

ICR ANNUAL REPORT

2019

Volume 26

Institute for Chemical Research
Kyoto University



ICR ANNUAL REPORT 2019 (Volume 26) - ISSN 1342-0321 -

This Annual Report covers from 1 January to 31 December 2019

Editors:

Professor: UESUGI, Motonari

Professor: YAMAGUCHI, Shinjiro

Associate Professor: MORIYAMA, Takahiro

Assistant Professor: MORI, Tomoya

Editorial Staff:

Public Relations Section: NAKAMURA, Kaori

NAKANO, Yukako

HAMAOKA, Meri

Published and Distributed by:

Institute for Chemical Research (ICR), Kyoto University

© 2020 Institute for Chemical Research, Kyoto University

Enquiries about copyright and reproduction should be addressed to:

ICR Annual Report Committee, Institute for Chemical Research, 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.html>

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
2019**



**Institute for Chemical Research
Kyoto University**
Volume 26



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 fulltime 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) *Spin-transfer Torques for Domain Wall Motion in Antiferromagnetically-coupled Ferrimagnets*; 2) *Major Lithogenic Contributions to the Distribution and Budget of Iron in the North Pacific Ocean*; 3) *Ultra-long Coherence Times Amongst Room-temperature Solid-state Spins*; 4) *Raman Optical Activity on a Solid Sample: Identification of Atropisomers of Perfluoroalkyl Chains Having a Helical Conformation and No Chiral Center*; 5) *A Purified, Solvent-Intercalated Precursor Complex for Wide-Process-Window Fabrication of Efficient Perovskite Solar Cells and Modules*; 6) *Strigolactone Perception and Deactivation by a Hydrolase Receptor DWARF14*. Some other topics were also presented in the 119th ICR Annual Symposium on December 13, 2019.

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. 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 69 official international collaboration agreements) and functioning as a Joint Usage/Research Center (2010–2018) and an International Joint Usage/Research Center (2018–) certified by MEXT. On the basis of highly evaluated activity in collaboration with Fudan University, China, ICR was approved by Kyoto University in 2019 to establish an On-site Laboratory “Kyoto University Shanghai Lab” in Shanghai, China as part of a strategy implemented under the education ministry’s Designated National University (DNU) program. 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 2020

TSUJII, Yoshinobu
Director

ICR News 2019

Introduction of the Incubation Support Laboratory

■ Prof WAKAMIYA, Atsushi

The Incubation Support Lab was founded in Uji Campus as an open incubation hub for electronics materials and devices research. The Incubation Support Lab facilitates the application and commercialization of Kyoto University's research achievements. The facility has a wealth of production equipment, including a dip-coater, large-size spin coater, screen printer, sputter deposition system, glove box, dry etching system, and laser scribe. There is advanced apparatus for measuring the Hall effect, absolute PL quantum yield, photoluminescence lifetime, and external quantum efficiency. A SQUID magnetometer and photoelectron yield spectrometer are also available, while electron beam lithography and vacuum deposition systems are accessible with joint usage agreements. These facilities can be used by researchers at Kyoto University as well as start-up companies. The Incubation Support Lab accelerates the exploration and commercialization of unique materials and functional devices at Kyoto University.



Sputter Deposition System



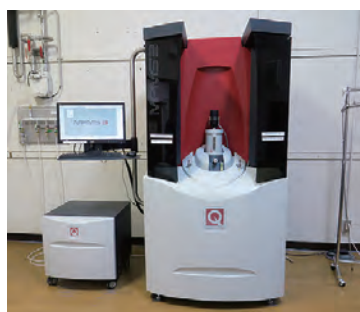
Glove Box



Dry Etching System



Hall Effect Measurement System



SQUID Magnetometer



Absolute PL Quantum Yield Measurement System

Ulaanbaatar Talent-Spot Event 2019

— KAPLAT, a JSPS-supported joint program by ICR, IAE (Kyoto U) and ISIR (Osaka U) —

■ Prof UESUGI, Motonari

The 2019 Talent-Spot Event series featured Ulaanbaatar, Mongolia. Like the previous events in Manila and Hanoi, the Ulaanbaatar event was convened on September 1 as a proactive strategy to recruit top talents from the region.

Sixteen shortlisted students were invited to attend tutorial lectures and one-on-one interviews with KAPLAT professors. Top three students received a travel award to undertake international research training in Uji campus.



Kyoto University Shanghai Lab, ICR's First On-Site Laboratory

■ Prof UESUGI, Motonari

In September 2019, ICR launched Kyoto University Shanghai Lab in partnership with Fudan University, one of the top-ranked universities in China.

As part of Kyoto University's "On-Site-Laboratory" initiatives, Shanghai Lab's missions are to expand its presence in the area and maintain competitiveness in the ever-changing academic research environment.

Shanghai lab functions as a vital chemistry hub for research collaboration, sharing equipment and resources, and research training.

In October, a kick-off meeting "Shanghai-Kyoto Chemistry Forum 2019" was held in Shanghai, where nine ICR professors exchanged ideas and tasks with the counterparts on the focused areas of New Materials, Energy Conversion and Chemical Biology.



19th Annual International Workshop on Bioinformatics and Systems Biology (IBSB 2019)

■ Prof MAMITSUKA, Hiroshi

The above workshop was held in Uji Campus of Kyoto University from 14 to 18 of July under the support of The Kyoto University Foundation and ICR (International Joint Usage/Research Center). This is an annual education-oriented event by four leading institutes world-wide: Bioinformatics Program of Boston University (USA), Systems Biology Group of Berlin (Germany), Human Genome Center, University of Tokyo and Bioinformatics Center, Kyoto University. The total number of participants, mainly PhD students and Postdocs, reached around 70, including four international invited speakers, 14 from USA and 11 from Germany. The main part of this event was around 20 oral and 30 poster presentations, bringing active scientific discussion and interchange, covering wide topics in bioinformatics and systems biology.



26th International Workshop on Oxide Electronics (iWOE26)

■ Prof SHIMAKAWA, Yuichi

The International Workshop on Oxide Electronics series has become an important venue to discuss recent advances and emerging trends in this developing field. The aim of the workshop is to provide an interdisciplinary forum for researchers—theorists as well as experimentalists—on understanding the fundamental electronic and structural properties and also on the design, synthesis, processing, characterization, and applications of (epitaxial) functional oxide materials. In this workshop, 170 scientists including world-leading professors, researchers, and students from all over the world participated. Results of critical scientific importance as well as studies revealing the technological potential of functional oxide thin films to create devices with enhanced performance were showcased.

■ <http://iwoe26.kuicr.kyoto-u.ac.jp/>



CONTENTS

Preface	iii
ICR News 2019	iv
ORGANIZATION	1
TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES	3
Division of Synthetic Chemistry	
Organoelement Chemistry	4
Structural Organic Chemistry	6
Synthetic Organic Chemistry	8
Advanced Inorganic Synthesis	10
Division of Materials Chemistry	
Chemistry of Polymer Materials	12
Polymer Controlled Synthesis	14
Inorganic Photonics Materials	16
Nanospintronics	18
Division of Biochemistry	
Biofunctional Design-Chemistry	20
Chemistry of Molecular Biocatalysts	22
Molecular Biology	24
Chemical Biology	26
Division of Environmental Chemistry	
Molecular Materials Chemistry	28
Hydrospheric Environment Analytical Chemistry	30
Chemistry for Functionalized Surfaces	32
Molecular Microbial Science	34
Division of Multidisciplinary Chemistry	
Polymer Materials Science	36
Molecular Rheology	38
Molecular Aggregation Analysis	40
Advanced Research Center for Beam Science	
Particle Beam Science	42
Laser Matter Interaction Science	44
Electron Microscopy and Crystal Chemistry	46
Atomic and Molecular Structures	48

International Research Center for Elements Science	
Synthetic Organotransformation	50
Advanced Solid State Chemistry	52
Organometallic Chemistry	54
Nanophotonics	56
Bioinformatics Center	
Chemical Life Science	58
Mathematical Bioinformatics	60
Bio-knowledge Engineering	62
HAKUBI RESEARCHERS' ACTIVITIES IN ICR	65
ACTIVITIES OF INTERNATIONAL JOINT USAGE/RESEARCH CENTER	67
iJURC Cooperative Research Subjects 2019	68
iJURC Publications (Selected Examples)	74
VISITING PROFESSORS' ACTIVITIES IN ICR	75
PERSONAL	77
Retirement	78
Awards	79
Paper Awards	85
Poster Awards	86
Obituary	89
PUBLICATIONS	92
INTERNATIONAL RESEARCH COLLABORATIONS	105
SELECTED GRANTS	107
THESES	112
THE 119TH ICR ANNUAL SYMPOSIUM	114
SEMINARS	117
MEETINGS AND SYMPOSIA	121
INDEX	123
NAME INDEX	124
KEYWORD INDEX	127

Abbreviations used in the columns

Prof Em	Professor Emeritus	Guest Scholar	Guest Scholar
Prof	Professor	Guest Res Assoc	Guest Research Associate
Vis Prof	Visiting Professor	SPD (JSPS)	Special Post-Doctoral Research Fellow (JSPS)
Assoc Prof	Associate Professor	PD	Post-Doctoral Research Fellow
Vis Assoc Prof	Visiting Associate Professor	Res	Researcher
Senior Lect	Senior Lecturer	Res Support Staff	Research Support Staff
Assist Prof	Assistant Professor	Proj Res	Project Researcher
Lect (pt)	Lecturer (part-time)	RF	Research Fellow
Specially Appointed Prof	Specially Appointed Professor	D 1~3	Doctoral Course (Program) 1~3
Program-Specific Assoc Prof	Program-Specific Associate Professor	M 1~2	Master's Course (Program) 1~2
Program-Specific Senior Lect	Program-Specific Senior Lecturer	RS	Research Student
Program-Specific Assist Prof	Program-Specific Assistant Professor	UG	Undergraduate Student
Program-Specific Res	Program-Specific Researcher	D Sc	Doctor of Science
Techn Staff	Technical Staff	D Eng	Doctor of Engineering
Assist Res Staff	Assistant Research Staff	D Agr	Doctor of Agricultural Science
Assist Techn Staff	Assistant Technical Staff	D Pharm Sc	Doctor of Pharmaceutical Science
		D Med Sc	Doctor of Medical Science
		D Inf	Doctor of Informatics
		D Human & Environmtl. Studies	Doctor of Human and Environmental Studies
		D Energy Sc	Doctor of Energy Science
		Ph D	Doctor of Philosophy
		(pt)	part-time



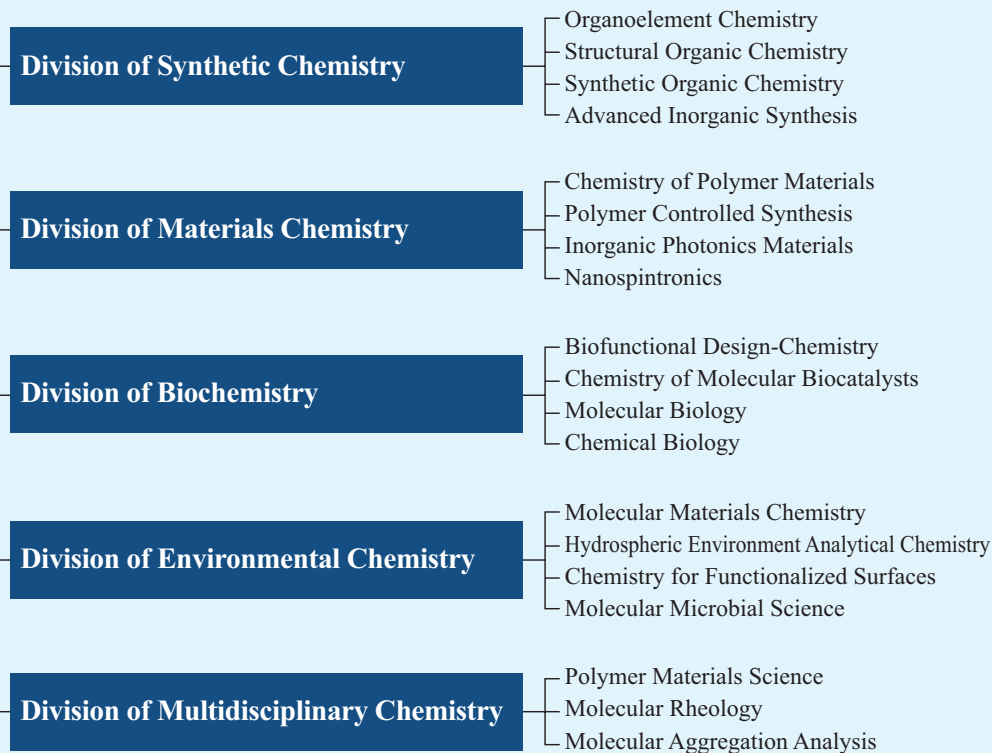
ORGANIZATION

Institute for Chemical Research

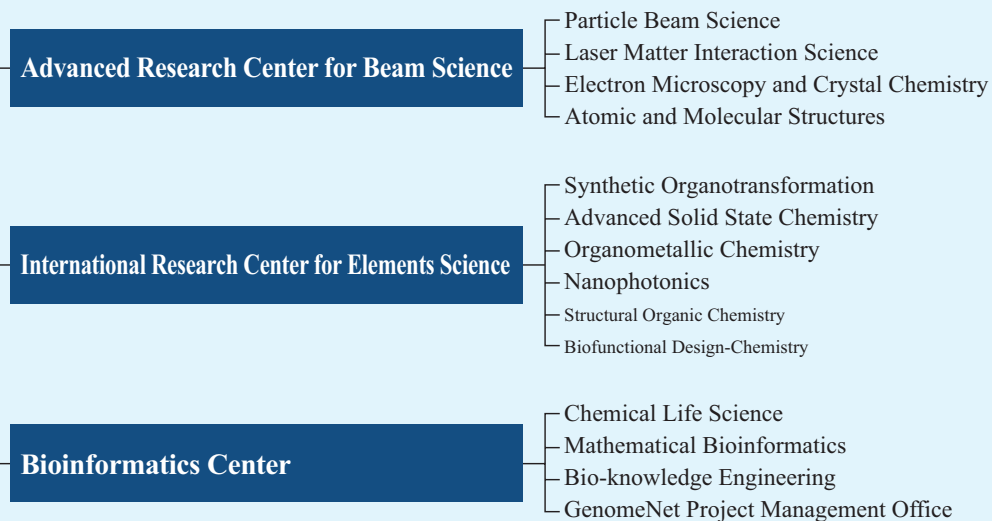
5 Divisions and 3 Centers

Laboratories

Research Divisions

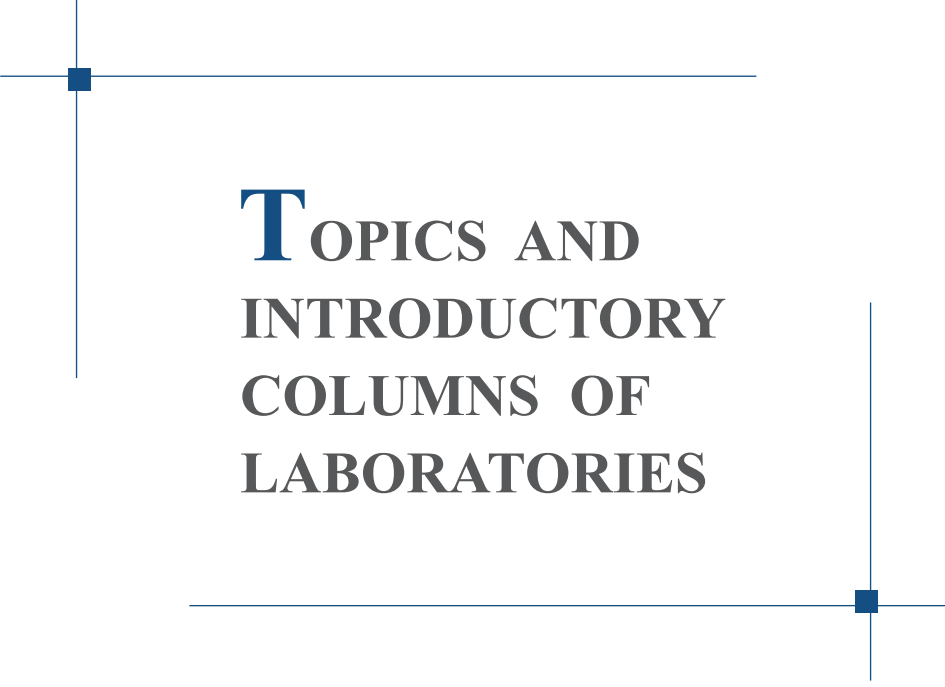


Research Centers



Visiting Divisions

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



TOPICS AND
INTRODUCTORY
COLUMNS OF
LABORATORIES

Division of Synthetic Chemistry – Organoelement Chemistry –

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



Prof

TOKITOH, Norihiro
(D Sc)



Assoc Prof

MIZUHATA, Yoshiyuki
(D Sc)



Assist Prof

YUKIMOTO, Mariko
(D Sc)



Techn

HIRANO, Toshiko

Students

YANAGISAWA, Tatsuya (D3)

OMATSU, Yamato (D2)

IWAI, Kento (D2)

JUN-I, Yuta (D1)

OSHIRO, Taku (D1)

TSUJI, Shingo (D1)

GARCIA, Julius (D1)

HONJO, Kazuma (M2)

JO, Minwoo (M2)

SASAYAMA, Ryuto (M1)

YASUI, Yuji (M1)

YANG, Yi (M1)

Guest Scholars

GLEIM, Florian Universität Bonn, Germany, 31 May–31 July

BECKER, David Universität Bonn, Germany, 9 September–4 November

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

Fujimori, S.; Mizuhata, Y.; Tokitoh, N., A Mixed-anion System Consisting of a Germyl Anion and Anions Delocalized on Conjugated Carbon Ring Skeletons, *Chem. Eur. J.*, **25**, 6284-6289 (2019).

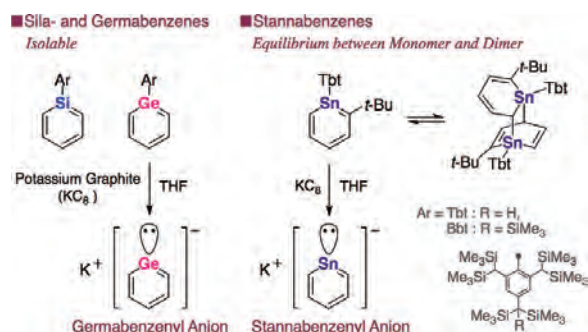
Yanagisawa, T.; Mizuhata, Y.; Tokitoh, N., Syntheses and Structures of Novel $\lambda^3\lambda^3$ -Phosphanylalumanes Fully Bearing Carbon Substituents and Their Substituent Effects, *Inorganics*, **7**, 132-143 (2019).

Sugahara, T.; Sasamori, T.; Tokitoh, N., The Formation of a 1,4-Disilabenzene and its Isomerization into a Disilabenzvalene Derivative, *Dalton Trans.*, **48**, 9053-9056 (2019).

Sugahara, T.; Guo, J.-D.; Hashizume, D.; Sasamori, T.; Tokitoh, N., Reversible Isomerizations between 1,4-Digerma-benzenes and 1,4-Digerma-dewar-benzenes: Air-stable Activators for Small Molecules, *J. Am. Chem. Soc.*, **141**, 2263-2267 (2019).

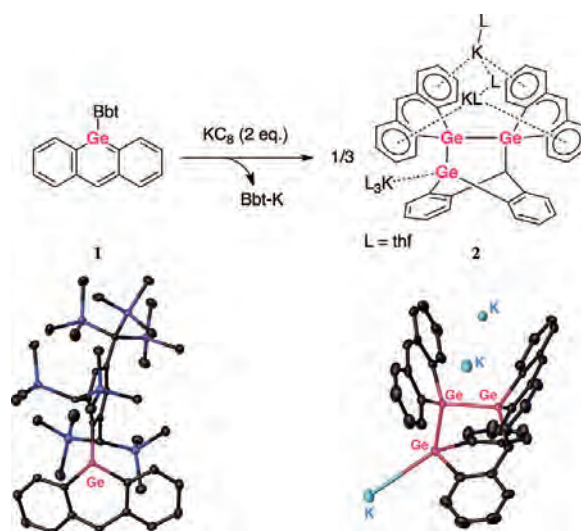
Heavy Aryl Anion Species

“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 $-200\text{ }^\circ\text{C}$. 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 germa- and stannabenzenylians, the heavier Group 14 element ($\text{E} = \text{Ge}, \text{Sn}$) analogues of phenyl anion as an isolable compound by the reaction of the corresponding isolated neutral germa- or stannabenzene having a Tbt group on the germanium or tin atom with potassium graphite (KC_8).



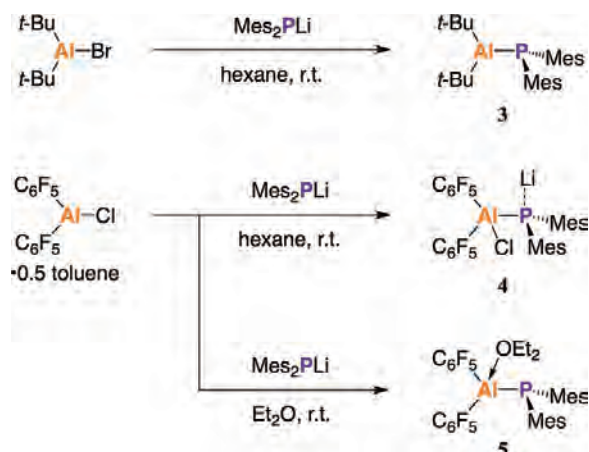
In this study, utilizing the successful method of synthesis of the germabenzenyl anion, we have reported the reduction of the previously reported 9-germaantracene, resulting in the formation of a mixed trianion, the trimer of 9-germaantracenyli anions. The reaction of 9-germaantracene **1** with 2 equivalents of potassium graphite in benzene at room temperature led to the elimination of Bbt group as benzylpotassium, BbtK, together with a purple precipitate. Washing the reaction mixture with *n*-hexane and benzene followed by extraction with THF gave the trianion **2**, a trimer of the 9-germaantracenyli anion, as a purple solid. The isolated trianion was characterized by X-ray crystallographic analysis, NMR spectroscopy and theoretical calculations. A trianion consisting of one germyl anion and two anions delocalized on conjugated carbon ring skeletons was synthesized by trimerization of the

germanium analogue of the anthryl anion, which exhibits high germylene character.



Novel Phosphanylalumanes

The bonding between group 13 (E) and group 15 (Pn) elements formulated as $\text{R}_2\text{E}-\text{PnR}_2$ have attracted much attention due to their relationship, including the vacant p orbital on E and the lone-pair electrons on Pn. In this study, we have reported synthesis of novel λ^3, λ^3 -, λ^4, λ^4 - and λ^4, λ^3 -Phosphanylalumanes **3-5**, Al-P single-bond species, by the reactions of aluminum monohalides [$(t\text{-Bu})_2\text{AlBr}$ and $(\text{C}_6\text{F}_5)_2\text{AlCl}$ (0.5 toluene)] with Mes_2PLi . Substituent effects on an Al atom were investigated, and the introduction of C_6F_5 groups on the Al atom substantially increased the Lewis acidity of aluminum. Based on the results of X-ray crystallographic analysis, theoretical calculations, and the reaction with benzophenone, λ^3, λ^3 -phosphanylalumane **3** was found to have a well-separated vacant p orbital on an Al atom and lone pairs on a P atom. Further studies on the reactivity of phosphanylalumanes are now under way.



Division of Synthetic Chemistry – Structural Organic Chemistry –

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



Prof
MURATA, Yasujiro
(D Eng)



Assoc Prof
HIROSE, Takashi
(D Eng)



Assist Prof
HASHIKAWA, Yoshifumi
(D Eng)



Program-Specific Res
IDE, Yuki
(D Sc)



Program-Specific Res
KIZAKI, Kazuro
(D Eng)



Researcher (pt)

ADACHI, Ayumi

Students

PD
ZHANG, Sheng
(Ph D)

HUANG, Guanglin (D1)
OKAMOTO, Shu (M2)
KANAYA, Taku (M1)

LI, Hui (M1)
LI, Jiayue (RS)
ZENG, Yuting (RS)

ZHU, Xiaotan (RS)
KOYAMA, Tomohisa (UG)
TANIGUCHI, Junichiro (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 Endohedral Fullerenes
Functional Materials Helical Structures
Radical Species



Selected Publications

Hashikawa, Y.; Murata, Y., Probing the Regioselectivity Using an Entrapped H_2 : Diels-Alder Reaction of a Cage Opened C_{60} Derivative with Anthracene, *Chem. Eur. J.*, **25**, 2482-2485 (2019).

Suzuki, H.; Nakano, M.; Hashikawa, Y.; Murata, Y., Rotational Motion and Nuclear Spin Interconversion of H_2O Encapsulated in C_{60} Appearing in the Low-Temperature Heat Capacity, *J. Phys. Chem. Lett.*, **10**, 1306-1311 (2019).

Fujii, S.; Cho, H.; Hashikawa, Y.; Nishino, T.; Murata, Y.; Kiguchi, M., Tuneable Single-Molecule Electronic Conductance of C_{60} by Encapsulation, *Phys. Chem. Chem. Phys.*, **21**, 12606-12610 (2019).

Hashikawa, Y.; Murata, Y., H_2O /Olefinic- π Interaction inside a Carbon Nanocage, *J. Am. Chem. Soc.*, **141**, 12928-12938 (2019).

Adachi, K.; Hirose, T.; Matsuda, K., Polymorphism of Porphyrin 2D Assemblies at the Liquid-Graphite Interface: Effect of Polar Solvent Additive and Flexible Spacer on the Face-On and Edge-On Type Molecular Arrangements, *Chem. Commun.*, **55**, 8836-8839 (2019).

Probing the Regioselectivity Using an Encapsulated H₂: Diels-Alder Reaction of a Cage Opened C₆₀ Derivative with Anthracene

We have studied the regioselectivity in the Diels-Alder reaction of an open-cage C₆₀ derivative with anthracene (Figure 1). By using an encapsulated H₂ molecule as a magnetic probe, we successfully evaluated the product population in detail, indicating the formation of ca. 10 compounds as major components. The NICS calculations showed the close resemblance to the observed ¹H NMR spectrum, which realizes facile characterization of the products. We further performed theoretical studies for forming all 29 possible anthracene-adducts. The results indicated that the regioselectivity is strongly governed by steric factor, frontier orbital coefficients, and thermodynamic stabilities. The single crystal X-ray analysis of the most dominant compound exhibited the supramolecular architecture between the anthracene moiety and the π-sphere of a neighbouring molecule.

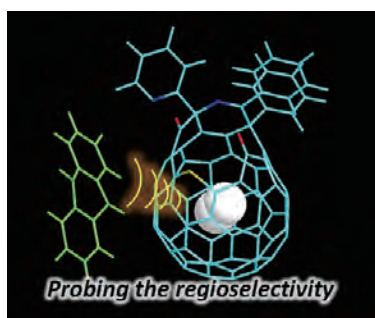


Figure 1. Regioselectivity on the Diels-Alder reaction of an open-cage C₆₀ derivative with anthracene, probed by an encapsulated H₂ molecule.

H₂O/Olefinic-π Interaction inside a Carbon Nanocage

The H₂O/CH₂=CH₂-type hydrogen-bonding (H-bonding) model was experimentally constructed using a water complex of an open-cage C₆₀ derivative, in which an olefinic double bond and a single molecule of H₂O are geometrically confined (Figure 2). To investigate OH/π-type H-bonding, that is, H₂O•••(C=C) interaction, we performed ¹H NMR spectroscopic studies that demonstrated the monotonic downfield shift of the proton signal corresponding to H₂O with remarkable rotational perturbation by lowering the temperature. From the temperature dependence of the angular momentum correlation time (τ₁), the interaction energy was quantitatively estimated to be ca. 0.3 kcal/mol. Based on comprehensive computational studies, the orientation of H₂O was found to play a prominent role to vary the bonding strength as well as contribution from the

electrostatic attraction and orbital-orbital interaction significantly driven by the favorable orbital overlap identified as π(C=C) → σ*(OH) interaction.

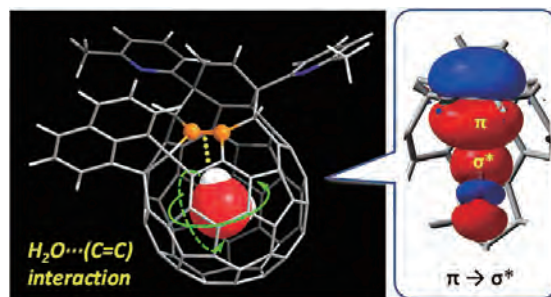


Figure 2. The experimental model of a water-olefin complex based on an open-cage C₆₀ derivative encapsulating a water molecule.

Polymorphism of Porphyrin 2D Assemblies at the Liquid–Graphite Interface: Effect of Polar Solvent Additive and Flexible Spacer on the Face-On and Edge-On Type Molecular Arrangements

Precise control over the intermolecular arrangement in ordered assemblies is of primary importance for the development of functional materials in the solid state. In the case where multiple crystal structures are obtained, i.e., so-called polymorphism is observed, selecting a specific molecular arrangement is a straightforward approach to control the solid state properties. In this study, we found that the molecular orientation of porphyrin two-dimensional assemblies at solid-liquid interfaces can be controlled by using intermolecular hydrogen bonds of amide groups (Figure 3). When phenyloctane was used as the solution phase, intermolecular hydrogen bonds were effectively formed and an edge-on orientation was selectively observed. On the other hand, only face-on orientation was observed when octanoic acid was used. Interestingly, the addition of only 0.5 vol% of a polar solvent was found to significantly affect the selectivity of molecular orientation.

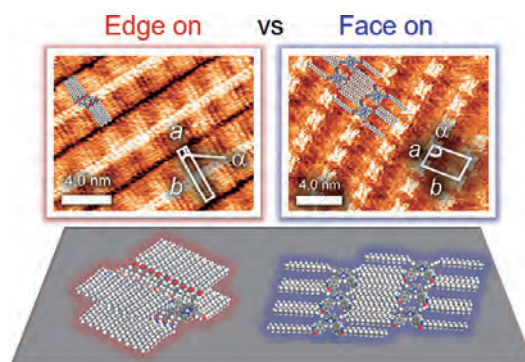


Figure 3. The two-dimensional polymorphs of porphyrin assembly at the liquid/solid interface.

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
CHANDA, Tanmoy
(Ph D)

Students

GONDOH, Naruhiro (D3)

SHIBAYAMA, Hiromitsu (D3)

MATAYOSHI, Aki (D3)

CHEN, Gong (D2)

XING, Yongning (D2)

NINOMIYA, Ryo (D2)

HASHIMOTO, Hisashi (D1)

MURAI, Takuya (D1)

YAMAMOTO, Satoru (M2)

SUGA, Akihisa (M2)

WATANABE, Yuji (M2)

GOTOH, Kengo (M2)

SATOH, Yuki (M2)

NABETA, Tomoki (M2)

EMI, Ryota (M1)

SHIGEMATSU, Hajime (M1)

FUJIMURA, Kouki (M1)

ICHIHARA, Tomoe (UG)

TANIGAKI, Yusuke (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 Memory of Chirality, *J. Am. Chem. Soc.*, **135**, 13294-13297 (2013).

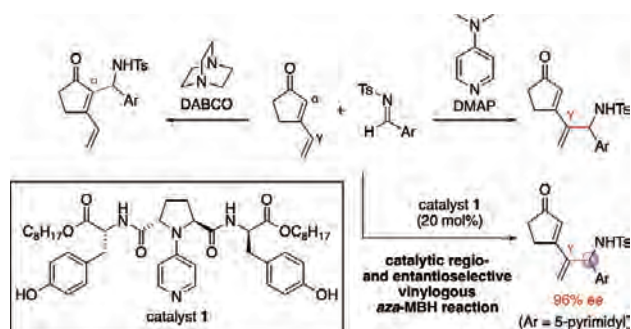
Yoshimura, T.; Tomohara, K.; Kawabata, T., Asymmetric Induction via Short-Lived Chiral Enolates with Chiral C-O Axis, *J. Am. Chem. Soc.*, **135**, 7102-7105 (2013).

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).

Organocatalytic Regio- and Enantioselective Vinyllogous *Aza*-Morita-Baylis-Hillman Reaction

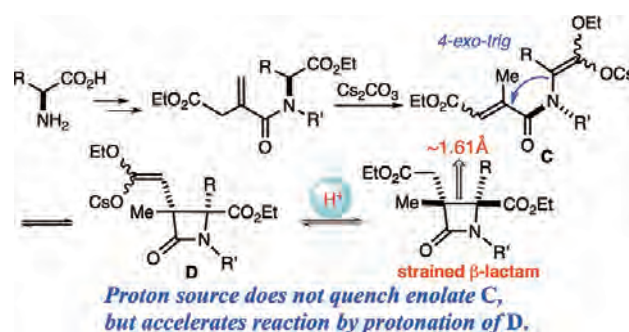
The *aza*-Morita-Baylis-Hillman (*aza*-MBH) reaction is an effective carbon-carbon bond-forming reaction between electron deficient alkenes and aldimines to give the corresponding allylamines. For the construction of further densely functionalized molecules, an advanced version of *aza*-MBH reactions using conjugated dienes with electron-withdrawing groups has been studied. We have reported the first example of regiodivergent vinyllogous *aza*-MBH reaction in a catalyst-controlled manner. Treatment of 3-vinylcyclopentenone with *N*-tosylaldimine and DABCO exclusively provided the α -adduct. In contrast, the corresponding reaction catalyzed by DMAP gave the γ -adduct selectively. Mechanistic analysis revealed that addition of proton sources accelerated the γ -selective reaction. Based on the findings, we designed original catalyst **1** possessing relatively acidic phenolic OH groups. Catalyst **1** successfully promoted enantioselective vinyllogous *aza*-MBH reaction to afford the γ -adduct regioselectively in up to 96% ee.



Asymmetric Synthesis of β -Lactams with Contiguous Tetrasubstituted Stereocenters from α -Amino Acids via Memory of Chirality

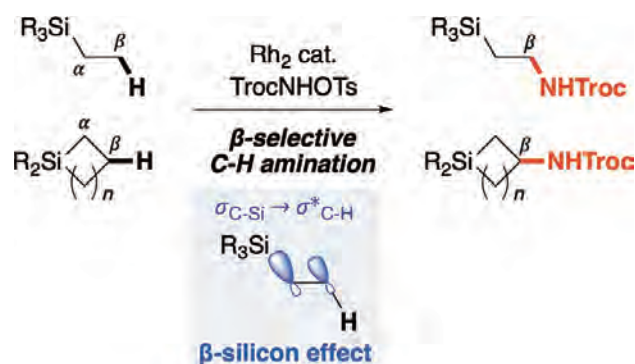
We have studied asymmetric reactions that proceed via enolate intermediates with dynamic chirality (memory of chirality: MOC). The major advantage of the strategy is the use of readily available α -amino acids as starting materials as well as the sole source of chirality. Since β -lactams still constitute one of the most important pharmacophores, and are useful as β -amino acid equivalents and chiral building blocks, development of synthetic methods for β -lactams is still of importance. Recently we developed a method for asymmetric synthesis of highly strained β -lactams with contiguous two tetrasubstituted stereocenters from readily available α -amino acids via a MOC strategy. In situ proton-

ation of the labile β -lactam enolate intermediates formed through 4-*exo-trig* cyclization of the axially chiral enolates seems to be the key to successfully produce highly strained β -lactams. A salient feature of this transformation is that proton source does not quench the axially chiral enolate **C**, but accelerate the overall reaction by protonation of the intermediary β -lactam enolate **D**.



Dirhodium-Catalyzed β -Selective C(sp³)-H Amination of Organosilicon Compounds

Metal-catalyzed nitrogen-group-transfer via C-H bond cleavage has become an important tool for the construction of C-N bonds. While site-selective C-H functionalization has been extensively studied in intramolecular reactions, the development of intermolecular site-selective C-H functionalization is a further challenge in current organic synthesis. We recently found a dirhodium-catalyzed, intermolecular β -selective C-H amination of organosilicon compounds. Primary C(sp³)-H bonds of silylethyl groups and secondary C(sp³)-H bonds of silacycloalkanes can be selectively converted to C-N bonds at the β -position of the silicon atoms. The experimental data and theoretical calculations indicate that the strong σ -donor ability of the carbon-silicon bonds is responsible for the β -selectivity. Because silicon can be considered a bioisostere of carbon, the present protocol is applicable to synthesizing multi-functionalized organosilicon compounds with the potential to be powerful tools for drug discovery.



Division of Synthetic Chemistry

– Advanced Inorganic Synthesis –

https://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
TAKAHATA, Ryo
(D Sc)



PD
LIU, Ming-Han
(Ph D)



PD
SUZUKI, Wataru
(Ph D)



PD
LIAN, Zichao
(D Sc)



PD
KIM, Jungryang
(D Energy Sc)



PD
PELICANO, Christian
(Ph D)

Students

MATSUMOTO, Kenshi (D3)
OKAMOTO, Yasuo (D2)
ZHANG, Jie (D2)
LI, Zhanzhao (D2)
TAKEKUMA, Haruka (D1)

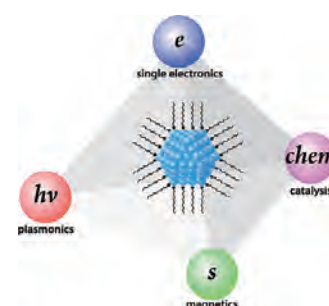
CHIGA, Yuuki (D1)
KANEKO, Ryota (M2)
KOSHI, Yuuki (M1)
NAKAGAWA, Fumiko (M1)
MANABE, Kouhei (M1)

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).

Formation of Strong $L1_0$ -FePd/ α -Fe Nanocomposite Magnets by Visualizing Efficient Exchange Coupling

Conceptual nanocomposite magnets (NCMs) composed of exchange-coupled hard/soft magnetic phases have been expected to show excellent magnetic performance based on simultaneous high coercivity (H_c) and high saturation magnetization (M_s). In our previous works, however, the H_c was considerably lower than its theoretical value (H_d), which prevented us from improving the performance of NCMs.

Here, we show that the H_c of isolated particulate $L1_0$ -FePd/ α -Fe NCMs is dominated by their phase segregation into core/shell-like structures versus Janus-like structures. Using first-order reversal curve (FORC) analysis, we clearly distinguished a microscopically undetectable difference in the phase-segregation structure in the NCMs, finding both efficient and inefficient exchange coupling. The nanostructurally controlled NCMs dominated by core/shell-like structure with efficient exchange coupling showed the largest energy product ($(BH)_{\max} = 17.5$ MGOe) in the Fe-Pd system and the highest H_c/H_a value (26.5%) among all NCM powders.

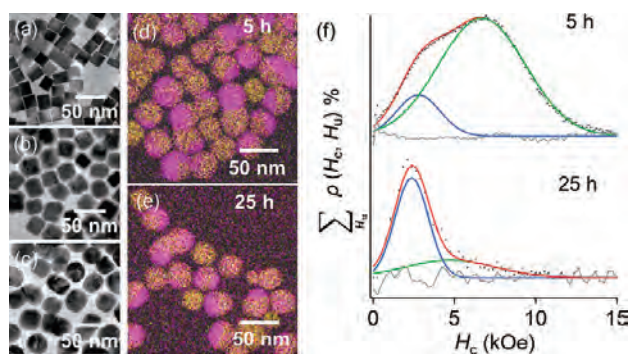


Figure 1. (a–c) TEM images of (a) Pd nanoparticles (NPs), (b) Pd@FeO_x core@shell NPs with Fe/Pd molar ratio of 66/34, and (c) $L1_0$ -FePd/ α -Fe NCMs obtained by reductive annealing of b at 540 °C for 5 h. (d, e) EDX elemental maps of $L1_0$ -FePd/ α -Fe NCMs synthesized by the annealing of b at 540 °C for (d) 5 h and (e) 25 h. (f) FORCs analysis for d and e. Blue and green curves are fitting curves by a Gaussian function, corresponding to inefficient and efficient exchange coupled NCMs, respectively, red curves are the sums of green and red curves, black dots are raw data, and gray curves are difference between red curves and black dots.

Plasmonic p–n Junction for Infrared Light to Chemical Energy Conversion

Solar light is an important energy resource for human society. The parts of the solar spectrum used for solar energy conversion, including photosynthesis and artificial photosynthesis, are limited to the ultraviolet (UV), visible, and a limited region of near infrared (NIR) light (700–1000 nm). IR light, which accounts for almost half of all solar energy, particularly IR light at wavelengths longer than 1000 nm, including shortwave IR (SWIR: 1400–3000 nm), represents a vast source of untapped energy. Developing artificial IR light-to-energy conversion systems would open up this resource for applications.

