviations and acronyms

JST : Japan Science and Technology Agency
MEXT : Ministry of Education, Culture, Sports, Science and Technology
METI : Ministry of Economy, Trade and Industry
NEDO : New Energy and Industrial Technology Development Organization

Mizuochi, N.
Creation of Innovative Sensor System by Advanced Control of Solid Quantum Sensor
QLEAP (Flagship Program of Quantum Leap)
1 November 2018–31 March 2028

Mizuochi, N.
Creation of Energy Innovation Based on Innovative Semiconductor Technology that Holds the Key to Achieving Super Smart Society
OPERA (Program on Open Innovation Platform with Enterprises, Research Institute and Academia)
1 November 2018–31 March 2023

— Nanospintronics —

Ono, T.
Spin-Orbitronics and Device Application
New Research Projects under Specially Promoted Research
1 April 2015–31 March 2020

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

Futaki, S.
New Strategies for Intracellular Delivery of Biopharmaceuticals
Grant-in-Aid for Science Research (A)
1 April 2015–31 March 2018

Imanishi, M.
Construction of Strategies for Sequence Specific Epigenomic Manipulation
Grant-in-Aid for Science Research (B)
1 April 2016–31 March 2019

Kawano, K.
Elucidation of the Mechanism at the Influx Point Occurrence of Membrane Penetrating Peptide Using Artificial Lipid Raft
Grants-in-Aid for Young Scientists
1 April 2018–31 March 2020

— Molecular Biology —

Aoyama, T.
Plant Epidermal Cell Differebtiation Regulated by the Transcription Factor GL2
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2020

Aoyama, T.
Mechanism for Establishment of Planar Polarity in Plant Cell Morphogenesis
Grant-in-Aid for Scientific Research (C), Special Field
1 April 2016–31 March 2019

Fujiwara-Kato, M.
Elucidation of Phospholipid Signaling for Root Hair Elongation in Plants
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2019

— Chemical Biology —

Uesugi, M.
Control and Analysis of Cells by Synthetic Small Molecules
Grant-in-Aid for Scientific Research (S)
30 May 2014–31 March 2019

Uesugi, M.
Chemical Biological Exploration of New Functions of Endogenous Lipid-related Morecules
AMED-CREST
1 October 2014–31 March 2020

Uesugi, M.
Chemical Signals of Synthetic Nutrient Conjugates
Grant-in-Aid for Scientific Research on Innovative Areas
1 July 2017–31 March 2022

DIVISION OF ENVIRONMENTAL CHEMISTRY

— Molecular Materials Chemistry —

Kaji, H.
Fundamental Science of Organic Devices Based on Detailed Structural Analysis and Theoretical Chemistry
Grant-in-Aid for Scientific Research (A)
1 April 2017–31 March 2020

Shizu, K.
Density Form of Electronic Transitions and Its Applications to Electroluminescent Materials
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2019

— Hydrospheric Environment Analytical Chemistry —

Sohrin, Y.
Development of Heavy Metal Stable Isotope Marine Chemistry to Understand Marine Environment and Ecosystem
Grant-in-Aid for Scientific Research (A)
1 April 2015–31 March 2018

Takano, S.
Development of the Method for Multi-Element Isotope Ratio Analysis for the Study of Trace Metals in the Marine Environment
Grant-in-Aid for Young Scientists
1 April 2018–31 March 2020

— Chemistry for Functionalized Surfaces —

Hasegawa, T.
Development of ROA Imaging and Its Application to Visualization of Atropisomers for a Study of Fluoroorganic Chemistry
Grant-in-Aid for Scientific Research (A)
1 April 2015–31 March 2020

Shimoaka, T.
Molecular Interaction Analysis for Understanding Perfluoroalkyl Compound-Specific Properties
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2020

— Molecular Microbial Science —

Kurihara, T.
Mechanism of Biogenesis of Membrane Microdomain Containing Polyunsaturated Fatty Acids in Bacteria and Its Physiological Functions
Grant-in-Aid for Scientic Research (B)
1 April 2015–31 March 2018

Kurihara, T.
Exploration and Development of Cold-Adapted Microorganisms Useful in Low-Temperature Biotechnology for Chemical Production and Environmental Conservation
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Kurihara, T.
Diversity of Acyl Groups of Phospholipids in Bacterial Cell Membranes: Its Generation Mechanism and Physiological Significance
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2021

Kurihara, T.
Elucidation of the Mechanism of Extracellular Membrane Vesicle Production with a Novel Bacterium That Abundantly Produces Vesicles and Their Application
Grant-in-Aid for Challenging Research (Exploratory)
29 June 2018–31 March 2020

Kawamoto, J.
Development of a Membrane Protein Production System by Using Tailor-made Membrane Vesicles Synthesized by Extremophiles
Grant-in-Aid for Challenging Exploratory Research
1 April 2016–31 March 2018

Ogawa, T.
Enzymatic Analysis of Molecular Basis for *de novo* Synthesis of Phosphatidic Acid
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2019

DIVISION OF MULTIDISCIPLINARY CHEMISTRY
— Polymer Materials Science —

Takenaka, M.
Nano-Control Technologies for DSA Nano-Patterning
Nano Defect Management Project
1 July 2016–31 March 2018

Ogawa, H.
Development of Visualizing Method through Cooperative Small Angle X-ray Scattering Coupled with Computed Tomography (SAXS-CT) and Information Science
Strategic Basic Research Programs, PRESTO, JST
1 September 2016–31 March 2020