Here, we synthesized an IR-responsive plasmonic energy conversion system composed of CdS/plasmonic Cu₇S₄ heterostructured nanocrystals (HNCs), which achieved highly efficient photocatalytic H₂ evolution (Figure 2a). Cu₇S₄ NCs, which exhibit localized surface plasmon resonance (LSPR) in IR region, can be applied to harvesting solar energy in the IR region (Figure 2b). The CdS/Cu₇S₄ HNCs exhibited an exceedingly high apparent quantum yield (AQY) of 3.8% at 1100 nm, which exceeds the current record for photocatalytic H₂ evolution under IR-light irradiation (Figure 2c). Furthermore, we demonstrated that our novel HNCs can convert energy from the solar spectrum up to the longest wavelengths (*i.e.*, 2000–2500 nm). Our spectroscopic investigations using femtosecond-laser flash photolysis reveal that the high catalytic activity of our system was related to efficient hot electron injection and long-lived charge separation (> 273 μ s) at the p–n heterojunction of the CdS/Cu₇S₄ HNCs, which is unlike a conventional Schottky junction at the heterointerface of plasmonic metal/semiconductor NCs. The present work should encourage further development of solar fuel generation systems driven by these previously untapped solar energy resources.

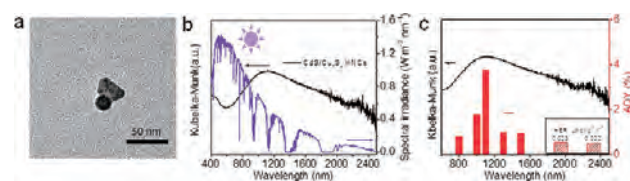


Figure 2. (a) TEM image of CdS/Cu₇S₄ HNCs. (b) Solar spectrum (purple line), and diffuse reflectance spectrum of CdS/Cu₇S₄ HNCs (black line). (c) Apparent quantum yield (AQY) of HER activity of CdS/Cu₇S₄ HNCs.

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
NAKAMICHI, Kimiyo
NAKAJIMA, Yuki

SEO, Haruna
YANADA, Mizuho

Proj Res

MATSUKAWA, Kimihiro (D Eng)*

*Res of Kyoto Inst Technol

Students

ISHIDA, Hisayuki (M2)
OHNO, Haruhisa (M2)
TAKEDA, Yusuke (M2)

HAN, Yutong (M1)
OKUBO, Ryo (M1)
TORIBUCHI, Taito (M1)

YOSHIKAWA, Shuhei (M1)
OKADA, Tasuku (UG)

KISHI, Keisuke (UG)
SAITO, Masahiro (UG)

Guest Res Assoc

BOUAD, Vincent
MORANDINI, Andrea

Ecole Nationale Supérieure de Chimie de Montpellier (ENSCM), France, 18 June–19 August
Università Ca' Foscari Venezia, Italy, 2 October 2019–3 February 2020

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).

pMAIRS Analysis on Chain-End Functionalization of Densely Grafted, Concentrated Polymer Brushes

The degree of chain-end functionality in a densely grafted, concentrated polymer brush is a critical parameter. In this study, *p*-polarized multiple-angle incidence resolution spectrometry (pMAIRS) technique was applied to monitor the emergence and disappearance of substituted azide (N_3) at the chain ends of polymer brushes, allowing accurate determination of the azide density and the click reaction efficacy. The peak separation of the N_3 absorption bands in the pMAIRS spectra showed that azide substitution occurred not only at the brush ends but also at underlying initiators that did not react during surface-initiated atom transfer radical polymerization (Figure 1). Hence, the density of each type of azide group and the efficiencies of the azidation and click reaction could successfully be estimated. Furthermore, a chain-end-selective click reaction was demonstrated for the azide-functionalized polymethacrylate-type polymer brushes based on size exclusion effects and polarity differences. Thus, the pMAIRS method provides important quantitative information that can expand applications of chain-end-functionalized polymer brushes.

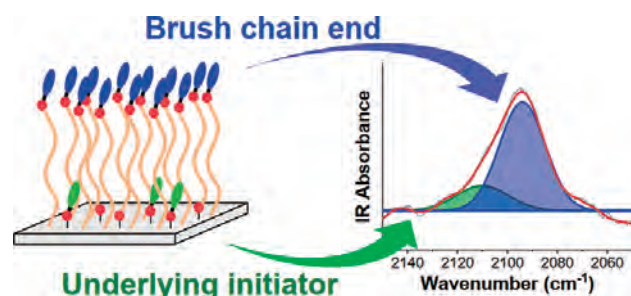


Figure 1. Peak separation of the N_3 absorption band in the pMAIRS spectra of an azide-functionalized polystyrene brush. Multiple Gaussian fitting highlights the peaks of brush-chain-end azides (blue) and azide-substituted initiators (green).

Main-Chain Stiffness of Cellulosic Bottlebrushes with Polystyrene Side Chains Introduced Regioselectively at the *O*-6 Position

We describe the conformational characteristics of a cellulosic bottlebrush, *i.e.*, a cellulose derivative of densely substituted side chains, in a dilute solution in order to clarify the effect of cellulosic main-chain stiffness and side-chain crowdedness. Novel cellulosic bottlebrushes **1** (Figure 2a) with polystyrene (PSt) side chains and methyl groups at the *O*-6 and *O*-2,3 positions, respectively, were highly regioselectively synthesized via a protecting group strategy in combination with a copper-catalyzed azide-

alkyne coupling click reaction, yielding densely graft polymers where PSt chains were introduced in every anhydroglucose repeating unit, *i.e.*, at a “constant” distance of 0.5 nm along the cellulose backbone. Small-angle X-ray scattering (SAXS) measurements of **1** in dimethylformamide revealed that the cross-sectional radius of gyration depended on the degree of polymerization (*DP*) of the PSt side chains in accordance with the power law with an exponent of 0.50, indicating that the PSt side chains adopted extended conformation owing to the inter-side-chain interaction, *i.e.*, the excluded volume effect among the neighboring side chains. Size exclusion chromatography–multi-angle light scattering (SEC-MALS) experiments were conducted to determine the main-chain stiffness. Despite the use of a poor solvent for PSt, the stiffness parameter λ^{-1} was almost independent of the *DP* of the PSt side chains up to 60 even in the brush regime of side-chains with inter-chain interaction and hence somehow stretched conformation. This behavior differs from those of previously reported bottlebrushes of flexible main chains and successfully demonstrated the cellulosic main chain intrinsically so stiff to form bottlebrushes of sufficiently long side chains with little effect on the main-chain conformation (Figure 2b). This would expand the diversity in design of bottlebrushes along with the chirality of cellulosic chain.

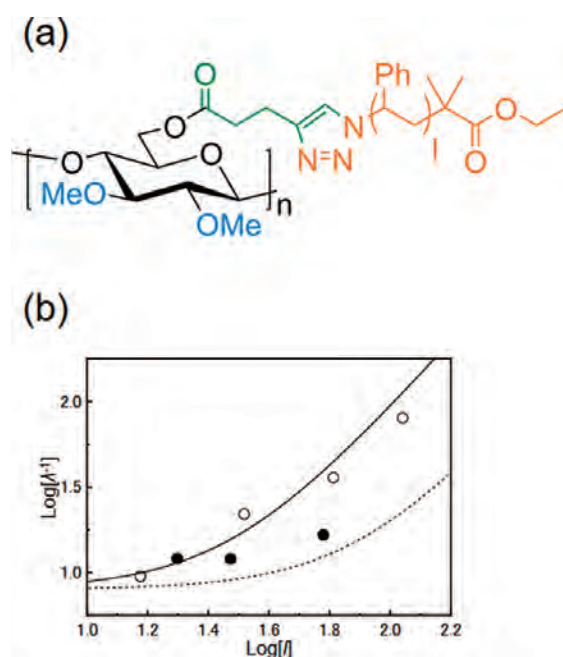


Figure 2. (a) Chemical structure of cellulosic bottlebrushes **1** with PSt side chains: $l = 60, 30,$ and 20 . (b) The dependence of λ^{-1} on the degree of polymerization (l) of the side chains for **1** in DMF/LiBr (filled circles) in this study and PSt-PSt bottlebrushes in cyclohexane (open circles) reported in literatures. The solid and broken lines represent theoretical curves for the PSt-PSt bottlebrush calculated with $h = 0.27$ nm (solid line) and $h = 0.52$ nm (broken line) in a Θ -solvent.

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*
LU, Yangtian
(D Eng)



PD
LI, Wenjuan
(Ph D)

Researcher (pt)

KATO, Tatsuhisa (D Sc)

Program-Specific Res

FUJITA, Takehiro

*New Research Field
Development Project

Students

SUN, Liansheng (D3)
FAN, Weijia (D3)
PARK, Beomsu (D3)
LI, Xiaopei (D2)
IMAMURA, Yuji (M2)

JIANG, Yuhan (M2)
ONOZUKA, Kota (M2)
ISHIDA, Kosuke (M1)
TERABAYASHI, Tomoaki (M1)
HE, Yu Zhong (M1)

MORI, Takahiro (RS)
WU, Jia-De (RS)
IKARI, Seiji (UG)
UEMURA, Seigo (UG)
ONCHI, Koshiro (UG)

KUNO, Taiki (UG)
TAKEUCHI, Hinako (UG)

Guest Res Assoc

CHEN, Dongyang University of St. Andrews, Scotland, 15 October–17 November
SOE, Myo Min University of Yangon, Myanmar, 16 November–13 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

Lu, Y.; Yamago, S., One-step Synthesis of Dendritic Highly Branched Polystyrenes by Organotellurium-mediated Copolymerization of Styrene and a Dienyl Telluride Monomer, *Angew. Chem. Int. Ed.*, **58**, 3952-3956 (2019).
Fan, W.; Yamago, S., Synthesis of Structurally Controlled Poly(N-vinyl amide)s and Poly(vinyl amine)s and Their Block Copolymers Using Organotellurium-mediated Radical Polymerization, *Angew. Chem. Int. Ed.*, **58**, 7113-7116 (2019).
Li, X.; Ogiwara, T.; Abe, M.; Nakamura, Y.; Yamago, S., The Effect of Viscosity on the Diffusion and Termination Reaction of Organic Radical Pairs, *Chem. Eur. J.*, **25**, 9846-9850 (2019).

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 Pt⁰ complex Pt(PPh₃)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.

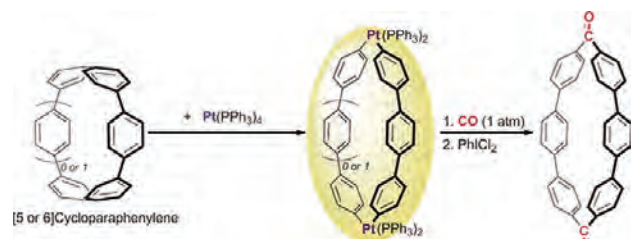


Figure 1. Carbon–Carbon Bond Activations of Cycloparaphenylenes by a Platinum Complex.

One-Step Synthesis of Dendritic Highly Branched Polystyrenes by Organotellurium-Mediated Copolymerization of Styrene and a Dienyl Telluride Monomer

By a one-step copolymerization of dienyly telluride (DT) and styrene (St) in the presence of organotellurium chain transfer agent (CTA) at thermal condition, dendritic highly branched polystyrenes (HB-PSts) were successfully synthesized. The molecular weight, branching density, and dendritic generation were easily controlled by the ratio of CTA, DT, and St with maintaining low dispersity ($D < 2.2$). The branching efficiency estimated by a deuterium-labeling experiment showed that DT quantitatively (>95%) served as the branching point. The end group fidelity was determined by the end group transformation to pyren derivative and was proved to be high (ca. 90%). Intrinsic viscosity of the HB-PSt was significantly lower than that of linear polystyrenes and were easily tuned by the branching number and branching density. The method is compatible of various functional groups, and furthermore, chloro and acetoxy-substituted styrenes were also used as comonomer. A tadpole block copolymer was also synthesized by starting from linear PSt as a macroinitiator.

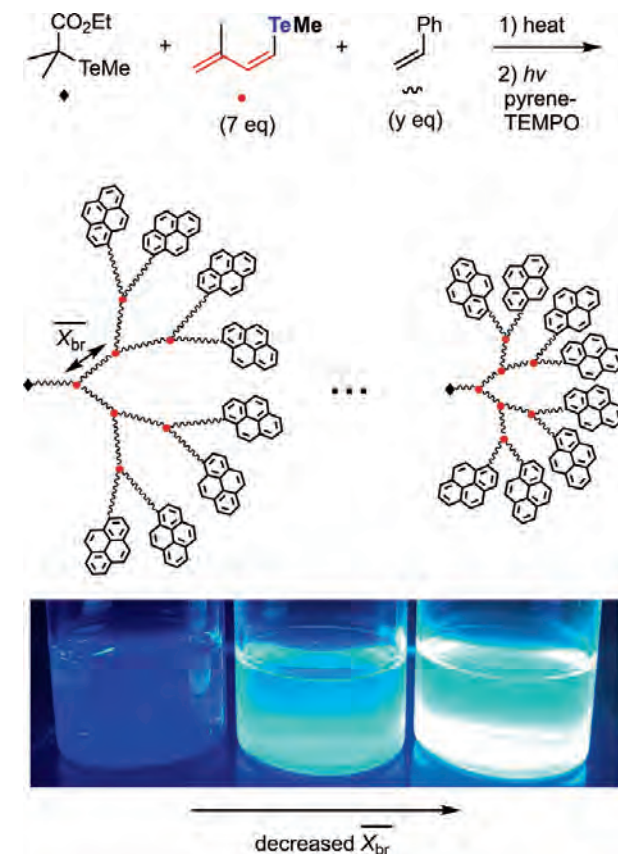


Figure 2. End group transformation of the highly branched polystyrene.

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 Assist Prof
HERBSCHLEB, Ernst David
(Ph D)



Program-Specific Res
OHKI, Izuru
(D Bioscience)



Program-Specific Res
TAKEMURA, Yuki



Res (pt)
HAYASHI, Kan
(D Sc)

Students

NISHIKAWA, Tetsuri (M2)

WATANABE, Akira (M2)

YAMASHITA, Shungo (M2)

NAKAMURA, Masaya (M1)

MORITA, Kouki (M1)

FU, Haining (RS)

FUJIE, Masahiro (UG)

MURAMATSU, Kanako (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 Materials
NV Center
Quantum Sensing
Quantum Information Science

Selected Publications

Herbschleb, E. D.; Kato, H.; Maruyama, Y.; Danjo, T.; Makino, T.; Yamasaki, S.; Ohki, I.; Hayashi, K.; Morishita, H.; Fujiwara, M.; Mizuochi, N., Ultra-long Coherence Times Amongst Room-temperature Solid-state Spins, *Nat. Commun.*, **10**, 3766 (2019).

Morishita, H.; Tashima, T.; Mima, D.; Kato, H.; Makino, T.; Yamasaki, S.; Fujiwara, M.; Mizuochi, N., Extension of the Coherence Time by Generating MW Dressed States in a Single NV Centre in Diamond, *Sci. Rep.*, **9**, 13318 (2019).

Tashima, T.; Morishita, H.; Mizuochi, N., Experimental Demonstration of Two-photon Magnetic Resonances in a Single-spin-system of a Solid, *Phys. Rev. A*, **100**, 023801 (2019).

Yamaguchi, T.; Matsuzaki, Y.; Saito, S.; Watanabe, H.; Mizuochi, N.; Ishi-Hayase, J., Bandwidth Analysis of AC Magnetic Field Sensing Based on Electronic Spin Double Resonance of Nitrogen-vacancy Centers in Diamond, *Jpn. J. Appl. Phys.*, **58**, 100901 (2019).

Ultra-long Coherence Times Amongst Room-temperature Solid-state Spins

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

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

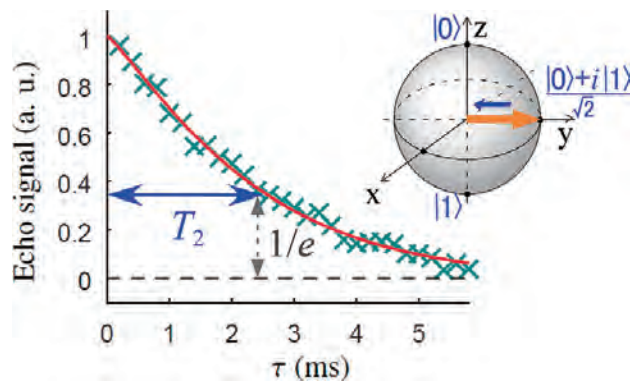


Figure 1. Echo signal of the single NV centre at room temperature. (Insert) Bloch sphere to show the coherence (superposition state).

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

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

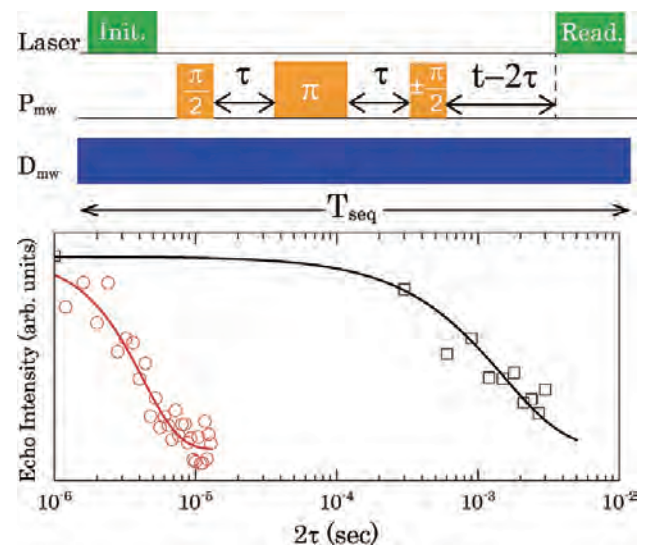


Figure 2. (Top) Pulse sequence to observe T_{2p} and T_2 with applying a phase cycle to the final $\pi/2$ pulse. (Bottom) Black and red plots show the results of T_{2p} and T_2 measurements, respectively. They are fitted by exponential decay curves described by black and red solid lines.

Division of Materials Chemistry

– Nanospintronics –

<https://www.scl.kyoto-u.ac.jp/~onoweb/>



Prof
ONO, Teruo
(D Sc)



Assoc Prof
MORIYAMA, Takahiro
(Ph D)



Assist Prof
SHIOTA, Yoichi
(D Eng)



Assist Prof*
HISATOMI, Ryusuke
(D Sc)

*New Research Field
Development Project

Students

ANDO, Fuyuki (D3)

OKUNO, Takaya (D3)

ODA, Kento (D3)

NISHIMURA, Tomoe (D3)

ISHIBASHI, Mio (D2)

HIRATA, Yushou (D2)

LI, Tian (D2)

IKEBUCHI, Tetsuya (D1)

HONG, Yu Min (D1)

IWAKI, Hiroyuki (M2)

FUNADA, Shinsaku (M2)

KOBAYASHI, Yuta (M1)

NODA, Kaoru (M1)

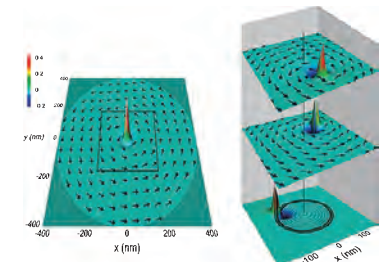
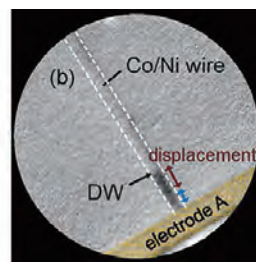
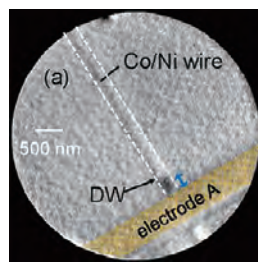
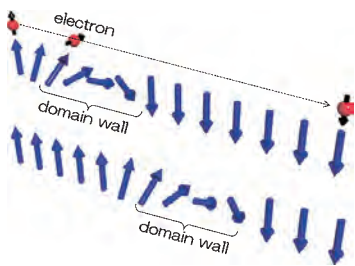
MIYASAKA, Yuta (M1)

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

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

Hirata, Y.; Kim, D.-H.; Kim, S. K.; Lee, D.-K.; Oh, S.-H.; Kim, D.-Y.; Nishimura, T.; Okuno, T.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Tserkovnyak, Y.; Shiota, Y.; Moriyama, T.; Choe, S.-B.; Lee, K.-J.; Ono, T., Vanishing Skyrmion Hall Effect at the Angular Momentum Compensation Temperature of a Ferrimagnet, *Nat. Nanotechnol.*, **14**, 232-236 (2019).

Moriyama, T.; Hayashi, K.; Yamada, K.; Shima, M.; Ohya, Y.; Ono, T., Intrinsic and Extrinsic Antiferromagnetic Damping in NiO, *Phys. Rev. Materials*, **3**, 051402 (2019).

Gray, I.; Moriyama, T.; Sivadas, N.; Stiehl, G. M.; Heron, J. T.; Need, R.; Kirby, B. J.; Low, D. H.; Nowack, K. C.; Schlom, D. G.; Ralph, D. C.; Ono, T.; Fuchs, G. D., Spin Seebeck Imaging of Spin-Torque Switching in Antiferromagnetic Pt/NiO Heterostructures, *Phys. Rev. X*, **9**, 041016 (2019).

Iino, T.; Moriyama, T.; Iwaki, H.; Aono, H.; Shiratsuchi, Y.; Ono, T., Resistive Detection of the Neel Temperature of Cr₂O₃ Thin Films, *Appl. Phys. Lett.*, **114**, 022402 (2019).

Spin-transfer-torque-driven Magnetic Domain Wall Motion in Antiferromagnetically Coupled Ferrimagnets

Magnetic domain wall (DW) racetrack memory is a next-generation, non-volatile and high-density magnetic memory, where the magnetic domain walls work as information bits and they are controlled by electric current via the effect of spin transfer torque (STT). Antiferromagnets are considered one of the material candidates for the racetrack memory. However, experimental explorations of STT in antiferromagnets remain elusive because of experimental difficulty accessing some of the magnetic properties. In this work, we instead examined the effects of STT in a ferrimagnetic material (a GdFeCo alloy), a more experimentally accessible material, which mimics an antiferromagnetic property at a certain temperature, the so-called angular momentum compensation temperature T_A . We measured the DW velocity under the application of electric current at various temperatures (see Figure 1 (a) for the experimental setup). We found that, as shown in Figure 1 (b), the DW velocity changes its sign in the vicinity of T_A . By fitting the experimental data with the theoretical model, we quantitatively determined the two components of STT, *i.e.* the adiabatic and non-adiabatic torques. Our result shows that the non-adiabatic STT in antiferromagnets is indeed quite large, suggesting that an energy-efficient DW racetrack memory may be possible with antiferromagnets.

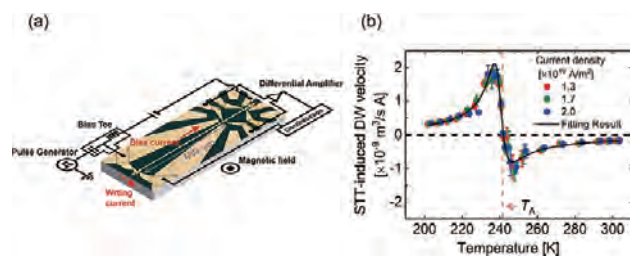


Figure 1. (a) Schematic illustration of the experimental setup. (b) The STT-induced DW velocity as a function of temperature. The dotted orange line represents the angular momentum compensation temperature T_A .

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 2(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.

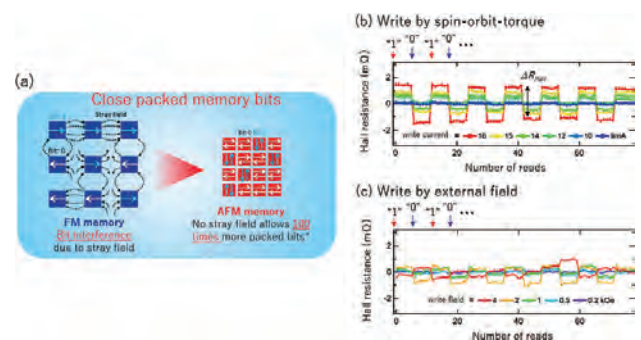


Figure 2. (a) Comparison between ferromagnetic bits and antiferromagnetic bits in terms of memory bit density. (b) After each write (“0”, “1”) by a spin-orbit-torque, the memory states were read by the Hall resistance. (c) After each write (“0”, “1”) by an external field, the memory states were read by the Hall resistance.

Division of Biochemistry – Biofunctional Design-Chemistry –

<https://www.scl.kyoto-u.ac.jp/~bfdc/index.html>



Prof
FUTAKI, Shiroh
(D Pharm Sc)



Assoc Prof
IMANISHI, Miki
(D Pharm Sc)



Assist Prof
KAWANO, Kenichi
(D Pharm Sc)



Program-Specific Assoc Prof
HIROSE, Hisaaki
(D Pharm Sc)

Students

MASUDA, Toshihiro (D3)

ARAFILES, Jan Vincent V. (D3)

SAKAMOTO, Kentarou (D2)

SAKAI, Takayuki (D1)

HIRAI, Yusuke (D1)

HSU, Wei-Yuan (M2)

NISHIMURA, Motoki (M2)

NOMURA, Yohei (M2)

SHINGA, Kenta (M2)

SUGIMOTO, Misaki (M2)

IWATA, Takahiro (M1)

KUROKI, Kakeru (M1)

NAGANO, Yuki (M1)

YOSHIDA, Atsuhiko (M1)

KURIYAMA, Masashi (UG)

MICHIBATA, Junya (UG)

OTONARI, Kenko (UG)

Scope of Research

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



KEYWORDS

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

Selected Publications

Masuda, T.; Baba, K.; Nomura, T.; Tsujita, K.; Murayama, T.; Itoh, T.; Takatani-Nakase, T.; Sokabe, M.; Inagaki, N.; Futaki, S., An Influenza-derived Membrane Tension-modulating Peptide Regulates Cell Movement and Morphology via Actin Remodeling, *Commun. Biol.*, **2**, 243 (2019).

Akishiba, M.; Futaki, S., Inducible Membrane Permeabilization by Attenuated Lytic Peptides: A New Concept for Accessing Cell Interiors through Ruffled Membranes, *Mol. Pharm.*, **16**, 2540-2548 (2019).

Kawaguchi, Y.; Ise, S.; Azuma, Y.; Takeuchi, T.; Kawano, K.; Le, T. K.; Ohkanda, J.; Futaki, S., Dipicolylamine/Metal Complexes that Promote Direct Cell-Membrane Penetration of Octaarginine, *Bioconjug. Chem.*, **30**, 454-460 (2019).

Sakai, T.; Kawano, K.; Iino, M.; Takeuchi, T.; Imanishi, M.; Futaki, S., Loosening of Lipid Packing by Cell-Surface Recruitment of Amphiphilic Peptides by Coiled-Coil Tethering, *Chembiochem*, **20**, 2151-2159 (2019).

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

Artificial Curvature Inducing Peptide Triggering Cellular Endocytic Uptake

Membrane curvature is no longer seen as a passive consequence of cellular activity but an active means to create membrane domains and to organize centres for membrane trafficking (McMahon & Gallop, *Nature*, (2005) 438, 590-596). The generation and maintenance of membrane curvature is of central importance for maintaining trafficking and cellular functions. It is therefore meaningful to develop a new tool for controlling membrane curvature to understand the fundamental aspects in cell homeostasis and the disorder. As a new tool candidate, we focused on amphipathic peptides. Some amphipathic peptides are known to induce membrane curvature by its interaction with membrane. We hypothesized that these amphipathic peptides can also induce membrane curvature in living cells by the interaction with plasma membranes and control cellular functions.

As a cellular activity which was regulated by membrane curvature, we focused on endocytic events. Plasma membrane curvature controls endocytosis events by affecting the activities of endocytic proteins (Zhao *et al.*, *Nat. Nanotech.*, (2017) 12, 750-756). Therefore, we hypothesized that amphipathic peptides can control endocytic events by inducing membrane curvature in living cells (Figure 1). To confirm the effects on endocytic events by amphipathic peptides, we measured the cellular uptake amount of fluorescent-labelled dextran, which is a fluid-phase endocytosis marker. In the amphipathic peptide-treated cells, increase in cellular uptake of fluorescent-labelled dextran was observed. Amphiphysin is a membrane curvature-sensing protein. The treatment of the cells with the amphipathic peptide increased the number of amphiphysin-derived puncta signals, suggesting that the amphipathic peptide may induce membrane curvature in living cells.

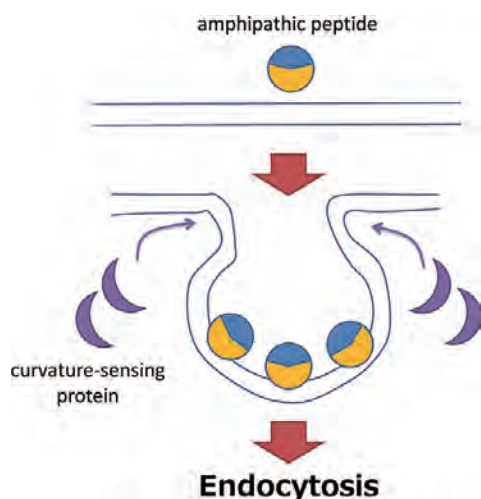


Figure 1. Mechanism of effect on endocytosis by amphipathic peptide.

Loosening of Lipid packing by Recruitment of Amphiphilic Peptides onto Cell Surface

Spatiotemporal membrane remodeling plays an important role in cellular events, including membrane trafficking, movement, growth and division. Alternations of the membrane structure are often accompanied by change of lipid packing. Establishment of means of controlling lipid packing may thus enable modification of various cellular functions and events.

Epsin-1 is an accessory protein involved in the induction of positive curvature necessary for clathrin-coated pit formation. We previously reported that an amphiphilic helical peptide corresponding to the N-terminus 18 residues (EpN18) has an ability to induce positive curvature^[1] and to loosen lipid packing of cell membranes.^[2] We have therefore focused on EpN18 as a means of manipulating lipid packing and the structure of the cell membranes.

In this study, we report a novel approach for recruitment of EpN18 onto cell surface using leucine-zipper peptides, E3 and K4, which form a stable heterodimer with a parallel coiled-coil structure.^[3] EpN18 was conjugated to the K4 segment, which specifically recognizes E3 segments expressed on cell surface. Live-cell confocal laser scanning microscopy analysis revealed that this cell-surface tethering of EpN18 yielded promotion of intracellular translocation of octaarginine and loosening of lipid packing. In addition, detachment of EpN18 from cell surface was accomplished by the treatment of excess amount of the K4 peptide without bearing EpN18. This approach thus shows promise for the modulation of lipid packing and related cellular events.^[4]

[1] S. Pujals *et al.* (2013) *ACS Chem. Biol.*, **8**, 1894-1899.

[2] T. Murayama *et al.* (2017) *Angew. Chem. Int. Ed.*, **56**, 7644-7647.

[3] Y. Yano *et al.* (2008) *ACS Chem. Biol.*, **3**, 341-345.

[4] T. Sakai *et al.* (2019) *ChemBioChem*, **20**, 2151-2159.

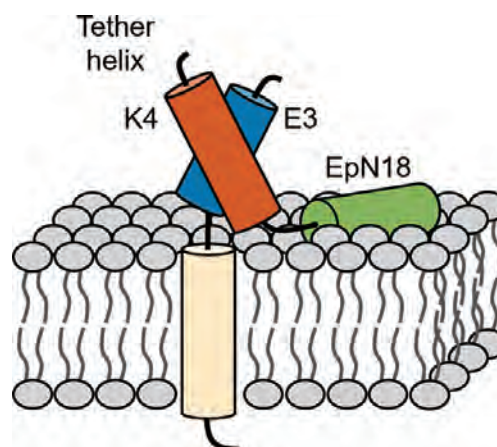


Figure 2. Tethering of EpN18 to cell-surface-expressed E3 segments by means of a coiled-coil heterodimer formation.

Division of Biochemistry – Chemistry of Molecular Biocatalysts –

<https://www.scl.kyoto-u.ac.jp/~bunta/index-j.html>



Prof

YAMAGUCHI, Shinjiro
(D Agr)



Assist Prof

WATANABE, Bunta
(D Agr)



Assist Prof

MASHIGUCHI, Kiyoshi
(D Agr)



PD

TAKEMOTO, Kodai
(D Sc)

Students

ISHIDA, Toshiaki (D1) KOBAYASHI, Takahiro (M1)
ISHIWARI, Kenji (M2) TAKEMOTO, Kiyoko (M1)
HIRANO, Rena (M2) HASE, Kanako (M1)

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

Yasui, R.; Seto, Y.; Ito, S.; Kawada, K.; Itto-Nakama, K.; Mashiguchi, K.; Yamaguchi, S., Chemical Screening of Novel Strigolactone Agonists that Specifically Interact with DWARF14 Protein, *Bioorg. Med. Chem. Lett.*, **29**, 938-942 (2019).
Seto, Y.; Yasui, R.; Kameoka, H.; Tamiru, M.; Cao, M.; Terauchi, R.; Sakurada, A.; Hirano, R.; Kisugi, T.; Hanada, A.; Umehara, M.; Seo, E.; Akiyama, K.; Burke, J.; Takeda-Kamiya, N.; Li, W.; Hirano, Y.; Hakoshima, T.; Mashiguchi, K.; Noel, J. P.; Kyojuka, J.; Yamaguchi, S., Strigolactone Perception and Deactivation by a Hydrolase Receptor DWARF14, *Nat. Commun.*, **10**, [191-1]-[191-10] (2019).
Burger, M.; Mashiguchi, K.; Lee, H. J.; Nakano, M.; Takemoto, K.; Seto, Y.; Yamaguchi, S.; Chory, J., Structural Basis of Karrikin and Non-natural Strigolactone Perception in *Physcomitrella patens*, *Cell Rep.*, **26**, 855-865 (2019).
Mashiguchi, K.; Hisano, H.; Takeda-Kamiya, N.; Takebayashi, Y.; Ariizumi, T.; Gao, Y.; Ezura, H.; Sato, K.; Zhao, Y.; Hayashi, K.; Kasahara, H., *Agrobacterium tumefaciens* Enhances Biosynthesis of Two Distinct Auxins in the Formation of Crown Galls, *Plant Cell Physiol.*, **60**, 29-37 (2019).

The Mechanism for Strigolactone Perception and Deactivation by a DWARF14 Receptor

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

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

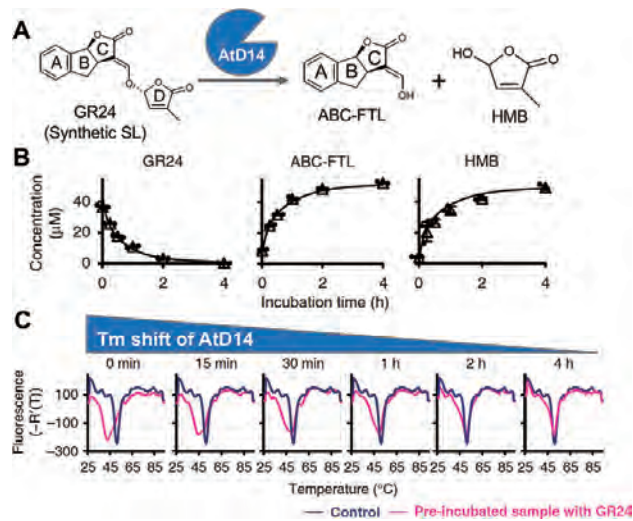


Figure 1. The time-course analyses of SL binding and hydrolysis by AtD14. (A) Hydrolysis reaction of SL (GR24) by AtD14. (B) Quantification of the hydrolysis reaction of GR24 (40 μ M) by AtD14. (C) The T_m shift of AtD14 incubated with GR24 (40 μ M) in DSF analysis. The maximum T_m shift was observed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

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

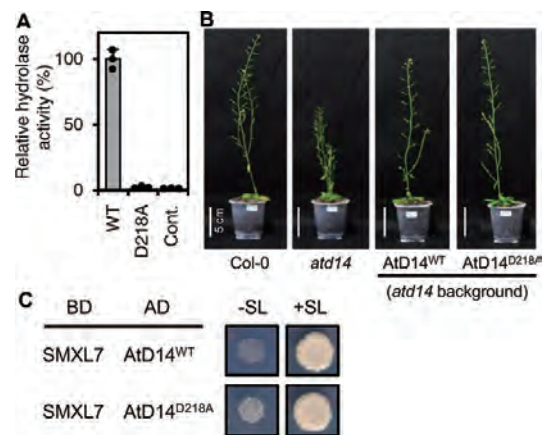


Figure 2. Functional analysis of the AtD14^{D218A} mutant. (A) The SL hydrolysis activities of maltose binding protein (MBP)-tagged wild-type of AtD14 protein (AtD14^{WT}) and the AtD14^{D218A} mutant. MBP was used in the control reaction. (B) The branching phenotype of Arabidopsis transgenic plants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

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

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

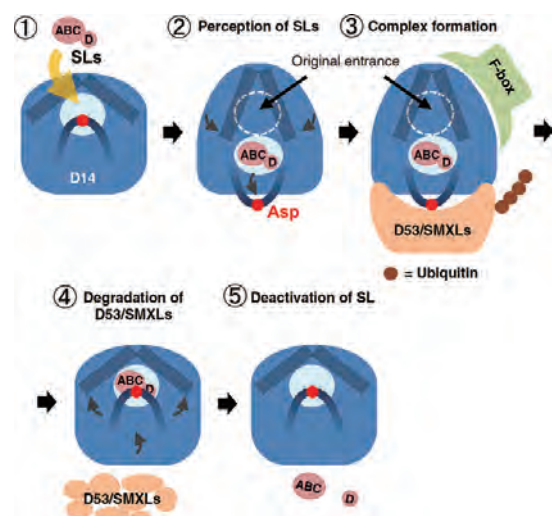


Figure 3. A proposed model of D14 in SL signaling. Bioactive SLs induce the conformational changes of D14, which triggers complex formation with the signaling partners. After the degradation of negative regulators of SL signaling (D53/SMXLs) and transmission of the SL signal, D14 reconstructs the catalytic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

Division of Biochemistry

– Molecular Biology –

<https://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

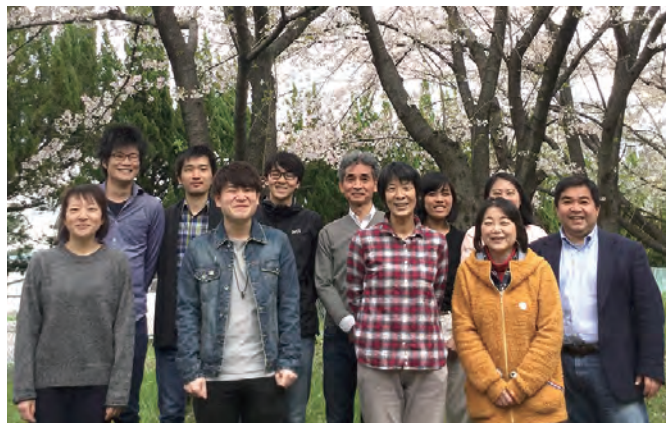
ZHANG, Xiao-Juan (D3) KURODA, Ryo (D3)
SHIMAMURA, Ryota (D3) AKAGI, Chika (D1)
WATARI, Machiko (D3) YAMADA, Koh (M2)

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 Signal Transduction
Phospholipid Signaling COP9 Signalosome
RNA



Selected Publications

Kato, M.; Tsuge, T.; Maeshima, M.; Aoyama, T., *Arabidopsis* PCaP2 Modulates the Phosphatidylinositol 4,5-bisphosphate Signal on the Plasma Membrane and Attenuates Root Hair Elongation, *Plant J.*, **99**, 610-625 (2019).
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 Ca²⁺-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).

PCaP2 Modulates Phosphoinositide Signaling on the Plasma Membrane

Arabidopsis plasma membrane-associated Ca²⁺-binding protein-2 (PCaP2), which belongs to a class of plant-unique Ca²⁺-binding proteins, also binds to phosphoinositides including phosphatidylinositol 4,5-bisphosphate [PtdIns(4,5)P₂]. PCaP2, together with PCaP1, was first characterized as a protein related to *Raphanus sativus* radish vacuole Ca²⁺-binding protein (RVCaB), and was later found to be associated with the plasma membrane *via* the *N*-myristoyl anchor and to bind Ca²⁺, the Ca²⁺/calmodulin complex, and phosphoinositides. Detailed biochemical analysis of PCaP2 has revealed that the 23-amino acid N-terminal polybasic region (PCaP2^{N23}) contains the *N*-myristoylation site and the sites of Ca²⁺/calmodulin- and phosphoinositide-binding activity, while the residual acidic region (PCaP2^{Δ23}) is the location of Ca²⁺-binding activity. In histochemical analysis, the *PCaP2* promoter was preferentially active in root hairs and pollen tubes, both of which are cellular structures formed by tip growth. While *pcap2* knockdown mutant exhibited longer root hairs than the wild type, root hair cell-specific overexpression of PCaP2^{N23} led to short-root-hair or no-root-hair phenotypes, and this defect was suppressed by overexpression of PIP5K3-YFP. These findings suggest that PCaP2 negatively modulates root hair elongation *via* its PtdIns(4,5)P₂-binding activity.

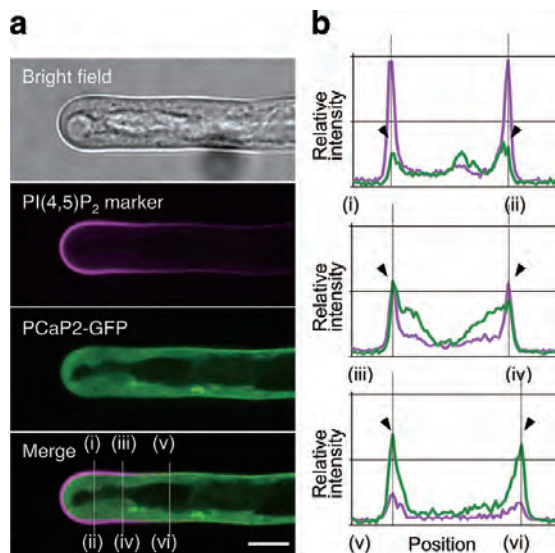


Figure 1. (a) Bright-field and fluorescence images (PCaP2-GFP and PI(4,5)P₂ marker) of elongating root hairs are shown. (b) The localization profiles of PCaP2-GFP (green) and the PI(4,5)P₂ marker (magenta) in the root hair apical region indicated in (a) are shown. In each column, a merged fluorescence image of PCaP2-GFP and the PI(4,5)P₂ marker, and their relative fluorescence intensities along the lines indicated in the image are shown. Dashed lines indicate the PI(4,5)P₂ marker localization on the plasma membrane. Arrowheads indicate the merge of PCaP2-GFP localization and PI(4,5)P₂ marker. Bars= 10 mm.

We focused on the function of PCaP2 *via* PtdIns(4,5)P₂-binding activity on the plasma membrane, and investigated the mechanism by which PCaP2 modulates root hair elongation. We found that the *pcap2* knockdown mutation caused a higher rate of root hair elongation than the wild type and partly suppressed the phenotype of a low elongation rate in the *pip5k3-2* mutant. Constitutively expressed 2xCHERRY-2xPH^{PLC}, a PtdIns(4,5)P₂ marker protein, and *PCaP2* promoter-driven PCaP2-GFP overlapped on the subapical plasma membrane of elongating root hairs (Figure 1). PCaP2^{N23}-GFP, which caused a low root hair elongation rate, exhibited a similar localization pattern on the plasma membrane to PCaP2-GFP. Inducibly overexpressed PCaP2-GFP, but not PCaP2^{Δ23}-GFP, replaced 2xCHERRY-2xPH^{PLC} on the plasma membrane in root meristematic epidermal cells (Figure 2), and suppressed FM4-64 internalization in elongating root hairs. Moreover, inducibly overexpressed PCaP2, but not PCaP2^{Δ23}, inhibited the endocytic recycling of PIN2-GFP, suggesting that PCaP2 affected the clathrin-mediated endocytosis involving the function of PtdIns(4,5)P₂ on the plasma membrane. Together, these results consistently support our idea that PCaP2 negatively modulates PtdIns(4,5)P₂ signaling on the subapical plasma membrane of elongating root hairs through competitive binding to PtdIns(4,5)P₂.

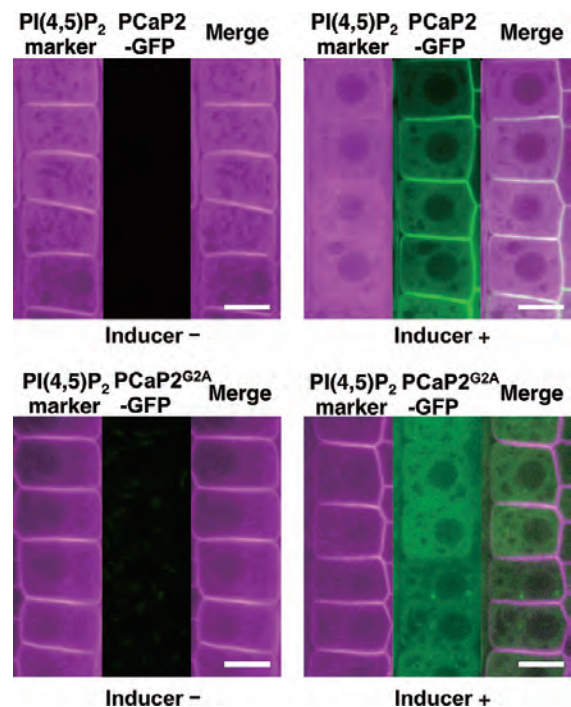


Figure 2. Fluorescence images of PCaP2-GFP (a) or PCaP2^{G2A}-GFP (b) expressed by an estradiol-inducible promoter, the PI(4,5)P₂ marker (magenta) expressed by the *UBIQUITIN10* promoter, and their merged images in meristematic root epidermal cells treated with (right panels) or without (left panels) 10 μM β-estradiol for 5 hours are shown. Bars = 10 mm.

Division of Biochemistry

– Chemical Biology –

<https://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)



Program-Specific Assist Prof
MAO, Di
(D Med Sc)



PD
TAKEMOTO, Misao
(D Eng)

Students

MENDOZA, Aileen de-Leon (D3)

HAKARIYA, Hayase (D2)

NODA, Naotaka (D2)

ADO, Genyir (D1)

JIN, Shuyu (D1)

NISHIO, Kosuke (D1)

PINEDA ARISTA, Karla Mariel (M2)

ZHAI, Peihong (M1)

SEGAWA, Shinsuke (M1)

SINGH, Vaibhav Pal (RS)

CRUZADO, Kevin Tan (RS)

Assist Techn Staffs

JUNG, Yejin PUNZALAN, Louvy Lynn Calvelo MANDAL, Sathi

Guest Res Assoc

CUI, Changyi

MAHAPATRA, Amarjyoti Das

DAO, Nhung Thi (Ph D)

Fudan University, China, P.R., 21 July–9 August

IIT Gandhinagar, India, 3 April–30 September

VNU University of Science, Vietnam National University, Vietnam, 25 November–20 December

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 Biology

Small Molecules

Chemical Library

Chemical Genetics

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).

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).

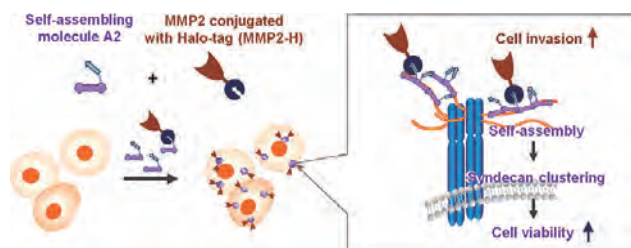
Furuta, T.; Mizukami, Y.; Asano, L.; Kotake, K.; Ziegler, S.; Yoshida, H.; Watanabe, M.; Sato, S.; Waldmann, H.; Nishikawa, M.; Uesugi, M., Nutrient-Based Chemical Library as a Source of Energy Metabolism Modulators, *ACS Chem. Biol.*, **14**, 1860-1865 (2019).

Takashima, I.; Kusamori, K.; Hakariya, H.; Takashima, M.; Vu, T. H.; Mizukami, Y.; Noda, N.; Takayama, Y.; Katsuda, Y.; Sato, S.; Takakura, Y.; Nishikawa, M.; Uesugi, M., Multifunctionalization of Cells with a Self-Assembling Molecule to Enhance Cell Engraftment, *ACS Chem. Biol.*, **14**, 775-783 (2019).

Nagata, A.; Akagi, Y.; Asano, L.; Kotake, K.; Kawagoe, F.; Mendoza, A.; Masoud, S. S.; Usuda, K.; Yasui, K.; Takemoto, Y.; Kittaka, A.; Nagasawa, K.; Uesugi, M., Synthetic Chemical Probes That Dissect Vitamin D Activities, *ACS Chem. Biol.*, **14**, 2851-2858 (2019).

Multifunctionalization of Cells with a Self-Assembling Molecule to Enhance Cell Engraftment

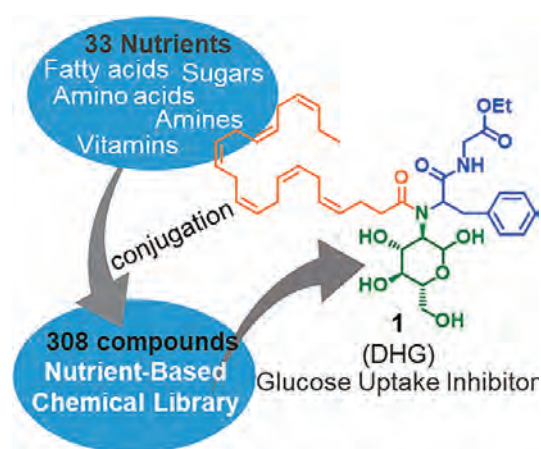
Cell-based therapy is a promising approach to restoring lost functions to compromised organs. However, the issue of inefficient cell engraftment remains to be resolved. Herein, we take a chemical approach to facilitate cell engraftment by using self-assembling molecules which modify two cellular traits: cell survival and invasiveness. In this system, the self-assembling molecule induces syndecan-4 clusters on the cellular surface, leading to enhanced cell viability. Further integration with Halo-tag technology provided this self-assembly structure with matrix metalloproteinase-2 to functionalize cells with cell-invasion activity. In vivo experiments showed that the pretreated cells were able to survive injection and then penetrate and engraft into the host tissue, demonstrating that the system enhances cell engraftment. Therefore, cell-surface modification via an alliance between self-assembling molecules and ligation technologies may prove to be a promising method for cell engraftment.



Nutrient-Based Chemical Library as a Source of Energy Metabolism Modulators

Covalent conjugates of multiple nutrients often exhibit greater biological activities than each individual nutrient and more predictable safety profiles than completely unnatural chemical entities. Here, we report the construction and application of a focused chemical library of 308 covalent conjugates of a variety of small-molecule nutrients. Screening of the library with a reporter gene of sterol reg-

ulatory element-binding protein (SREBP), a master regulator of mammalian lipogenesis, led to the discovery of a conjugate of docosahexaenoic acid (DHA), glucosamine, and amino acids as an inhibitor of SREBP (molecule 1, DHG). Mechanistic analyses indicate that molecule 1 impairs the SREBP activity by inhibiting glucose transporters and thereby activating AMP-activated protein kinase (AMPK). Oral administration of molecule 1 suppressed the intestinal absorption of glucose in mice. These results suggest that such synthetic libraries of nutrient conjugates serve as a source of novel chemical tools and pharmaceutical seeds that modulate energy metabolism.



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 & Environmtl. Studies)



Techn Staff *
OHMINE, Kyoko



Techn Staff
MAENO, Ayaka

*Re-employed Staff

Researcher

NAKAGAWA, Hiromichi (D Eng)

Program-Specific Res

GELDSTZER, Jan (Ph D)

Students

WADA, Yoshimasa (D3)
REN, Yongxia (D1)
SAWADA, Ayaka (M2)

MISONO, Tomoya (M2)
MORIWAKI, Kazuki (M1)
HU, Weizhe (M1)

KUSAKABE, Yu (M1)
LIU, Xingyuan (RS)
MATSUMOTO, Soma (UG)

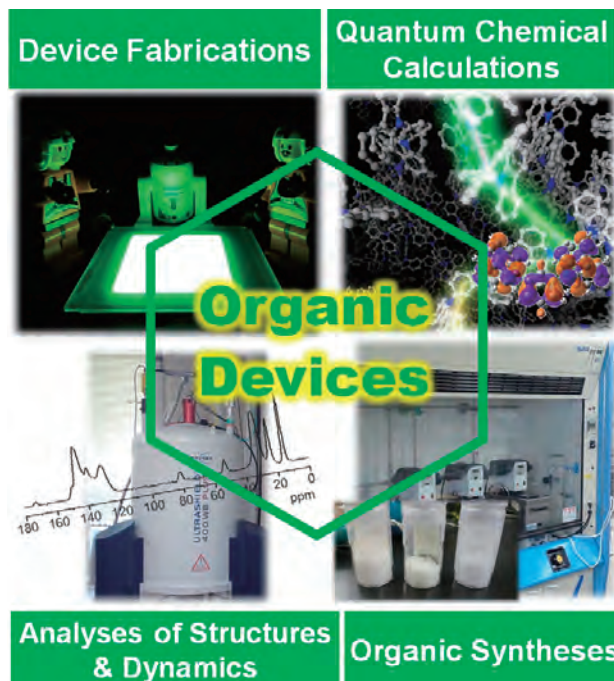
MURAMATSU, Tomomi (UG)
SAKAI, Kahori (UG)

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
Solid-State NMR
Quantum Chemical Calculation
Amorphous Materials
Dynamic Nuclear Polarization Enhanced NMR



Selected Publications

Zhang, D. D.; Suzuki, K.; Song, X. Z.; Wada, Y.; Kubo, S.; Duan, L. A.; Kaji, H., Thermally Activated Delayed Fluorescent Materials Combining Intra- and Intermolecular Charge Transfers, *ACS Appl. Mater. Interfaces*, **11**, 7192-7198 (2019).

Fukushima, T.; Ishibashi, H.; Suemasa, D.; Nakamura, R.; Yomogida, M.; Isono, T.; Satoh, T.; Kaji, H., Synthesis and Characterization of Cyclic P3HT as a Donor Polymer for Organic Solar Cells, *J. Polym. Sci., PartB: Polym. Phys.*, **57**, 266-271 (2019).

Kusaka, Y.; Hasegawa, T.; Kaji, H., Noise Reduction in Solid-State NMR Spectra Using Principal Component Analysis, *J. Phys. Chem. C*, **123**, 10333-10338 (2019).

Thermally Activated Delayed Fluorescent Materials Combining Intra- and Intermolecular Charge Transfers

A novel thermally activated delayed fluorescent (TADF) compound, 9-(3-((4,6-diphenyl-1,3,5-triazin-2-yl)oxy)phenyl)-3,6-diphenyl-9H-carbazole (PhCz-o-Trz), with a donor- σ -acceptor (D- σ -A) motif is developed. A flexible small space σ -junction is adopted to partly suppress the intramolecular charge transfer (intra-CT) while inversely enhancing the intermolecular charge transfer (inter-CT) between D/A moieties, realizing the coexistence of both intra-CT and inter-CT in an amorphous aggregate (Figure 1). The coexistence of dual CTs increases the complexity of the singlet and triplet state mixing, enhancing the triplet-to-singlet spin-flip transition and thereby the TADF emission. Additionally, PhCz-o-Trz is evaluated not only as an emitter but also as a sensitizing host for fluorescent and phosphorescent dopants.

With increasing the PhCz-o-Trz concentration, red-shift of fluorescence spectra was observed. Also, it is observed that both the intra- and inter-CT emissions coexist from 20 wt % to nearly 100 wt %. These results indicate the coexistence of the intra-CT and inter-CT, facilitating the triplet-to-singlet spin-flip transition. The device with DPEPO: 40% PhCz-o-Trz as the EML provided an EQEmax of 8.5%. Furthermore, devices with PhCz-o-Trz as the single host for fluorescence, phosphorescence, and TADF dopants were evaluated, realizing an maximum external quantum efficiency of 11.9, 27.1, and 20.2%, respectively. Our

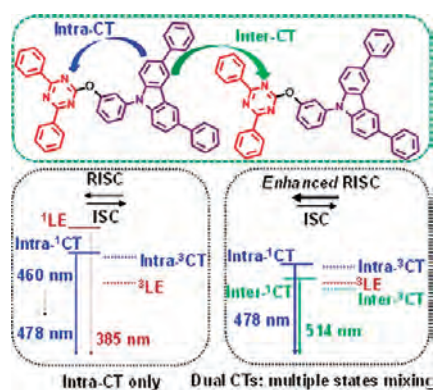


Figure 1. Molecular structure and mechanism of intra- and inter molecular charge transfer.

results here will shed new light on developing novel TADF materials with tunable intra- and inter-CT states, enabling not only TADF emitters with dual CT states but also single-molecule exciplex-type hosts with an easy device fabrication procedure, and may also deepen our understanding about TADF mechanisms.

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.

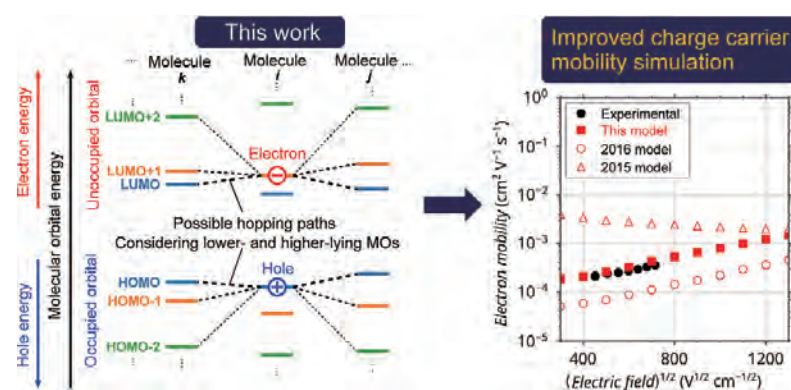


Figure 2. The charge transport simulation model for this work and electric field dependence of electron mobility.

Division of Environmental Chemistry

– Hydrospheric Environment Analytical Chemistry –

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



Prof
SOHRIN, Yoshiki
(D Sc)



Assist Prof
TAKANO, Shotaro
(D Sc)



Assist Prof
ZHENG, Linjie
(D Sc)



Techn Staff
IWASE, Misato



Guest Res Assoc*
GUNDIGA PUTTOJIRAO,
Gurumurthy
(Ph D)

Students

TSUJISAKA, Makoto (D3)
FUJIWARA, Yuta (M2)

TSUCHIYA, Mao (M2)
CHAN, Cheuk-Yin (M1)

NAGAE, Ayumi (M1)

*Geochemistry Research Lab, Birbal
Sahni Institute of Palaeosciences,
India, 25 January–25 July

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

- Zheng, L.; Minami, T.; Konagaya, W.; Chan, C.-Y.; Tsujisaka, M.; Takano, S.; Norisuye, K.; Sohrin, Y., Distinct Basin-scale-distributions of Aluminum, Manganese, Cobalt, and Lead in the North Pacific Ocean, *Geochim. Cosmochim. Acta*, **254**, 102-121 (2019).
- Zheng, L.; Sohrin, Y., Major Lithogenic Contributions to the Distribution and Budget of Iron in the North Pacific Ocean, *Sci. Rep.*, **9**, [11652-1]-[11652-9] (2019).
- 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.*, **511**, 494-509 (2019).
- Tanaka, Y.; Tsujisaka, M.; Zheng, L.; Takano, S.; Sohrin, Y., Application of NOBIAS Chelate-PA 1 Resin to the Determination of Zirconium, Niobium, Hafnium, and Tantalum in Seawater, *Anal. Sci.*, **35**, 1015-1020 (2019).
- Yang, S.-C.; Welter, L.; Kolatkar, A.; Nieva, J.; Waitman, K. R.; Huang, K.-F.; Liao, W.-H.; Takano, S.; Berelson, W. M.; West, A. J.; Kuhn, P.; John, S. G., A New Anion Exchange Purification Method for Cu Stable Isotopes in Blood Samples, *Anal. Bioanal. Chem.*, **411**, 765-776 (2019).

Major Lithogenic Contributions to the Distribution and Budget of Iron in the North Pacific Ocean

Recent studies have elucidated that iron (Fe) is a critical trace metal that influences the productivity of marine ecosystems and the biogeochemical cycles of other elements in the modern ocean. However, our understanding of the biogeochemistry of Fe remains incomplete. Herein, we report basin-scale and full-depth sectional distributions of total dissolvable iron (tdFe), dissolved iron (dFe), and labile particulate iron (lpFe = tdFe – dFe) in the North Pacific Ocean, as observed during three cruises of the GEOTRACES Japan program. We found that lpFe dominates tdFe and is significantly correlated with labile particulate aluminum (lpAl): $lpFe \text{ [nmol kg}^{-1}] = (0.544 \pm 0.005) lpAl \text{ [nmol kg}^{-1}] + 0.11 \pm 0.04$, $r^2 = 0.968$, $n = 432$. The results indicate a major lithogenic contribution to the distribution of particulate Fe. For dFe, the unique distribution is attributed to the combined effects of biogeochemical cycling, manganese reduction, and lithogenic contribution. Based on concurrent observations of Fe, Al, and manganese (Mn), we infer that the width of the boundary scavenging zone is approximately 500 km off the Aleutian shelf. We estimate the inventory of tdFe in the North Pacific as 1.1×10^{12} mol, which is approximately four times that of dFe. Our results emphasize the potential importance of lpFe in the ocean's iron cycle.

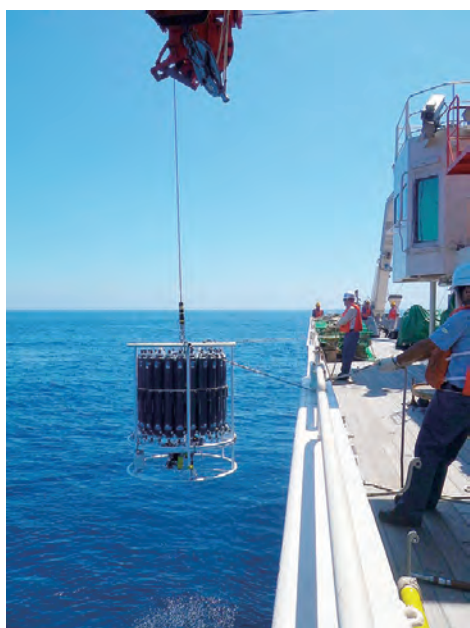


Figure 1. Clean water sampling during the KH-12-4 cruise.

Precise Analysis of the Concentrations and Isotopic Compositions of Molybdenum and Tungsten in Geochemical Reference Materials

Molybdenum (Mo) is a redox-sensitive element and its concentrations and stable isotope compositions are widely used as a redox proxy in paleoceanography. Tungsten (W) is an emerging new isotope proxy, which has potential as a tracer for hydrothermal and early diagenetic processes. We present a new method for the precise and accurate analysis of Mo and W concentrations and isotope compositions from one single sample aliquot, thus saving mass of a sample and making the results directly comparable without concerns related to analytical or natural sample heterogeneity. After acid digestion, Mo and W are separated from the sample matrix using chelating resin NOBIAS Chelate-PA1 and anion exchange resin AG1 X8. Matrix removal is highly efficient: the remaining percentage is 10^{-2} to $10^{-5}\%$ with respect to the initial weight. Subsequently, samples are measured for Mo and W concentrations and isotope compositions using multi-collector inductivity coupled plasma mass spectrometry (MC-ICP-MS). For mass bias correction and determination of concentrations, we use standard-sample bracketing and in addition an external correction method employing ruthenium (Ru) for Mo and rhenium (Re) for W. This double correction approach results in an external reproducibility of or below 0.10‰ (2SD) for $\delta^{98}\text{Mo}$ and 0.05‰ for $\delta^{186}\text{W}$. We present data for Mo and W in 12 geological reference materials including igneous rocks, sedimentary rocks, marine sediments, and manganese nodules. For Mo our method reproduces published values for the geological standard materials within analytical error of published values. For W, although published data do not always agree for a given geological standard material, our data agree within error with more recent data. We interpret a cause of the deviations is due to unknown effects of a desolvating nebulizer for MC-ICP-MS.

Division of Environmental Chemistry – Chemistry for Functionalized Surfaces –

<https://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 (D1)

FUJII, Masamichi (M1)

FUKUMI, Aki (M2)

YAMAGUCHI, Yuta (M1)

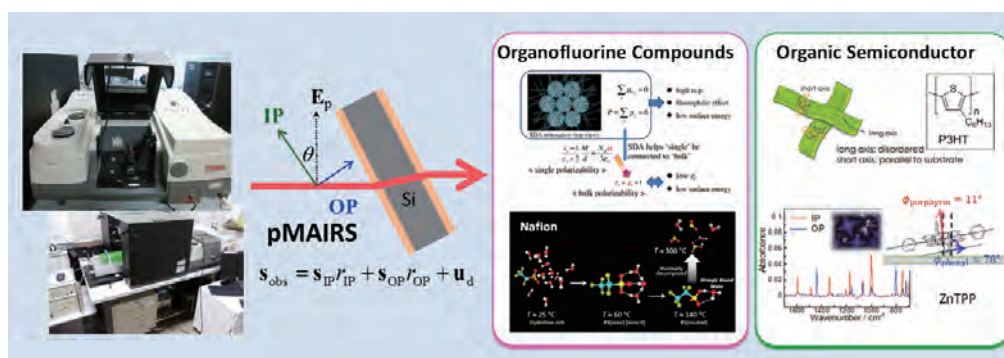
FUJIWARA, Ryoji (M2)

Scope of Research

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

KEYWORDS

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



Selected Publications

Shioya, N.; Murdey, R.; Nakao, K.; Yoshida, H.; Koganezawa, T.; Eda, K.; Shimoaka, T.; Hasegawa, T., Alternative Face-on Thin Film Structure of Pentacene, *Sci. Rep.*, **9**, 579 (2019).

Nakamura, T.; Shioya, N.; Shimoaka, T.; Nishikubo, R.; Hasegawa, T.; Saeki, A.; Murata, Y.; Murdey, R.; Wakamiya, A., Molecular Orientation Change in Naphthalene Diimide Thin Films Induced by Removal of Thermally Cleavable Substituents, *Chem. Mater.*, **31**, 1729-1737 (2019).

Shimoaka, T.; Sonoyama, M.; Amii, H.; Takagi, T.; Kanamori, T.; Hasegawa, T., Raman Optical Activity on Solid Sample: Identification of Atropisomers of Perfluoroalkyl Chains Having a Helical Conformation and No Chiral Center, *J. Phys. Chem. A*, **123**, 3985-3991 (2019).

Shioya, N.; Tomita, K.; Shimoaka, T.; Hasegawa, T., Second Generation of Multiple-Angle Incidence Resolution Spectrometry, *J. Phys. Chem. A*, **123**, 7177-7183 (2019).

Wang, C.; Sharma, S. K.; Olaluwoye, O. S.; Alrashdi, S. A.; Hasegawa, T.; Leblanc, R. M., Conformation Change of α -Synuclein(61-95) at the Air-Water Interface and Quantitative Measurement of the Tilt Angle of the Axis of its α -Helix by Multiple Angle Incidence Resolution Spectroscopy, *Colloids Surf. B*, **183**, 110401 (2019).

Sakakibara, K.; Nishiumi, K.; Shimoaka, T.; Hasegawa, T.; Tsujii, Y., pMAIRS Analysis on Chain-End Functionalization of Densely Grafted, Concentrated Polymer Brushes, *Macromolecules*, **52**, 6673-6682 (2019).

Alternative Face-on Thin Film Structure of Pentacene

Rod-shaped molecules represented by pentacene are known to form a highly ordered structure in a thin film, in which the molecular long axis aligns perpendicularly to the substrate surface, *i.e.*, end-on orientation. The face-on oriented thin film, on the other hand, where the molecular plane is parallel to the substrate, has never been found on an inert substrate represented by SiO₂. As a result, the face-on orientation has long been believed to be generated only on specific substrates such as a metal single crystal. In the present study, the face-on orientation grown on a SiO₂ surface has first been identified by means of visible and infrared p-polarized multiple-angle incidence resolution spectrometry (pMAIRS). The combination of the multiple techniques reveals that the face-on phase is definitely realized as the dominant component. The face-on film is obtained when the film growth is kinetically restricted to be prevented from transforming into the thermodynamically stable structure, *i.e.*, the end-on orientation. This concept is useful for controlling the molecular orientation in general organic semiconductor thin films.

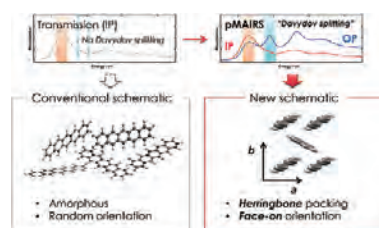


Figure 1. Face-on thin-film structure of pentacene revealed by Vis pMAIRS.

Raman Optical Activity on a Solid Sample: Identification of Atropisomers of Perfluoroalkyl Chains Having a Helical Conformation and No Chiral Center

Perfluoroalkyl (R_f) chains have a specific helical conformation due to the steric repulsion between the adjacent CF₂ units. Although R_f chains have no chiral center, two chiral structures, *i.e.*, the right-handed (R) and left-handed (L) helices, are available as the most stable conformations, which are atropisomers to each other. According to the stratified dipole array (SDA) theory, the helical structure about the chain axis plays a key role in the spontaneous molecular aggregation of R_f chains in a two-dimensional manner, and the R_f chains having the same chirality tend to be aggregated spontaneously to generate molecular domains. This implies that an R_f compound in a solid state should be a mixture of the R and L domains, and each domain should exhibit distinguishable optical activity. To

identify molecular domains with different atropisomers, in this study, Raman optical activity (ROA) measurements were performed on a Raman imaging spectrometer. Through the ROA measurements of recrystallized solid samples of an R_f compound, each particle exhibits an apparent optical activity, and the two atropisomers were readily distinguished. As a result, an R_f compound with the same helicity is found to be spontaneously aggregated as expected by the SDA theory.

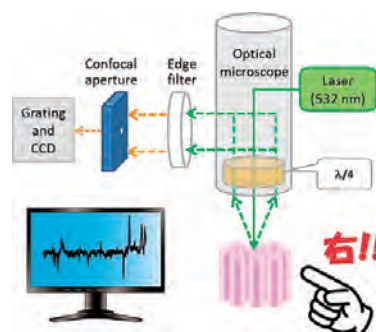


Figure 2. Overall view of the apparatus for Raman and ROA measurements.

Second Generation of Multiple-Angle Incidence Resolution Spectrometry

Infrared (IR) surface spectroscopic techniques commonly have long-term issues that 1) the multiple reflections of light in the substrate yield optical interference fringes in the absorption spectrum, and 2) the double-modulation of light at the interferometer in FT-IR makes a water-vapor-subtraction impossible. These measurement troubles often disturb the quantitative analysis of chemical bands of the analyte thin film. To overcome the long-term common issues, in the present study, an advanced MAIRS technique named “MAIRS2” is proposed: the angle of incidence is fixed at a larger angle to avoid the two problems; whereas the polarization angle is changed instead. With this simple conceptual change of MAIRS, as a result, we are ready for concentrating on spectral analysis only without concerning about the measurement troubles.

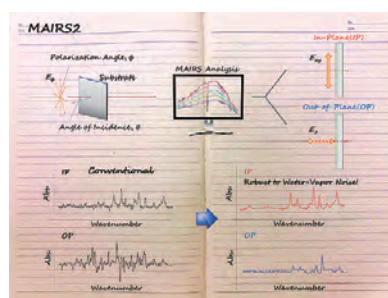


Figure 3. MAIRS2 realizes ideal IR measurements of a thin film for accurate molecular orientation analysis, which is highly robust to water-vapor and optical fringes.

Division of Environmental Chemistry – Molecular Microbial Science –

https://www.scl.kyoto-u.ac.jp/~mmsier/mmstojp/Top_en.html



Prof

KURIHARA, Tatsuo
(D Eng)



Assoc Prof

KAWAMOTO, Jun
(D Agr)



Assist Prof

OGAWA, Takuya
(D Agr)

Students

MARUOKA, Naruyuki (D3)

YOKOYAMA, Fumiaki (D3)

YUSUF, Yustina (D3)

KAMASAKA, Kouhei (D1)

SUWANAWAT, Nittikarn (D1)

CHEN, Mengyi (M2)

HIROSE, Kazuki (M2)

KUBOSHIMA, Misaki (M2)

KUREBAYASHI, Toshiki (M2)

LIU, Yuing (M2)

YONEDA, Yuki (M2)

HAYASHI, Kyosuke (M1)

KISHI, Shintaro (M1)

NARITA, Asuka (M1)

ZHU, Mengshan (M1)

WANG, Jue (RS)

Reseachers (pt)

KAWAI, Soichiro

CHEN, Chen

Assist Res Staff

KITAYAMA, Kaori

Scope of Research

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



KEYWORDS

Extremophiles

Phospholipid Acyltransferase

Bacterial Cold-adaptaion Mechanism

Extracellular Membrane Vesicle

Polyunsaturated Fatty Acid

Selected Publications

Kawai, S.; Kawamoto, J.; Ogawa, T.; Kurihara, T., Development of a Regulatable Low-temperature Protein Expression System Using the Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10, as the Host, *Biosci. Biotechnol. Biochem.*, **83**, 2153-2162 (2019).

Casillo, A.; Di Guida, R.; Carillo, S.; Chen, C.; Kamasaka, K.; Kawamoto, J.; Kurihara, T.; Corsaro, M. M., Structural Elucidation of a Novel Lipooligosaccharide from the Cold-Adapted Bacterium OMVs Producer *Shewanella* sp. HM13, *Mar. Drugs*, **17**, E34 (2019).

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).

Bacterial Regulation of Vesicle Production and Biofilm Dispersion in Response to Extracellular Environment

Extracellular membrane vesicles (EMVs) secreted by many kinds of bacteria have various roles in survival such as inter-cellular communication and biofilm formation. Therefore, the amounts and components of EMVs should be tuned in response to their growing environment. Although several vesiculation mechanisms are suggested, it remains largely unknown how bacteria regulate vesiculation in response to the environments. We are focusing on a sensor protein, HM1275, identified in EMVs of *Shewanella vesiculosa* HM13, a cold-adapted Gram-negative bacterium.

Addition of Lys to a poor nutrient medium increased the vesicle production by the parent strain in a dose-dependent manner, whereas the effect of Lys addition on the *hm1275*-disrupted mutant was less significant. HM1275 has approximately 40% sequence identity to BdlA, which is known as a protein for biofilm dispersion. The amount of biofilm of the parent decreased over time probably due to biofilm dispersion and was lower than that of the mutant in the poor medium containing additional Lys (Figure 1).

Together, HM1275 is involved in regulation of both vesicle production and biofilm dispersion in response to Lys in the poor nutrient medium. There may be a linkage between these two phenomena, where HM1275-containing EMVs released by the Lys-sensing cells are delivered to other cells to induce biofilm dispersion for collective cell behavior.

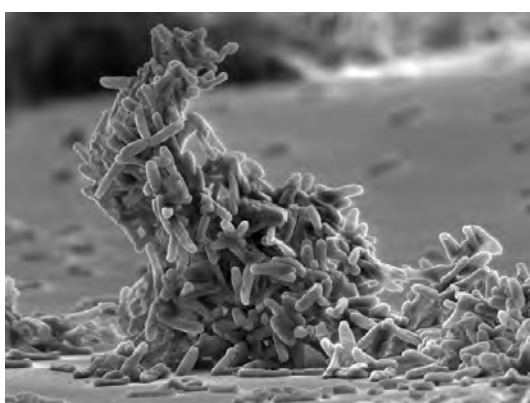


Figure 1. Side-view of SEM image of $\Delta hm1275$ biofilm.

Bioconversion of DHA into EPA

The psychrotrophic bacterium *Shewanella livingstonensis* Ac10 produces eicosapentaenoic acid (EPA) at cold temperatures. The EPA-less mutant that is deficient of *de novo*

EPA biosynthesis showed cold-sensitive phenotypes such as growth retardation and abnormal cell filamentation, and these phenotypes were suppressed by supplementation of EPA and of docosahexaenoic acid (DHA). The interesting finding was that the EPA-less mutant produced EPA when grown in the presence of DHA, suggesting the presence of the unidentified metabolic pathway that converts DHA into EPA (Figure 2A). The biosynthesis of EPA/DHA in marine bacteria has been intensively studied, whereas the other metabolic route including degradation and bioconversion are poorly understood. To understand the DHA conversion mechanism in *S. livingstonensis* Ac10, we carried out mutagenesis experiments of genes of β -oxidation enzymes and their homologs. We found that the disruption of *sl_1351* gene that putatively encodes 2,4-dienoyl-CoA reductase (FadH) resulted in the decreased conversion level (Figure 2B). FadH is an auxiliary enzyme of β -oxidation pathway and essential to degrade Δ^4 -unsaturated fatty acids, like DHA. As *Sl_1351* is highly homologous to a well-studied FadH from *Escherichia coli*, the DHA conversion is likely mediated through a typical β -oxidation pathway. On the other hand, possible β -oxidation intermediates other than EPA (e.g. octadecapentaenoic and hexadecatetraenoic acids) were not detected on the supplementation of DHA. It suggests that *S. livingstonensis* Ac10 metabolizes DHA to preferentially form EPA, which is an important biofactor for the bacterium.

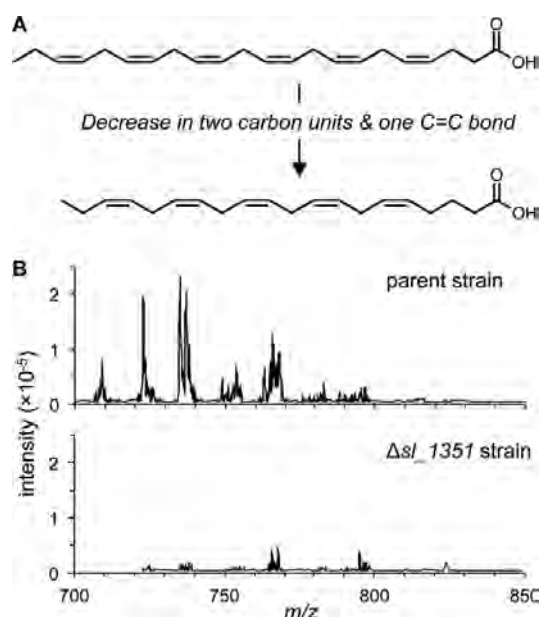


Figure 2. (A) The schematic view of the bioconversion from DHA to EPA. (B) Mass spectrometry analysis of EPA-containing phospholipids from the parent and Δsl_1351 cells. The precursor ion scans for the target ion of m/z 301 (corresponding to $[M-H]^-$ ion for EPA) are shown.

Division of Multidisciplinary Chemistry – Polymer Materials Science –

<https://www.scl.kyoto-u.ac.jp/~polymat/index.html>



Prof
TAKENAKA, Mikihiro
(D Eng)



Assoc Prof
OGAWA, Hiroki
(D Eng)

Students

KISHIMOTO, Mizuki (D2)
WATANABE, Yuki (D2)
IKEDA, Yuta (M2)
HIKAMI, Yuichi (M2)

ODA, Tappei (M1)
MITANI, Kenta (M1)
KUMAGAWA, Daiki (M1)
AOKURA, Shuta (UG)

KUWATA, Satoshi (UG)
MANDAI, Yuji (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

Nishitsuji, S.; Takenaka, M., Viscoelastic Effects on Dynamics of Concentration Fluctuations in Semi-dilute Polymer Solution in the Good Solvent Regime, *Polymer*, **179**, 121622 (2019).

Hashimoto, T.; Amino, N.; Nishitsuji, S.; Takenaka, M., Hierarchically Self-organized Filler Particles in Polymers: Cascade Evolution of Dissipative Structures to Ordered Structures, *Polym. J.*, **51(2)**, 109-130 (2019).

Ono, K.; Masuda, S.; Ogawa, H., Polymer-brush-decorated Colloidal Platelets: Precision Synthesis and Self-assembly, *Polym. Chem.*, **10**, 2686-2696 (2019).

Kinose, Y.; Sakakibara, K.; Ogawa, H.; Tsujii, Y., Main-Chain Stiffness of Cellulosic Bottlebrushes with Polystyrene Side Chains Introduced Regioselectively at the O-6 Position (in press).

In-situ Measurement of Self-assembling Block Copolymer Thin Film with GISAXS

Directed self-assembly (DSA) of block copolymers (BCPs) has been one of the most promising next generation lithography candidates. In order to use the DSA lithography for advanced semiconductor device manufacturing, we need to mitigate defects in the DSA materials and processes and to clarify the defect generation mechanism by using in-situ measurement of the self-assembling processes of BCPs. In this study, we, thus, observed the process of the self-assembly of a diblock copolymer by grazing incident angle small angle X-ray scattering (GISAXS) during heating process. Figure 1 shows a two-dimensional images of GISAXS for the self-assembling of Polystyrene-*b*-Poly methyl-methacrylate (PS-*b*- PMMA) ($M_n = 29800-28700$, M_n : number-averaged molecular weight) during heating processes at incident angles with 0.05° and 0.12° . An isotropic structure was induced near the glass transition temperature, and transformation to lamella structure was observed at 135°C . The lamellar structure has a larger period than isotropic structure. The structure gradually grew according to the temperature, and it turned out that the whole film had a vertical lamellar structure at 145°C . At higher temperature the long-range order of vertical lamellar structure was developed with temperature.