— Molecular Aggregation Analysis —

Wakamiya, A.
Development of Film Photovoltaics
COI STREAM (Center of Innovation Science and Technology Based Radical Innovation and Entrepreneurship Program), JST
1 April 2013–31 March 2021

Wakamiya, A.
High Performance Pb-Free Perovskite Solar Cells
ALCA (Advanced Low Carbon Technology Research and Development Program), JST
16 November 2016–31 March 2021

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE
— Laser Matter Interaction Science —

Sakabe, S.
Proof of Concept for Electron Optical System Using Intense Laser-driven Surface Wave
Grant-in-Aid for Scientific Research (A)
1 April 2016–31 March 2019

Hashida, M.
Stable Formation of Advanced Functionality on Metal Surface Produced by High Electric Field of Laser Pulse
Grant-in-Aid for Scientific Research (C)
1 April 2016–31 March 2019

Hashida, M.
Surface Structures on Solar Cells by Adavnced Laser Processing for Improving the Performance
The Amada Foundation AF-2018203-A3
1 October 2018–31 March 2022

Hashida, M.
Operand Measurement by Advanced Beams for the Nanostructure Formation Mechanism
Q-LEAP Flagship Program, Basic and Fundamental Research
1 November 2018–31 March 2028

Inoue, S.
Time-resolved Radiograph Measurement for Ultrafast Transient Electromagnetic Fields with Intense Laser-accelerated Short Pulse Electron
Grant-in-Aid for Scientific Research (C)
1 April 2018–31 March 2021

Kojima, S.
Anomalous Heating of High Dense Fusion Plasma with Crossing Fast Electron Beams
Grant-in-Aid for JSPS Research Fellow
26 April 2017–31 March 2020

Kojima, S.
Probing Ultrafast Motion of Critical Surface Pushed by Multi-pico-second Relativistic Radiation Pressure
Grant-in-Aid for Early-Career Scientists
1 April 2018–31 March 2020

— Electron Microscopy and Crystal Chemistry —

Kurata, H.
Advanced Characterization Nanotechnology Platform at Kyoto University
Nanotechnology Platform Project, MEXT
2 July 2012–31 March 2022

Kurata, H.
Development of Precise Spatially Resolved EELS and Analysis of Interfacial Electronic States
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Kurata, H.
State Analysis of Organic Nanomaterials by High-Resolution EELS
Grant-in-Aid for Challenging Exploratory Research
1 April 2016–31 March 2018

Haruta, M.
Electronic State Mapping Using Oxygen
Grant-in-Aid for Young Scientists (A)
1 April 2014–31 March 2018

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Synthetic Organotransformation —

Nakamura, M.
Development of Selective Woody Molecular Transformations for Forest Chemical Industry
Grant-in-Aid for Challenging Research (Exploratory)
29 June 2018–31 March 2020

Takaya, H.
Artificial Enzymes Base on Metalated Peptides
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Iwamoto, T.
Development of Novel Halogenation by Photocatalyst
Grant-in-Aid for Early-Career Scientists
1 April 2018–31 March 2020

— Advanced Solid State Chemistry —

Shimakawa, Y.
Solid-state Chemistry for Transition-metal Oxides: Exploring for New Materials with Novel Functionalities
JSPS Core-to-Core Program
1 April 2016–31 March 2020

— Nanophotonics —

Kanemitsu, Y.
Design of Next-generation Flexible Photonic Devices Based on Metal-halide Perovskites
CREST(Core Research for Evolutional Science and Technology), JST
1 October 2016–31 March 2022

Kanemitsu, Y.
Higher Harmonic Generation in Semiconductor Nanomaterials and Strong Electric Field Nonlinear Optics
Grant-in-Aid for Scientific Research (A)
1 April 2018–31 March 2021

BIOINFORMATICS CENTER

— Chemical Life Science —

Ogata, H.
Deciphering the Mechanisms of Virus-Host Co-Existence in Aquatic Environments
Grant-in-Aid for Scientific Research on Innovative Area “Neovirology, the Raison d’Etre of Viruses”
30 June 2016–31 March 2021

Ogata, H.
Probabilistic and Statistical Theory on Non-Abelian Topological Semigroup A* and Its Application to Environmental Microbiology and Bioengineering
Grant-in-Aid for Scientific Research (B)
19 July 2016–31 March 2019

Ogata, H.
Deep Understanding of the Diversity and Ecology of Giant Viruses in Aquatic Microbial Communities
The Kyoto University Foundation
1 July 2017–31 March 2018

Ogata, H.
Comprehensive Understanding of the Role of Giant Viruses in Aquatic Ecosystems
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2022

Ogata, H.
Innovative Foundation of Viral Oceanography Based on a Comprehensive Virome Study
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Ogata, H.
Elucidation of the Origin and Mechanism of Success of Diatoms through Comparative Biological Analyses between Ancient Centric Diatoms and Their Sister Paramales
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Ogata, H.
Comprehensive Study and Establishment of Application Foundation of Carboxydotrophic Bacteria through Spatio-Temporal Search
Grant-in-Aid for Scientific Research (S)
1 April 2016–31 March 2021

Blanc-Mathieu, R.
Unraveling Evolutionary Mechanisms That Led to the Success of Diatoms
The Kyoto University Foundation
1 July 2018–31 March 2019