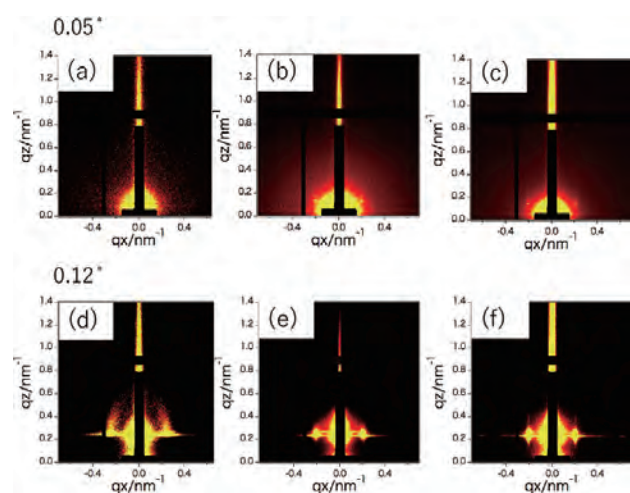


Figure 1. Two-dimensional GISAXS images of PS-*b*- PMMA in stepwise annealing process. these are at (a)135, (b)145, (c)180 °C with the incident angle of 0.12° and (d)135, (e)145, (f)180 °C with the incident angle of 0.05° .

Improving GISAXS-CT Images by Total Variation Minimization

Grazing incidence small-angle X-ray scattering (GISAXS) coupled with computed tomography (CT) has enabled visualizing the spatial distribution of nanostructures in thin films. The two-dimensional GISAXS images are obtained by scanning along the perpendicular direction to the X-ray beam at each rotation angle. Because the intensities at q positions contain nanostructural information, reconstructed CT images individually represent the spatial distributions of this information (*e.g.* size, shape, surface, characteristic length). These images are reconstructed from the intensities which are acquired at the angular intervals over 180° , though, it prolongs total measurement time. Moreover, this is often to increase with the radiation dosage and can cause damage to the sample. One way to reduce the overall measurement time is simply that scanning GISAXS measurement is performed along the perpendicular direction to the X-ray beam with a limited interval angle. Using filtered back-projection, CT images are reconstructed from the images of sinogram with the limited interval angles from $\Delta 3^\circ$ to $\Delta 48^\circ$ (FBP-CT images). However, these images are blurred and result in lower image quality. In this study, to optimize CT image quality, the total variation (TV) regularization is introduced to minimize sinogram image denoising and artifacts. In comparison with the FBP-CT images, we propose that the TV method can apply to down-sampling sinograms for improving CT images (TV-CT images).

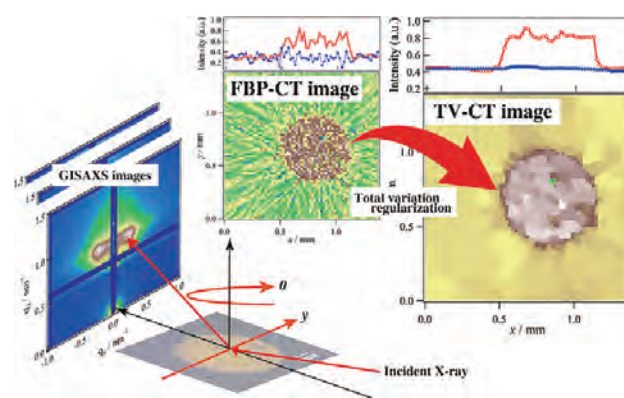


Figure 2. An overview of the FBP-CT and TV-CT images.

Division of Multidisciplinary Chemistry – Molecular Rheology –

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



Prof

WATANABE, Hiroshi
(D Sc)



Assoc Prof

MATSUMIYA, Yumi
(D Eng)

Students

MARUYAMA, Tatsuki (UG)

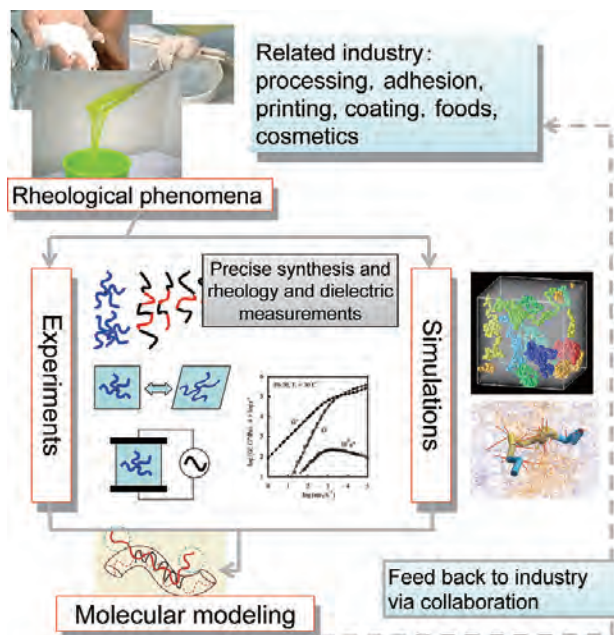
MOTEKI, Wataru (UG)

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

Kwon, Y.; Matsumiya, Y.; Watanabe, H., Dielectric Relaxation of Type-A Chains Undergoing Head-to-Tail Association/Dissociation: Difference from Head-to-Head Case and Correlation with Viscoelastic Relaxation, *Macromolecules*, **52**, 8484-8502 (2019).

Morelly, S. L.; Palmese, L.; Watanabe, H.; Alvarez, N. J., Effect of Finite Extensibility on Nonlinear Extensional Rheology of Polymer Melts, *Macromolecules*, **52**, 915-922 (2019).

Dielectric Relaxation of Type-A Chains Undergoing Head-to-Tail Association/Dissociation: Difference from Head-to-Head Case and Correlation with Viscoelastic Relaxation

Dielectric relaxation of type-A chains reflects global motion of the chains but is also affected by relative alignment of the dipoles along the chain backbone, namely, by the dipole inversion. Head-to-head association of type-A unimers gives a symmetrically dipole-inverted dimer, and the association/dissociation equilibrium of these unimers and dimer results in motional coupling of these chains, thereby affecting the dielectric behavior. In fact, for this head-to-head case, eigenmode analysis has been reported in the literature to reveal that motional coupling results in moderate retardation and acceleration of the dielectric relaxation of the unimer and dimer obeying the reptation dynamics. In contrast, the coupling has no effect on the dielectric relaxation of the Rouse unimer and dimer, namely, the effect of motional coupling on the dielectric relaxation changes with the type of chain dynamics. This effect was not clarified for head-to-tail associating unimers and their dimer having no dipole inversion (Figure 1). Thus, for completeness, this study makes the eigenmode analysis of the dielectric relaxation for this case of head-to-tail reac-

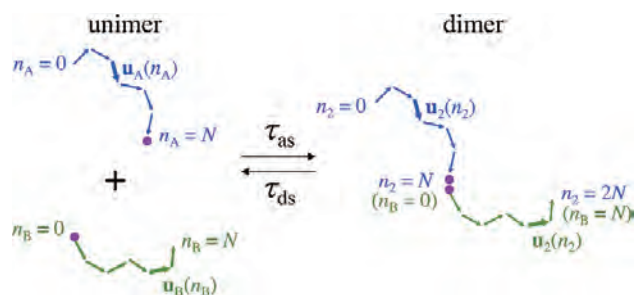


Figure 1. Illustration of head-to-tail associating unimers and dissociating dimer at equilibrium. Purple circles at N -th and 0 -th segments of the blue and green unimers (A and B) indicate the associative head and tail, respectively. The unimers and dimer have type-A dipoles aligned along the chain backbone without inversion.

tion. For the unimer and dimer obeying either Rouse or reptation dynamics, the analysis indicates that the retardation and acceleration of the dielectric relaxation of the unimer and dimer are much more significant for the head-to-tail case than for the head-to-head case irrespective of the chain dynamics, and that the dielectric relaxation function for the former case exactly coincides with the viscoelastic relaxation function if the unimer and dimer obey the reptation dynamics (Figure 2). This result suggests an interesting method of resolving some detail of the chain dynamics under the reaction through comparison of dielectric and viscoelastic responses of the associative type-A chains.

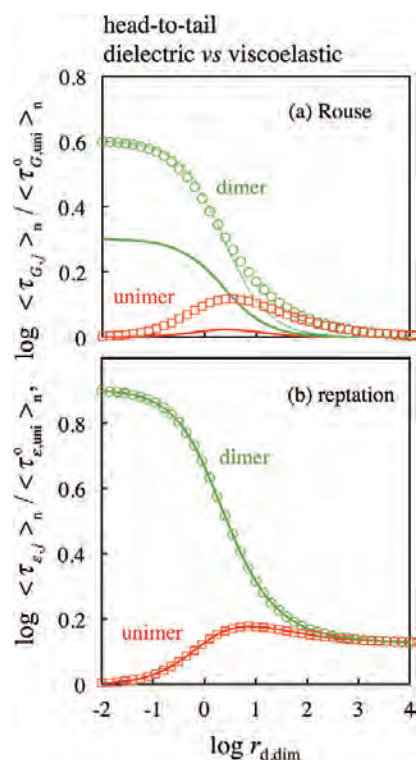


Figure 2. Terminal viscoelastic and dielectric relaxation times, $\langle \tau_{G,j} \rangle_n / \langle \tau_{G,uni} \rangle_n$ and $\langle \tau_{e,j} \rangle_n / \langle \tau_{e,uni} \rangle_n$ (solid curves and symbols), of the unimer and dimer undergoing head-to-tail reaction plotted against normalized dissociation rate $r_{d,dim}$ (set identical to $r_{a,dim}$). For comparison, $\{ \langle \tau_{G,2} \rangle_n / \langle \tau_{G,uni} \rangle_n \}^2$ for the Rouse dimer is shown with the dashed green curve in the top panel.

Division of Multidisciplinary Chemistry – Molecular Aggregation Analysis –

<https://www.scl.kyoto-u.ac.jp/~wakamiya/english/index.html>



Prof
WAKAMIYA, Atsushi
(D Eng)



Assist Prof
MURDEY, Richard
(Ph D)



Assist Prof
NAKAMURA, Tomoya
(D Eng)



PD
LIU, Jiewei
(Ph D)



PD
OHASHI, Noboru
(D Eng)



PD
TRUONG, Minh Anh
(D Eng)

PD

RAFIEH, Alwani Imanah
KIM, Kyusun

Researchers (pt)

SHIMAZAKI, Ai
ISHIKURA, Yasushi
TANABE, Masanaga
SUZUKI, Yoshie

Assist Techn Staffs

IWASAKI, Yasuko
MATSUSHIGE, Yuko

Students

OTSUKA, Kento (M1)
HASHIMOTO, Ruito (M1)
HU, Shuaifeng (RS)

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

Ozaki, M.; Shimazaki, A.; Jung, M.; Nakaike, Y.; Maruyama, N.; Yakumaru, S.; Rafieh, A. I.; Sasamori, T.; Tokitoh, N.; Ekanayake, P.; Murata, Y.; Murdey, R.; Wakamiya, A., A Purified, Solvent-Intercalated Precursor Complex for Wide Process Window Fabrication of Efficient Perovskite Solar Cells and Modules, *Angew. Chem. Int. Ed.*, **58**, 9389-9393 (2019).

Ozaki, M.; Ishikura, Y.; Truong, M. A.; Liu, J.; Okada, I.; Tanabe, T.; Sekimoto, S.; Ohtsuki, T.; Murata, Y.; Murdey, R.; Wakamiya, A., Iodine-rich Mixed Composition Perovskites Optimised for Tin(IV) Oxide Transport Layers: the Influence of Halide Ion Ratio, Annealing Time, and Ambient Air Aging on Solar Cell Performance, *J. Mater. Chem. A*, **7**, 16947-16953 (2019).

Nakamura, T.; Shioya, N.; Shimoaka, T.; Nishikubo, R.; Hasegawa, T.; Saeki, A.; Murata, Y.; Murdey, R.; Wakamiya, A., Molecular Orientation Change in Naphthalene Diimide Thin Films Induced by Removal of Thermally Cleavable Substituents, *Chem. Mater.*, **31**, 1729-1737 (2019).

Truong, M. A.; Lee, J.; Nakamura, T.; Seo, J.-Y.; Jung, M.; Ozaki, M.; Shimazaki, A.; Shioya, N.; Hasegawa, T.; Murata, Y.; Zakeeruddin, S. M.; Gratzel, M.; Murdey, R.; Wakamiya, A., Influence of Alkoxy Chain Length on the Properties of Two-Dimensionally Expanded Azulene Core-Based Hole-Transporting Materials for Efficient Perovskite Solar Cells, *Chem. Eur. J.*, **25**, 6741-6752 (2019).

Ozaki, M.; Nakaike, Y.; Shimazaki, A.; Jung, M.; Maruyama, N.; Yakumaru, S.; Rafieh, A. I.; Ekanayake, P.; Saito, T.; Shimakawa, Y.; Sasamori, T.; Murata, Y.; Murdey, R.; Wakamiya, A., How to Make Dense and Flat Perovskite Layers for >20% Efficient Solar Cells: Oriented, Crystalline Perovskite Intermediates and their Thermal Conversion, *Bull. Chem. Soc. Jpn.*, **92**, 1972-1979 (2019).

Influence of Alkoxy Chain Length on the Properties of Two Dimensionally Expanded Azulene-Core-Based Hole-Transporting Materials for Efficient Perovskite Solar Cells

A series of two-dimensionally expanded azulene-core-based π systems have been synthesized with different alkyl chain lengths in the alkoxy moieties connected to the partially oxygen-bridged triarylamine skeletons. The thermal, photophysical, and electronic properties of each compound were evaluated to determine the influence of the alkyl chain length on their effectiveness as hole-transporting materials (HTMs) in perovskite solar cells (PSCs). All the synthesized molecules showed promising material properties, including high solubility, the formation of flat and amorphous films, and optimal alignment of energy levels with perovskites. In particular, the derivatives with methyl and *n*-butyl in the side chains retained amorphous stability up to 233 and 159 °C, respectively. Such short alkoxy chains also resulted in improved electrical device properties. The PSC device fabricated with the HTM with *n*-butyl side chains showed the best performance with a power conversion efficiency of 18.9%, which compares favorably with that of spiroOMeTAD-based PSCs (spiro-OMeTAD = 2,2',7,7'-tetrakis[N,N-bis(p-methoxyphenyl)amino]-9,9'-spirobifluorene).

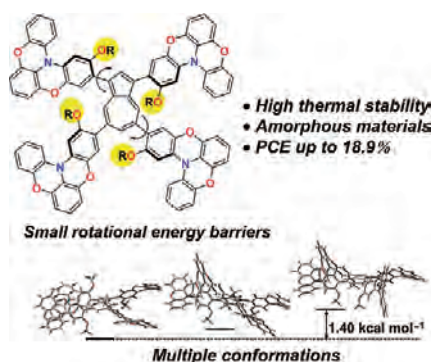


Figure 1. Molecular structures of the azulene-core-based two-dimensionally expanded π -system derivatives.

A Purified, Solvent-Intercalated Precursor Complex for Wide-Process Window Fabrication of Efficient Perovskite Solar Cells and Modules

A high-purity methylammonium lead iodide complex with intercalated dimethylformamide (DMF) molecules, $\text{CH}_3\text{NH}_3\text{PbI}_3 \cdot \text{DMF}$, is introduced as an effective precursor material for fabricating high-quality solution-processed perovskite layers. Spin-coated films of the solvent-intercalated complex dissolved in pure dimethyl sulfoxide

(DMSO) yielded thick, dense perovskite layers after thermal annealing. The low volatility of the pure DMSO solvent extended the allowable time for low-speed spin programs and considerably relaxed the precision needed for the antisolvent addition step. An optimized, reliable fabrication method was devised to take advantage of this extended process window and resulted in highly consistent performance of perovskite solar cell devices, with up to 19.8% power-conversion efficiency (PCE). The optimized method was also used to fabricate a 22.0 cm², eight cell module with 14.2% PCE (active area) and 8.64 V output (1.08 V/cell).

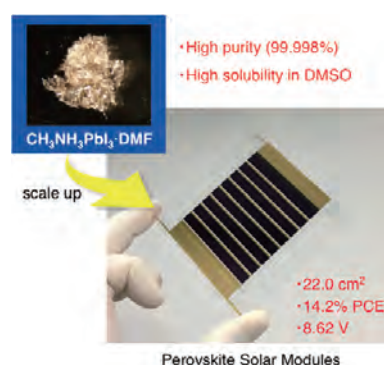


Figure 2. Photograph of $\text{CH}_3\text{NH}_3\text{PbI}_3 \cdot \text{DMF}$ complex and the perovskite solar modules.

Iodine-rich Mixed Composition Perovskites Optimized for Tin(IV) Oxide Transport Layers: the Influence of Halide Ion Ratio, Annealing Time, and Ambient Air Aging on Solar Cell Performance

Iodine-rich mixed composition metal-halide perovskites were developed to improve the performance of perovskite solar cell devices incorporating tin(IV) oxide substrates for electron transport layers by optimizing the I/Br halide ion ratio. Device performance was further enhanced by exposing to ambient atmosphere over several days, which correlated with a shift of the energy levels in the perovskite and significant suppression of charge carrier recombination. A high power conversion efficiency of 20.6% was obtained for the aged device.

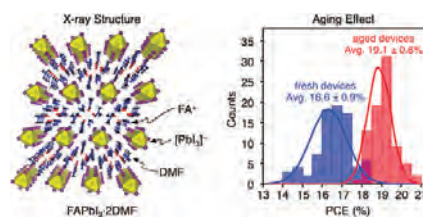


Figure 3. X-ray crystal structure of $\text{FAPbI}_3 \cdot \text{DMF}$ complex and the performance of perovskite solar cells.

Advanced Research Center for Beam Science – Particle Beam Science –

<http://www.kuicr.kyoto-u.ac.jp/www/index-e.html>



Prof

WAKASUGI, Masanori
(D Sc)



Assoc Prof

IWASHITA, Yoshihisa
(D Sc)



Techn Staff

TONGU, Hiromu

Lect (pt)

UESAKA, Tomohiro (D Sc) Nishina Center, RIKEN

Students

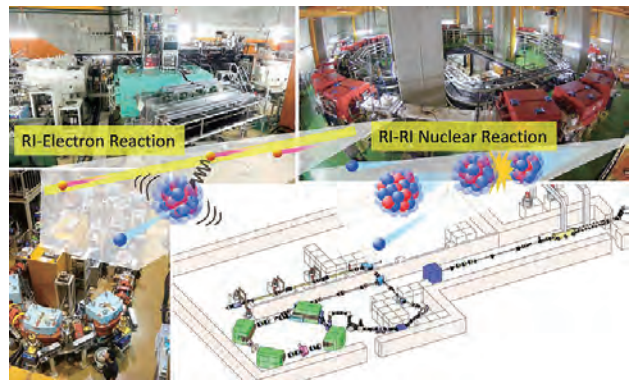
ABE, Masashi (M2)
YAKO, Tomoki (M2)
TAKAGI, Shu (M1)

Scope of Research

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

KEYWORDS

Beam Physics	Accelerator Physics
Neutron Optics	Storage Ring
Unstable Nuclear Physics	



Selected Publications

Wakasugi, M.; Togasaki, M.; Ohnishi, T.; Kurita, K.; Toba, R.; Watanabe, M.; Yamada, K., FRAC: Fringing-RF-Field-Activated DC-to-Pulse Converter for Low-Energy Ion Beam, *Rev. Sci. Instrum.*, **89**, 095107 (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).

Tsukada, K.; Enokizono, A.; Ohnishi, T.; Adachi, K.; Fujita, T.; Hara, M.; Hori, M.; Hori, T.; Ichikawa, S.; Kurita, K.; Matsuda, K.; Suda, T.; Tamae, T.; Togasaki, M.; Wakasugi, M.; Watanabe, M.; Yamada, K., First Elastic Electron Scattering from ^{132}Xe at the SCRIT Facility, *Phys. Rev. Lett.*, **118**, 262501 (2017).

Kitaguchi, M.; Iwashita, Y.; Shimizu, H. M., Concentration of the Velocity Distribution of Pulsed Neutron Beams, *Prog. Theor. Exp. Phys.*, **2017**, 043D01 (2017).

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

Launch of KAKEN-RNC Collaboration and Relocation of Heavy-Ion Storage Ring (s-LSR) to RIKEN

We launched KAKEN-RNC collaboration to drive a new research field in unstable nuclear science. One of the attempts in the collaboration is a co-development of a *beam recycling* technique in a heavy-ion storage ring. That aims to a study for nuclear reaction especially for rarely-produced radio-active isotopes (RI) and RI-RI collision experiments not yet realized.

What is a *beam recycling*? In a nuclear reaction study, we observe what happen when a high-energy-nuclear beam hits a thin fixed target. Normally, only a tiny part of the injected nuclei participates in the collision with the target nuclei. Conversely, the most of them are thrown away without any reactions with the target nuclei, because the nuclear reaction cross section is extremely small. In a heavy-ion storage ring in which a high-energy nuclear beam is accumulated, nuclear reactions can be observed when we provide a thin target in the beam-circulation orbit. Unlike a conventional way, the beam passing through the target without any reaction is recirculated in the ring and the accumulated beam hits target turn by turn. It is wonderful that the beam can keep turning around until nuclear reaction takes place. This is a *beam recycling*. The *beam recycling* technique should greatly contribute to an effective use of beam especially for the rarely produced unstable nuclei. We believe that a *beam recycling* technology open up new research area such as an RI-RI collision experiment.

There are some technical challenges to establish the *beam recycling*. We need to compensate turn by turn the energy loss and the emittance growth taken placed at the internal target to keep the steady beam circulation. In KAKEN-RNC collaboration, we will develop jointly the new technology required for *beam recycling*. We are convinced that the heavy-ion cooler storage ring (s-LSR) constructed at KAKEN more than ten years ago is perfectly

suitable for the R&D study. Therefore, we disassembled s-LSR and carried them to RIKEN RI Beam Factory (RIBF) in this year (see Figure 1).



Figure 1. Reassembling of s-LSR at KAKEN accelerator facility.

We are going to reconstruct s-LSR as a new storage ring named RUNBA (Recycled-Unstable-Nuclear Beam Accumulator) at the ISOL (Isotope Separator On-Lin) facility in RIKEN RIBF where low-energy radioactive-isotope (RI) beams are provided for nuclear physics research (see Figure 2). Rough sketch of RUNBA planned at RIKEN RIBF is shown in Figure 2. The RI beam from ISOL will be transported to a charge breeder, which converts the incoming singly-charged ions to highly-charged ions, and fully stripped RI ion beams are injected into RUNBA. The RI ion beam is accelerated up to 10 MeV/u in RUNBA for being ready for nuclear fusion reaction. We plan to accumulated ${}^6\text{He}$ beam produced by ${}^7\text{Li}(\gamma, p)$ reaction in the day-one experiment. We are now developing infrastructure and working on design study for RUNBA and technical design for the required components in RUNBA.

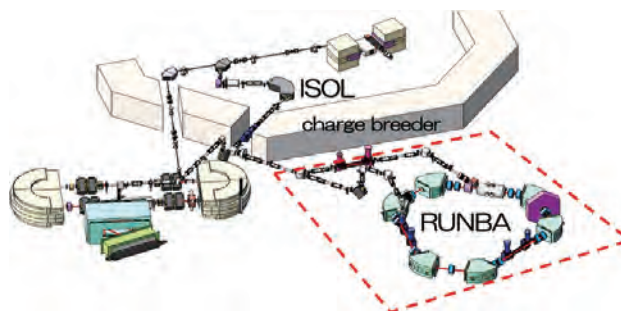


Figure 2. Sketch of RUNBA reconstructed at RIKEN RIBF.

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)



Proj Res*
NAKAMIYA, Yoshihide
(D Sc)

Students

FURUKAWA, Yuki (D2)

HOSOKAWA, Chikai (M2)

YAMANAKA, Takashi (M2)

KONGO, Ryota (M1)

TANAKA, Yohei (M1)

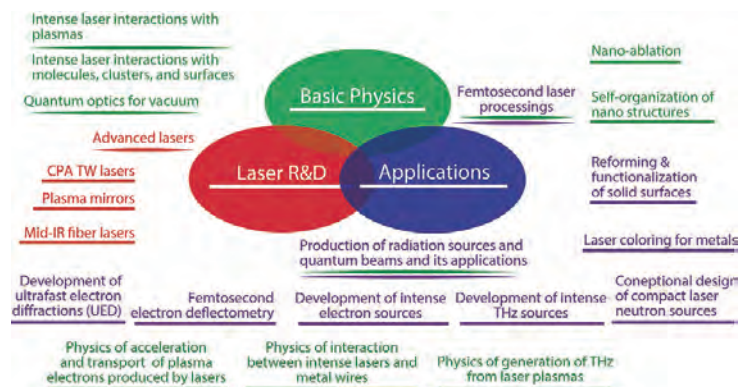
*Postdoctoral Research Assistant of
Extreme Light Infrastructure-Nuclear
Physics (ELI-NP) / Horia Hulubei
National Institute for R&D in Physics
and Nuclear Engineering (IFIN-HH)

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

Mori, K.; Hashida, M.; Nagashima, T.; Li, D.; Teramoto, K.; Nakamiya, Y.; Inoue, S.; Sakabe, S., Increased Energy of THz Waves from a Cluster Plasma by Optimizing Laser Pulse Duration, *AIP Advances*, **9**, [015134-1]-[015134-4] (2019).

Nishiura, Y.; Inoue, S.; Kojima, S.; Teramoto, K.; Furukawa, Y.; Hashida, M.; Sakabe, S., Detection of Alpha Particles from ${}^7\text{Li}(p, \alpha){}^4\text{He}$ and ${}^{19}\text{F}(p, \alpha){}^{16}\text{O}$ Reactions Induced by Laser-accelerated Protons Using CR-39 with Potassium Hydroxide–ethanol–water Etching Solution, *Rev. Sci. Instrum.*, **90**, 083307 (2019).

Takenaka, K.; Tsukamoto, M.; Hashida, M.; Masuno, S.; Sakagami, H.; Kusaba, M.; Sakabe, S.; Inoue, S.; Furukawa, Y.; Asai, S., Ablation Suppression of a Titanium Surface Interacting with a Two-color Double-pulse Femtosecond Laser Beam, *Appl. Surf. Sci.*, **478**, 882–886 (2019).

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, *Phys. Rev. Accel. Beams*, **21**, [041302-1]-[041302-6] (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**, 023204 (2018).

Development of Intense Terahertz Light Source for Forming Periodic Structures on Material Surface

When solid materials are irradiated with intense terahertz waves, periodic structures are formed on their surface. The inter space of these structures is about 1/20 of terahertz wavelength, and mechanism of structures formation has not been clarified yet. Getting clues of formation mechanism, we develop an intense terahertz light source to form structures and intend to observe the formation process by pump-probe method during a terahertz wave irradiation.

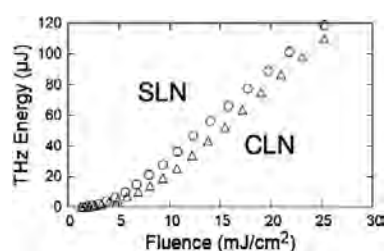


Figure 1. Terahertz energy dependence on laser fluence.

Uniform LIPSS on Titanium Irradiated by Two-color Double-pulse Beam of Femtosecond Laser

We produced the uniform LIPSS (Laser Induced Periodic Surface Structures) on titanium surfaces with using the use of two-color femtosecond double-pulse laser irradiation. The double-pulse beam consisted of 800 nm pulses with duration of 150 fs and 400 nm pulses with duration of > 150 fs. For double-pulse beam irradiation in which the laser fluence is close to the ablation threshold, it was found that the longer-wavelength laser pulse is responsible for LIPSS formation, while the shorter-wavelength laser pulse is responsible for improving LIPSS uniformity. Relatively uniform LIPSS characterized by the fundamental wavelength were obtained using a double-pulse beam with fluences of $1.5F_{400\text{th}} + 0.9F_{800\text{th}}$ and delay of $\Delta t = 0-2$ ps.

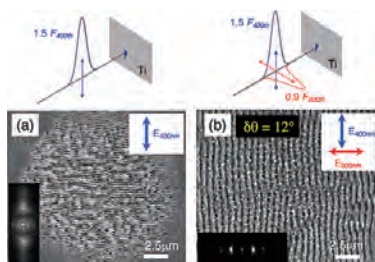


Figure 2. SEM images of titanium surfaces irradiated with (a) only the fundamental wavelength pulse with $N = 60$ pulses and (b) the two-color double-pulse beam with delay of $\Delta t = 0$ and $N = 60$ pairs of pulses. The LIPSS uniformity ($\delta\theta$) shows the LIPSS characterized by the 800 nm pulse.

Detection of Alpha Particles from ${}^7\text{Li}(p,\alpha){}^4\text{He}$ and ${}^{19}\text{F}(p,\alpha){}^{16}\text{O}$ Reactions Induced by Laser-accelerated Protons Using CR-39 with PEW Etching Solution

With the development of high-intensity lasers in recent years, applied research on laser-accelerated ions has attracted considerable interest in fields where nuclear reactions are used or studied and in industrial applications. In studies of laser plasma and laser ion acceleration, electrostatic or magnetic ion analyzers such as the Thomson parabola spectrometer (TPS) are widely used to monitor the primary and secondary ions emitted from laser plasmas and nearby targets. The TPS is an effective instrument for measuring the energy spectra of laser plasma ions, but it has difficulty detecting small numbers of secondary ions, such as those generated by nuclear reactions with a small cross section, and this limitation is primarily attributable to the solid angle of the TPS entrance aperture from the ion source. Solid-state nuclear track detectors (SSNTDs) can be used to detect even a single ion and are insensitive to radiation other than ions. Furthermore, SSNTDs are easy to handle owing to their compact nature and can be cut into arbitrary sizes and shapes. These features of high sensitivity and easy handling allow for convenient measurements of high-intensity laser-produced ions with extremely large solid angles. However, SSNTDs exhibit high sensitivity for all ion species, making the fractionation of ion species a key issue for SSNTD. In particular, when CR-39 is used, one of the most popular SSNTD in laser plasma physics, the sensitivity must be controlled to be sufficiently high for the secondary ions and sufficiently low for the primary protons.

We have reported the control of the sensitivity of the CR-39 for radioactive particles, and the selective detection of Alpha particles generated by ${}^7\text{Li}(p,\alpha){}^4\text{He}$ and ${}^{19}\text{F}(p,\alpha){}^{16}\text{O}$ reactions in the presence of abundant primary protons by reducing the proton sensitivity of CR-39 using potassium hydroxide–ethanol–water (PEW) etching solution. These nuclear reactions are induced in a LiF crystal using the laser-accelerated protons (4×10^{11} protons/pulse with a maximum energy of 3.3 MeV) generated and accelerated by the interaction of a 40-fs laser pulse with a polyethylene thin film target at a peak intensity of 5×10^{19} W/cm². Subsequent etching of the CR-39 in PEW solution (KOH: 17 wt %; C₂H₅OH: 25 wt %; H₂O: 58 wt %) permits the selective detection of 4.0 MeV alpha particles, which is independently confirmed by an experiment using alpha particles from an ${}^{241}\text{Am}$ source. The described method is expected to be useful for research into nuclear reactions in laser plasma.

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)



Assoc Prof
HARUTA, Mitsutaka
(D Sc)



Assist Prof
NEMOTO, Takashi
(D Sc)



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



Program-Specific Res*
KIYOMURA, Tsutomu

*Nanotechnology Platform

Researcher (pt)

YAMAGUCHI, Atsushi

Students

LAI, Ming Wei (D3)

SHINYA, Tomoki (M2)

TOBA, Tomohito (M2)

IWASHIMIZU, Chisaki (M2)

KAWAGUCHI, Tomoki (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

Extremely Low Count Detection

Gain Normalized Spectrum

Read-out Noise

Selected Publications

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 $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4+\delta}$, *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).

Haruta, M.; Fujiyoshi, Y.; Nemoto, T.; Ishizuka, A.; Ishizuka, K.; Kurata, H., Extremely Low Count Detection for EELS Spectrum Imaging by Reducing CCD Read-out Noise, *Ultramicroscopy*, **207**, [112827-1]-[112827-6] (2019).

Extremely Low Count Detection for EELS Spectrum Imaging by Reducing CCD Read-out Noise

Electron energy-loss spectroscopy (EELS) combined with scanning transmission electron microscopy (STEM) is useful for examining local chemical elements, electronic structure, and optical excitation with high spatial resolution. However, it is not easy to obtain high signal-to-noise ratio (SNR) spectra with high spatial resolution without sample damage. Summation of many spectra obtained by multiple spectrum imaging (SI) measurement with low dose rate is often used to prevent the sample damage. In the present contribution, we report a systematic statistical study on the reduction of CCD noise for EELS using our original method.

STEM-EELS experiments were carried out on a JEM-ARM200F (200 kV, JEOL) using a GIF Quantum ERS (Gatan) for EELS acquisition and Gatan Microscopy Suite (GMS, Gatan) for the analysis. 2048×260 2D CCD signals are binned by hardware/software along y direction to produce 2048 channel 1D EELS spectrum.

In general, an EELS spectrum is acquired in the gain normalized mode. In this mode, the obtained spectrum I_G is described as

$$I_G = \sum_y ([S_{x,y} + D_{x,y}] - D_{x,y}^s) G_{x,y},$$

where $S_{x,y}$ is an EELS signal derived from incident electrons, $D_{x,y}$ is dark reference, $D_{x,y}^s$ is a single frame dark reference measured with beam blanking and $G_{x,y}$ is a gain correction, which is saved as the reciprocal of the gain reference image measured with the uniform radiation condition in the TEM mode. $[\]$ indicates integer processing by analog-to-digital conversion. The main component of the dark reference is read-out offset and read-out noise. Unfortunately, this common process inevitably gives rise to fixed pattern noise derived from the difference between the average of the dark reference $[D_{x,y}]$ and $D_{x,y}^s$. To remove such fixed pattern noise, recent GMS software has added a HQ (high-quality) dark reference option in post-processing. The HQ spectrum HQI_G is

$$HQI_G = \{I_G + \sum_y (D_{x,y}^s G_{x,y})\} - \sum_y (\langle [D_{x,y}] \rangle G_{x,y}),$$

where $\langle [D_{x,y}] \rangle$ is the average dark reference image. However HQI_G cannot completely remove the above noise due to the integer process. As an alternative, we obtain the ultra-high-quality (UHQ) dark subtracted spectrum $UHQI_D$ by subtracting the UHQ dark reference $UHQD_U = \sum_y [D_{x,y}]$ from the experimental spectra I_U in the unprocessed mode without the integer process:

$$UHQI_D = I_U - UHQD_U = \sum_y [S_{x,y} + D_{x,y}] - \sum_y [D_{x,y}].$$

In this case, if $UHQD_U$ is the population mean of the dark reference, the noise derived from the dark reference

could be suppressed by the summation. The UHQ gain normalized spectrum $UHQI_G$ is obtained by using the average gain reference data generated by averaging the vertical 260 channels of the gain correction image:

$$UHQI_G = UHQI_D \times \sum_y G_{x,y}.$$

A histogram of the intensity of the dark read-out at a single channel is close to a Gaussian distribution. This means that if the population mean of the dark read-out at individual channels was subtracted, the noise could be suppressed by a summation over many measurements. The noise standard deviation of the dark read-out over 2048 spectral channels after subtraction of $UHQD_U$ (using n_a frames) as a function of the accumulation number n_s become much less than one count above $n_s = 5000$ for $n_a \geq 5000$. Therefore, it may be possible to visualize even a single signal count per spectrum by summation of the spectrum, if we use a good averaged dark reference.

As a test experiment, the Ti $L_{2,3}$ -edge was measured from SrTiO₃. $UHQD_U$ was estimated using 20,000 spectra. Figure 1(a) shows a single frame Ti $L_{2,3}$ -edge spectrum of $UHQI_G$ in the SI data obtained with a very low dose. Figure 1(b) shows 12,000-frame summed spectra after different spectral treatments. The average peak intensity of the first peak was about 1.2 counts, which corresponds to 0.15 electrons per dwell time. This is a demonstration of the detection of a single inelastic electron per channel in a spectrum during the dwell time. The result of gain averaging by shifting the spectrum over 200 channels after $UHQI_G$ shows a further improvement of the noise standard deviation (0.092 counts), and this process is very effective. A combination of the subtraction of the $UHQD_U$ and the gain averaging is the best method. Even a single-electron core-loss signal per spectrum can be visualized as a high-SNR spectrum using the present technique.

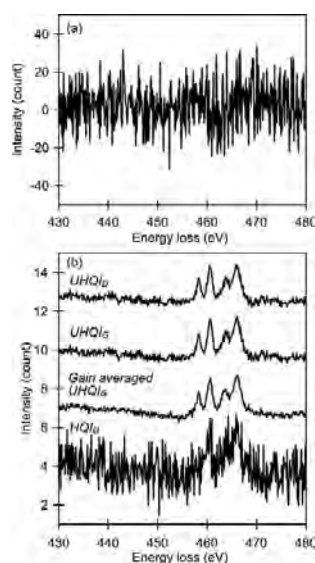


Figure 1. (a) A single-frame $UHQI_G$ of the Ti $L_{2,3}$ -edge spectrum of SrTiO₃ extracted from SI data obtained with a very weak signal. (b) Spectra averaged over 12,000 frames after different spectral treatments. The spectral intensities were normalized as a single spectrum. Each spectrum is vertically shifted by 3 counts except for the bottom spectrum (HQI_G).



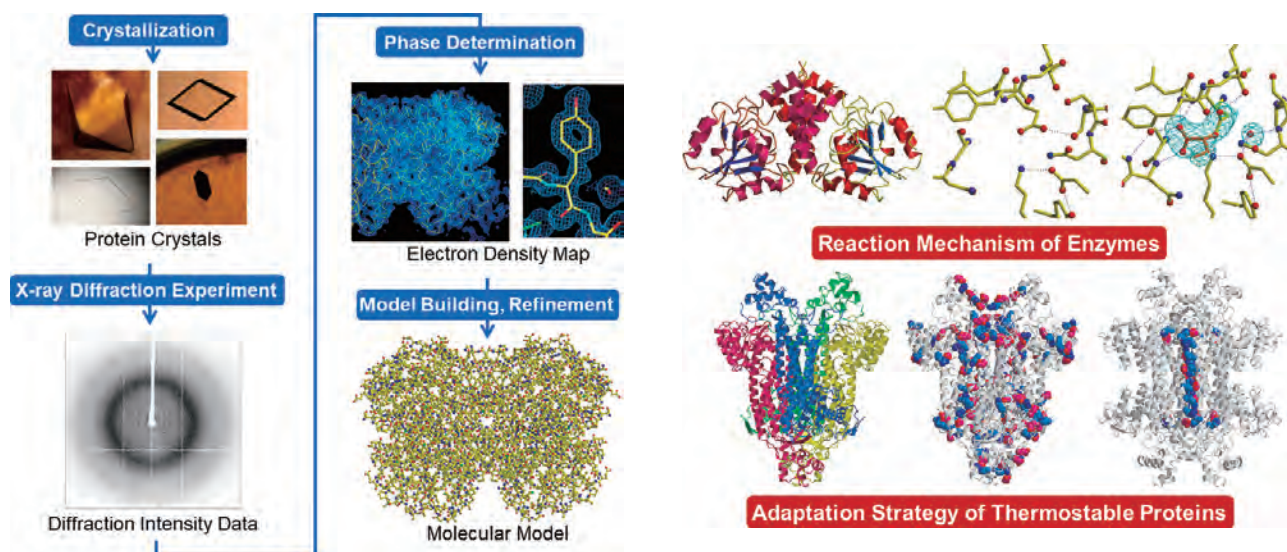
Assist Prof
FUJII, Tomomi
(D Sc)

Scope of Research

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

KEYWORDS

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



Selected Publications

- Fujii, T.; Sato, A.; Okamoto, Y.; Yamauchi, T.; Kato, S.; Yoshida, M.; Oikawa, T.; Hata, Y., The Crystal Structure of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005 Provides Insights into the Reaction Mechanism of Enzymes in Its Original Family, *Proteins: Structure, Function, and Bioinformatics*, **84**, 1029-1042 (2016).
- 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).
- Fujii, T.; Goda, Y.; Yoshida, M.; Oikawa, T.; Hata, Y., Crystallization and preliminary X-ray Diffraction Studies of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **64**, 737-739 (2008).
- Fujii, T.; Oikawa, T.; Muraoka, I.; Soda, K.; Hata, Y., Crystallization and Preliminary X-ray Diffraction Studies of Tetrameric Malate Dehydrogenase from the Novel Antarctic Psychrophile *Flavobacterium frigidimaris* KUC-1, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **63**, 983-986 (2007).
- Fujii, T.; Sakai, H.; Kawata, Y.; Hata, Y., Crystal Structure of Thermostable Aspartase from *Bacillus* sp. YM55-1: Structure-based Exploration of Functional Sites in the Aspartase Family, *J. Mol. Biol.*, **328**, 635-654 (2003).