— Mathematical Bioinformatics —

Tamura, T.
Developing Control Methods for Biological Networks on Mathematical Models
Grant-in-Aid for Scientific Research (C)
1 April 2016–31 March 2019

Akutsu, T.
Analysis and Application of Discrete Preimage Problems
Grant-in-Aid for Scientific Research (A)
2 April 2016–31 March 2023

Mori, T.
Development of a Detailed Cell Classification and Evaluation Method Based on DNA Methylation Information
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2019

— Bio-knowledge Engineering —

Mamitsuka, H.
Reinforcement of Resiliency of Concentrated Polymer Brushes and Its Tribological Applications
Strategic Basic Research Program, ACCEL, JST
1 September 2015–31 March 2020

Mamitsuka, H.
Efficiently Inferring Factors Embedded in Multiple Data Matrices
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2019

Yotsukura, S.
Computational Breeding Design of Least Allergen Crops
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2017–31 October 2018

Nguyen, C. H.
Machine Learning on Large Graphs
Grant-in-Aid for Scientific Research (C)
1 April 2018–31 March 2021

THESES

ARAI, Kenta
D Pharm Sc, Kyoto University
"Catalytic Site-Selective C-H Amination Mediated by Rhodium Nitrenoids"
Supervisor: Prof KAWABATA, Takeo
25 September 2018

LIAN, Zichao
D Sc, Kyoto University
"Synthesis and Plasmonic Properties of Copper-based Nanocrystals"
Supervisor: Prof TERANISHI, Toshiharu
1 June 2018

MIHARA, Tomoko
D Pharm Sc, Kyoto University
"Development and Application of Bioinformatics Tools in Virus Research"
Supervisor: Prof OGATA, Hiroyuki
25 September 2018

NAKANISHI, Yohei
D Eng, Kyoto University
"Fundamental and Applied Studies on Self-assembling of Polymer-brush-modified Nanoparticles in Ionic Liquid"
Supervisor: Prof TSUJII, Yoshinobu
26 March 2018

ONUKI, Ritsuko
D Sc, Kyoto University
"Genome-wide Study of the Diversity of Disease-related Traits through Identification of Ancient Haplotype Blocks"
Supervisor: Prof OGATA, Hiroyuki
25 September 2018

SHIOYA, Nobutaka
D Sc, Kyoto University
"Development of Analytical Technique of Molecular Orientation in a Thin Film and Its Application to Low-Crystallinity Organic Thin Films Having a Surface Roughness"
Supervisor: Prof HASEGAWA, Takeshi
26 March 2018

SUGIURA, Miwa
D Agr, Kyoto University
"Effects of Eicosapentaenoic Acid-Containing Phospholipids on the Formation of Membrane Proteins from *Shewanella livingstonensis* Ac10"
Supervisor: Prof KURIHARA, Tatsuo
25 September 2018

SUZUKI, Yuko
D Sc, Kyoto University
"Synthesis and Property of the Redox-active Divalent Germanium Compounds"
Supervisor: Prof TOKITOH, Norihiro
26 March 2018

TAGUCHI, Hiro-omi
D Eng, Kyoto University
"Studies on PNP-Pincer Type Phosphaalkene Complexes Stabilized by a Fused-Ring Bulky Protection Group"
Supervisor: Prof OZAWA, Fumiyuki
23 May 2018

TANAKA, Kensho
D Sc, Kyoto University
"Spin Injection and Spin Current Generation in Ferromagnetic Multilayers"
Supervisor: Prof ONO, Teruo
18 January 2018

TANIGUCHI, Takuya
D Sc, Kyoto University
"Domain Wall Motion in Perpendicularly Magnetized Ferromagnetic Nanowires"
Supervisor: Prof ONO, Teruo
18 January 2018

TOKUNAGA, Tomohisa
D Agr, Kyoto University
"Synthesis and Application of ω-Ethynyl Fatty Acids to Analyze the Physiological Functions of Eicosapentaenoic Acid"
Supervisor: Prof KURIHARA, Tatsuo
26 March 2018

XIONG, Peng
D Sc, Kyoto University
"Cation Substituion-induced Changes in Structural and Physical Properties of Perovskite Oxides Having Unusually High Valent Fe"
Supervisor: Prof SHIMAKAWA, Yuichi
26 March 2018

ZHENG, Linjie
D Sc, Kyoto University
"Distributions of Bioactive Trace Metals in the North Pacific Ocean"
Supervisor: Prof SOHRIN, Yoshiki
26 March 2018

THE 118TH ICR ANNUAL SYMPOSIUM

SEMINARS MEETINGS AND SYMPOSIA

THE 118TH ICR ANNUAL SYMPOSIUM

(30 November 2018)

ORAL PRESENTATION

UEDA, Yoshihiro (Synthetic Organic Chemistry)
"Total Synthesis of Natural Glycosides Based on Site-Selective Functionalization of Unprotected Carbohydrates"

TAKANO, Shotaro (Hydrospheric Environment Analytical Chemistry)
"Development of a New Method for Simultaneous Analysis of Ni, Cu and Zn Isotope Ratios in Seawater and Its Application to Chemical Oceanography"

HASHIDA, Masaki (Laser Matter Interaction Science)
"Surface Nanostructures Induced by Short Laser Pulse and Its Applications"

SAKAKIBARA, Keita (Chemistry of Polymer Materials)
"Development of Soft and Resilient Tribology (SRT) Systems"

KAYAHARA, Eiichi (Polymer Controlled Synthesis)
"Synthesis of New Cyclic Curved π-Conjugated Molecules Using Reactivity of Cycloparaphenylenes"