Crystal Structure Analysis of GraC Protein from *Rhizobium* sp. Strain MTP-10005 in Complex with Coenzyme

Rhizobium is a genus of tubercle-forming bacteria. It grows in the root of a plant in symbiosis with other bacteria to fix nitrogen from the air. Although considerable attention has been paid to *Rhizobium* genes and gene products, there is still little information available on the molecular structure, function, and detailed properties of the enzymes involved in its metabolic pathways. In the course of a screening experiment, *Rhizobium* sp. strain MTP-10005 was isolated from natural river water. Enzymological and genetic studies showed that products of the *graA*, *graB*, *graC*, and *graD* genes in the bacterium are involved in the degradation pathway of resorcinol. In order to reveal the structures and functions, we have been performing X-ray structural studies of the enzymes. Maleylacetate reductase (GraC) catalyzes NADH- or NADPH-dependent reduction of maleylacetate to 3-oxoadipate. We have determined the GraC-coenzyme complex structure.

N-terminal His-tagged GraC was overexpressed in *Escherichia coli*, purified, and used for crystallization. The protein solution consisted of 2.5 mg/ml GraC, 5 mM NADH, and 50 mM Tris-HCl pH 8.0. Initial crystallization experiments were performed by the sitting-drop vapor-diffusion method using several screening kits. Small crystals were obtained after several days with several conditions. Particularly, thin plate-shaped adequately sized crystals for X-ray diffraction experiments were obtained using a reservoir solution consisting of 20% (w/v) PEG1500 and 0.1 M Bis-Tris pH 6.5. Diffraction experiments were performed on beamline BL-5A, Photon Factory, KEK, Japan. The crystal was mounted with a cryoloop and cooled with a cold stream of nitrogen. Diffraction data were collected up to 2.5 Å resolution. The crystal belonged to space group *P1*. The structure was determined by molecular replacement using an apo-type GraC crystal structure as a starting model and refined at 2.5 Å resolution.

In the present crystal, one homodimer GraC molecule exists in the unit cell and each subunit binds an NADH molecule (Figure 1). The subunit of GraC molecule consists of two domains: an N-terminal domain, residues 1–159, adopting an α/β structure and a C-terminal α -helical domain, residues 160–351. The active site is located in the cleft between the domains of the subunit. The NADH molecule is located in the active site cleft and mainly binds to the N-terminal domain (Figure 2). The subunit of the GraC-coenzyme complex has a closed conformation that may be adopted on binding the coenzyme. However, one subunit of apo-type GraC binds no other ligand except two

sulfate anion. It has an open conformation, as is the case before the enzymatic reaction. Thus, the two types of GraC crystal structures reveal the structures of maleylacetate reductase both in the coenzyme-binding state and in the ligand-free state, which suggests that the structure of GraC must change from the open conformation to the closed conformation in the course of enzymatic reaction (Figure 3).

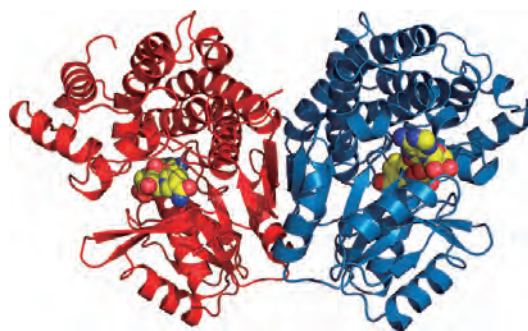


Figure 1. Dimeric molecular structure of GraC-coenzyme complex.

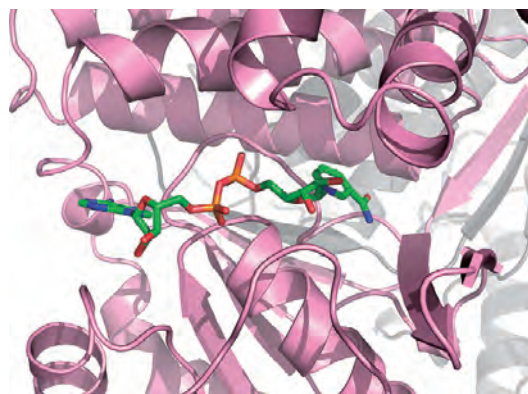


Figure 2. Structure of coenzyme-binding site of GraC-coenzyme complex.

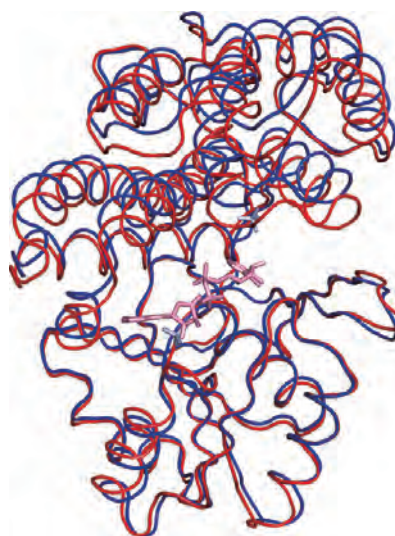


Figure 3. Superposition of GraC subunits. Subunit-A of GraC-coenzyme complex and Subunit-B of apo-type GraC are shown in red and blue, respectively.

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, Katsuhiko
(D Eng)



Assist Prof*
IWAMOTO, Takahiro
(D Eng)



Program-Specific Senior Lect
PINCELLA, Francesca
(Ph D)



Program-Specific Res
SHARMA, Akhilesh Kumar
(Ph D)



Program-Specific Res
AGATA, Ryosuke
(D Eng)

*Project for Iron-Catalyzed
Selective Organotransformation

Researchers (pt)

MATSUDA, Hiroshi
NAKAMURA, Yuki

Students

KAWASAKI, Hiroto (M2)
LU, Siming (M2)

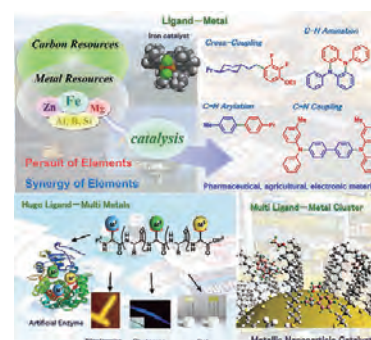
NAKATANI, Yuya (M1)
YAMAMOTO, Atsushi (M1)

WANG, Jun (M1)
ZHANG, Yaqi (RS)

YIN, Haozhi (RS)
NOMURA, Satsuki (UG)

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

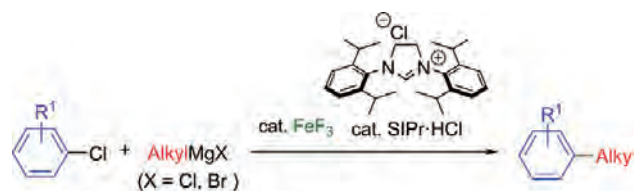
Selective Organic Reaction Iron Catalyst Metalated Peptide Metallic Nanoparticle Catalyst Solution-Phase XAS Analysis

Selected Publications

- Iwamoto, T.; Hosokawa, A.; Nakamura, M., Endergonic Addition of N-methylamines to Aromatic Ketones Driven by Photochemical Offset of the Entropic Cost, *Chem. Commun.*, **55**, 11683-11686 (2019).
- Aoki, Y.; O'Brien, H. M.; Kawasaki, H.; Takaya, H.; Nakamura, M., Ligand-Free Iron-Catalyzed C–F Amination of Diarylamines: A One-Pot Regioselective Synthesis of Diaryl Dihydrophenazines, *Org. Lett.*, **21**, 461-464 (2019).
- Agata, R.; Kawamura, S.; Isozaki, K.; Nakamura, M., Iron-catalyzed Alkyl–Alkyl Negishi Coupling of Organoaluminum Reagents, *Chem. Lett.*, **48**, 238-241 (2019).
- Agata, R.; Takaya, H.; Matsuda, H.; Nakatani, N.; Takeuchi, K.; Iwamoto, T.; Hatakeyama, T.; Nakamura, M., Iron-Catalyzed Cross Coupling of Aryl Chlorides with Alkyl Grignard Reagents: Synthetic Scope and Fe^{II}/Fe^{IV} Mechanism Supported by X-ray Absorption Spectroscopy and Density Functional Theory Calculations, *Bull. Chem. Soc. Jpn.*, **92**, 381-390 (2019).
- Iwamoto, T.; Okuzono, C.; Adak, L.; Jin, M.; Nakamura, M., Iron-Catalysed Enantioselective Suzuki–Miyaura Coupling of Racemic Alkyl Bromides, *Chem. Commun.*, **55**, 1128-1131 (2019).

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 iron-catalyzed cross coupling of aryl chlorides with alkyl Grignard reagents (Figure 1a). By using X-ray absorption spectrometry and DFT calculations, we revealed that the reaction proceeds via the formation of Fe-Mg dinuclear intermediate (Figure 1b).



ArCl: including deactivated aryl chlorides
 AlkylMgX: with or without β -hydrogens

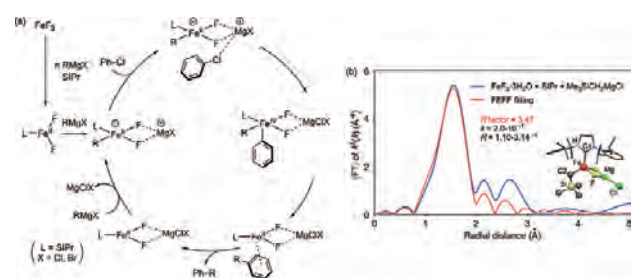


Figure 1. Iron-catalyzed cross coupling of aryl chlorides with alkyl Grignard reagents. (a) Proposed mechanism and (b) EXAFS fitting of Fe-Mg dinuclear intermediate.

Moreover, we developed iron-catalyzed C-F amination reaction of various diarylamines for the one-pot diastereoselective synthesis of diaryl dihydrophenazines, which are of significant research interest due to the potent applicability as organic luminescent materials and photoredox catalysts (Figure 2).

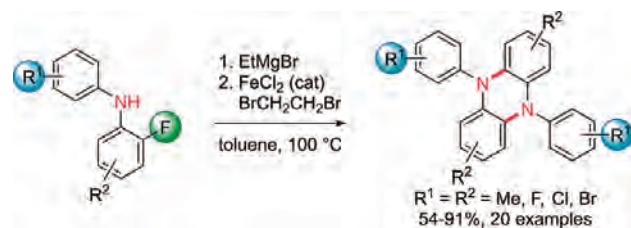


Figure 2. One-pot regioselective synthesis of diaryl dihydrophenazines by iron-catalyzed C-F amination of diarylamines.

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

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

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 –

<https://www.scl.kyoto-u.ac.jp/~shimakgr/indexE.html>



Prof
SHIMAKAWA, Yuichi
(D Sc)



Assoc Prof
KAN, Daisuke
(D Sc)



Assist Prof
GOTO, Masato
(D Sc)



Program-Specific Assist Prof *
AMANO PATINO, Midori Estefani
(Ph D)



Techn Staff
ICHIKAWA, Noriya
(D Eng)

*Research Unit for Development
of Global Sustainability

Students

KOEDTRUAD, Anucha (D3)
TAN, Zhenhong (D2)
SANTO, Jyunya (M2)

KOSUGI, Yoshihisa (M2)
SUGANO, Satoshi (M2)
OKAZAKI, Masato (M1)

SUZUKI, Ikumi (M1)
SEMBA, Yuna (M1)
SHEN, Yufan (RS)

Scope of Research

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



KEYWORDS

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

Selected Publications

Denis Romero, F.; Shimakawa, Y., Charge Transitions in Perovskite Oxides Containing Unusually High-valent Fe, *Chem. Comm.*, **55**, 3690-3696 (2019).

Goto, M.; Saito, S.; Shimakawa, Y., Unusual Ferromagnetic Metal: A-Site-Layer-Ordered Double Perovskite YBaCo_2O_6 with Unusually High Valence $\text{Co}^{3.5+}$, *Chem. Mater.*, **30**, 8702-8706 (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 $\text{CaCu}_3\text{Fe}_2\text{Re}_2\text{O}_{12}$ 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).

Unusual Ferromagnetic Metal: A-site-Layer-Ordered Double Perovskite YBaCo₂O₆ with Unusually High Valence Co^{3.5+}

A-site cation order in the double perovskites is much less common than B-cation order and a few compounds with the A-site-layered order were reported. Among them, layer-ordered oxygen-deficient perovskites, RBaCo₂O₅ (R: Y or lanthanoid) with mixed-valence Co^{2.5+}, are structurally interesting compounds. The layer ordering of R³⁺ and Ba²⁺ induces the layer ordering of oxygen vacancies along the stacking direction, giving an apically connected double layer of corner-sharing CoO₅ square pyramids (Figure 1). In this class of compounds, extra oxygen δ can be introduced into the R-layer, changing them into RBaCo₂O_{5+ δ} with CoO₅ pyramids and CoO₆ octahedra. The extra oxygen δ not only modifies the local oxygen coordination but also increases the valence state of the Co ions. As a result, the electronic structures of the compounds and spin states of the Co ions are significantly changed, giving rise to a wide variety of physical properties

In this study, we have synthesized a fully oxygenated polycrystalline sample of YBaCo₂O₆ by low-temperature topochemical ozone oxidation of the precursor YBaCo₂O₅ (Figure 1). Structure analysis with synchrotron X-ray diffraction data revealed that YBaCo₂O₆ crystallizes in a tetragonal structure at room temperature and shows an orthorhombic distortion below approximately 140 K. At the structural transition temperature, a ferromagnetic transition is induced, which suggests strong spin-lattice coupling. YBaCo₂O₆ contains unusual high valence Co^{3.5+} and the spins order ferromagnetically below 140 K. Low temperature electronic heat capacity data revealed that the compound is a metal with strong electronic correlation. The DFT calculation clarified that the up-spin band mainly contributes the metallic property in the spin polarized electronic structure. Therefore, the present A-site-layer-ordered double perovskite YBaCo₂O₆ with unusual high valence Co^{3.5+} is concluded to be an unusual ferromagnetic metal with strong electron correlation.

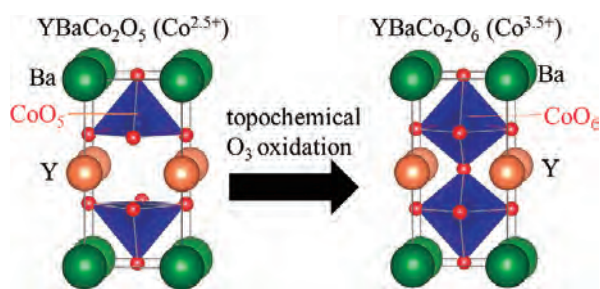


Figure 1. Crystal structures of YBaCo₂O₅ and YBaCo₂O₆.

Selective Growth of α -Fe₂O₃, γ -Fe₂O₃ and Fe₃O₄ at Low Temperatures and Under Ambient Pressure

Various functional properties for transition metal oxides are closely tied to the oxides' structural phases and the valence states of the constituent transition metals. Engineering crystal structures and cations' valence states is therefore a key for exploring functional properties, and developing techniques for such engineering has been one of the central issues in materials science research. In this study, we utilized mist chemical vapor deposition (mist CVD), in which ultrasonically atomized chemical solutions of precursors are used as starting materials and are transferred to the substrate surface under ambient conditions, enabling ones to (epitaxially) grow polymorphs of various binary oxides at relatively low temperatures.

Our focuses are on binary iron oxides which are well-known to have various structural phases and to accommodate +2 and +3 valence states of Fe. Here we show that that using mist CVD to synthesize iron oxides at relatively low temperatures (~400 °C) and under ambient (non-vacuum) conditions enables their crystal structures and Fe valence states (hematite, maghemite and magnetite) to be selectively controlled (Figure 2). We found that the structural phases (polymorphs) and preferred orientation of the iron oxides are strongly influenced by the surface structure of the substrate, while the valence states of Fe depend on the solvent in which the Fe precursor is dissolved (water or methanol). α -Fe₂O₃ and γ -Fe₂O₃ films, both of which contain iron that is in only its +3 valence state, are grown by atomizing the aqueous solution of the Fe precursor and transferring them to the (001) Al₂O₃ and (001) SrTiO₃ substrates. On the other hand, Fe₃O₄ films in which Fe³⁺ and Fe²⁺ coexist were grown from the mist made from the alcoholic solution. We also show that the fabricated films exhibit distinct magnetic properties depending on their crystal structures and the Fe valence states.

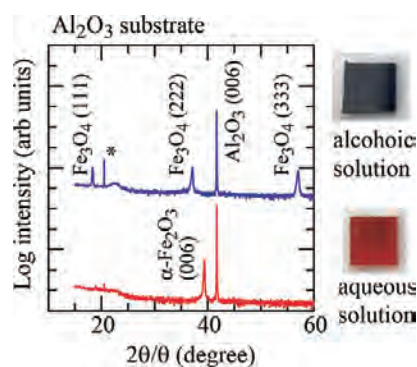


Figure 2. Photographs and X-ray 2 θ / θ profiles for (upper) Fe₃O₄ and (lower) α -Fe₂O₃ films grown on (001) Al₂O₃ substrates.



Assist Prof
WAKIOKA, Masayuki
(D Eng)

Students

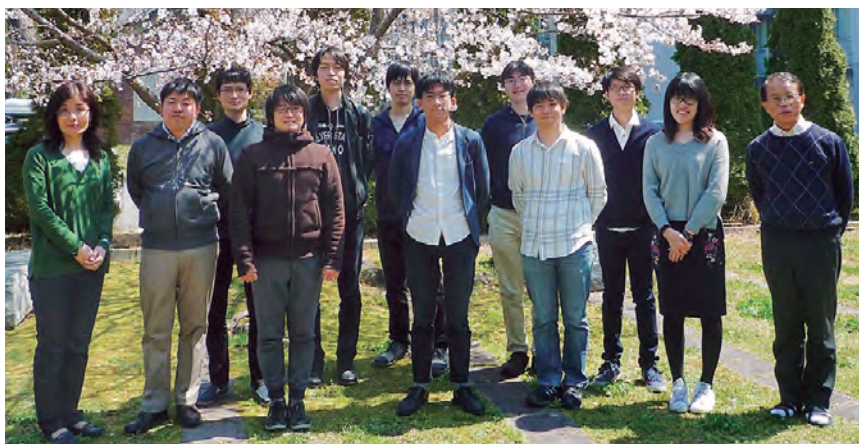
ISHIZUKA, Risa (M2)
MAEDA, Junya (M2)

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.; Ichihara, N.; Kitano, Y.; Ozawa, F., A Highly Efficient Catalyst for the Synthesis of Alternating Copolymers with Thieno[3,4-*c*]pyrrole-4,6-dione Units via Direct Arylation Polymerization, *Macromolecules*, **47**, 626-631 (2014).

Wakioka, M.; Nakamura, Y.; Montgomery, M.; Ozawa, F., Remarkable Ligand Effect of P(2-MeOC₆H₄)₃ on Palladium-Catalyzed Direct Arylation, *Organometallics*, **34**, 198-205 (2015).

Iizuka, E.; Wakioka, M.; Ozawa, F., Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Effective Prevention of Structural Defects Using Diamines, *Macromolecules*, **49**, 3310-3317 (2016).

Wakioka, M.; Takahashi, R.; Ozawa, F., Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Highly Selective Synthesis of π -Conjugated Polymers with Diketopyrrolopyrrole Units, *Macromolecules*, **50**, 927-934 (2017).

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

Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Synthesis of Donor–Acceptor Polymers Containing Unsubstituted Bithiophene Units

The combined use of P(2-MeOC₆H₄)₃ (**L1**) and TMEDA as ligands effectively prevents defect formation in palladium-catalyzed direct arylation polymerization (DAP) to give donor-acceptor type alternating copolymers (DA polymers) with unsubstituted 2,2'-bithiophene units (Figure 1). When only **L1** is used as the ligand, the reaction of **1a-Br** with 2,2'-bithiophene (**2-H**) in toluene at 100 °C forms a notable amount of insoluble materials via branching and cross-linking. In contrast, in the presence of **L1** and TMEDA, the formation of insoluble materials is completely suppressed, and poly(**1a-alt-2**) with well-controlled structure and high molecular weight is obtained ($M_n = 88,100$). Similarly, the reaction of **1b-Br** with **2-H** in toluene at 110 °C forms poly(**1b-alt-2**) with $M_n = 43,800$. The resulting polymers function as good components of bulk-heterojunction type organic solar cells (OSCs) using PC₇₁BM. In particular, poly(**1b-alt-2**) exhibits the best performance among DAP polymers reported so far (power conversion efficiency (PCE) = 9.0(1)%).

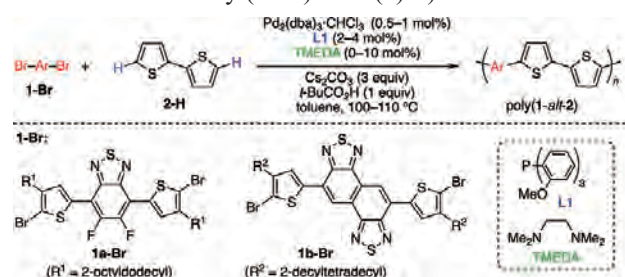


Figure 1. DAP synthesis of DA polymers containing bithiophene units.

Synthesis of π -Conjugated Polymers Containing Benzodithiophene and Benzotriazole Units via Highly Selective Direct Arylation Polymerization (DAP): Effects of Homocoupling Defects on Photovoltaic Performance

As shown above, recently, we have developed a highly selective catalyst that produces donor–acceptor-type alternating copolymers (DA polymers) with well-controlled structure via direct arylation polymerization (DAP). In this study, we applied this catalyst to investigate the effects of homocoupling defects on photovoltaic performance of DA polymers (PBDTBTz) containing benzodithiophene (BDT) and benzotriazole (BTz) units. Specifically, we prepared three types of polymers via DAP and compared their performance in bulk-heterojunction organic solar

cells (OSCs). One is a nearly perfect alternating copolymer, whereas the other two each contain one of the two kinds of homocoupling defects (BDT-BDT or BTz-BTz) (**P1**: $M_n = 31,500$, homocoupling defect < 0.1%; **P2**: $M_n = 22,800$, BDT-BDT defect = 19.3%; **P3**: $M_n = 22,800$, BTz-BTz defect = 18.5%). It was found that BDT-BDT defects significantly deteriorate the OSC performance, whereas BTz-BTz defects little affect the performance. It was also found that PBDTBTz prepared by Migita–Stille cross-coupling polymerization ($M_n = 32,100$) contains a large amount of BTz-BTz defects (13.1%). However, the polymer shows the OSC performance comparable to **P1** (PCE up to 9.9%) because the deterioration due to BTz-BTz defects is small.

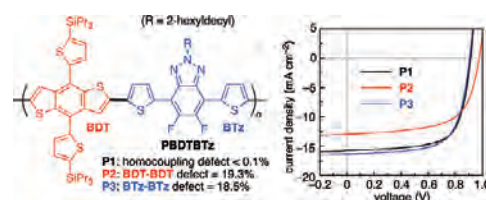


Figure 2. Structure of PBDTBTz and photovoltaic characteristics of PBDTBTz ($J-V$ curves).

Synthesis and Properties of T-Shaped π -Conjugated Polymers

π -Conjugated polymers including poly(3-hexylthiophene) (P3HT) have attracted much attention due to their solution processability and good mechanical properties, which allow easy access to the next generation of large-area devices such as organic solar cells (OSCs) and perovskite solar cells (PSCs). To improve the performance of these devices, the π -conjugated polymers should adopt face-on orientation to the substrate, since the charges are generally transported through the intermolecular overlap of π -orbitals. Although a variety of polymers that exhibit face-on orientation have been found, the guiding principles for controlling the orientation of polymers have not yet been established. In this study, we examined T-shaped π -conjugated polymers composed of a thiazole-fused benzothiadiazole (TBT) core and three P3HT side-chains (**T-10** and **T-20**). We found that this molecular geometry could prevent the edge-on orientation and cause face-on orientation, as confirmed by 2D-GIXD.

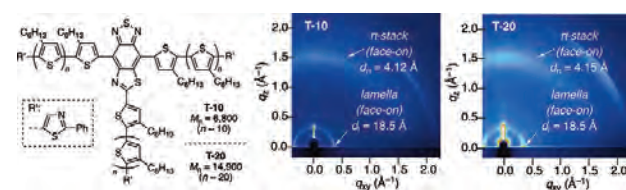


Figure 3. 2D-GIXD patterns of T-shaped π -conjugated polymers (**T-10** and **T-20**) in thin film.

International Research Center for Elements Science – Nanophotonics –

<https://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)



Program-Specific Res
YAMADA, Takumi
(D Sc)



Program-Specific Res
SEKIGUCHI, Fumiya
(D Sc)

Students

HANDA, Taketo (D3)

SANARI, Yasuyuki (D2)

OHARA, Keiichi (M2)

MASADA, Sojiro (M2)

KOBIYAMA, Etsuki (M1)

CHO, Kenichi (M1)

NAKAGAWA, Kotaro (M1)

ZHANG, Zhenya (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

Handa, T.; Tahara, H.; Aharen, T.; Kanemitsu, Y., Large Negative Thermo-optic Coefficients of a Lead Halide Perovskite, *Sci. Adv.*, **5**, [eaax0786-1]-[eaax0786-8] (2019).

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).

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).

Yamada, T.; Aharen, T.; Kanemitsu, Y., Near-Band-Edge Optical Responses of CH₃NH₃PbCl₃ Single Crystals: Photon Recycling of Excitonic Luminescence, *Phys. Rev. Lett.*, **120**, [057404-1]-[057404-6] (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).

Negative Thermo-optic Coefficient in Metal Halide Perovskites

Metal halide perovskites have been the subject of considerable research efforts due to their potential applications in optoelectronics. Understanding the refractive index and its change upon temperature rise is very important for the optimum design of semiconductor photonic devices. We found that the halide perovskite $\text{CH}_3\text{NH}_3\text{PbCl}_3$ shows a decrease in the refractive index with temperature, *i.e.*, negative thermo-optic coefficient. This negative thermo-optic coefficient is opposite to the positive coefficients in conventional inorganic semiconductors. Therefore, the halide perovskite works as a compensator of temperature-induced optical phase shift that inevitably occurs in inorganic semiconductors. To prove this compensation, we measured the optical phase shifts for conventional inorganic semiconductor ZnSe with and without $\text{CH}_3\text{NH}_3\text{PbCl}_3$ compensator (Figure 1(a)). As shown in Figure 1(b), we found that $\text{CH}_3\text{NH}_3\text{PbCl}_3$ actually compensates the optical phase shift of ZnSe. This discovery of the negative thermo-optic coefficient is of great importance for practical applications and adds new functionalities to the halide perovskites.

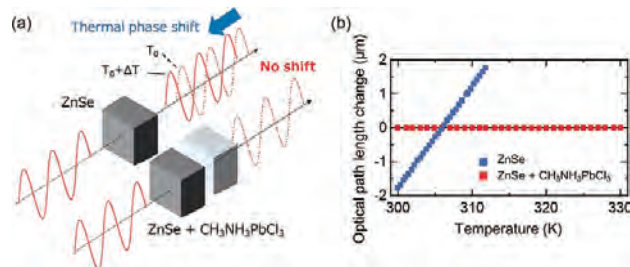


Figure 1. (a) Schematic of compensation measurement of optical phase shift. (b) Experimental results of optical phase shifts.

High Harmonic Generation from Metal Halide Perovskites

Light with a much higher photon energy than an input photon energy is generated by illuminating a solid with intense pulse laser. This phenomenon is called high-order harmonic generation (HHG). HHG originates from non-linear currents that are caused by strong driving of electrons and holes by a high-intensity electric field, but the detailed mechanism is still unclear. In addition, exploration of materials with high generation efficiency is necessary from the viewpoint of photonic device application. We observed high efficiency HHGs up to the 13th order from organic-inorganic hybrid perovskite $[\text{MAPbX}_3]$ ($\text{MA} = \text{CH}_3\text{NH}_3$, $\text{X} = \text{Cl, Br, I}$). Here, the mid-infrared laser pulse centered at energy of 0.35 eV with a maximum peak elec-

tric field of 10 MV/cm was used for photoexcitation. This finding is quite important for application to HHG light sources, since halide perovskite thin films are easily fabricated over a large area.

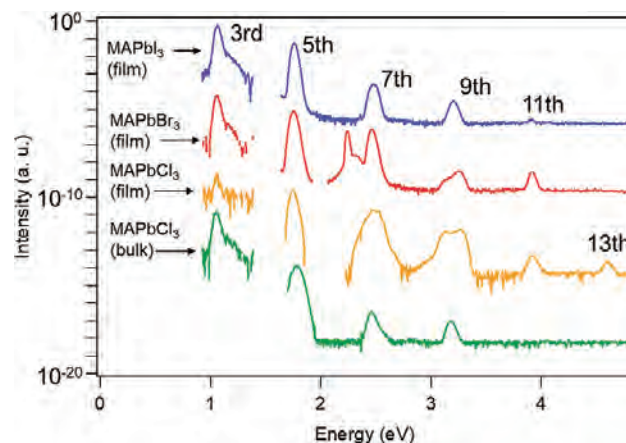


Figure 2. High harmonic generation spectra from methylammonium lead halide perovskite thin films.

Ionization and Neutralization Processes in Metal Halide Perovskite Nanocrystals Studied by Double Pump Spectroscopy

Lead halide perovskite CsPbX_3 ($\text{X} = \text{Cl, Br, I}$) nanocrystals have excellent properties such as very high luminescence efficiencies and efficient optical gain, then, are expected for various light-emitting device applications. Trions (charged excitons) in nanocrystals have a disadvantage of reducing luminescence efficiencies, but also have an advantage of lowering the optical gain threshold. Therefore, a detailed understanding of the trion generation and relaxation dynamics is required for device applications. We studied the ionization and neutralization processes of CsPbBr_3 nanocrystals by using double-pump transient absorption spectroscopy. It is clarified that photo-ionization processes are attributed to the radiative and non-radiative Auger recombination of biexcitons and trions, and neutralization processes are governed by the fast (~ 990 ps) and slow (~ 12 μs) process (Figure 3).

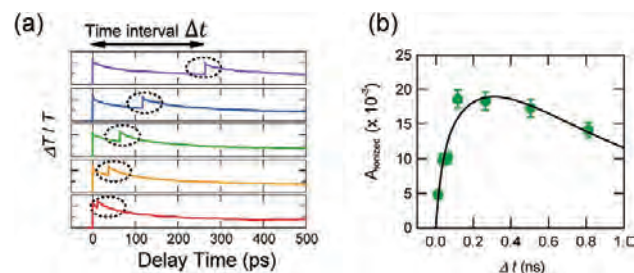


Figure 3. (a) Double pump transient absorption signals for various time intervals. (b) Time interval dependence of signal amplitude of ionized nanocrystals.

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 (D3)

NISHIYAMA, Hiroki (D3)

PRODINGER, Florian (D3)

KANEKO, Hiroto (D1)

MENG, Lingjie (D1)

XIA, Jun (D1)

YOSHIDA, Koki (M2)

BAN, Hiroki (M1)

GARCIA, Kimberly Gacayon (RS)

ZHANG, Ruixuan (RS)

SUN, Weiyu (RS)

FANG, Yue (RS)

MIYAZAKI, Urara (UG)

HASHIMOTO, Kentaro (UG)

Guest Res Assoc

GRIMSLEY, Nigel (Ph D)

DELMONT, Tom (Ph D)

Sorbonne University, France, 21–26 July

Centre National de la Recherche Scientifique, France, 31 August–24 September

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

Aramaki, T.; Blanc-Mathieu, R.; Endo, H.; Ohkubo, K.; Kanehisa, M.; Goto, S.; Ogata, H., KofamKOALA: KEGG Ortholog Assignment Based on Profile HMM and Adaptive Score Threshold, *Bioinformatics*, **btz859**, doi: 10.1093/bioinformatics/btz859 (2019).

Ibarbalz, F. M.; Henry, N.; Brandão, M. C.; Martini, S.; Busseni, G.; Byrne, H.; Coelho, L. P.; Endo, H.; Gasol, J. M.; Gregory, A. C.; Mahé, F.; Rigonato, J.; Royo-Llonch, M.; Salazar, G.; Sanz-Sáez, I.; Scalco, E.; Soviadan, D.; Zayed, A. A.; Zingone, A.; Labadie, K.; Ferland, J.; Marec, C.; Kandels, S.; Picheral, M.; Dimier, C.; Poulain, J.; Pisarev, S.; Carmichael, M.; Pesant, S.; Tara Oceans Coordinators; Babin, M.; Boss, E.; Iudicone, D.; Jaillon, O.; Acinas, S. G.; Ogata, H.; Pelletier, E.; Stemmann, L.; Sullivan, M. B.; Sunagawa, S.; Bopp, L.; de Vargas, C.; Karp-Boss, L.; Wincker, P.; Lombard, F.; Bowler, C.; Zinger, L., Global Trends in Marine Plankton Diversity Across Kingdoms of Life, *Cell*, **179**, 1084-1097 (2019).

Endo, H.; Suzuki, K., Spatial Variations in Community Structure of Haptophytes Across the Kuroshio front in the Tokara Strait, *Nagai, T., Saito, H., Suzuki, K., Takahashi, M.(eds.), Kuroshio Current: Physical, Biogeochemical and Ecosystem Dynamics, AGU Geophysical Monograph Series, AGU-Wiley*, 207-221 (2019).

Li, Y.; Endo, H.; Gotoh, Y.; Watai, H.; Ogawa, N.; Blanc-Mathieu, R.; Yoshida, T.; Ogata, H., The Earth is Small for “leviathans”: Long Distance Dispersal of Giant Viruses Across Aquatic Environments, *Microbes Environ.*, **34**, 334-339 (2019).

Yoshikawa, G.; Blanc-Mathieu, R.; Song, C.; Kayama, Y.; Mochizuki, T.; Murata, K.; Ogata, H.; Takemura, M., Medusavirus, A Novel Large DNA Virus Discovered from Hot Spring Water, *J. Virol.*, **93**, e02130-18 (2019).

Comparing Two Megaviridae Communities Using Meta-barcode During a Red Tide Period in an Enclosed Bay

“Megaviridae” is a proposed family of giant viruses infecting unicellular eukaryotes. They are very abundant and ubiquitous in the sea water and affect marine microbial community by their lytic infection cycle. However, only a few Megaviridae members have been explored in the marine environments, and their ecological roles in marine ecosystems remains unknown.

To study the differences of Megaviridae community in two different kind of water, surface sea water samples (0.22–3 μm) were collected from an enclosed bay (Uranouchi Inlet, Kochi) during a red tide period. A set of degenerated primers (called “MEGAPRIMER”), which target family B DNA polymerase genes of Megaviridae, was used to assess the composition of Megaviridae community. Bioinformatic analysis was applied after sequencing. As a result, hundreds of operational taxonomic units (OTUs) were identified in each sample. When we compared the Megaviridae structures between within and without red-tide waters, there was a clear difference between these two samples in a community variation analysis. The difference was also visible in dominant OTU proportions (Figure 1) between the two types of samples. Phylogenetic analysis based on a maximum-likelihood method showed that almost all of the OTUs belong to unknown Megaviridae branches (Figure 1). Future study will mainly focus on the host-virus interactions and the relationship between viral community and environmental factors, that may reveal ecological functions of Megaviridae in a coastal ecosystem.

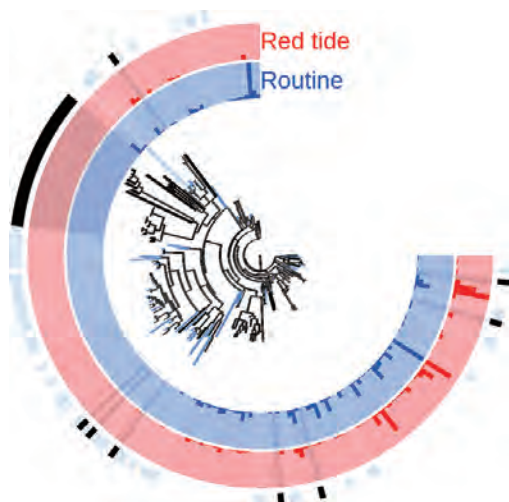


Figure 1. Phylogenetic tree of Megaviridae OTUs (97% identity) based on ML method. Relative abundances of Megaviridae in routine and red-tide samples were also shown in blue and red colors, respectively. Reference sequences-black; other pelagic sea water sequences-light blue.

An Assessment of NCLDV Host Prediction Based on Co-occurrence Analysis

Nucleocytoplasmic large DNA viruses (NCLDVs) form a monophyletic group of viruses and our understanding of these virus-host systems is limited. Co-culture with their host is the “Gold Standard” for the identification of virus-host relationship but limited by our ability to cultivate microorganisms (thus hosts). Therefore, consideration should be put into cultivation-independent approaches.

In our research, we used deeply sequenced metagenomic and amplicon data generated by the *Tara* Oceans project to examine if the use of co-occurrence approaches can provide virus-host relationship for this group of viruses. Samples were collected from the surface (SRF) and deep chlorophyll maximum (DCM) layers of global oceans. The abundance matrices of NCLDVs and eukaryotes were constructed from pico-size fraction (0.22–1.6 or 0.22–3.0 μm) and four larger size fractions (0.8–5, 3–20, 5–20, 20–180 and 180–2000 μm), respectively. Co-occurrence analysis was carried out by Flashweave. As a result, we got a large number of associations between NCLDVs and eukaryotes (Figure 2). However, because of the deficiency of information about known NCLDVs, it will be necessary to quantitatively evaluate the FlashWeave host-virus relationship predictions. Furthermore, the prediction of the NCLDV-host pairs by abundance-based methods may be improved by combining with other data, such as phylogenetic relationships among various viruses. These bioinformatic tools eventually will help us to understand the natural diversity, life cycle, interactions and co-evolution of NCLDVs and their host.

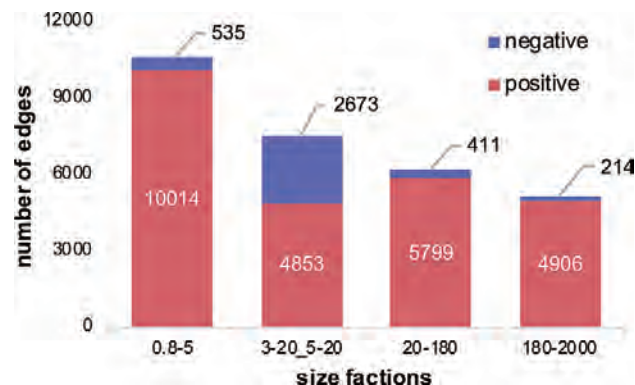


Figure 2. Number of edges between NCLDVs and eukaryotes in inferred network by size fraction. Red: edges with positive weight; Blue: edges with negative weight.

Bioinformatics Center – Mathematical Bioinformatics –

<https://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)



Program-Specific Res
MÜNZNER,
Ulrike Tatjana Elisabeth
(Ph D)

Students

LIU, Pengyu (D3)

YU, Coleman (D3)

TAKAGI, Motoshige (D3)

LI, Ruiming (D2)

WANG, Feiqi (D2)

OHTOMO, Masahiro (D2)

NAKASHIMA, Shogo (D1)

KUMANO, Sou (M2)

YANG, Ziwei (RS)

MA, Yier (RS)

Guest Res Assoc

LEE, Jung-Yu (Ph D)

CHEN, Yun-Ti (Ph D)

LIN, Xiang-Yu (Ph D)

National Chiao Tung University, China, P.R., 18 November–6 December

National Chiao Tung University, China, P.R., 18 November–6 December

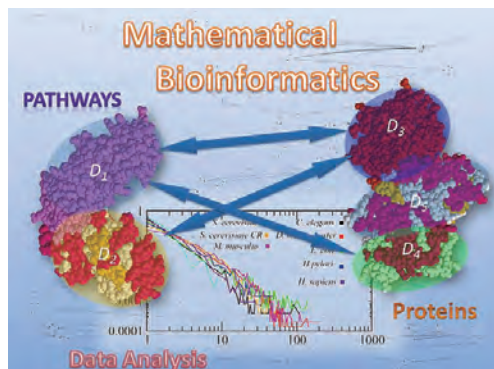
National Chiao Tung University, China, P.R., 18 November–6 December

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.; Melkman, A. A., Identification of the Structure of a Probabilistic Boolean Network from Samples Including Frequencies of Outcomes, *IEEE Transactions on Neural Networks and Learning Systems*, **30**, 2383-2396 (2019).

Schwartz, J.-M.; Otokuni, H.; Akutsu, T.; Nacher, J. C., Probabilistic Controllability Approach to Metabolic Fluxes in Normal and Cancer Tissues, *Nat. Commun.*, **10**, [2725-1]-[2725-9] (2019).

Itami-Matsumoto, S.; Hayakawa, M.; Uchida-Kobayashi, S.; Enomoto, M.; Tamori, A.; Mizuno, K.; Toyoda, H.; Tamura, T.; Akutsu, T.; Ochiya, T.; Kawada, N.; Murakami, Y., Circulating Exosomal miRNA Profiles Predict the Occurrence and Recurrence of Hepatocellular Carcinoma in Patients with Direct-Acting Antiviral-Induced Sustained Viral Response, *Biomedicines*, **7**, [81-1]-[81-14] (2019).

Marini, S.; Vitali, F.; Rampazzi, S.; Demartini, A.; Akutsu, T., Protease Target Prediction via Matrix Factorization, *Bioinformatics*, **35**, 923-929 (2019).

Hou, W.; Ruan, P.; Ching, W.-K.; Akutsu, T., On the Number of Driver Nodes for Controlling a Boolean Network When the Targets Are Restricted to Attractors, *J. Theor. Biol.*, **463**, 1-11 (2019).

Identification of the Structure of a Probabilistic Boolean Network from Probability Distribution of Samples

In order to understand dynamical behavior of biological systems, various kinds of mathematical models have been utilized. Among them, the Boolean network (BN) is one of the simplest non-linear models, in which 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. In a BN, each node corresponds to a gene or neuron, and 1 and 0 mean that genes/neurons are active and inactive, respectively. Although BN is an old model proposed more than 50 years ago, extensive studies are still being done. However, real biological systems contain noise and other stochastic factors. In order to cope with these stochastic factors, the probabilistic Boolean network (PBN) has been proposed and utilized, 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 (Figure 1). We have been studying 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 our previous work, we studied the identification of the structure (*i.e.*, set of Boolean functions assigned for each node) of a PBN using information only on the occurrences of samples. In this work, we make use of additional information obtainable from samples: the frequencies of occurrences of sub-tuples. We show that under this model, it is possible to identify a PBN for much broader classes of PBNs. In particular, we prove under a reasonable assumption that the structure of a PBN can be identified from among the class of PBNs that have at most three functions assigned to each node, but that identification may be impossible if four or more functions are assigned to each node. We also present an efficient algorithm for the identification of a PBN consisting of threshold functions from samples.

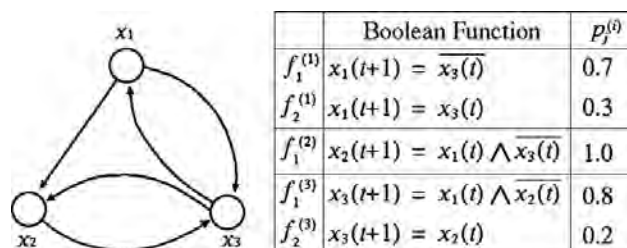


Figure 1. Example of a probabilistic Boolean threshold network. Boolean functions are independently selected at each time step according to the prescribed probabilities shown in the table.

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.

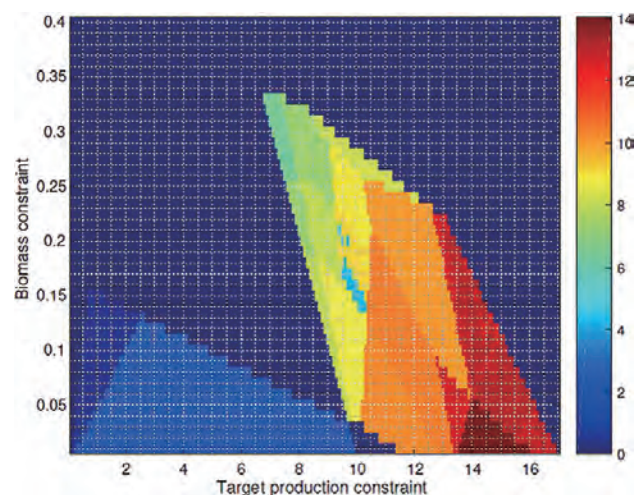


Figure 2. An example of the production rate heatmap for a target metabolite where each grid represents constraints for the ranges by the production rate and the growth rate.

Bioinformatics Center – Bio-knowledge Engineering –

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



Prof

MAMITSUKA, Hiroshi
(D Sc)



Senior Lect

NGUYEN, Hao Canh
(D Knowledge Science)



Program-Specific Res

WIMALAWARNE, Kishan
(D Eng)



Program-Specific Res

SUN, Lu
(D Eng)

Students

NGUYEN, Dai Hai (D3) NGUYEN, Duc Anh (D2)

Guest Scholar

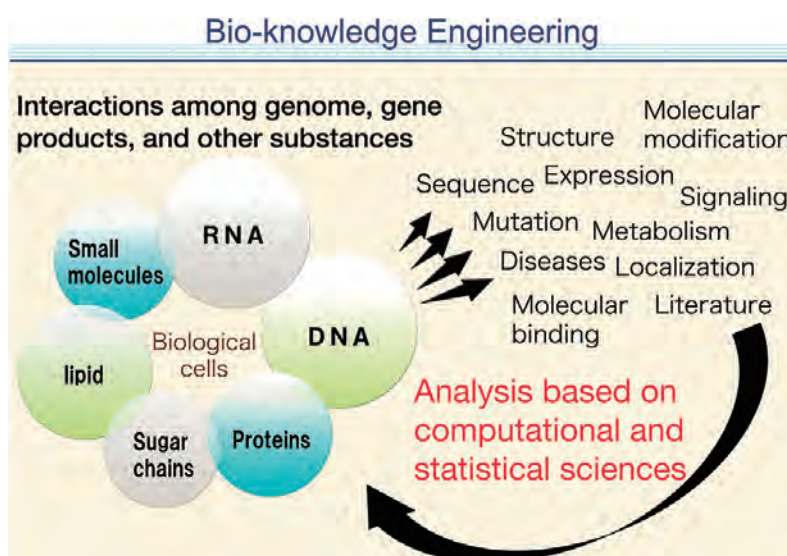
KASKI, Samuel (Ph D) Aalto University, Finland, 2 April–31 May

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

- Sun, L.; Nguyen, C. H.; Mamitsuka, H., Multiplicative Sparse Feature Decomposition for Efficient Multi-View Multi-Task Learning, *Proceedings of the 28th International Joint Conference on Artificial Intelligence (IJCAI 2019)*, 3506-3512 (2019).
- Sun, L.; Nguyen, C. H.; Mamitsuka, H., Fast and Robust Multi-View Multi-Task Learning via Group Sparsity, *Proceedings of the 28th International Joint Conference on Artificial Intelligence (IJCAI 2019)*, 3499-3505 (2019).
- You, R.; Yao, S.; Xiong, Y.; Huang, X.; Sun, F.; Mamitsuka, H.; Zhu, S., NetGO: Improving Large-scale Protein Function Prediction with Massive Network Information, *Nucleic Acids Res.*, **47**, W379-W387 (2019).
- Nguyen, D. H.; Nguyen, C. H.; Mamitsuka, H., ADAPTIVE: leArning DAta-dePendentT, ConcIse Molecular VEctors for Fast, Accurate Metabolite Identification from Tandem Mass Spectra, *Bioinformatics (Proceedings of the 27th International Conference on Intelligent Systems for Molecular Biology (ISMB/ECCB 2019))*, **35** (14), i164-i172 (2019).
- Gillberg, J.; Marttinen, P.; Mamitsuka, H.; Kaski, S., Modelling G×E with Historical Weather Information Improves Genomic Prediction in New Environments, *Bioinformatics*, **35**(20), 4045-4052 (2019).

Advanced Machine Learning for Metabolite Identification from Mass Spectrometry

Metabolites are small molecules and play important functions in living cells such as energy transport, signaling, building blocks of cells and so on. Identifying their biochemical characteristics or so-called metabolite identification is an essential task in metabolomics to increase the knowledge of biological systems. However, it is still a challenging task due to the size or coverage of spectra libraries. Mass spectrometry is a widely used technique in analytical chemistry for dealing with metabolite identification task. In detail, a chemical compound is decomposed into fragments, of which mass-to-charge ratios (m/z) are measured to obtain a mass spectrum. The spectrum can also be represented by a list of peaks, each of which corresponds to a fragment captured by MS. The MS spectra provide structural information about the measured compound, which makes MS more useful for tackling the task of metabolite identification.

Computational methods proposed for identifying metabolites from MS data can be categorized into three main groups: (i) spectra library search; (ii) *in silico* fragmentation; and (iii) machine learning [1]. Our research focuses on machine learning based approach, where the common scheme is to predict a chemical structure of a given spectrum through an intermediate representation called molecular fingerprints. It consists of two steps: (i) predicting molecular fingerprints from spectra; (ii) searching molecular structures in database corresponding to the predicted fingerprints. Molecular fingerprints are often binary feature vectors, which should be large to cover all possible substructures and chemical properties, and therefore heavily redundant, in the sense of having many substructures irrelevant to the task, causing limited predictive performance and computational efficiency.

We propose a machine learning framework for metabolite identification task, named ADAPTIVE [2], which allows to learn representation for molecular structures, which we call molecular vectors, instead of using molecular fingerprints to characterize or represent molecules. It has two subtasks in learning step: (i) learning a mapping from structures to molecular representation vectors and (ii) learning another mapping from spectra to molecular vectors as illustrated in Figure 1. In Subtask 1, ADAPTIVE learns a mapping to generate molecular vectors for metabolites using their chemical structures and these vectors are specific to both data and task, and therefore less redundant. The mapping is parameterized by a model, namely message passing neural network (MPNN), and its parameters are trained so that the correlation (measured by Hilbert-

Schmidt Independence Criterion, HSIC) between spectra and molecular vectors are maximized. For Subtask 2, ADAPTIVE use IOKR [3], standing for Input Output Kernel Regression, to learn another mapping from spectra to molecular vectors generated by the Subtask 1.

We conducted experiments using a benchmark data to evaluate the proposed method against existing ones in terms of predictive performance and computational efficiency. As shown in Figure 2, ADAPTIVE achieved the best predictive performance, outperforming the second best method, IOKR, with the difference of around 3–5% of *top-20* under the same conditions. Furthermore, ADAPTIVE was significantly faster than IOKR (4–7 times) because molecular vectors by ADAPTIVE are much more concise and adaptive to given data and task than molecular fingerprints used in existing methods.

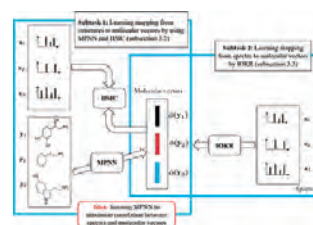


Figure 1. Overview of ADAPTIVE. It has two subtasks: (i) Subtask 1: estimate parameters of a mapping from structures to molecular vectors, given a set of spec-structure pairs; (ii) Subtask 2: learn another mapping from spectra to molecular vectors, generated by subtask 1.

Method	Vec. size	MKL	Accuracies (mean/SD %)		
			Top 1	Top 10	Top 20
FingerID	2763	None	17.74	49.59	58.17
CSiFingerID	2763	ALIGNF	24.82	60.47	68.20
CSiFingerID	2763	ALIGNF	28.84	66.07	73.07
Platz					
IOKR linear	2765	UNIMKL	30.58/2.23	65.99/2.46	73.53/2.47
		ALIGNF	28.54/2.54	65.77/2.39	73.19/3.11
ADAPTIVE linear	100	UNIMKL	29.42/2.83	70.01/2.79	77.48/2.98
		ALIGNF	29.19/3.21	69.52/2.89	77.64/3.23
		UNIMKL	29.57/3.96	69.38/3.05	76.93/2.98
IOKR Gaussian	2765	UNIMKL	29.11/3.45	69.53/2.72	77.56/2.43
		ALIGNF	30.22/3.47	70.48/2.72	78.18/2.67
		UNIMKL	30.61/3.23	70.51/2.52	78.23/2.75
ADAPTIVE Gaussian	100	UNIMKL	30.66/3.34	66.51/2.87	73.94/2.54
		ALIGNF	29.59/2.58	66.13/2.09	73.62/1.85
		UNIMKL	29.47/3.21	70.01/2.83	77.51/2.11
IOKR	2765	UNIMKL	29.37/3.21	69.91/2.64	77.48/2.33
		ALIGNF	29.44/3.86	69.84/2.78	77.08/2.95
		UNIMKL	28.98/3.32	69.65/2.71	77.15/2.74
ADAPTIVE	100	UNIMKL	30.31/3.48	71.10/2.73	78.51/2.65
		ALIGNF	31.03/3.40	70.89/2.74	78.52/2.52
		UNIMKL	30.31/3.48	71.10/2.73	78.51/2.65

Method	Mol. vec. size	prediction time (ms/example)	
		Linear	Gaussian
IOKR	2765	140.22	3332.4
ADAPTIVE	100	20.32	802.6
	200	39.88	844.33
	300	54.14	1071.8

Figure 2. Evaluation of ADAPTIVE against existing methods in terms of *top-k* ($k = 1, 10$ and 20) accuracies and computation time.

- [1] Nguyen, D. H. *et al.*, Recent Advances and Prospects of Computational Methods for Metabolite Identification: a Review with Emphasis on Machine Learning Approaches, *Brief. Bioinf.*, doi:10.1093/bib/bby066 (2018).
- [2] Nguyen, D. H. *et al.*, Adaptive: Learning Data-dependent, Concise Molecular Vectors for Fast, Accurate Metabolite Identification from MS/MS, *Bioinformatics*, **35**, i164-i172 (2019).
- [3] Brouard, C. *et al.*, Fast Metabolite Identification with Input Output Kernel Regression, *Bioinformatics*, **32**, i28-i36 (2016).



**HAKUBI RESEARCHERS’
ACTIVITIES IN ICR**

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





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
INTERNATIONAL **J**OINT
USAGE/**R**ESEARCH
CENTER

iJURC Cooperative Research Subjects 2019

(1 April 2019 ~ 31 March 2020)

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

Ultra Directional Neutron Beam Generation by Using Laser Driven X-ray and Spin Polarized Deuterium Target
ARIKAWA, Yasunobu, Institute of Laser Engineering, Osaka University
Host in iJURC INOUE, Shunsuke I

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

Development of New Target Material Using CNT
OHNISHI, Tetsuya, Nishina Center for Accelerator Based Science, RIKEN
Host in iJURC WAKASUGI, Masanori

Laser Driven Ion Acceleration Experiment Using Carbonized Thin Tape Target
KONDO, Kotaro, Kansai Photon Science Institute, National Institutes for Quantum and Radiological Science and Technology
Host in iJURC HASHIDA, Masaki

Catalysis Research of Transition Metal Oxides
GUO, Haichuan, Ningbo Institute of Industrial Technology (CNITECH) of the Chinese Academy of Sciences
Host in iJURC SHIMAKAWA, Yuichi I

Development of Iron-catalyzed Strategies for Diversity Oriented Synthesis of Heterocycles and Carbocycles
HAJRA, Alakananda, Department of Chemistry, Visva-Bharati University
Host in iJURC NAKAMURA, Masaharu I

Iron-Catalyzed Carbometalation of Heterobicyclic Alkenes: Development of Asymmetric Reactions and Application to Synthesis of Polycyclic Aromatic Hydrocarbons
ITO, Shingo, School of Physical and Mathematical Sciences, Nanyang Technological University
Host in iJURC NAKAMURA, Masaharu I

Open-cage Fullerenes Incorporating Hydrogen as n-Type Composite Materials for Polymer Solar Cell Applications
CHUANG, Shih-Ching, Department of Applied Chemistry, National Chiao Tung University
Host in iJURC MURATA, Yasujiro I

Development of Mid-infrared Laser and Applications to Nano-material Sciences
ITATANI, Jiro, The Institute for Solid State Physics, The University of Tokyo
Host in iJURC KANEMITSU, Yoshihiko

Study on the Mechanism for the Stability of an In-doped Novel Fe-Pd Phase
TATETSU, Yasutomi, Liberal Arts Organization, Meio University
Host in iJURC TERANISHI, Toshiharu

Development of the Novel Functional Paint Using Metallic Uru-shiol Complexes
TACHIBANA, Yoichi, Kyoto Municipal Institute of Industrial Technology and Culture
Host in iJURC NAKAMURA, Masaharu

Photocurrent of Pb Perovskite Solar Cells by Heterodyne Interference Spectroscopy
OGAWA, Yoshihiro, Joetsu University of Education
Host in iJURC KANEMITSU, Yoshihiko

Network Analyses for Data-driven Exploration and Hypothesis Testing in Microbial Ecology
CHAFFRON, Samuel, Laboratoire des Sciences du Numérique de Nantes (LS2N), Centre National de la Recherche Scientifique (CNRS)
Host in iJURC BLANC-MATHIEU, Romain I

Distribution of Prasinoviruses and Their Association with Natural Hosts in the Global Ocean
GRIMSLEY, Nigel, Sorbonne University
Host in iJURC ENDO, Hisashi I

Viral Impacts on Microbial Ecosystems in the Highly-enclosed Inlet, Uranouchi Bay, Kochi
NAGASAKI, Keizo, Faculty of Agriculture and Marine Science, Kochi University
Host in iJURC ENDO, Hisashi

Isolation of New Giant Viruses and Their Genomic and Transcriptomic Characterization
TAKEMURA, Masaharu, Faculty of Science, Tokyo University of Science
Host in iJURC OGATA, Hiroyuki

Concentration of Bloom Forming Algae from Environmental Samples and Identification of the Viruses Infecting the Alga
YOSHIDA, Takashi, Faculty of Agriculture, Kyoto University
Host in iJURC OGATA, Hiroyuki

Exhaustive Analysis of Local Structural Changes of Biological Networks
SHIGA, Motoki, Informatics Course, Department of Electrical, Electronic and Computer Engineering, Faculty of Engineering, Gifu University
Host in iJURC MAMITSUKA, Hiroshi

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

Application of s-Tetrazines in Guanidine Functionalization of Fullerenes
MARGETIC, Davor, Division of Organic Chemistry and Biochemistry, Rudjer Boskovic Institute
Host in iJURC MURATA, Yasujiro I

I: International Joint Research

F: Female PI

Preparation of Novel Branched Block Copolymer with Well-controlled Stereoregularity and Evaluation of Its Molecular Aggregation State

HIRAI, Tomoyasu, Department of Applied Chemistry, Osaka Institute of Technology

Host in iJURC TAKENAKA, Mikihito

Study of Anchoring Behavior of Chiral Nematic Liquid Crystal

AKAGI, Kazuo, Research Organization of Science and Technology, Ritsumeikan University

Host in iJURC TSUJII, Yoshinobu

Application of $\delta^{98/95}\text{Mo}$ and $\delta^{186/184}\text{W}$ Isotopes Ratios for the Reconstruction of Late Miocene Oxygenation in the Arabian Sea

GUNDIGA PUTTOJIRAO, Gurumurthy, Geochemistry Research Lab, Birbal Sahni Institute of Palaeosciences

Host in iJURC SOHRIN, Yoshiki

Investigation on the Decay Process of Hot Carriers in Heavily Doped Semiconductor Nanocrystals

DOUHAL, Abderrazzak A., Physical Chemistry, University of Castilla-La Mancha (UCLM)

Host in iJURC SAKAMOTO, Masanori

Elongational Rheology of Telechelic-type Ionomers

CHEN, Quan, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences (CAS)

Host in iJURC MATSUMIYA, Yumi

Study on Transportation and Separation of Metal Ions Through a Liquid Membrane Using Ionic Liquid

MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education

Host in iJURC SOHRIN, Yoshiki

Study on Gelation Behaviors of Polymer Oleogels

OSAKA, Noboru, Graduate School of Science, Okayama University of Science

Host in iJURC TAKENAKA, Mikihito

Investigation on the Carrier Relaxation Processes of Quantum Dots Protected with Functional Organic Molecules

TAMAI, Naoto, School of Science and Technology, Kwansai Gakuin University

Host in iJURC SAKAMOTO, Masanori

Preparation and Mechanical Properties of Noncovalent Bonded Elastomers Based on Styrenic Block Copolymers

NORO, Atsushi, Graduate School of Engineering, Nagoya University

Host in iJURC WATANABE, Hiroshi

EXPANDING SUBJECTS

(IN SPECIFIC FIELDS CHOSEN BY iJURC)

Advanced Functionality on Materials Induced by Intense THz Pulse Irradiation

NAGASHIMA, Takeshi, Faculty of Science and Engineering, Setsunan University

Host in iJURC HASHIDA, Masaki

Research on the High-performance Superconducting Cavity and the Cost Reduction by Noble Inner-surface Processes

SAEKI, Takayuki, Accelerator Division VI, High Energy Accelerator Research Organization

Host in iJURC 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, Advanced Industrial Science and Technology

Host in iJURC IWASHITA, Yoshihisa

Controlling Chiral Structure of Au Nanowires by Enantiomeric Excess

KAWAI, Takeshi, Faculty of Engineering, Tokyo University of Science

Host in iJURC KURATA, Hiroki

Crystal Structure Analysis of GraE Protein from Root-Nodule-Forming Bacterium

OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University

Host in iJURC FUJII, Tomomi

Enhanced Production of Fast Ions by TNSA with Pre-pulse Laser

SUNAHARA, Atsushi, Institute of Laser Engineering, Osaka University

Host in iJURC INOUE, Shunsuke

Fundamental Study on Micro-fabrication of Si with Controlling Laser Absorption

KUSABA, Mitsuhiro, Electronics, Information and Communication Engineering, Osaka Sangyo University

Host in iJURC HASHIDA, Masaki

Development of a Fast and Efficient Neutron Trigger Device for Electron-RI Scattering Experiments

ENOKIZONO, Akitomo, Nishina Center for Accelerator Based Science, RIKEN

Host in iJURC WAKASUGI, Masanori

Optimization of 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 iJURC IWASHITA, Yoshihisa

High Pressure Approach to the Synthesis of Novel Ferroelectric Photovoltaic Transition Metal Oxides

CHEN, Wei-Tin, Center for Condensed Matter Sciences, National Taiwan University

Host in iJURC SHIMAKAWA, Yuichi

Small Molecule Activation Using Anionic Crypto-FLPs

STREUBEL, Rainer, Institute for Inorganic Chemistry, University of Bonn

Host in iJURC TOKITOH, Norihiro

Development of Unsymmetrical π -Electron Systems of Heavier Main Group Elements and Elucidation of Their Property

IWAMOTO, Takeaki, Department of Chemistry, Tohoku University

Host in iJURC TOKITOH, Norihiro

Mechanistic Studies of C-H Bond Functionalization Reactions Catalyzed by 3d Transition Metals

YOSHIKAI, Naohiko, Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University

Host in iJURC NAKAMURA, Masaharu

Study on Nickelate Complexes Constructed by a Monoanionic Tridentate Pincer-type Ligand

YAMAGUCHI, Yoshitaka, Faculty of Engineering, Division of Materials Science and Chemical Engineering, Yokohama National University

Host in iJURC NAKAMURA, Masaharu

Mechanistic and Synthetic Studies of Poly((meth)acrylonitrile) Chain End Radicals

NAKAMURA, Yasuyuki, Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science

Host in iJURC YAMAGO, Shigeru

Creation of Effective Oxidation Scavenger for Efficient Perovskite-based Solar Cells

SASAMORI, Takahiro, Graduate School of Natural Sciences, Nagoya City University

Host in iJURC WAKAMIYA, Atsushi

Integrating Omics Data and Module-based Network with Deep Learning to Develop Cancer Type Predictive Models

YANG, Jinn-Moon, Department of Biological Science and Technology/Institute of Bioinformatics & Systems Biology, National Chiao Tung University

Host in iJURC AKUTSU, Tatsuya

Next-generation Bioinformatics Approaches for the Accurate Identification of Protease-specific Substrate Cleavage Sites

SONG, Jiangning, Monash Biomedicine Discovery Institute, Monash University

Host in iJURC AKUTSU, Tatsuya

Statistical Machine Learning Methods for Molecular Network Analysis

KAYANO, Mitsunori, Research Center for Global Agromedicine, Obihiro University of Agriculture and Veterinary Medicine

Host in iJURC MAMITSUKA, Hiroshi

Coupling of Planar and Curved π -Systems for the Development of Novel Functional Materials

NARITA, Akimitsu, Max Planck Institute for Polymer Research

Host in iJURC HIROSE, Takashi

Design, Synthesis, and Characterization of Charge Transport Materials for Non-lead Perovskite

SAEKI, Akinori, Department of Applied Chemistry, Graduate School of Engineering, Osaka University

Host in iJURC WAKAMIYA, Atsushi

Development of Novel π -Conjugated Polymers and Their Application to Organic Photovoltaics

OSAKA, Itaru, Graduate School of Engineering, Hiroshima University

Host in iJURC WAKIOKA, Masayuki

Molecular Engineering of Organic Semiconductors Toward the Control of Molecular Packing in Thin Films via a Thermal Precursor Approach

SUZUKI, Mitsuharu, Graduate School of Engineering, Osaka University

Host in iJURC MURATA, Yasujiro

Synthesis and Properties of π -Conjugated Zwitterions Composed of an Electron-Donating Anion and an Electron-Accepting Cation

SHIMIZU, Akihiro, Department of Materials Engineering Science Graduate School of Engineering Science, Osaka University

Host in iJURC HIROSE, Takashi

The Elemental and Isotopic Composition of Particulate Trace Metals in the Subarctic Pacific Ocean: Sources and Internal Cycling

HO, Tung-Yuan, Research Center for Environmental Changes, Academia Sinica

Host in iJURC SOHRIN, Yoshiki

Development of Photocatalytic Materials by Quantitative Charge Carrier Dynamics and Structural Analysis

TACHIBANA, Yasuhiro, School of Engineering, RMIT University

Host in iJURC TERANISHI, Toshiharu

High Frequency Rheological and Dielectric Response of Polymeric Liquids

SUKUMARAN, Sathish K., Graduate School of Organic Materials Science, Yamagata University

Host in iJURC WATANABE, Hiroshi

Study on the Origin and Generation Mechanism of Urban Atmospheric Aerosol

NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kindai University

Host in iJURC SOHRIN, Yoshiki

Characterization of Physical Properties and Structure of Partially Fluorinated Phospholipid Membrane

SONOYAMA, Masashi, Faculty of Science and Technology, Gunma University

Host in iJURC HASEGAWA, Takeshi

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

Role of PX-PH-type Phospholipase Ds in Plant Intracellular Membrane Traffic

OHASHI, Yohei, MRC Laboratory of Molecular Biology, University of Cambridge

Host in iJURC AOYAMA, Takashi

Proteomic Approach to Discovering Specific Inhibitors for Bile-Acid Interacting Enzymes

LEI, Xiaoguang, College of Chemistry and Molecular Engineering, Peking University

Host in iJURC UESUGI, Motonari

Micro- and Nano-structural Characterization by Advanced Transmission Electron Microscopy of Novel Functional Materials for Battery Development

CHAIRUANGSRI, Torranin, Industrial Chemistry, Chiang Mai University

Host in iJURC KURATA, Hiroki

Construction of Low-temperature Protein Expression System by Using Cold-adapted Microorganisms

DAI, Xianzhu, College of Resources and Environment, Southwest University

Host in iJURC KURIHARA, Tatsuo

Determine the Three-dimensional Structure of ^{13}C Labeled α -Synuclein(61-95) in the Langmuir-Blodgett Film and Supported Phospholipids Bilayers by p-MAIRS FT-IR

WANG, Chengshan, Middle Tennessee State University

Host in iJURC HASEGAWA, Takeshi

Effect of Dipole Alignment along Chain Backbone on Dielectric Relaxation of Type-A Polymers at Association/Dissociation Equilibrium

KWON, Youngdon, School of Chemical Engineering, Sungkyunkwan University

Host in iJURC MATSUMIYA, Yumi I

Study on the Regulatory Network of Plant Epidermal Cell Differentiation

TOMINAGA, Rumi, Graduate School of Biosphere Science, Hiroshima University

Host in iJURC AOYAMA, Takashi F

Investigation of Magnetic and Electric Properties of Cobalt Ferrite Films for Development of High Spin-polarized Current Source

TANAKA, Masaaki, Department of Physical Science and Engineering, Nagoya Institute of Technology

Host in iJURC ONO, Teruo

Giant Isotope Effects of Deuterium Atoms Terminating on Nanocrystalline Silicon and Their Use

MATSUMOTO, Takahiro, School of Design and Architecture, Graduate School of Design and Architecture, Nagoya City University

Host in iJURC KANEMITSU, Yoshihiko

Synthesis and Biological Evaluation of Antitumor Cyclic Octadepsipeptide Containing α -Fluorinated Amino Acid

NAGASAWA, Hideko, Gifu Pharmaceutical University

Host in iJURC KAWABATA, Takeo F

Studies on Total Synthesis of Gonytolides

YOSHIMURA, Tomoyuki, Graduate School of Medical Sciences, Kanazawa University

Host in iJURC KAWABATA, Takeo

Studies on the Physiological Significance of Two Alanine Dehydrogenases in *Geobacillus kaustophilus*

OMORI, Taketo, Faculty of Engineering, Osaka Institute of Technology

Host in iJURC KURIHARA, Tatsuo

Synthesis and Study of Oxides with Unusually High-valent Cation

SAITO, Takashi, Institute of Materials Structure Science, High Energy Accelerator Research Organization KEK

Host in iJURC SHIMAKAWA, Yuichi

Application of Surfactant for Extraction of Platinum Group Elements Using Solvent Impregnated Resin

KURAHASHI, Kensuke, Environmental and Materials Chemistry Course, Osaka Prefecture University College of Technology

Host in iJURC SOHRIN, Yoshiki

Manipulation of Three Dimensional Structure of Porous Polymer Composites Controlled by Additive Manufacturing

MURASE, Hiroki, Faculty of Home Economics, Kyoritsu Women's University

Host in iJURC TSUJII, Yoshinobu

Investigation of New Anti-lust Surfactant Containing a Perfluoroalkyl Chain and an Amino Acid Head Group

YAMADA, Norihiro, Faculty of Education, Chiba University

Host in iJURC HASEGAWA, Takeshi

Ring-size-dependent Excitation Dynamics of Cycloparaphenylenes

FUJITSUKA, Mamoru, The Institute of Scientific and Industrial Research, Osaka University

Host in iJURC YAMAGO, Shigeru

Nonlinear Rheology of Semiflexible Polymer Solutions

INOUE, Tadashi, Graduate School of Science, Osaka University

Host in iJURC MATSUMIYA, Yumi

Analysis of Soret Effect for DNA in Molecular-Scale Temperature Gradient

SHIMADA, Ryoko, Department of Mathematical and Physical Sciences, Faculty of Science, Japan Women's University

Host in iJURC WATANABE, Hiroshi F

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 iJURC AOYAMA, Takashi I

Site-Selective Protein Acetylation by a Small Molecule

ZHOU, Lu, School of Pharmacy, Fudan University

Host in iJURC UESUGI, Motonari I

Study of Magnonic Properties of Ferrimagnets

KIM, Kab-Jin, Department of Physics, Korea Advanced Institute of Science and Technology

Host in iJURC ONO, Teruo I

Development of Highly Efficient and Stable Blue Organic Light Emitting Diodes Using Thermally Activated Delayed Fluorescent Materials as Sensitizer

ZHANG, Dongdong, Department of Chemistry, Tsinghua University

Host in iJURC KAJI, Hironori I

Highly Efficient Blue Thermally Activated Delayed Fluorescence Emitters Using Sterically Hindered Donor Skeleton

KWON, Jang Hyuk, Department of Information Display, Kyung Hee University

Host in iJURC KAJI, Hironori I

Structural Analysis of Organic Amorphous Thin Films Using Solid Effect Dynamic Nuclear Polarization NMR

KOBAYASHI, Takeshi, Ames National Laboratory, U.S. Department of Energy

Host in iJURC KAJI, Hironori I

Memory of Chirality Using Flow Electrochemistry

WIRTH, Thomas, School of Chemistry, Cardiff University

Host in iJURC KAWABATA, Takeo I

Creation of Functional Molecules Based on Hydrogen Bond Networks

CLAYDEN, Jonathan, School of Chemistry, University of Bristol

Host in iJURC KAWABATA, Takeo I

Structural and Functional Analysis of the Surface Components of Bacterial Outer Membrane Vesicles

CORSARO, Maria Michela, Department of Chemical Sciences, University of Naples Federico II

Host in iJURC KURIHARA, Tatsuo I F

Search for Four-wave-mixing in the Vacuum –Unveiling Dark Components in the Universe–

HOMMA, Kensuke, Graduate School of Science, Hiroshima University

Host in iJURC SAKABE, Shuji I

Development of Biosensors by Combining Stimuli-Responsive Polymer Brushes with Electrochemical Analysis
MA, Ying, Department of Chemistry and Chemical Engineering, South China University of Technology
Host in iJURC OHNO, Kohji I

Exploring New Polyether Nanocomposite Electrolytes to Enhance Energy Storage of Lithium Ion Batteries
FERRIER, Robert C., Chemical Engineering and Materials Science, Michigan State University
Host in iJURC OHNO, Kohji I

Fluorinated Polymer-Brush-Grafted Nanoparticles: Precise Synthesis and Applications to Membrane Technology
LADMIRAL, Vincent, Institut Charles Gerhardt (ICGM), CNRS
Host in iJURC OHNO, Kohji I

Real-time Imaging of Single-molecule mRNA with Different Methylation States
STASEVICH, Timothy J., Department of Biochemistry and Molecular Biology, Colorado State University
Host in iJURC IMANISHI, Miki I

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

Research of Multi-qubit Diamond Quantum Processors
DOHERTY, W. Marcus, Research School of Physics and Engineering, Australian National University
Host in iJURC MIZUOCHI, Norikazu I

Research on Shallow NV Center in Diamond
BALASUBRAMANIAN, Gopalakrishnan, Max-Planck Institute for Biophysical Chemistry
Host in iJURC MIZUOCHI, Norikazu I

New Cellular Functions of Acyldopamine
ITO, Akihiro, School of Life Sciences, Tokyo University of Pharmacy and Life Sciences
Host in iJURC UESUGI, Motonari

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

Development of the Epitaxial Thin Film of Weyl Semimetal Mn₃Sn
NAGAHAMA, Taro, Faculty of Engineering, Hokkaido University
Host in iJURC ONO, Teruo

Effect of Microstructure on Damping Constant in Polycrystalline Bi-YIG Thin Films Prepared by Sol-Gel Method
YAMADA, Keisuke, Faculty of Engineering, Gifu University
Host in iJURC ONO, Teruo

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

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

Fine Synthesis of Polymer Brush on Ferromagnetic Nano-Platelet for Ferromagnetic Photonic LC
UCHIDA, Yoshiaki, Department of Materials Engineering Science, Graduate School of Engineering Science, Osaka University
Host in iJURC OHNO, Kohji

Ferromagnetic Single-electron Transistor
MAJIMA, Yutaka, Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology
Host in iJURC TERANISHI, Toshiharu

Development of NanoBRET-based Screening System for Peptidic CXCR4 Ligands
NOMURA, Wataru, School of Pharmaceutical Sciences, Hiroshima University
Host in iJURC FUTAKI, Shiroh

Establishment of Cell Penetrating Peptide (CPP)-based Delivery System into Resident Cancer Stem Cells in Deep Cancer Tissue
OHASHI, Wakana, Graduate School of Medicine and Pharmaceutical Sciences for Research, University of Toyama
Host in iJURC FUTAKI, Shiroh F

Manufacture of Shallow NV Centers in Diamond
TOKUDA, Norio, Nanomaterials Research Institute, Kanazawa University
Host in iJURC MIZUOCHI, Norikazu

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 iJURC MIZUOCHI, Norikazu

SUBJECTS FOCUSING OF JOINT USAGE OF iJURC/ICR FACILITIES

Atomic Level Analysis and Fabrication of Highly Stable Perovskite Films and Light Emitting Diodes
QIAO, Juan, Department of Chemistry, Tsinghua University
Host in iJURC KAJI, Hironori I F

High-pressure Synthesis of Potential Multiferroic Oxides
ATTFIELD, J. Paul, Centre for Science at Extreme Conditions and School of Chemistry, University of Edinburgh
Host in iJURC SHIMAKAWA, Yuichi I

Synthesis and Characterization of Novel Organoselenium and -Tellurium Compounds
MINOURA, Mao, College of Science, Department of Chemistry, Rikkyo University
Host in iJURC TOKITOH, Norihiro I

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 iJURC KURATA, Hiroki

Plasmon-exciton Coupling on a Plasmonic Crystal
SAITO, Hikaru, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University
Host in iJURC KURATA, Hiroki

Design of Flat Silicene with Perfect π -Conjugate 2D Sheet
TAKAHASHI, Masae, Graduate School of Agricultural Science, Tohoku University
Host in iJURC TOKITOH, Norihiro F

Synthesis and Structures of Acene Molecules Bearing Chalcogenopyrylium Units
NAGAHORA, Noriyoshi, Department of Chemistry, Faculty of Science, Fukuoka University
Host in iJURC TOKITOH, Norihiro

Synthesis and Structural Characterization of Divalent Species of Heavier Group 14 Elements
MATSUO, Tsukasa, Faculty of Science and Engineering, Kindai University
Host in iJURC TOKITOH, Norihiro

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 Materials Science and Engineering, College of Engineering, Ibaraki University
Host in iJURC TOKITOH, Norihiro; MIZUHATA, Yoshiyuki

High Sensitive Imaging Mass Spectrometry Targeting the Carbonyl Compounds Derived from Biological Tissues
HATANO, Osamu, Department of Anatomy and Cell Biology, Nara Medical University
Host in iJURC ISOZAKI, Katsuhiko

SUBJECTS ENCOURAGING JOINT PROGRAM

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

Synthesis of Structurally Controlled Polymers Having Green Fluorescence Protein Chromophore and Their Photophysical Properties in Solution
YANG, Jye-Shane, Department of Chemistry, National Taiwan University
Host in iJURC YAMAGO, Shigeru I

Vinyl Azides as New Monomers of Radical Polymerization for the Fabrication of Green Polymers Having Chemically- and Biodegradable Properties
CHIBA, Shunsuke, Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University
Host in iJURC YAMAGO, Shigeru I

The 15th International Workshop for East Asian Young Rheologists
INOUE, Tadashi, Graduate School of Science, Osaka University
Host in iJURC MATSUMIYA, Yumi I

The 8th Japanese-Sino Symposium on Organic Chemistry for Young Scientists
HAMASHIMA, Yoshitaka, School of Pharmaceutical Sciences, University of Shizuoka
Host in iJURC KAWABATA, Takeo

26th International Workshop on Oxide Electronics
MATSUNO, Jobu, Department of Physics, Osaka University
Host in iJURC KAN, Daisuke

iJURC Publications (Selected Examples)

(until 31 May 2019)

2,5-Digermaselenophenes: Germanium Analogues of Selenophenes

Sugahara, T.; Sasamori, T.; Tokitoh, N., *J. Am. Chem. Soc.*, **140**, 11206-11209 (2018).

Abstract

A stable crystalline 2,5-digermaselenophene was synthesized. In contrast to hitherto reported selenophenes, this digermaselenophene exhibits a *trans*-pyramidalized structure, which is due to its electronic properties. The practical utility of this 2,5-digermaselenophene is reflected in its ability to activate dihydrogen and acetylene at room temperature in the absence of a transition-metal complex, and this behavior can be rationalized on the basis of its physicochemical properties, which are characterized by considerable electron-donating and -accepting abilities.

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

Kayahara, E.; Hayashi, T.; Takeuchi, K.; Ozawa, F.; Ashida, K.; Ogoshi, S.; Yamago, S., *Angew. Chem. Int. Ed.*, **57**, 11418-11421 (2018).

Abstract

The carbon–carbon (C–C) bond activation of [*n*]cycloparaphenylenes ([*n*]CPPs) by a transition-metal complex is herein reported. The Pt⁰ complex Pt(PPh₃)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 reveal 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.

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

Wada, Y.; Kubo, S.; Kaji, H., *Adv. Mater.*, **30**, [1705641-1]-[1705641-8] (2018).

Abstract

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'Éclairage (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.