— ICR Award for Young Scientists —
HASHIKAWA, Yoshifumi (Structural Organic Chemistry)
"Facile Access to Azafullerenyl Cation $C_{59}N^+$ and Specific Interaction with Entrapped Molecules"

TAHARA, Hirokazu (Nanophotonics)
"Quantum Coherence of Multiple Excitons Governs Absorption Cross-sections of PbS/CdS Core/shell Nanocrystals"

— ICR Award for Graduate Students —
HASEGAWA, Shota (Structural Organic Chemistry)
"Construction of a Metal-Free Electron Spin System by Encapsulation of an NO Moleculeinside an Open-Cage Fullerene C_{60} Derivative"

LU, Yangtian (Polymer Controlled Synthesis)
"Synthesis of Structurally Controlled Hyperbranched Polymers Using a Monomer Having Hierarchical Reactivity"

MIZUNO, Hayato (Nanospintronics)
"Electric-field-induced Modulation of the Anomalous Hall Effect in a Heterostructured Itinerant Ferromagnet $SrRuO_3$"

HANDA, Taketo (Nanophotonics)
"Radiative Recombination and Electron-phonon Coupling in Lead-free $CH_3NH_3SnI_3$ Perovskite Thin Films"

NGUYEN, Dai Hai (Bio-knowledge Engineering)
"SIMPLE:Sparse Interaction Model over Peaks of moLEcules for Fast, Interpretable Metabolite Identification from MS/MS"

— ICR Grants for Promoting Integrated Research —
OGAWA, Takuya (Molecular Microbial Science)
"Development of an Inhibitor Targeting 1-acylglycerol-3-phosphate Acyltransferase for Crystal Structure Analysis and Antimicrobial Drug Discovery"

HERBSCHLEB, Ernst David (Inorganic Photonics Materials)
"Research on the Advanced Quantum Device by the Single NV Center in Diamond"

POSTER PRESENTATIONS

LW : Laboratory Whole Presentation
LT : Laboratory Topic
GE : General Presentation

— Organoelement Chemistry —

LW “Studies on the Synthesis and Properties of Novel Organic Compounds Containing Heavier Elements”

GE YANAGISAWA, Tatsuya; MIZUHATA, Yoshiyuki; TOKITOH, Norihiro
“Synthesis and Reactivity of Novel Phosphinoalumanes”

— Structural Organic Chemistry —

LW “Research Activities in Structural Organic Chemistry Laboratory”

GE ZHANG, Sheng; HASHIKAWA, Yoshifumi; MURATA, Yasujiro
“Development of a Novel Cage-Expansion Method from C_{60} to $C_{65}N$ and $C_{64}N$ Skeletons”

— Synthetic Organic Chemistry —

LW “The Latest Research in the Division of Fine Synthetic Organic Chemistry”

GE MORISAKI, Kazuhiro; UEDA, Yoshihiro; KAWABATA, Takeo
“Remote Asymmetric Induction by Catalytic C–H Bond Amination”

GE HASHIMOTO, Hisashi; YOSHIDA, Keisuke; IMAYOSHI, Ayumi; MORISAKI, Kazuhiro; UEDA, Yoshihiro; KAWABATA, Takeo
“Remote Asymmetric Desymmetrization of σ-Symmetric 1,7-Diols by Catalytic Silylation”

— Advanced Inorganic Synthesis —

LW “Recent Progress of Advanced Inorganic Synthesis Laboratory”

GE MATSUMOTO, Kenshi; SATO, Ryota; TERANISHI, Toshiharu
“Formation of Novel Fe–Pd Ordered Alloy Nanoparticles Induced from Third Element”

GE OKAMOTO, Yasuo; SAKAMOTO, Masanori; TERANISHI, Toshiharu
“Control of Geometric Anisotropy of Janus Porphyrin Coordinated Gold Clusters”

— Chemistry of Polymer Materials —

LW “Research Activities in Chemistry of Polymer Materials Laboratory”

GE EGUCHI, Hiroshi; SAKAKIBARA, Keita; TSUJII, Yoshinobu
“Lubrication Properties Analysis of Concentrated Polymer Brushes by Optical Interferometry Method”

— Polymer Controlled Synthesis —

GE LIN, Yiming; LU, Yangtian; YAMAGO, Shigeru
“Synthesis of Structurally Controlled Core-shell Block Copolymers with Thermal Responsive Solution Properties”

GE YAMAMOTO, Koji; KAYAHARA, Eiichi; YAMAGO, Shigeru
“Cycloaddition Reaction of Cycloparaphenylenes with 1,2,4-Triazoline-3,5-dione”

GE NAKANO, Masaya; SUN, Liansheng; KAYAHARA, Eiichi; YAMAGO, Shigeru
“Transformation of Tetrahydroxy [10]Cycloparaphenylene by Transition Metal Catalyzed Reactions”

GE SHIGEKI, Erika; TOSAKA, Masatoshi
“The Model of Shape-Memory State Appearing in Natural Rubber”

— Inorganic Photonics Materials —

LW “Research Topics of Inorganic Photonics Lab”

— Nanospintronics —

GE ANDO, Fuyuki
“Microscopic Origin of Electric-field-induced Modulation of Curie Temperature in Pt/Co Film”

GE OKUNO, Takaya
“Spin-transfer Torques in the Vicinity of the Angular Momentum Compensation Temperature of Ferrimagnets”