Viscoelastic and Dielectric Relaxation of Reptating Type-A Chains Affected by Reversible Head-to-Head Association and Dissociation

Watanabe, H.; Matsumiya, Y.; Kwon, Y., *Macromolecules*, **51**, 6476-6496 (2018).

Abstract

For entangled linear polymer having type A dipoles and undergoing head-to-head association and dissociation reaction, viscoelastic and dielectric behavior is theoretically analyzed on the basis of the reptation dynamics combined with the reaction kinetics. Specifically, for the dissociated unimer and associated dimer (indexed with $j = 1$ and 2, respectively), the normalized complex modulus $g_j^*(\omega)$ and the normalized complex dielectric permittivity $\tilde{\epsilon}_j^*(\omega)$ are analytically calculated via eigenfunction expansion of the orientational anisotropy and orientational memory defined in terms of the bond vectors \mathbf{u} of entanglement segments. The reaction activates mutual conformational transfer between the unimer and dimer. Multiple coupling occurs for the anisotropy decay modes of the unimer and dimer due to this transfer, and the viscoelastic g_1^* and g_2^* of the unimer and dimer, respectively, exhibit considerably retarded and accelerated relaxation compared to the pure reptation case. In contrast, the memory decay modes of the unimer and dimer are only pairwise coupled, so that the reaction-induced acceleration and retardation for the dielectric $\tilde{\epsilon}_1^*$ and $\tilde{\epsilon}_2^*$ are much weaker than those seen for the viscoelastic g_1^* and g_2^* . The orientational anisotropy is the tensorial, second-moment average of \mathbf{u} associated with no cancellation in the conformational transfer, whereas the orientational memory is the vectorial, first-moment average accompanied by partial cancellation, which results in the difference between g_j^* and $\tilde{\epsilon}_j^*$. This difference between g_j^* and $\tilde{\epsilon}_j^*$ is noted also for the associating/dissociating Rouse chains. Nevertheless, the reaction-induced retardation of the viscoelastic relaxation is stronger for the reptating unimer than for the Rouse unimer, whereas the reaction-induced acceleration is similar, in magnitude, for the reptating dimer and Rouse dimer. These features of g_j^* of the unimer and dimer are discussed in relation to the motional coherence along the chain backbone being present and absent in the reptation and Rouse dynamics.

Half-cycle Terahertz Surface Waves with MV/cm Field Strengths Generated on Metal Wires

Teramoto, K.; Tokita, S.; Terao, T.; Inoue, S.; Yasuhara, R.; Nagashima, T.; Kojima, S.; Kawanaka, J.; Mori, K.; Hashida, M.; Sakabe, S., *Appl. Phys. Lett.*, **113**, 051101 (2018).

<https://doi.org/10.1063/1.5031873>

Reproduced from [FULL CITATION], with the permission of AIP Publishing.

Abstract

Irradiating a metal wire with an intense femtosecond laser pulse induces a terahertz (THz) surface wave that travels along the wire. Here, the characteristics of the THz surface wave generated by the laser–wire interaction are investigated in detail by using an electro-optical method to determine the dependence of surface wave properties on laser energy and wire diameter. The surface wave is distributed by the Hankel function in the wire radial direction. On the wire surface, the electric field is estimated to be MV/cm. The peak electric field of the surface wave and the conversion efficiency from laser energy to surface wave energy are found to be proportional to the laser energy raised to the power of 0.67 and 0.3, respectively.



VISITING PROFESSORS'
ACTIVITIES IN ICR



Vis Prof
TOMOOKA, Katsuhiko
(D Sc)

Laboratory of Synthetic Organic Chemistry
Professor, Institute for Materials Chemistry and Engineering, Kyushu University (6-1 Kasuga-koen, Kasuga, Fukuoka 816-8580)

Lecture at ICR
Discovery of Novel Chiral Molecules and Development of Asymmetric Synthesis



Vis Prof
KASAHARA, Hiroyuki
(D Eng)

Laboratory of Chemistry of Molecular Biocatalysts
Professor, Institute of Global Innovation Research, Tokyo University of Agriculture and Technology (3-5-8 Saiwaicho, Fuchu-shi, Tokyo 183-8509)

Lecture at ICR
Coordination in the Regulation of Indole-3-acetic Acid and Phenylacetic Acid Metabolism in Arabidopsis



Vis Prof
ISHIDA, Yasuhiro
(D Eng)

Laboratory of Molecular Aggregation Analysis
Team Leader, Center for Emergent Matter Science, RIKEN (2-1 Hirosawa, Wako, Saitama 351-0198)

Lecture at ICR
More Haste, Less Speed: Precision Synthesis of Soft Materials



Vis Prof
OIWA, Akira
(D Sc)

Laboratory of Nanophotonics
Professor, The Institute of Scientific and Industrial Research, Osaka University (8-1 Mihogaoka, Ibaraki, Osaka 567-0047)

Lecture at ICR
A Poincaré Interface Based on Photon-electron Spin Quantum State Conversion



Vis Prof
CAI, Hongmin
(Ph D)

Laboratory of Mathematical Bioinformatics
Professor, South China University of Technology (Room B5-514 School of Computer Science & Engineering South China University of Technology Guangzhou Higher Education Mega Centre 510006, Guangzhou, China, P.R.)

Lecture at ICR
Identification of Gene-drug and Multi-omics Regulatory Modules Through Integrative Analysis



Vis Assoc Prof
TOKITA, Masatoshi
(D Eng)

Laboratory of Chemistry of Polymer Materials
Associate Professor, Department of Chemical Science and Engineering, Tokyo Institute of Technology (Ookayama, Meguro-ku, Tokyo 152-8550)

Lecture at ICR
Soft Matter Science Developed from a Junction between Polymer and Liquid Crystal



Vis Assoc Prof
KOSONO, Saori
(D Eng)

Laboratory of Molecular Microbial Science
Project Associate Professor, Biotechnology Research Center, The University of Tokyo (1-1-1 Yayoi, Bunkyo-ku, Tokyo 113-8657)

Lecture at ICR
Metabolic Regulation via Protein Acylation in Bacteria



Vis Assoc Prof
SANNO, Tomokazu
(D Eng)

Laboratory of Laser Matter Interaction Science
Associate Professor, Graduate School of Engineering, Osaka University (Yamadaoka, Suita, Osaka 560-8532)

Lecture at ICR
Fundamentals and Applications of Material Modification by Femtosecond Laser Induced Shock Waves



Vis Assoc Prof
SAIGO, Hiroto
(D Inf)

Laboratory of Mathematical Bioinformatics
Associate Professor, Graduate School and Faculty of Information Science and Electrical Engineering, Kyushu University (744 Motooka, Nishi-ku, Fukuoka 819-0395)

Lecture at ICR
Prediction Models that Consider Variable Interactions



Prof Em KANEHISA, Minoru (D Sc)
Appointed as Res (pt) at ICR,
1 April 2012–31 March 2020



PERSONAL

Retirement

Professor SAKABE, Shuji
Advanced Research Center for Beam Science
– Laser Matter Interaction Science –



On 31 March 2020, Dr. SAKABE, Shuji retired from Institute for Chemical Research (ICR), Kyoto University after about 17 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Sakabe was born in Hyogo Prefecture in September 1954. He graduated from Faculty of Engineering, Osaka University in 1978, and went on the graduate school at Osaka University to study the sciences of laser plasma and laser nuclear fusion under the supervision of the late Professor Chiyo Yamanaka at Institute of Laser Engineering (ILE). He was employed as Assistant Professor at ILE, Osaka University in 1982, and was awarded the degree of Doctor of Engineering for the thesis titled “Research on energy absorption and implosion uniformity for laser nuclear fusion” in 1985. In 1983–1985, he served as a group leader to lead the project for the construct of the world’s largest output-power laser facility “GekkoXII” at the time. In 1985 he was employed as researcher at Max-Planck Institute for Quantum Optics, Federal Republic of Germany (West Germany), the division of laser plasma physics directed by Drs. Sibert Witkowski and Richard Sigel. He was re-employed as assistant professor at ILE, in 1986, moved to Graduate School of Engineering, Osaka University in 1989, and was promoted to Associate Professor in 1996. He was appointed as Visiting Associate Professor at National Institute for Fusion Science of MEXT in 1997–2002. He spent months in 2002 as Visiting Professor at Technical University of Vienna. In 2003, he was employed as full-professor at ICR. Since the reorganization of ICR in 2002 he has held the chair of the Laboratory for Laser Matter Interaction Science in Advanced Research Center for Beam Science. He served as the director of Advanced Research Center for Beam Science in 2009–2011 and 2017–2019.

Throughout his academic career, Dr. Sakabe has been engaged in the fundamental research on the physics of high-intensity laser interaction with matter (plasmas), and its applications such as quantum beam generation and laser processing, and has achieved significant results. In particular, during the inception of laser fusion science research in Japan, he made pioneering contributions in the field of high-intensity laser science, such as physical elucidation of laser plasma absorption and fast ion generation, demonstration of indirect laser implosion, construction of the world’s largest output-power laser facility, and the database construction of atom-ion collision cross section for laser isotope separation.

It should be noted that he constructed ultra-intense short-pulse laser system by the wisdom that he has cultivated so far, opened the research facility for the physics of the interaction between high-intensity lasers and materials and its application in the Advanced Beam Nanoscience Center, ICR, and established a base for high-intensity laser science infrastructure. From this facility, he achieved many remarkable results, including:

- Demonstration of laser proton acceleration

- Demonstration of laser-induced cluster coulomb explosion
- Exploring the possibility of applying explosive accelerated ions to compact neutron sources
- Physics of interaction between high-intensity short-pulse laser and large molecules
- Demonstration of terahertz wave generation from clusters induced by laser
- Development of laser accelerated electron source and its application
- Demonstration of compression method of laser accelerated electron pulse
- Development of ultrafast electron diffraction/deflection method using laser accelerated electron pulses
- Discovery of electron generation and induction by laser
- Generation of high-intensity surface electromagnetic waves by laser
- Observation of ultra-high-speed phenomena by deflection method using laser-accelerated electron pulses
- Investigation of the physics of nano-ablation with femtosecond laser
- Investigation of the physics of self-organization of nano periodical structure on matter surface with femtosecond laser
- Applications of femtosecond laser to laser matter processing

In addition, he made the high-performance laser with high availability and high quality, and provided the facility use as a joint use / research center, and conducted many joint researches.

As described above, he made extensive contributions to the foundation of high-intensity laser science by conducting extensive research on high-intensity laser material interactions and their applications. His achievements were highly regarded internationally and he gave invited talks at many international conferences. These achievements have been published as 126 original papers and 15 reviews papers in academic journals, 6 books (edited and co-authored), 183 international conference lectures, and 432 domestic conference lectures. He is also active in international activities such as the chair of the organizing committee of OPIC (Optics and Photonics International Congress). He also holds important positions at academic societies in Japan, such as the Vice President of the Laser Society of Japan.

His educational contribution to Kyoto University is also noteworthy. He has guided 34 graduate students and sent many valuable human resources to universities and academia society.

For his achievements, he was awarded from the Laser Society of Japan, Achievement Award for Excellent Paper in 1989, 2016 and 2017, Achievement Award for Excellent Progress in 2007, Fellow in 2015 and The Laser Society Achievement Award in 2018.

Dr. Sakabe’s contribution to Kyoto University and ICR and academic societies through his scientific, educational and administrative activities is hereby gratefully acknowledged.

Awards

TOKITOH, Norihiro



8th Award of the Society of Silicon Chemistry JAPAN

“Exploration of Uncharted Chemistry of Silicon and Heavier Group 14 Elements Compounds”

The Society of Silicon Chemistry JAPAN

2 November 2019

MURATA, Yasujiro



The Chemical Society of Japan Award for Creative Work

The 99th Annual Meeting of the Chemical Society of Japan

“Realization of Isolated Chemical Species by Organic Synthesis of Endohedral Fullerenes”

The Chemical Society of Japan

17 March 2019

MIZUHATA, Yoshiyuki



2019 Kansai Branch Award of the Society of Synthetic Organic Chemistry, Japan

“Development of Heavy Aryl Anions Containing Heavy Group 14 Elements on Benzene Skeleton”

The Society of Synthetic Organic Chemistry, Japan

22 November 2019

HIROSE, Takashi



Outstanding Reviewer for Chemical Communications in 2018

Chemical Communications, RSC

20 March 2019

Publons Peer Review Awards 2019

Publons

17 September 2019

FUJIMORI, Shiori



The 11th Kyoto “Tachibana” Award

“Synthesis and Characterization of Phenylanion Species Containing Heavier Group 14 Elements in the Skeleton”

Kyoto University

4 March 2019

L'ORÉAL-UNESCO For Women in Science Awards

“Synthesis and Characterization of Heavy Phenylanions”

L'ORÉAL Japan

4 July 2019

UEDA, Yoshihiro



CSJ Presentation Award

The 99th Annual Meeting of the Chemical Society of Japan

“Total Synthesis of Ellagitannins Based on Sequential Site-Selective Functionalization of D-Glucose”

The Chemical Society of Japan

9 April 2019

GONDOH, Naruhiro



The Best Oral Presentation Award

The 45th Symposium on Progress in Organic Reactions and Syntheses

“Catalytic Acylative Parallel Kinetic Resolution of Diols and Kinetic Resolution of tertiary-Alcohols”

Division of Organic Chemistry, The Pharmaceutical Society Japan

29 October 2019

SHIBAYAMA, Hiromitsu



The Best Presentation Award

139th Annual Meeting of the Pharmaceutical Society of Japan

“Total Synthesis of Punicafolin Based on Sequential Site-Selective Functionalization of D-Glucose”

The Pharmaceutical Society of Japan

31 March 2019

NINOMIYA, Ryo



The Best Presentation Award

139th Annual Meeting of the Pharmaceutical Society of Japan

“Dirhodium-Catalyzed β -Selective C(sp³)-H Amination of Organosilicon Compounds”

The Pharmaceutical Society of Japan

31 March 2019

MURAI, Takuya



The Best Presentation Award

139th Annual Meeting of the Pharmaceutical Society of Japan

“Chalcogen-Bond Assisted Dirhodium Complex -Development of Stereoselective Intramolecular C-H Insertion and Total Synthesis of Naturally Occurring γ -Lactones-”

The Pharmaceutical Society of Japan

31 March 2019

MATSUMOTO, Kenshi



CSJ Student Presentation Award 2019

The 99th Annual Meeting of the Chemical Society of Japan

“Formation of Novel Ordered Fe–Pd Alloy Nanoparticles Caused by the Elemental Miscibility of Trace Third Elements”

The Chemical Society of Japan

9 April 2019

SAKAKIBARA, Keita



The Cellulose Society of Japan Progress Award for 2018

“Control of Dispersion and Network Formation of Cellulose Nanofiber in Polymer Composite Materials”

The Cellulose Society of Japan

11 July 2019

YAMAGO, Shigeru



The Award of the Society of Polymer Science, Japan

The 67th SPSJ Annual Meeting

“Development and Application of Controlled Radical Polymerization Using Organic Tellurium Compounds”

The Society of Polymer Science, Japan

30 May 2019

KAYAHARA, Eiichi



The CSJ Award for Young Chemist

The 99th Annual Meeting of the Chemical Society of Japan

“Practical Synthesis and Development of New Functions of Cyclic Curved π -Conjugated Molecules”

The Chemical Society of Japan

17 March 2019

HERBSCHLEB, Ernst David



Presentation Award

“Ultra-long Coherence Times of NV Centres in n-Type Diamond”
The First International Forum on Quantum Sensing
19 February 2019

ICR Award for Young Scientists

“Ultra-long Coherence Times Amongst Room-temperature Solid-state Spins”
Institute for Chemical Research, Kyoto University
13 December 2019

OKUNO, Takaya



ICR Award for Graduate Students

“Spin-transfer Torques for Domain Wall Motion in Antiferromagnetically-coupled Ferrimagnets”
Institute for Chemical Research, Kyoto University
13 December 2019

FUTAKI, Shiroh



Honorary Member of Hungarian Academy of Sciences

Hungarian Academy of Sciences
10 May 2019

SAKAMOTO, Kentarou



The Excellent Presentation Award

The 66th Annual Meeting of the Japanese Biochemical Society, Kinki Branch
“Development of Cytosolic Delivery Systems of Macromolecules by Peptides”
The Japanese Biochemical Society, Kinki Branch
25 May 2019

YAMAGUCHI, Shinjiro



The Olchemim Award 2019

2019 Gibberellins
“Research on Plant Hormones Gibberellins”
Olchemim s.r.o.
2 July 2019

2019 Highly Cited Researcher

Clarivate Analytics
19 November 2019

HAKARIYA, Hayase



Leave a Nest Grant IKEDA SCIENTIFIC Award

LNest Grant
“Cell Surface Modification with a Self-assembling Molecule to enhance the Engraftment of Cardiomyocytes derived from iPSCs”
Leave a Nest Co., Ltd. & IKEDA SCIENTIFIC Co., Ltd.
16 November 2019

MORIWAKI, Kazuki



Lecture Encouragement Award

The 28th Japan OLED Forum Annual Meeting
“Analysis of Charge Transport Characteristics of Host-guest Amorphous System by Multi-scale Simulation”
Japan OLED Forum
21 November 2019

SOHRIN, Yoshiki



12th Prime Minister's Commendations for Contributors to Promote the Country as a "Maritime Nation"

“Elucidation of the Modern and Past Ocean by Using Trace Elements and Their Isotopes”
Cabinet Office, Government of Japan
22 August 2019

SHIMOAKA, Takafumi



The Spectroscopical Society of Japan Award for Young Scientists

“Development of Vibrational Spectroscopy for Revealing Molecular Aggregation Structure of Organofluorine Compounds”

The Spectroscopical Society of Japan

15 May 2019

The Japan Society for Analytical Chemistry Award for Young Researchers

“Structural and Quantitative Analysis of Adsorbed Water Molecules in Nafion Membrane and the Role of Organofluorine Chain”

The Japan Society for Analytical Chemistry

12 September 2019

TOMITA, Kazutaka



Young Scientist Presentation Award

The 66th JSAP Spring Meeting 2019

“Polymorphism of Tetrphenylporphyrin in a Spin Coated Film”

The Japan Society of Applied Physics

9 March 2019

Young Scientist Presentation Award

Annual Meeting of the Spectroscopical Society of Japan 2019

“Understanding of Polymorphism of Tetrphenylporphyrin in a Solution Processed Film by Using pMAIRS and GIXD Techniques”

The Spectroscopical Society of Japan

16 May 2019

YOKOYAMA, Fumiaki



Best Oral Presentation Award

The 66th Annual Meeting of the Japanese Biochemical Society, Kinki Branch

“Regulation of Bacterial Vesicle Production by a Sensor Protein Homolog Involved in Biofilm Dispersion”

The Japanese Biochemical Society, Kinki Branch

25 May 2019

YUSUF, Yustina



Young Scientist Award

The 92nd Annual Meeting of the Japanese Biochemical Society

“Polyunsaturated Fatty Acid Conversion in *Shewanella livingstonensis* Ac10”

The Japanese Biochemical Society

18 September 2019

KAMASAKA, Kouhei



Best Oral Presentation Award

The 66th Annual Meeting of the Japanese Biochemical Society, Kinki Branch

“Function of Cell Surface Structure in Protein Secretion Mechanism via Bacterial Extracellular Membrane Vesicles in *Shewanella* sp. HM13”

The Japanese Biochemical Society, Kinki Branch

25 May 2019

Young Scientist Award

The 92nd Annual Meeting of the Japanese Biochemical Society

“Role of Cell Surface Structure in Selective Protein Secretion via Bacterial Extracellular Membrane Vesicles”

The Japanese Biochemical Society

20 September 2019

WATANABE, Yuki



The Best Young Oral Presentation Award

Annual Meeting of the Society of Rubber Science and Technology, Japan

“Study for Hierarchical Structure of Rubber Filled with Carbon Black by Anomalous Small-angle X-ray Scattering”

The Society of Rubber Science and Technology, Japan

23 May 2019

WAKAMIYA, Atsushi



4th Yoshida Prize Symposium Lecturer (Distinguished Lecturer)

International Organic Chemistry Foundation (IOCF)

19 November 2019

KOSUGI, Yoshihisa



Student Award for Outstanding Presentation

Autumn Meeting of the Japan Society of Powder and Powder Metallurgy, 2019

“Tuning Charge Transition Temperatures of $LnCu_3Fe_4O_{12}$ by *A*-site Substitution”

Japan Society of Powder and Powder Metallurgy

24 October 2019

PINCELLA, Francesca



CSJ Presentation Award 2019

The 99th Annual Meeting of the Chemical Society of Japan

“Microwave-assisted Facile Conversion of Lignin to Fluorescent Imidazole Compounds”

The Chemical Society of Japan

9 April 2019

KANEMITSU, Yoshihiko



Shimadzu Prize 2018

“Pioneering Study on Optical Properties of Semiconductors by Luminescence Spectroscopy”

Shimadzu Science Foundation

15 February 2019

Kato Memorial Award

“Pioneering Study on Optical Properties and Functions of Nanostructured Semiconductors”

Kato Foundation for Promotion of Science

15 November 2019

GOTO, Masato



Inoue Research Award for Young Scientists

“Various Ground States and Magnetic Field Induced Phase Transitions in Kagome-Lattice Transition-Metal Fluorides”

Inoue Foundation for Science

4 February 2019

TAHARA, Hirokazu



The 45th (2018 Autumn) JSAP Presentation Award

“Optical Phase Shifter Using Metal Halide Perovskite”

The Japan Society of Applied Physics

9 March 2019

Ando Incentive Prize for the Study of Electronic

“Discovery of Coherent Phenomena Related to Efficient Photoelectric Conversion of Semiconductor Nanoparticles”

The Foundation of ANDO Laboratory

29 June 2019

AMANO PATINO, Midori Estefani



CSJ Presentation Award 2019

The 99th Annual Meeting of the Chemical Society of Japan

“Magnetic Order of *A'*-site Iron Spins in $CaFe_3Ti_4O_{12}$ and Field-induced Switching”

The Chemical Society of Japan

9 April 2019

YOSHIKAWA, Genki



ICR Award for Graduate Students

“Medusavirus, a Novel Large DNA Virus Discovered from Hot Spring Water”

Institute for Chemical Research, Kyoto University

13 December 2019

MENG, Lingjie



The Best Oral Presentation Award

Workshop on Environmental Viruses

“NCLDV Host Prediction with Marker Gene Co-occurrence Analysis in Marine Metagenomes”

Japanese Society of Microbial Ecology

2 November 2019

PRODINGER, Florian



The Best Presentation Award

2019 JSME Annual Meeting

“Linking Seasonal Dynamics of Megaviridae and Bloom Forming Eukaryotic Phytoplankton in Uranouchi Inlet, Japan”

Japanese Society of Microbial Ecology

12 September 2019

Paper Awards

TOSAKA, Masatoshi



The Award for the Outstanding Paper in JFST
Annual Meeting 2019

“Formation of Crystallites with Low Surface Energy
—A Key to Understand the Crystallization of Oriented Polymer”
The Society of Fiber Science and Technology, Japan

6 June 2019

ONO, Teruo;



MORIYAMA, Takahiro;



ODA, Kento

MSJ Distinguished Paper Award

“Magnetoresistance in Bilayers of Heavy
Metal and Non-collinear Antiferromagnet”

The Magnetics Society of Japan

26 September 2019



MATSUMIYA, Yumi



The Journal of the Society of Rheology, Japan Paper Award

The 46th Annual Meeting of the Society of Rheology, Japan

“Rheology of Nano-Cellulose Fiber Suspension”

The Society of Rheology, Japan

8 May 2019

HASHIDA, Masaki



Encouragement Award

“Study on Modification of Ablation Rate for Femtosecond
Laser Material Processing”

The Amada Foundation

24 April 2019

NAKAMURA, Masaharu;



TAKAYA, Hikaru;



IWAMOTO, Takahiro;



AGATA, Ryosuke;

MATSUDA, Hiroshi;

NAKATANI, Naoki¹;

TAKEUCHI, Katsuhiko²;



HATAKEYAMA, Takuji³

BCSJ Award

“Iron-Catalyzed Cross Coupling of Aryl Chlorides with Alkyl
Grignard Reagents: Synthetic Scope and Fe^{II}/Fe^{IV} Mechanism
Supported by X-ray Absorption Spectroscopy and Density
Functional Theory Calculations”

The Chemical Society of Japan

15 February 2019

¹Department of Chemistry, Graduate School of Science, Tokyo
Metropolitan University

²National Institute of Advanced Industrial Science and Technology

³Department of Chemistry, School of Science and Technology,
Kwansei Gakuin University

KANEMITSU, Yoshihiko;



HANDA, Taketo



Award for Best Review Paper

41st JSAP AWARDS

The 41st Japan Society of Applied Physics

“Photophysics of Metal Halide Perovskites: From Materials to
Devices”

The Japan Society of Applied Physics

18 September 2019

Poster Awards

YANAGISAWA, Tatsuya



Best Poster Award

13th International Conference on Heteroatom Chemistry
“Addition Reactions of Phosphinoaluminanes to C–C
Unsaturated Bonds”

13th International Conference on Heteroatom Chemistry
5 July 2019

NINOMIYA, Ryo



Chemistry Letters Young Award

The 8th Japanese-Sino Symposium on Organic Chemistry for
Young Scientists

“Dirhodium-Catalyzed β -Position-Selective C(sp³)-H
Amination of Alkylsilanes”

The Organizing Committee of Japanese-Sino Symposium on
Organic Chemistry

20 September 2019

OMATSU, Yamato



Poster Award

The 23rd Symposium on the Society of Silicon Chemistry
JAPAN

“Synthesis and Reactivity of Cyclic Oligosilanes Having
Bulky Alkyl Substituents”

The Society of Silicon Chemistry JAPAN
2 November 2019

SAKAKIBARA, Keita



PMF Excellent Presentation Award

27th Polymer Material Forum

“Preparation of Novel Monolith Particles for Next-Generation
Chromatographic Separations”

The Society of Polymer Science, Japan

30 May 2019

UEDA, Yoshihiro



Poster Award for Excellence

The 47th Naito Conference on C-H Bond Activation and
Transformation

“Dirhodium-Catalyzed Site-Selective C-H Amination:
para-Selectivity in C(sp²)-H Amination of Alkoxyarenes and
 β -Selectivity in C(sp³)-H Amination of Organosilanes”

The Naito Foundation
5 July 2019

EGUCHI, Hiroshi



Award for Encouragement of Research

28th Annual Meeting of MRS-J

“Simultaneous Evaluation of Friction and Lubrication Gap of
Concentrated Polymer Brush for Well Understanding Its
Tribological Characteristics”

The Materials Research Society of Japan

31 January 2019

OKUBO, Ryo



Excellent Poster Award

2019 the Annual Kobe Polymer Research Symposium, Japan
“Preparation and Functionalization of Epoxy-based Monolith Particles for Chromatographic Application”
The Society of Polymer Science, Kansai Regional Chapter, Japan

12 July 2019

ONOZUKA, Kota



Poster Award

The 30th Symposium on Physical Organic Chemistry
“Synthesis and Identification of Cycloparaphenylene Derivatives with Twisted Structures and Their Oxidized Species”
The Society of Physical Organic Chemistry, Japan

27 September 2019

MORISHITA, Hiroki



Poster Award

“Room-Temperature Electrically Detected ^{14}N Nuclear Spins Coherence in Ensemble of NV Centers”
The First International Forum on Quantum Sensing

19 February 2019

HERBSCHLEB, Ernst David



Poster Award

“AC Magnetic-field Quantum-sensor with Unlimited Dynamic-range”
The Second International Forum on Quantum Metrology and Sensing

18 December 2019

YAMASHITA, Shungo



Best Poster Presentation Award

“Extension of Coherence Time with the Dressed States of Ensemble of NV Centers in Diamond”
The Second International Forum on Quantum Metrology and Sensing

18 December 2019

YOKOYAMA, Fumiaki



Best Poster Award

The 20th Annual Meeting of Japanese Society for Extremophiles
“Regulation of Vesicle Production and Biofilm Dispersion by a Sensor Protein of a Cold-Adapted Bacterium, *Shewanella vesiculosa* HM13”
The Japanese Society for Extremophiles

16 November 2019

SOMA, Kae



The Best Presentation Award for Short Oral Papers

“Uniaxial Elongation Viscosity of Poly(4-n-Alkylstyrene)s”
14th International Workshop for East Asian Young Rheologists

24 January 2019

OTSUKA, Kento



Poster Prize

The 4th Frontier Solar Cell Seminar
“Fabrication and Characterization of Tin-based Perovskite Semiconductor Films Prepared from High Purity Materials”
The Executive Committee of the 4th Frontier Solar Cell Seminar

26 November 2019

AGATA, Ryosuke



GSC Poster Award 2019

The 8th JACI/GSC Symposium

“Iron-Catalyzed Cross Coupling Reaction of Aryl Chlorides with Alkyl Grignard Reagents”

Japan Association for Chemical Innovation

25 June 2019

OHARA, Keiichi



Student Presentation Award of the Physical Society of Japan Division 5

The Physical Society of Japan 2019 Autumn Meeting

“Excitonic Optical Nonlinearities of Perovskite $\text{CH}_3\text{NH}_3\text{PbCl}_3$ Single Crystals”

The Physical Society of Japan

19 October 2019

KOEDTRUAD, Anucha



CSJ Poster Presentation Award 2019 for Excellent Research

9th CSJ Chemistry Festa

“Synthesis, Crystal Structures, Properties and their Relations in Ag-Bi-I Solar Cell Compounds”

The Chemical Society of Japan

20 November 2019

MÜNZNER, Ulrike Tatjana Elisabeth



Best Poster Award

4th Annual SysMod Meeting ISMB/ECCB 2019 in Basel

“A Mechanistically Detailed Model of the Cell Cycle in *Saccharomyces Cerevisiae*”

ISMB/ECCB 2019

22 July 2019

HANDA, Taketo



Student Presentation Award of the Physical Society of Japan Division 5

The Physical Society of Japan 2019 Autumn Meeting

“Observation of Negative Thermo-Optic Coefficients and Photo-Induced Refractive Index Change in Lead Halide Perovskites”

The Physical Society of Japan

19 October 2019

Obituary

Professor Emeritus

Dr. KATAYAMA, Ken-ichi (1927–2019)



Dr. Ken-ichi Katayama, Professor Emeritus of Kyoto University, passed away on March 29, 2019, at the age of 91.

Dr. Katayama was born in Osaka on August 25, 1927. He graduated from the Faculty of Science, Kyoto University, on March, 1950, with his major in physics. After graduation, he served as a staff member in Osaka Municipal Technical Research Institute from June of the same year till February 1952, when he moved to the Asahi Chemical Industry Co., Ltd. He joined the Institute for Chemical Research, Kyoto University, as an associate professor on April, 1972. He received a doctoral degree of science from Kyoto University in 1961 for his structural study on polymer crystals by X-ray diffraction.

Dr. Katayama was promoted to a full professor of the Institute in January, 1978, to direct the Laboratory of Polymer Crystals. He has given lectures on polymer crystals since 1973 at the Graduate School of Engineering and supervised dissertation works of many graduate students. Dr. Katayama served also a visiting lecturer at several universities such as Osaka University, Okayama University, Gifu University and Nagoya Institute of Technology. Dr. Katayama retired from Kyoto University in March 1991 and was honored with the title of Professor Emeritus, Kyoto University in April of the same year. After the retirement, he was appointed as a principal at Takuma National College of Technology from April 1991 to March 1996, and as a professor at Heian Jogakuin College from April 1996 to March 1998.

During his research career, Dr. Katayama devoted himself to the study on the structure and morphology of polymers in the solid state by X-ray and electron diffraction and by electron microscopy. He developed a system for the quick and accurate measurements of the intensity of X-ray diffraction and to elucidate the formation process of polymer solid structures. He applied the system for the clarification of the fine structures formed during fiber spinning. By using a high power X-ray source to examine its process *in situ* dynamically, he clarified that the structure formation

is already started before the onset of crystallization. For this pioneering work, he received The Award of The Society of Fiber Science and Technology, Japan in 1979.

Dr. Katayama also worked on high-resolution electron microscopy of polymer crystals as a powerful method to observe the arrangement of individual molecules in the crystal structure. In 1982, he succeeded in obtaining the high-resolution electron micrograph of single crystals of poly-*p*-xylylene, revealing an array of chain molecules. Subsequently, he clarified the local disorder structures in crystals of poly(*p*-phenylene sulfide), syndiotactic polystyrene, and so on, on the basis of the high-resolution micrographs; such local structures could not be analyzed by other methods at that time. In this way, he opened up the field of high-resolution electron microscopy of polymer crystals.

Dr. Katayama was instrumental in managing the Institute for Chemical Research. He worked as a member and chairman of various standing committees and contributed for the development of the Institute. He served as a vice-President of the Society of Fiber Science and Technology, Japan, for two years since April, 1988. He actively participated in International Conferences inside and outside Japan as a member of the executive committee, and contributed greatly to the development of international scientific exchanges. He also contributed to edit scientific journals such as *Polymer Journal* as an executive editor, *Journal of Macromolecular Science* as a member of advisory board and *Journal of Polymer Engineering* as a member of editorial board. Because of his contribution to the education and to the development of polymer science, Dr. Katayama was awarded The Order of the Sacred Treasure, Gold Rays with Neck Ribbon from the Japanese Cabinet Office in 2005.

Dr. Katayama was respected by his students, colleagues and friends because of his sincere, thoughtful and warm personality.



PUBLICATIONS

INTERNATIONAL
RESEARCH
COLLABORATIONS

SELECTED GRANTS

THESSES



PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Hayashi, S.; Uegaito, M.; Nishide, T.; Tanaka, E.; Nakanishi, W.; Sasamori, T.; Tokitoh, N.; Minoura, M., Nature of the E...E' Interactions (E, E' = O, S, Se, and Te) at Naphthalene 1,8-Positions with Fine Details of the Structures: Experimental and Theoretical Investigations, *New J. Chem.*, **43**, 14224-14237 (2019).

Miki, K.; Noda, T.; Gon, M.; Tanaka, K.; Chujo, Y.; Mizuhata, Y.; Tokitoh, N.; Ohe, K., Near-infrared Circularly Polarized Luminescence through Intramolecular Excimer Formation of Oligo (p-phenyleneethynylene)-based Double Helicates, *Chem. Eur. J.*, **25**, 9211-9216 (2019).

Ozaki, M.; Shimazaki, A.; Jung, M.; Nakaike, Y.; Maruyama, N.; Yakumaru, S.; Rafieh, A. I.; Sasamori, T.; Tokitoh, N.; Ekanayake, P.; Murata, Y.; Murdey, R.; Wakamiya, A., A Purified, Solvent-intercalated Precursor Complex for Wide-process-window Fabrication of Efficient Perovskite Solar Cells and Modules, *Angew. Chem. Int. ed.*, **58**, 9389-9393 (2019).

Sugahara, T.; Sasamori, T.; Tokitoh, N., The Formation of a 1,4-Disilabenzene and Its Isomerization into a Disilabenzvalene Derivative, *Dalton Trans.*, **48**, 9053-9056 (2019).

Fujimori, S.; Mizuhata, Y.; Tokitoh, N., A Mixed-anion System Consisting of a Germyl Anion and Anions Delocalized on Conjugated Carbon Ring Skeletons, *Chem. Eur. J.*, **25**, 6284-6289 (2019).

Agou, T.; Suzuki, S.; Kanno, Y.; Hosoya, T.; Fukumoto, H.; Mizuhata, Y.; Tokitoh, N.; Suda, Y.; Furukawa, S.; Saito, M.; Kubota, T., Synthesis and Properties of Perfluoroalkylated TIPS-pentacenes, *Tetrahedron*, **75**, 130678 (2019).

Sugahara, T.; Guo, J.-D.; Hashizume, D.; Sasamori, T.; Tokitoh, N., Reversible Isomerizations between 1,4-Digerma-benzenes and 1,4-Digerma-Dewar-benzenes: Air-stable Activators for Small Molecules, *J. Am. Chem. Soc.*, **141**, 2263-2267 (2019).

Yanagisawa, T.; Mizuhata, Y.; Tokitoh, N., Dibromometalloyl-iron Complexes Generated by the Recombination of an Alumannyl-iron Complex with EBr₃ (E = Al, Ga), *Heteroat. Chem.*, **29**, e21465 (2018).

Yanagisawa, T.; Mizuhata, Y.; Tokitoh, N., Syntheses and Structures of Novel λ^3, λ^3 -Phosphanylalumanes Fully Bearing Carbon Substituents and Their Substituent Effects, *Inorganics*, **7**, 132-143 (2019).

— Structural Organic Chemistry —

Ozaki, M.; Ishikura, Y.; Truong, M. A.; Liu, J.; Okada, I.; Tanabe, T.; Sekimoto, S.; Ohtsuki, T.; Murata, Y.; Murdey, R.; Wakamiya, A., Iodine-rich Mixed Composition Perovskites Optimised for Tin(IV) Oxide Transport Layers: How Starting Material Stability, Halide Ion Ratio, and Aging in Ambient Air Influence Solar Cell Performance, *J. Mater. Chem. A*, **7**, 16947-16953 (2019).

Fujii, S.; Cho, H.; Hashikawa, Y.; Nishino, T.; Murata, Y.; Kiguchi, M., Tunable Single-Molecule Electronic Conductance of C₆₀ by Encapsulation, *Phys. Chem. Chem. Phys.*, **21**, 12606-12610 (2019).

Hashikawa, Y.; Murata, Y., H₂O/Olefinic- π Interaction inside a Carbon Nanocage, *J. Am. Chem. Soc.*, **141**, 12928-12938 (2019).

Tsukao, M.; Hashikawa, Y.; Toyama, N.; Muraoka, M.; Murata, M.; Sasamori, T.; Wakamiya, A.; Murata, Y., Propeller-Shaped Aluminum Complexes with an Azaperylene Core in the Ligands, *Inorganics*, **7**, 109 (2019).

Ozaki, M.; Shimazaki, A.; Jung, M.; Nakaike, Y.; Maruyama, N.; Yakumaru, S.; Rafieh, A. I.; Sasamori, T.; Tokitoh, N.; Ekanayake, P.; Murata, Y.; Murdey, R.; Wakamiya, A., A Purified, Solvent-Intercalated Precursor Complex for Wide Process Window Fabrication of Efficient Perovskite Solar Cells and Modules, *Angew. Chem. Int. Ed.*, **58**, 9389-9393 (2019).

Nakamura, T.; Shioya, N.; Hasegawa, T.; Murata, Y.; Murdey, R.; Wakamiya, A., Phthalimide-Based Transparent Electron Transport Materials with Oriented-Amorphous Structure from Solution-Processed Precursor Films, *ChemPlusChem*, **84**, 1396-1404 (2019).

Truong, M. A.; Lee, J.; Nakamura, T.; Seo, J.-Y.; Jung, M.; Ozaki, M.; Shimazaki, A.; Shioya, N.; Hasegawa, T.; Murata, Y.; Zakeeruddin, S. M.; Gratzel, M.; Murdey, R.; Wakamiya, A., Influence of Alkoxy Chain Length on the Properties of Two-Dimensionally Expanded Azulene-Core-Based Hole-Transporting Materials for Efficient Perovskite Solar Cells, *Chem. Eur. J.*, **25**, 6741-6752 (2019).

Nakamura, T.; Arakawa, N.; Ishikura, Y.; Hori, M.; Satou, M.; Endo, M.; Masui, H.; Fuse, S.; Takahashi, T.; Murata, Y.; Murdey, R.; Wakamiya, A., Donor-Acceptor Polymers Containing Thiazole-Fused Benzothiadiazole Acceptor Units for Organic Solar Cells, *RSC Adv.*, **9**, 7107-7114 (2019).

Nakamura, T.; Shioya, N.; Shimoaka, T.; Nishikubo, R.; Hasegawa, T.; Saeki, A.; Murata, Y.; Murdey, R.; Wakamiya, A., Molecular Orientation Change in Naphthalene Diimide Thin Films Induced by Removal of Thermally Cleavable Substituents, *Chem. Mater.*, **31**, 1729-1737 (2019).

Suzuki, H.; Nakano, M.; Hashikawa, Y.; Murata, Y., Rotational Motion and Nuclear-Spin Interconversion of H₂O Encapsulated in C₆₀ Appeared in the Low-Temperature Heat Capacity, *J. Phys. Chem. Lett.*, **10**, 1306-1311 (2019).

Hashikawa, Y.; Murata, Y., Probing the Regioselectivity by Encapsulated H₂: Diels-Alder Reaction of a Cage-Opened C₆₀ Derivative with Anthracene, *Chem. Eur. J.*, **25**, 2482-2485 (2019).