GE NISHIMURA, Tomoe
“Correlation between Magnetic Properties and Depinning Field in Field-Driven Domain Wall Dynamics in GdFeCo Ferrimagnets”

GE ODA, Kento
“Exchange Bias Controlled by Electric Current: Interplay of Joule Heating and the Induced Field”

— Biofunctional Design-Chemistry —

LW “Research Activities in Laboratory of Biofunctional Design Chemistry”

GE AKISHIBA, Misao; FUTAKI, Shiroh
“Mechanism of Peptide-mediated Intracellullar Delivery of Biomacromolecules”

— Chemistry of Molecular Biocatalysts —

LW “Research Activities in Laboratory of Chemistry of Molecular Biocatalysts”

— Molecular Biology —

LW “Research of Molecular Biology Laboratory”

— Chemical Biology —

LW “Create New World of Bioactive Synthetic Molecules”

— Molecular Materials Chemistry —

GE WAKISAKA, Yasuaki; WADA, Yoshimasa; KAJI, Hironori
"Photophysical Properties and Device Performances of a Blue Thermally Activated Delayed Fluorescence Material Which Shows Highly Efficient TADF in Various Hosts"

— Hydrospheric Environment Analytical Chemistry —

LT TSUCHIYA, Mao; TAKANO, Shotaro; TSUJISAKA, Makoto; IMAI, Shoji; YAMAMOTO, Yuhei; SHIN, Ki-Cheol; SOHRIN, Yoshiki
"Isotope Ratios of Ni, Cu and Zn in Rainwater Collected in Western Japan"

GE TANAKA, Yuriko
"An Advanced Method for the Determination of Zr, Hf, Nb, and Ta in Seawater and Its Application to Seawater Samples from the North Pacific Ocean"

— Chemistry for Functionalized Surfaces —

GE TOMITA, Kazutaka; SHIOYA, Nobutaka; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
"Polymorphic Control in a Spin-Coated Film of a Porphyrin Derivative"

GE FUJIWARA, Ryoi; SHIOYA, Nobutaka; TOMITA, Kazutaka; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
"Analysis of Structual Conversion of a Pentacene Precursor Thin Film Using pMAIRS"

GE FUKUMI, Aki; SHIMOAKA, Takafumi; SHIOYA, Nobutaka; HASEGAWA, Takeshi
"*In situ* Observation of Aggregation Structure and Orientation Change of Perfluoroalkane in a Monolayer on Water Surface"

— Molecular Microbial Science —

LW "Laboratory of Molecular Microbial Science"

GE KAMASAKA, Kouhei; CHEN, Chen; YOKOYAMA, Fumiaki; IMAI, Tomoya; KAWAMOTO, Jun; KURIHARA, Tatsuo
"Elucidation of a Vesiculation-mediated Protein Secretion Mechanism of *Shewanella* sp. HM13"

— Polymer Materials Science —

LW "Polymer Materials Science"

GE MATSUNAGA, Tsubasa; OGAWA, Hiroki; TAKENAKA, Mikihito; MIYAZAKI, Tsukasa; KABE,Taizo
"Direct Observation of Spin Coating Process of Polystyrene-b-poly(2-vinylpyridine) Thin Film Under Selective Solvent"

GE OMOSU, Takuya; TAKENAKA, Mikihiro; OGAWA, Hiroki
"*In-situ* Measurement of Self-assembling Blockcopolymer Thin Film with GISAXS"

GE NISHIMURA, Yu; TAKENAKA, Mikihito
"Study on Dynamics of Aggregates in Rubber Filling System"

GE FUWA, Takuto; OGAWA, Hiroki; TAKENAKA, Mikihito; KANAYA, Toshiji; YAMADA, Norifumi
"Neutron Reflectivity Measurement for Phase Separation and Dewetting in dPS/P2ClS Thin Films"

— Molecular Rheology —

LW "Introduction of Laboratory of Molecular Rheology"

— Molecular Aggregation Analysis —

LW "Design and Fabrication of Molecular Aggregates for Organic Electronics"

GE NAKAMURA, Tomoya; SHIOYA, Nobutaka; SHIMOAKA, Takafumi; HASEGAWA, Takeshi; MURATA, Yasujiro; WAKAMIYA, Atsushi
"Directed Molecular Orientation of N-type Organic Semiconductors Controlled by Hydrogen Bond Networks"

GE OZAKI, Masashi; SHIMAZAKI, Ai; MURATA, Yasujiro; MURDEY, Richard; WAKAMIYA, Atsushi
"Fabrication of Efficient Perovskite Solar Cells and Modules from a Highly-Purified Precursor Complex"

GE YAKUMARU, Shinya; LIU, Jiewei; OZAKI, Masashi; HANDA, Taketo; KANEMITSU, Yoshihiko; MURATA, Yasujiro; MURDEY, Richard; WAKAMIYA, Atsushi
"Development of Highly Reproducible Perovskite Layer Deposition Method for Efficient Lead-free Perovskite Solar Cells"

— Particle Beam Science —

LW "Research Topics in Accelerator Laboratory"

GE TAKEUCHI, Yusuke; TONGU, Hiromu; IWASHITA, Yoshihisa
"Compact ECR H^+ Ion Source with Permanent Magnet"

GE YAKO, Tomoki; ABE, Masashi; IWASHITA, Yoshihisa; TONGU, Hiromu; KATAYAMA, Ryo; TAKEUCHI, Yusuke; TERUNUMA, Nobuhiro; FUWA, Yasuhiro
"Design Study of Main Dipole Magnet and Correction Magnet Using Permanent Magnet for ILC Damping Ring"

— Laser Matter Interaction Science —

LW "Research Activities in Laboratory of Laser Matter Science"

GE NISHINO, Shogo; HASHIDA, Masaki; SHIMIZU, Masahiro; FURUKAWA, Yuki; INOUE, Shunsuke; KOJIMA, Sadaoki; TSUKAMOTO, Masahiro; TAKENAKA, Keisuke; SAKABE, Shuji
"Dot Coloring on Titanium Surface by Femtosecond-laser Double-pulse Irradiation"

GE YOSHIDA, Masahiro; KOJIMA, Sadaoki; INOUE, Shunsuke; FURUKAWA, Yuuki; HASHIDA, Masaki; SAKABE, Shuji
"Fast Time-resolved Imaging Method with Pump-probe Ellipsometry"

GE NISHIURA, Yosuke; INOUE, Shunsuke; KOJIMA, Sadaoki; FURUKAWA, Yuuki; HASHIDA, Masaki; SAKABE, Shuji
"Detection of α Particles Generated by Nuclear Reaction with Laser Accelerated Protons by Two-step Etching of CR-39"

GE FURUKAWA, Yuki; NISHINO, Shogo; KOJIMA, Sadaoki; INOUE, Shunsuke; HASHIDA, Masaki; SAKABE, Shuji
"Ablation for Titanium by Double-pulse Femtosecond Laser Irradiation"

GE KOJIMA, Sadaoki; INOUE, Shunsuke; HASHIDA, Masaki; SAKABE, Shuji
"Probing Ultrafast Motion of Critical Surface Pushed by Multi-pico-second Relativistic Radiation Pressure"

— Electron Microscopy and Crystal Chemistry —

LW "Research Activities in the Division of Electron Microscopy and Crystal Chemistry"

GE YAMAGUCHI, Atsushi; NEMOTO, Takashi; KURATA, Hiroki
"Analysis of Carbon K Edge ELNES of Copper Phthalocyanine Crystalline by First-principles Band Calculation"

— Atomic and Molecular Structures —

LW "Introduction of Atomic and Molecular Structures Laboratory"

— Synthetic Organotransformation —

LW "Research of Synthetic Organotransformation"

GE SHANOH, Takafumi; TAKAYA, Hikaru; TAKEDA, Yoshihiko; NAKATANI, Yuuya; ITO, Masato; NAKAMURA, Masaharu
"Iron-Catalyzed Oxidative Depolymerization of Lignin"

GE HOSOKAWA, Atsushi; IWAMOTO, Takahiro; NAKAMURA, Masaharu
"Light-Driven Intermolecular Coupling of Amines and Ketones"

— Advanced Solid State Chemistry —

LW "Introduction of Advanced Solid State Chemistry Laboratory"

— Organometallic Chemistry —

LW "Activity Report: Organometallic Chemistry Laboratory"

GE TORII, Naohiro; WAKIOKA, Masayuki; SAITO, Masahiko; OSAKA, Itaru; OZAWA, Fumiyuki
"Synthesis of Donor-Acceptor Alternating Copolymers Containing Benzodithiophene Units via Highly Selective Direct Arylation Polymerization"

— Nanophotonics —

LW "Recent Research Topics of Nanophotonics Group"

— Chemical Life Science —

LW "Introduction of Laboratory of Chemical Life Science"

— Mathematical Bioinformatics —

LT LI, Ruiming
"Deep Learning with Evolutionary and Genomic Profiles for Identifying Cancer Subtypes"

— Bio-knowledge Engineering —

LT NGUYEN, Dai Hai; NGUYEN, Canh Hao; MAMITSUKA, Hiroshi
"Sparse Interaction Model Over Peaks of moLEcules for Fast, Interpretable Metabolite Identification from Tandem Mass Spectra"

SEMINARS

Prof ABE, Manabu
Hiroshima University, Hiroshima, Japan
"Is π Single Bond (C - π - C) Possible?"
8 May 2018

Dr ANTOINE, Claire Z.
Cea Saclay, France
"Material and Surface Aspects in SRF Technology"
21–22 November 2018

Dr ARUMUGAM, Sri Ranjini
Max-Plank Institute for Biophysical Chemistry, Germany
"Single Molecule Spectroscopic Approach to Study DNA Replication Machinery"
19 October 2018

Dr BALASUBRAMANIAN, Gopalakrishnan
Max-Plank Institute for Biophysical Chemistry, Germany
"Precision Metrology at the Nanoscale"
15 October 2018

Prof BALSARA, Nitash
University of California, Berkeley, U.S.A.
"Block Copolymers in Lithium Batteries"
29 June 2018

Dr BHUVANESH, Ramakrishna
Department of Physics, Indian Institute of Technology Hyderabad, India
"Ultla High Intense Laser Matter Interaction and Their Applications"
12 July 2018

Prof BOYER, Cyrille A.
University New South Wales, Australia
"Seeing the Light: Advancing Polymer Synthesis"
20 November 2018

Dr CHAFFRON, Samuel
Center National de la Recherche Scientifique/Laboratoire des Sciences du Numerique de Nants, France
"An Eco-systems View of Complex Microbiomes"
14 September 2018

Prof CHOE, Sug-Bong
Soul National University, Korea, R.
"DMI Measurement Schemes Based on Domain-Wall Dynamics in Ferromagnetic Thin Films"
28 November 2018

Dr CHU, Ming-Wen
Center for Condensed Matter Sciences, National Taiwan University, Taiwan
"Atomic-Scale Unraveling of Transition Pathway, Hidden Order Parameter, and Domain Topology in Improper Ferroelectrics"
27 August 2018

Prof COLBY, Ralph
Penn State University, U.S.A.
"Linear Viscoelasticity of Ionic Polymers: Ionomers and Polyelectrolytes"
20 June 2018

Assoc Prof DUKKA, Bahadur K. C.
Computational Science and Engineering Department North Carolina A&T State University Greensboro, U.S.A.
"Computational Prediction of Post-translational Modification Sites"
24 July 2018

Prof GOTO, Susumu
Database Center for Life Science, The University of Tokyo, Tokyo, Japan
"Life Science Database Integration Based on Semantic Web Technology"
18 October 2018

Dr GUIGO, Roderic
Center for Genomic Regulation, Spain
"The Molecular Anatomy of the Human Body"
23 August 2018

Prof GUY, C. Lloyd-Jones FRS
The University of Edinburgh, U.K.
"An in Situ Journey from Reactants to (side) Products"
3 March 2018

Senior Researcher HAAR, Stefan
Head of MExICo Team, INRIA Saclay Center, France
"Let's Have a New Update on Boolean Networks !"
26 October 2018

Prof HALEY, Michael M.
University of Oregon, U.S.A.
"Modular Supramolecular Fluorescent Receptors: Functional Materials and Applications as Probes for Anions"
19 November 2018

Prof HE, Junpo
The State Key Laboratory of Molecular Engineering of Polymers, Fudan University, China, P.R.
"Synthesis of Amphiphilic Dendrimer-like Polymers and Application as Unimolecular Nanoreactors"
10 December 2018

Proj Assoc Prof HIROTA, Katsuya
Osaka University, Osaka, Japan
"Compact Accelerator Driven Neutron Source and Its Application 1"
29 November 2018

Assit Prof HUANG, Possu
Department of Bioengineering, Stanford University, U.S.A.
"De Novo Design of Novel Molecular Platforms"
7 September 2018

Dr IDZUCHI, Hiroshi
Harvard University, U.S.A.
"How to Characterize Spin Current in Mesoscopic System?"
26 March 2018

Assoc Prof ISHIDA, Shintaro
Department of Chemistry, Graduate School of Science, Tohoku University, Miyagi, Japan
“Novel Transformation of Stable Low-coordinate Silicon Compounds”
15 November 2018

Prof ITO, Akichika
Faculty of Pharmaceutical Science, Gifu Pharmaceutical University, Gifu, Japan
“Development of Photo-oxidation Reactions with Molecular Oxygen and Visible Light”
23 February 2018

Prof JUNG, Myung-Hwa
Sogang University, China, P.R.
“Rare-earth Doped Magnetic Topological Insulators”
4 December 2018

Dr KITAYAMA, Kenji
Daicel Chemical Industries Ltd., Tokyo, Japan
“Synthetic Organic Technology for Product Development: for Your Own Way in The Future”
7 September 2018

Dr KUPCZOK, Anne
Institute of General Microbiology, Kiel University, Germany
“Evolutionary Rate Estimation for Bacteriophages Based on Time Series Data Sets”
26 July 2018

Prof LAUREAN, Llies
Department of Chemistry, Graduate School of Science, The University of Tokyo, Tokyo, Japan
“Catalysis with Earth-abundant Metals: C-H Functionalization and Other Stories”
26 February 2018

Prof LIU, Zhi-Quan
Chinese Academy of Sciences, China, P.R.
“Property-Related Morphological and Orientation Characterization of Nanomaterials Using TEM”
24 January 2018

Prof MARTIN, Kotora
Department of Organic Chemistry, Charles University, Czech R.
“Catalytic Cycloadditions with Alkynes: Synthesis of Various Aromatic and Heteroaromatic Compounds”
13 March 2018

Prof MARTIN, Oestreich
Technische Universität Berlin, Germany
“Wheland Intermediates in Catalysis”
28 September 2018

Dr MASSUE, Julien
University of Strasbourg, France
“Optimized Fluorescent Emitters Based on A Hydroxybenzazole or Anil Scaffold”
13 March 2018

Prof MATSUSHIMA, Toshinori
Kyushu University, Fukuoka, Japan
“Optoelectronic Devices Using Metal Halide Perovskites”
4 July 2018

Prof MOTOME, Yukitoshi
The University of Tokyo, Tokyo, Japan
“Splitting Spins”
12 June 2018

Prof OGOSHI, Sensuke
Osaka University, Osaka, Japan
“Asymmetric Carbon-carbon Bond Positive Reaction by Optically Active Nickel Catalyst”
27 April 2018

Junior Research Fellow PETSCHNER, Peter
Department of Pharmacodynamics, Semmelweis University, Hungary
“Complexity of Environment-dependent Genetic Effects in Major Depression through the Scope of 5-HTTLPR”
10 July 2018

Prof RINALDO, Poli
CNRS, Laboratoire de Chimie de Coordination, Toulouse, France
“Ligand-functionalized, Well-definedpolymeric Nanoreactors: Metal Coordination, Polymer Dynamics and Applications in Aqueous Biphasic Catalysis”
23 January 2018

Dr ROMERO-NIETO, Carlos
University of Heidelberg, Germany
“From Phosphaphenalenes to Diphosphahexaarenes: Fused Six-membered Phosphorus Heterocycles”
29 November 2018

Dr RUBIO, Vicente
Centro Nachional de Biotecnologia-CSIC, Spain
“DET1 Complexes Control Photomorphogenesis by Acting at the Interface between Light Signalind and Epigenome Dynamics”
21 June 2018

Prof SANDAA, Ruth-Anne
Marine Microbiology Group, Department of Biological Science, Bergen University, Norway
“Living with the Enemy: Virus-host Relationship in the Ocean”
24 April 2018

Prof SASAMORI, Takahiro
Nagoya City University, Aichi, Japan
“Active Chemical Species of Heavier Main Group Elements and Lead-Free Perovskites”
7 July 2018

Assoc Prof SHIBATOMI, Kazutaka
Department of Environmental and Life Sciences, Toyohashi University of Technology, Aichi, Japan
“Enantioselective Halogenation Reactions Catalyzed by Chiral Amines”
28 February 2018

Prof SHIMIZU, M. Hirohiko
Nagoya University, Aichi, Japan
“Compact Neutron Source and Its Industrial Application”
17 May 2018
“Neutron Oscillation”
11 October 2018

Leader Researcher SHIMONO, Masanori
Graduate School of Medicine, Kyoto University, Kyoto, Japan
“Connecting Multi-scale Networks in the Brain”
24 April 2018

Assist Prof SLJOKA, Adnan
Department of Informatics, School of Science and Technology, Kwansei Gakuin University, Osaka, Japan
“Lifting the Curtain: Probing Allostery and Other Biological Secrets with High Throughput Rigidity Analysis”
25 April 2018

Prof SOKOLOV, Alexei
University of Tennessee and Oak Ridge National Laboratory, U.S.A.
"Why Many Polymers are So Fragile: The Final Answer?"
20 June 2018

Senior Research Fellow and Group Leader SONG, Jiangning
Monash Biomedicine Discovery Institute (BDI), Monash University, Australia
"Harnessing the Power of Machine-learning Techniques to Address Sequence Classification Problems in the Era of Biomedical Big Data"
25 September 2018

Prof STASEVICH, Tim
Department of Biochemistry and Molecular Biology, Colorado State University, U.S.A.
"Imaging Canonical and Non-Canonical Single mRNA Translation Dynamics in Living Cells"
29 June 2018

Dr SUGAWARA, Koto
Material Analysis Research Center, Teijin Limited, Tokyo, Japan
"Structural Analysis of Polylactic Acid for Material Development"
25 May 2018

Prof SUKBOK, Chang
Korea Advanced Institute Science and Technology, Korea, R.
"Development of Direct C-H Amination Reactions: Inner- versus Outer-Sphere Pathways"
16 April 2018

Dr TOMARU, Yuji
National Research Institute of Fisheries and Environment of Inland Sea, Japan Fisheries Research and Education Agency, Hiroshima, Japan
"Ecological Studies on Marine Diatom and Their Infectious Viruses"
25 May 2018

Prof WOLFGANG, Brutting
Institute of Physics, University of Augsburg, Germany
"Molecular Orientation as Key Parameter in Organic Optoelectronics"
18 September 2018

Assoc Prof XING, Bengang
School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore
"Unique Fluorescent Imaging Probes for Specific Manipulation of Cellular Functions and Localized Theranostics"
26 July 2018

Prof YANG, Jye-Shane
National Taiwan University, Taiwan
"Stimuli-Responsive π-Conjugated Oligomers"
23 January 2018

MEETINGS AND SYMPOSIA

The 12th International Workshop for East Asian Young Rheologists (IWEAYR-13)
Co-organized by WATANABE, Hiroshi
24–27 January 2018 (Jeju, Korea, R.)

38th Anniversary Meeting of Prof. Masayoshi Ishibashi, Research Institute of Oceanochemistry Foundation
Organized by SOHRIN, Yoshiki
28 April 2018 (Kyoto, Japan)

The 74th Meeting of the Collegium of Rheology in Kansai
Organized by MATSUMIYA, Yumi
20 June 2018 (Kyoto, Japan)

The 15th International Symposium on Inorganic Ring Systems
Organized by TOKITOH, Norihiro
24–29 June 2018 (Kyoto, Japan)

Environmental Virus Meeting 2018
Organized by OGATA, Hiroyuki
27 October 2018 (Kyoto, Japan)

The 18th IEEE International Conference on BioInformatics and Bioengineering
PC co-chair by AKUTSU, Tatsuya
29–31 October 2018 (Taichung, Taiwan)

72nd Annual Autumn Meeting of Research Institute of Oceanochemistry Foundation
Organized by SOHRIN, Yoshiki
10 November 2018 (Kyoto, Japan)

The 10th International Peptide Symposium
Organized by FUTAKI, Shiroh
3–7 December 2018 (Kyoto, Japan)

The JPS City Forum 2018
Organized by KAWANO, Kenichi
5 December 2018 (Kyoto, Japan)

The 24th Peptide Forum in Kyoto
Organized by FUTAKI, Shiroh
8 December 2018 (Kyoto, Japan)

The 3rd pMAIRS Workshop
Organized by HASEGAWA, Takeshi
14 December 2018 (Kyoto, Japan)

INDEX

NAME INDEX

KEYWORD INDEX

Institute for
Chemical
Research

Kyoto University