Ozaki, M.; Nakaike, Y.; Shimazaki, A.; Jung, M.; Maruyama, N.; Yakumaru, S.; Rafieh, A. I.; Ekanayake, P.; Saito, T.; Shimakawa, Y.; Sasamori, T.; Murata, Y.; Murdey, R.; Wakamiya, A., How to Make Dense and Flat Perovskite Layers for >20% Efficient Solar Cells: Oriented, Crystalline Perovskite Intermediates and Their Thermal Conversion, *Bull. Chem. Soc. Jpn.*, **92**, 1972-1979 (2019).

Nishitani, N.; Hirose, T.; Matsuda, K., 2-D Self-assembly of Alkyl-substituted Oligophenylene Derivatives at the Liquid/Solid Interface: Influence of Core Size and Hydrogen Bonds on the Nucleation–Elongation Process, *Chem. Lett.*, **48**, 253-256 (2019).

Nishitani, N.; Hirose, T.; Matsuda, K., Self-Assembly of Photochromic Diarylethene–Peptide Conjugates Stabilized by β -Sheet Formation at the Liquid/Graphite Interfac, *Chem. Commun.*, **55**, 5099-5102 (2019).

Bretel, G.; Le Grogne, E.; Jacquemin, D.; Hirose, T.; Matsuda, K.; Felpin, F.-X., Fabrication of Robust Spatially Resolved Photochromic Patterns on Cellulose Papers by Covalent Printing for Anticounterfeiting Applications, *ACS Appl. Polym. Mater.*, **1**, 1240-1250 (2019).

Adachi, K.; Hirose, T.; Matsuda, K., Polymorphism of Porphyrin 2D Assemblies at the Liquid–Graphite Interface: Effect of Polar Solvent Additive and Flexible Spacer on the Face-On and Edge-On Type Molecular Arrangements, *Chem. Commun.*, **55**, 8836-8839 (2019).

[Others]

Faiz, J.; Murata, Y., Cleaving Double Bonds in Fullerene Derivatives, *ChemViews*, doi:10.1002/chemv.201900013 (2019).

— Synthetic Organic Chemistry —

Yanagi, M.; Ueda, Y.; Ninomiya, R.; Imayoshi, A.; Furuta, T.; Mishiro, K.; Kawabata, T., Synthesis of 4-Deoxy Pyranosides via Catalyst-Controlled Site-Selective Toluoylation of Abundant Sugars, *Org. Lett.*, **21**, 5006-5009 (2019).

Kawabata, T., Potential in Acylation, *Journal of Synthetic Organic Chemistry, Japan*, **77**, 268-271 (2019) (in Japanese).

Kondo, Y.; Morisaki, K.; Hirazawa, Y.; Morimoto, H.; Ohshima, T., A Convenient Preparation Method for Benzophenone Imine Catalyzed by Tetrabutylammonium Fluoride, *Org. Process Res. Dev.*, **28**, 1718-1724 (2019).

Irie, Y.; Hanaki, M.; Murakami, K.; Imamoto, T.; Furuta, T.; Kawabata, T.; Kawase, T.; Hirose, K.; Minobe, Y.; Akagi, K.; Yanagita, R. C.; Irie, K., Synthesis and Biochemical Characterization of Quasi-Stable Trimer Models Full-Length Amyloid β 40 with a Toxic Conformation, *Chem. Commun.*, **55**, 182-185 (2019).

— Advanced Inorganic Synthesis —

Sakamoto, M.; Kawawaki, T.; Kimura, M.; Vequizo, J. J. M.; Matsunaga, H.; Ranasinghe, C. S. K.; Yamakata, A.; Matsuzaki, H.; Furube, A.; Teranishi, T., Clear and Transparent Nanocrystals for Infrared-Responsible Carrier Transfer, *Nat. Commun.*, **10**, [406-1]-[406-7] (2019).

Choi, Y. Y.; Teranishi, T.; Majima, Y., Robust Pt-based Nanogap Electrodes with 10-nm-scale Ultrafine Linewidth, *Appl. Phys. Express*, **12**, [025002-1]-[025002-5] (2019).

Matsumoto, K.; Sato, R.; Trinh, T. T.; Sakuma, N.; Shoji, T.; Haruta, M.; Kurata, H.; Teranishi, T., Formation of Strong L10-FePd/ α -Fe Nanocomposite Magnets by Visualizing Efficient Exchange Coupling, *Nanoscale Adv.*, **1**, 2598-2605 (2019).

Kawawaki, T.; Sakamoto, M.; Nakagawa, T.; Teranishi, T., Carrier-selective Blocking Layer Synergistically Improves the Plasmonic Enhancement Effect, *J. Am. Chem. Soc.*, **141**, 8402-8406 (2019).

Kim, J.; Wu, H.-L.; Hsu, S.; Matsumoto, K.; Sato, R.; Teranishi, T., Nanoparticle Approach to the Formation of $\text{Sm}_2\text{Fe}_{17}\text{N}_3$ Hard Magnetic Particles, *Chem. Lett.*, **48**, 1054-1057 (2019).

Sakamoto, M.; Kim, H.-D.; Eguchi, D.; Chang, I.-Y.; Tanaka, D.; Tahara, H.; Furube, A.; Minagawa, Y.; Majima, Y.; Kanemitsu, Y.; Teranishi, T., Impact of Orbital Hybridization at Molecular-Metal Interface on Carrier Dynamics, *J. Phys. Chem. C*, **123**, 25877-25882 (2019).

Nakahara, S.; Ohara, K.; Tahara, H.; Yumoto, G.; Kawawaki, T.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Ionization and Neutralization Dynamics of CsPbBr_3 Perovskite Nanocrystals Revealed by Double-Pump Transient Absorption Spectroscopy, *J. Phys. Chem. Lett.*, **10**, 4731-4736 (2019).

Lian, Z.; Sakamoto, M.; Kobayashi, Y.; Tamai, N.; Ma, J.; Sakurai, T.; Seki, S.; Nakagawa, T.; Lai, M.; Haruta, M.; Kurata, H.; Teranishi, T., Anomalous Photo-Induced Hole Transport in Type-I Core/Mesoporous-Shell Nanocrystals for Efficient Photocatalytic H_2 Evolution, *ACS Nano*, **13**, 8356-8363 (2019).

Lian, Z.; Sakamoto, M.; Vequizo, J. J. M.; Ranasinghe, C. S. K.; Yamakata, A.; Nagai, T.; Kimoto, K.; Kobayashi, Y.; Tamai, N.; Teranishi, T., Plasmonic p–n Junction for Infrared Light to Chemical Energy Conversion, *J. Am. Chem. Soc.*, **141**, 2446-2450 (2019).

[Others]

Ohara, K.; Nakahara, S.; Tahara, H.; Yumoto, G.; Kawawaki, T.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Charging and Neutralization Dynamics in CsPbBr_3 Nanocrystals Studied by Double Pump Transient Absorption Spectroscopy, *The Proceedings of the Japan Society of Applied Physics Spring Meeting 2019 (CD-ROM)*, **66**, ROMBUNNO.11p-S223-11 (2019) (in Japanese).

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

Yahata, Y.; Kimura, K.; Nakanishi, Y.; Marukane, S.; Sato, T.; Tsujii, Y.; Ohno, K., Control of Phase Separation in Polystyrene/Ionic Liquid-Blended Films by Polymer Brush-Grafted Particles, *Langmuir*, **35**, 3733-3747 (2019).

Sakakibara, K.; Moriki, Y.; Tsujii, Y., Preparation of High-Performance Polyethylene Composite Materials Reinforced with Cellulose Nanofiber: Simultaneous Nanofibrillation of Wood Pulp Fibers during Melt-Compounding Using Urea and Diblock Copolymer Dispersant, *ACS Appl. Polym. Mater.*, **1**, 178-187 (2019).

Shimizu, Y.; Sakakibara, K.; Akimoto, S.; Tsujii, Y., Effective Reinforcement of Poly(methyl methacrylate) Composites with a Well-Defined Bacterial Cellulose Nanofiber Network, *ACS Sustainable Chem. Eng.*, **7**, 13351-13358 (2019).

Sakakibara, K.; Nishiumi, K.; Shimoaka, T.; Hasegawa, T.; Tsujii, Y., pMAIRS Analysis on Chain-End Functionalization of Densely Grafted, Concentrated Polymer Brushes, *Macromolecules*, **52**, 6673-6682 (2019).

Mizukami, M.; Gen, M.; Hsu, S.-Y.; Tsujii, Y.; Kurihara, K., Dynamics of Lubricious, Concentrated PMMA Brush Layers Studied by Surface Forces and Resonance Shear Measurements, *Soft Matter*, **15**, 7765-7776 (2019).

- Yoshikawa, C.; Sakakibara, K.; Nakaji-Hirabayashi, T.; Yamazaki, T.; Tsujii, Y., Well-Defined Monolith Morphology Regulates Cell Adhesion and its Functions, *Mater. Sci. Eng. C*, **105**, [110108-1]-[110108-8] (2019).
- Sato, O.; Okuno, H.; Adachi, I.; Watanabe, J.; Tokita, M.; Sakakibara, K.; Kinose, Y.; Goto, A.; Tsujii, Y., Novel In-plane Switching Liquid Crystal Display with an Extremely High Transmittance Using a Well-designed Bottlebrush as a Zero-azimuth Anchoring Material, *Jpn. J. Appl. Phys.*, **58**, [066503-1]-[066503-7] (2019).
- Yahata, Y.; Marukane, S.; Sato, T.; Tsujii, Y.; Ohno, K., Controlling the Thermally Induced Phase Separation of Polymer/Ionic Liquid Blended Films with Concentrated-Polymer-Brush-Decorated Hybrid Particles, *Langmuir*, **35**, 14566-14575 (2019).
- Kinose, Y.; Sakakibara, K.; Ogawa, H.; Tsujii, Y., Main-Chain Stiffness of Cellulosic Bottlebrushes with Polystyrene Side Chains Introduced Regioselectively at the O-6 Position, *Macromolecules*, **52**, 8733-8740 (2019).
- Ohno, K.; Yahata, Y.; Sakaue, M.; Ladmiral, V., Grafting of Polymer Brushes from Xanthate-Functionalized Silica Particles, *Chem. Eur. J.*, **25**, 2059-2068 (2019).
- Ohno, K.; Masuda, S.; Ogawa, H., Polymer-brush-decorated Colloidal Platelets: Precision Synthesis and Self-assembly, *Polym. Chem.*, **10**, 2686-2696 (2019).
- Yamazawa, Y.; Kato, H.; Nakaji-Hirabayashi, T.; Yoshikawa, C.; Kitano, H.; Ohno, K.; Saruwatari, Y.; Matsuoka, K., Bioinactive Semi-interpenetrating Network Gel Layers: Zwitterionic Polymer Chains Incorporated in a Cross-linked Polymer Brush, *J. Mater. Chem. B*, **7**, 4280-4291 (2019).
- Koski, J. P.; Krook, N. M.; Ford, J.; Yahata, Y.; Ohno, K.; Murray, C. B.; Frischknecht, A. L.; Composto, R. J.; Riggelman, R. A., Phase Behavior of Grafted Polymer Nanocomposites from Field-Based Simulations, *Macromolecules*, **52**, 5110-5121 (2019).
- Pamvouxoglou, A.; Bogri, P.; Nagele, G.; Ohno, K.; Petekidis, G., Structure and Dynamics in Suspensions of Soft Core-shell Colloids in the Fluid Regime, *J. Chem. Phys.*, **151**, [024901-1]-[024901-19] (2019).
- Ohno, K.; Zhao, C.; Nishina, Y., Polymer-Brush-Decorated Graphene Oxide: Precision Synthesis and Liquid-Crystal Formation, *Langmuir*, **35**, 10900-10909 (2019).
- Shimizu, Y.; Sakakibara, K.; Yasuda, S.; Tsujii, Y., Lubrication Characteristics of Epoxy Resin-Based Monolithic Thin Films with a Well-Defined Porous Morphology, *Adv. Eng. Mater.*, **21**, [1900683-1]-[1900683-5] (2019).
- Okubo, H.; Tadokoro, C.; Sakakibara, K.; Nakano, K.; Sasaki, S.; Tsujii, Y., Super-Low Friction of Thermal-Treatment-Concentrated Polymer Brushes (TT-CPBs) under Boundary Lubrication: A Practical Method to Shorten the Swelling Time of CPBs in Solvents, *Tribol. Online*, **14**, 226-236 (2019).
- Polymer Controlled Synthesis —
- Duy, L. N.; Sekiya, R.; Tosaka, M.; Yamago, S.; Matsumoto, T.; Nishino, T.; Ichikawa, T.; Haino, T., Organogelators of 5,17-Difunctionalized Calix[4]arenes, *Chem. Lett.*, **48**, 43-46 (2019).
- Lu, Y.; Yamago, S., One-step Synthesis of Dendritic Highly Branched Polystyrenes by Organotellurium-mediated Copolymerization of Styrene and a Dienyl Telluride Monomer, *Angew. Chem. Int. Ed.*, **58**, 3952-3956 (2019).
- Fan, W.; Yamago, S., Synthesis of Structurally Controlled Poly(N-vinyl amide)s and Poly(vinyl amine)s and Their Block Copolymers Using Organotellurium-mediated Radical Polymerization, *Angew. Chem. Int. Ed.*, **58**, 7113-7116 (2019).
- Li, X.; Ogihara, T.; Abe, M.; Nakamura, Y.; Yamago, S., The Effect of Viscosity on the Diffusion and Termination Reaction of Organic Radical Pairs, *Chem. Eur. J.*, **25**, 9846-9850 (2019).
- Fujitsuka, M.; Lu, C.; Zhuang, B.; Kayahara, E.; Yamago, S.; Majima, T., Size-Dependent Relaxation Processes of Photo-Excited [n]Cycloparaphenylenes (n = 5–12): Significant Contribution of Internal Conversion in Smaller Rings, *J. Phys. Chem. A*, **123**, 4737-4742 (2019).
- Gros, A.; Huneau, B.; Verron, E.; Tosaka, M., A Physically-based Model for Strain-induced Crystallization in Natural Rubber. Part I: Life Cycle of a Crystallite, *J. Mech. Phys. Solids*, **125**, 164-177 (2019).
- Tosaka, M.; Maruyama, T., Multiple Structural Changes Found around Crack Tip of Carbon Black-filled Natural Rubber Vulcanizate, *Nippon Gomu Kyokaishi*, **92**, 171-173 (2019) (in Japanese).
- Yamago, S.; Kayahara, E., Synthesis and Reactions of Carbon Nanochoop, *J. Synth. Org. Chem. Jpn.*, **77**, 1147-1158 (2019).
- Inorganic Photonics Materials —
- Tashima, T.; Morishita, H.; Mizuochi, N., Experimental Demonstration of Two-photon Magnetic Resonances in a Single-spin System of a Solid, *Phys. Rev. A*, **100**, [023801-1]-[023801-8] (2019).
- Herbschleb, E. D.; Kato, H.; Maruyama, Y.; Danjo, T.; Makino, T.; Yamasaki, S.; Ohki, I.; Hayashi, K.; Morishita, H.; Fujiwara, M.; Mizuochi, N., Ultra-long Coherence Times Amongst Room-temperature Solid-state Spins, *Nat. Commun.*, **10**, [3766-1]-[3766-6] (2019).
- Yamaguchi, T.; Matsuzaki, Y.; Saito, S.; Saijo, S.; Watanabe, H.; Mizuochi, N.; Ishi-Hayase, J., Bandwidth Analysis of AC Magnetic Field Sensing Based on Electronic Spin Double-resonance of Nitrogen-vacancy Centers in Diamond, *Jpn. J. Appl. Phys.*, **58**, [100901-1]-[100901-5] (2019).
- Morishita, H.; Tashima, T.; Mima, D.; Kato, H.; Makino, T.; Yamasaki, S.; Fujiwara, M.; Mizuochi, N., Extension of the Coherence Time by Generating MW Dressed States in a Single NV Centre in Diamond, *Sci. Rep.*, **9**, [13318-1]-[13318-8] (2019).
- Nanospintronics —
- Kim, K.-J.; Mochizuki, M.; Ono, T., Prediction of Topological Hall Effect in a Driven Magnetic Domain Wall, *Appl. Phys. Express*, **12**, 053006 (2019).
- Moriyama, T.; Hayashi, K.; Yamada, K.; Shima, M.; Ohya, Y.; Ono, T., Intrinsic and Extrinsic Antiferromagnetic Damping in NiO, *Phys. Rev. Materials*, **3**, [051402-1]-[051402-5] (2019).

- Pradipto, A.-M.; Yakushiji, K.; Ham, W. S.; Kim, S.; Shiota, Y.; Moriyama, T.; Kim, K.-W.; Lee, H.-W.; Nakamura, K.; Lee, K.-J.; Ono, T., Enhanced Perpendicular Magnetocrystalline Anisotropy Energy in an Artificial Magnetic Material with Bulk Spin-momentum Coupling, *Phys. Rev. B*, **99**, [180410-1]-[180410-6] (2019).
- Kim, K.-J.; Li, T.; Kim, S.; Moriyama, T.; Koyama, T.; Chiba, D.; Lee, K.-J.; Lee, H.-W.; Ono, T., Possible Contribution of High-energy Magnons to Unidirectional Magnetoresistance in Metallic Bilayers, *Appl. Phys. Express*, **12**, 063001 (2019).
- Kim, D.-H.; Haruta, M.; Ko, H.-W.; Go, G.; Park, H.-J.; Nishimura, T.; Kim, D.-Y.; Okuno, T.; Hirata, Y.; Futakawa, Y.; Yoshikawa, H.; Ham, W.; Kim, S.; Kurata, H.; Tsukamoto, A.; Shiota, Y.; Moriyama, T.; Choe, S.-B.; Lee, K.-J.; Ono, T., Bulk Dzyaloshinskii-Moriya Interaction in Amorphous Ferrimagnetic Alloys, *Nat. Mater.*, **18**, 685-690 (2019).
- Moriyama, T.; Oda, K.; Ono, T., Choking Nonlocal Magnetic Damping in Exchange-Biased Ferromagnets, *Phys. Rev. Applied*, **11**, [011001-1]-[011001-5] (2019).
- Iino, T.; Moriyama, T.; Iwaki, H.; Aono, H.; Shiratsuchi, Y.; Ono, T., Resistive Detection of the Neel Temperature of Cr₂O₃ Thin Films, *Appl. Phys. Lett.*, **114**, 022402 (2019).
- Yamamoto, T.; Nozaki, T.; Imamura, H.; Shiota, Y.; Ikeura, T.; Tarnaru, S.; Yakushiji, K.; Kubota, H.; Fukushima, A.; Suzuki, Y.; Yuasa, S., Write-Error Reduction of Voltage-Torque-Driven Magnetization Switching by a Controlled Voltage Pulse, *Phys. Rev. Applied*, **11**, [014013-1]-[014013-8] (2019).
- Hirata, Y.; Kim, D.-H.; Kim, S. K.; Lee, D.-K.; Oh, S.-H.; Kim, D.-Y.; Nishimura, T.; Okuno, T.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Tserkovnyak, Y.; Shiota, Y.; Moriyama, T.; Choe, S.-B.; Lee, K.-J.; Ono, T., Vanishing Skyrmion Hall Effect at the Angular Momentum Compensation Temperature of a Ferrimagnet, *Nat. Nanotechnol.*, **14**, 232-236 (2019).
- Kim, D.-H.; Okuno, T.; Kim, S. K.; Oh, S.-H.; Nishimura, T.; Hirata, Y.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Tserkovnyak, Y.; Shiota, Y.; Moriyama, T.; Kim, K.-J.; Lee, K.-J.; Ono, T., Low Magnetic Damping of Ferrimagnetic GdFeCo Alloys, *Phys. Rev. Lett.*, **122**, [127203-1]-[127203-6] (2019).
- Yamamoto, T.; Nozaki, T.; Imamura, H.; Shiota, Y.; Tamaru, S.; Yakushiji, K.; Kubota, H.; Fukushima, A.; Suzuki, Y.; Yuasa, S., Improvement of Write Error Rate in Voltage-driven Magnetization Switching, *J. Phys. D: Appl. Phys.*, **52**, 164001 (2019).
- Shiota, Y.; Moriyama, T.; Ono, T., Magnetic Properties of Ferrimagnetic Tb/CoFeB/MgO Films, *Appl. Phys. Express*, **12**, [083002-1]-[083002-3] (2019).
- Funada, S.; Nishimura, T.; Shiota, Y.; Kasukawa, S.; Ishibashi, M.; Moriyama, T.; Ono, T., Spin Wave Propagation in Ferrimagnetic Gd_xCo_{1-x}, *Jpn. J. Appl. Phys.*, **58**, [080909-1]-[080909-4] (2019).
- Okuno, T.; Kim, D.-H.; Oh, S.-H.; Kim, S. K.; Hirata, Y.; Nishimura, T.; Ham, W. S.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Tserkovnyak, Y.; Shiota, Y.; Moriyama, T.; Kim, K.-J.; Lee, K.-J.; Ono, T., Spin-transfer Torques for Domain Wall Motion in Antiferromagnetically Coupled Ferrimagnets, *Nat. Electron.*, **2**, 389-393 (2019).
- Okuno, T.; Kim, S. K.; Moriyama, T.; Kim, D.-H.; Mizuno, H.; Ikebuchi, T.; Hirata, Y.; Yoshikawa, H.; Tsukamoto, A.; Kim, K.-J.; Shiota, Y.; Lee, K.-J.; Ono, T., Temperature Dependence of Magnetic Resonance in Ferrimagnetic GdFeCo Alloys, *Appl. Phys. Express*, **12**, [093001-1]-[093001-5] (2019).
- Ohkochi, T.; Kim, K.-J.; Kim, S.; Yoshimura, Y.; Tanigawa, H.; Ohshima, N.; Koyama, T.; Kotsugi, M.; Chiba, D.; Ono, T.; Kinoshita, T., Real-space and Pulse-by-pulse Analysis of Domain Wall Creep Induced by Spin-Hall Torque, *Jpn. J. Appl. Phys.*, **58**, [023001-1]-[023001-3] (2019).
- Lee, H. Y.; Kim, S.; Park, J. Y.; Oh, Y. W.; Park, S. Y.; Ham, W.; Kotani, Y.; Nakamura, T.; Suzuki, M.; Ono, T.; Lee, K.-J.; Park, B. G., Enhanced Spin-orbit Torque via Interface Engineering in Pt/CoFeB/MgO Heterostructures, *APL Mater.*, **7**, 031110 (2019).
- Hirata, Y.; Kim, D.-H.; Kim, S. K.; Lee, D. K.; Oh, S.-H.; Kim, D. Y.; Nishimura, T.; Okuno, T.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Tserkovnyak, Y.; Shiota, Y.; Moriyama, T.; Choe, S. B.; Lee, K.-J.; Ono, T., Vanishing Skyrmion Hall Effect at the Angular Momentum Compensation Temperature of a Ferrimagnet, *Nat. Nanotechnol.*, **14**, 232-236 (2019).
- Kim, D.-H.; Okuno, T.; Kim, S. K.; Oh, S.-H.; Nishimura, T.; Hirata, Y.; Futakawa, Y.; Yoshikawa, H.; Tsukamoto, A.; Tserkovnyak, Y.; Shiota, Y.; Moriyama, T.; Kim, K.-J.; Lee, K.-J.; Ono, T., Low Magnetic Damping of Ferrimagnetic GdFeCo Alloys, *Phys. Rev. Lett.*, **122**, [127203-1]-[127203-6] (2019).

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

- Masuda, T.; Baba, K.; Nomura, T.; Tsujita, K.; Murayama, T.; Itoh, T.; Takatani-Nakase, T.; Sokabe, M.; Inagaki, N.; Futaki, S., An Influenza-derived Membrane Tension-modulating Peptide Regulates Cell Movement and Morphology via Actin Remodeling, *Commun. Boil.*, **2**, 243 (2019).
- Kawaguchi, Y.; Ise, S.; Azuma, Y.; Takeuchi, T.; Kawano, K.; Le, T. K.; Ohkanda, J.; Futaki, S., Dipicolylamine/Metal Complexes that Promote Direct Cell-Membrane Penetration of Octaarginine, *Bioconjugate Chem.*, **30**, 454-460 (2019).
- Okuda, A.; Tahara, S.; Hirose, H.; Takeuchi, T.; Nakase, I.; Ono, A.; Takehashi, M.; Tanaka, S.; Futaki, S., Oligoarginine-Bearing Tandem Repeat Penetration-Accelerating Sequence Delivers Protein to Cytosol via Caveolae-Mediated Endocytosis, *Biomacromolecules*, **20**, 1849-1859 (2019).
- Akishiba, M.; Futaki, S., Inducible Membrane Permeabilization by Attenuated Lytic Peptides: A New Concept for Accessing Cell Interiors through Ruffled Membranes, *Mol. pharm.*, **16**, 2540-2548 (2019).
- Ichimizu, S.; Watanabe, H.; Maeda, H.; Hamasaki, K.; Ikegami, K.; Chuang, V. T. G.; Kinoshita, R.; Nishida, K.; Shimizu, T.; Ishima, Y.; Ishida, T.; Seki, T.; Katsuki, H.; Futaki, S.; Otagiri, M.; Maruyama, T., Cell-penetrating Mechanism of Intracellular Targeting Albumin: Contribution of Macropinocytosis Induction and Endosomal Escape, *J. Control. Release*, **304**, 156-163 (2019).
- Kawano, K.; Ogushi, M.; Masuda, T.; Futaki, S., Development of a Membrane Curvature-sensing Peptide Based on a Structure-activity Correlation Study, *Chem. Pharm. Bull.*, **67**, 1131-1138 (2019).

Sakai, T.; Kawano, K.; Iino, M.; Takeuchi, T.; Imanishi, M.; Futaki, S., Loosening of Lipid Packing by Cell-Surface Recruitment of Amphiphilic Peptides by Coiled-Coil Tethering, *ChemBiochem*, **20**, 2151-2159 (2019).

Futaki, S.; Matsuzaki, K.; Goto, Y., Meeting Peptides in Kyoto, *ChemBiochem*, **20**, 2015-2016 (2019).

Nakase, I.; Katayama, M.; Hattori, Y.; Ishimura, M.; Inaura, S.; Fujiwara, D.; Takatani-Nakase, T.; Fujii, I.; Futaki, S.; Kirihata, M., Intracellular Target Delivery of Cell-penetrating Peptide-conjugated Dodecaborate for Boron Neutron Capture Therapy (BNCT), *Chem. Commun.*, **55**, 13955-13958 (2019).

Tsuji, S.; Imanishi, M., Modified Nucleobase-Specific Gene Regulation Using Engineered Transcription Activator-like Effectors, *Adv. Drug Deliv. Rev.*, **147**, 59-65 (2019).

— Chemistry of Molecular Biocatalysts —

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

Bürger, M.; Mashiguchi, K.; Lee, H. J.; Nakano, M.; Takemoto, K.; Seto, Y.; Yamaguchi, S.; Chory, J., Structural Basis of Karrikin and Non-natural Strigolactone Perception in *Physcomitrella patens*, *Cell Rep.*, **26**, 855-865 (2019).

Yasui, R.; Seto, Y.; Ito, S.; Kawada, K.; Itto-Nakama, K.; Mashiguchi, K.; Yamaguchi, S., Chemical Screening of Novel Strigolactone Agonists that Specifically Interact with DWARF14 Protein, *Bioorg. Med. Chem. Lett.*, **29**, 938-942 (2019).

Yoshida, S.; Kim, S.; Wafula, E. K.; Tanskanen, J.; Kim, Y. M.; Honaas, L.; Yang, Z.; Spallek, T.; Conn, C. E.; Ichihashi, Y.; Cheong, K.; Cui, S.; Der, J. P.; Gundlach, H.; Jiao, Y.; Hori, C.; Ishida, J. K.; Kasahara, H.; Kiba, T.; Kim, M. S.; Koo, N.; Laohavisit, A.; Lee, Y. H.; Lumba, S.; McCourt, P.; Mortimer, J. C.; Mutuku, J. M.; Nomura, T.; Sasaki-Sekimoto, Y.; Seto, Y.; Wang, Y.; Wakatake, T.; Sakakibara, H.; Demura, T.; Yamaguchi, S.; Yoneyama, K.; Manabe, R. I.; Nelson, D. C.; Schulman, A. H.; Timko, M. P.; dePamphilis, C. W.; Choi, D.; Shirasu, K., Genome Sequence of *Striga asiatica* Provides Insight into the Evolution of Plant Parasitism, *Curr. Biol.*, **29**, 3041-3052 (2019).

Mashiguchi, K.; Hisano, H.; Takeda-Kamiya, N.; Takebayashi, Y.; Ariizumi, T.; Gao, Y.; Ezura, H.; Sato, K.; Zhao, Y.; Hayashi, K.; Kasahara, H., *Agrobacterium tumefaciens* Enhances Biosynthesis of Two Distinct Auxins in the Formation of Crown Galls, *Plant Cell Physiol.*, **60**, 29-37 (2019).

Fujiyama, K.; Hino, T.; Kanadani, M.; Watanabe, B.; Jae Lee, H.; Mizutani, M.; Nagano, S., Structural Insights into a Key Step of Brassinosteroid Biosynthesis and Its Inhibition, *Nat. Plants*, **5**, 589-594 (2019).

Suwannarach, N.; Kumla, J.; Watanabe, B.; Matsui, K.; Lumyong, S., Characterization of Melanin and Optimal Conditions for Pigment Production by an Endophytic Fungus, *Spissiomycetes endophytica* SDBR-CMU319, *PLoS One*, **14**, [e0222187-1]-[e0222187-15] (2019).

Koyama, T.; Tsubota, A.; Sawano, T.; Tawa, M.; Watanabe, B.; Hiratake, J.; Nakagawa, K.; Matsumura, Y.; Ohkita, M., Involvement of γ -Glutamyl Transpeptidase in Ischemia/Reperfusion-Induced Cardiac Dysfunction in Isolated Rat Hearts, *Biol. Pharm. Bull.*, **42**, 1947-1952 (2019).

— Molecular Biology —

Kato, M.; Tsuge, T.; Maeshima, M.; Aoyama, T., Arabidopsis PCaP2 Modulates the Phosphatidylinositol 4,5-bisphosphate Signal on the Plasma Membrane and Attenuates Root Hair Elongation, *Plant J.*, **99**, 610-625 (2019).

— Chemical Biology —

Takashima, I.; Kusamori, K.; Hakariya, H.; Takashima, M.; Vu, T. H.; Mizukami, Y.; Noda, N.; Takayama, Y.; Katsuda, Y.; Sato, S. I.; Takakura, Y.; Nishikawa, M.; Uesugi, M., Multifunctionalization of Cells with a Self-Assembling Molecule to Enhance Cell Engraftment, *ACS Chem. Biol.*, **14**, 775-783 (2019).

Furuta, T.; Mizukami, Y.; Asano, L.; Kotake, K.; Ziegler, S.; Yoshida, H.; Watanabe, M.; Sato, S.; Waldmann, H.; Nishikawa, M.; Uesugi, M., Nutrient-Based Chemical Library as a Source of Energy Metabolism Modulators, *ACS Chem. Biol.*, **14**, 1860-1865 (2019).

Abo, M.; Weerapana, E., Chemical Probes for Redox Signaling and Oxidative Stress, *Antioxidants & Redox Signaling*, **30**, 1369-1386 (2019).

Kawagoe, F.; Mototani, S.; Yasuda, K.; Nagasawa, K.; Uesugi, M.; Sakaki, T.; Kittaka, A., Introduction of Fluorine Atoms to Vitamin D3 Side-chain and Synthesis of 24,24-Difluoro-25-hydroxyvitamin D3, *J. Steroid Biochem. Mol. Biol.*, **195**, 105477 (2019).

Nagata, A.; Akagi, Y.; Asano, L.; Kotake, K.; Kawagoe, F.; Mendoza, A.; Masoud, S. S.; Usuda, K.; Yasui, K.; Takemoto, Y.; Kittaka, A.; Nagasawa, K.; Uesugi, M., Synthetic Chemical Probes That Dissect Vitamin D Activities, *ACS Chem. Biol.*, **14**, 2851-2858 (2019).

Kawagoe, F.; Yasuda, K.; Mototani, S.; Sugiyama, T.; Uesugi, M.; Sakaki, T.; Kittaka, A., Synthesis and CYP24A1-Dependent Metabolism of 23-Fluorinated Vitamin D3 Analogues, *ACS Omega*, **4**, 11332-11337 (2019).

Chen, I. S.; Liu, C.; Tateyama, M.; Karbat, I.; Uesugi, M.; Reuveny, E.; Kubo, Y., Non-sedating Antihistamines Block G-protein-gated Inwardly Rectifying K⁺ Channels, *Br. J. Pharmacol.*, **176**, 3161-3179 (2019).

Nagata, A.; Akagi, Y.; Masoud, S. S.; Yamanaka, M.; Kittaka, A.; Uesugi, M.; Odagi, M.; Nagasawa, K., Stereoselective Synthesis of Four Calcitriol Lactone Diastereomers at C23 and C25, *J. Org. Chem.*, **84**, 7630-7641 (2019).

Kawagoe, F.; Sugiyama, T.; Yasuda, K.; Uesugi, M.; Sakaki, T.; Kittaka, A., Concise Synthesis of 23-Hydroxylated Vitamin D3 Metabolites, *J. Steroid Biochem. Mol. Biol.*, **186**, 161-168 (2019).

Nishikawa, Y.; Kodama, Y.; Shiokawa, M.; Matsumori, T.; Marui, S.; Kuriyama, K.; Kuwada, T.; Sogabe, Y.; Kakiuchi, N.; Tomono, T.; Mima, A.; Morita, T.; Ueda, T.; Tsuda, M.; Yamauchi, Y.; Sakuma, Y.; Ota, Y.; Maruno, T.; Uza, N.; Uesugi, M.; Kageyama, R.; Chiba, T.; Seno, H., Hes1 Plays an Essential Role in Kras-driven Pancreatic Tumorigenesis, *Oncogene*, **38**, 4283-4296 (2019).

DIVISION OF ENVIRONMENTAL CHEMISTRY — **Molecular Materials Chemistry** —

Cai, M.; Zhang, D.; Xu, J.; Hong, X.; Zhao, C.; Song, X.; Qiu, Y.; Kaji, H.; Duan, L., Unveiling the Role of Langevin and Trap-Assisted Recombination in Long Lifespan OLEDs Employing Thermally Activated Delayed Fluorophore, *ACS Appl. Mater. Interfaces*, **11**, 1096-1108 (2019).

Zhang, D. D.; Suzuki, K.; Song, X. Z.; Wada, Y.; Kubo, S.; Duan, L. A.; Kaji, H., Thermally Activated Delayed Fluorescent Materials Combining Intra- and Intermolecular Charge Transfers, *ACS Appl. Mater. Interfaces*, **11**, 7192-7198 (2019).

Cai, M.; Zhang, D.; Xu, J.; Hong, X.; Zhao, C.; Song, X.; Qiu, Y.; Kaji, H.; Duan, L., Correction to Unveiling the Role of Langevin and Trap-Assisted Recombination in Long-Lifespan OLEDs Employing Thermally Activated Delayed Fluorophores, *ACS Appl. Mater. Interfaces*, **11**, 6663 (2019).

Fukushima, T.; Ishibashi, H.; Suemasa, D.; Nakamura, R.; Yomogida, M.; Isono, T.; Satoh, T.; Kaji, H., Synthesis and Characterization of Cyclic P3HT as a Donor Polymer for Organic Solar Cells, *J. Polym. Sci., Part B: Polym. Phys.*, **57**, 266-271 (2019).

Ghosh, S.; Tsutsui, Y.; Suzuki, K.; Kaji, H.; Honjo, K.; Uemura, T.; Seki, S., Impact of the Position of Imine-Linker over Optoelectronic Performance of π -Conjugated Organic Frameworks, *Mol. Syst. Des. Eng.*, **4**, 325-331 (2019).

Shiota, K.; Toda, T.; Oshita, K.; Fujimori, T.; Kaji, H.; Maeno, A.; Takaoka, M., The Effect of Gas Emission on the Strength of Composite Products Derived Using Alkali-activated Municipal Solid Waste Incineration Fly Ash/pyrophyllite-Based Systems, *Chemosphere*, **228**, 513-520 (2019).

Zu, G. Q.; Kanamori, K.; Maeno, A.; Kaji, H.; Nakanishi, K.; Shen, J., Ambient-dried Highly Flexible Copolymer Aerogels and Their Nanocomposites with Polypyrrole for Thermal Insulation, Separation, and Pressure Sensing, *Polym. Chem.*, **10**, 4980-4990 (2019).

Kusaka, Y.; Hasegawa, T.; Kaji, H., Noise Reduction in Solid-State NMR Spectra Using Principal Component Analysis, *J. Chem. Phys. A*, **123**, 10333-10338 (2019).

— **Hydrospheric Environment Analytical Chemistry** —

Zheng, L.; Minami, T.; Konagaya, W.; Chan, C.-Y.; Tsujisaka, M.; Takano, S.; Norisuye, K.; Sohrin, Y., Distinct Basin-scale-distributions of Aluminum, Manganese, Cobalt, and Lead in the North Pacific Ocean, *Geochim. Cosmochim. Acta*, **254**, 102-121 (2019).

Zheng, L.; Sohrin, Y., Major Lithogenic Contributions to the Distribution and Budget of Iron in the North Pacific Ocean, *Sci. Rep.*, **9**, [11652-1]-[11652-9] (2019).

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.*, **511**, 494-509 (2019).

Tanaka, Y.; Tsujisaka, M.; Zheng, L.; Takano, S.; Sohrin, Y., Application of NOBIAS Chelate-PA 1 Resin to the Determination of Zirconium, Niobium, Hafnium, and Tantalum in Seawater, *Anal. Sci.*, **35**, 1015-1020 (2019).

Yang, S.-C.; Welter, L.; Kolatkar, A.; Nieva, J.; Waitman, K. R.; Huang, K.-F.; Liao, W.-H.; Takano, S.; Berelson, W. M.; West, A. J.; Kuhn, P.; John, S. G., A New Anion Exchange Purification Method for Cu Stable Isotopes in Blood Samples, *Anal. Bioanal. Chem.*, **411**, 765-776 (2019).

Tsujisaka, M.; Takano, S.; Murayama, M.; Sohrin, Y., Precise Analysis of the Concentrations and Isotopic Compositions of Molybdenum and Tungsten in Geochemical Reference Materials, *Anal. Chim. Acta*, **1091**, 146-159 (2019).

— **Chemistry for Functionalized Surfaces** —

Kise, R.; Fukumi, A.; Shioya, N.; Shimoaka, T.; Sonoyama, M.; Amii, H.; Takagi, T.; Kanamori, T.; Eda, K.; Hasegawa, T., Fluorous Property of a Short Perfluoroalkyl-Containing Compound Realized by Self-Assembled Monolayer Technique on a Silicon Substrate, *Bull. Chem. Soc. Jpn.*, **92**, 785-789 (2019).

Shioya, N.; Murdey, R.; Nakao, K.; Yoshida, H.; Koganezawa, T.; Eda, K.; Shimoaka, T.; Hasegawa, T., Alternative Face-on Thin Film Structure of Pentacene, *Sci. Rep.*, **9**, [579-1]-[579-7] (2019).

Nakamura, T.; Shioya, N.; Shimoaka, T.; Nishikubo, R.; Hasegawa, T.; Saeki, A.; Murata, Y.; Murdey, R.; Wakamiya, A., Molecular Orientation Change in Naphthalene Diimide Thin Films Induced by Removal of Thermally Cleavable Substituents, *Chem. Mater.*, **31**, 1729-1737 (2019).

Truong, M. A.; Lee, J.; Nakamura, T.; Seo, J.-Y.; Jung, M.; Ozaki, M.; Shimazaki, A.; Shioya, N.; Hasegawa, T.; Murata, Y.; Zakeeruddin, S. M.; Grätzel, M.; Murdey, R.; Wakamiya, A., Influence of Alkoxy Chain Length on the Properties of Two-Dimensionally Expanded Azulene-Core-Based Hole-Transporting Materials for Efficient Perovskite Solar Cells, *Chem. Eur. J.*, **25**, 6741-6752 (2019).

Wang, C.; Hosomi, T.; Nagashima, K.; Takahashi, T.; Zhang, G.; Kanai, M.; Hao, Z.; Mizukami, W.; Shioya, N.; Shimoaka, T.; Tamaoka, T.; Yoshida, H.; Takeda, S.; Yasui, T.; Baba, Y.; Aoki, Y.; Terao, J.; Hasegawa, T.; Yanagida, T., Rational Method of Monitoring Molecular Transformations on Metal-Oxide Nanowire Surfaces, *Nano Lett.*, **19**, 2443-2449 (2019).

Shimoaka, T.; Sonoyama, M.; Amii, H.; Takagi, T.; Kanamori, T.; Hasegawa, T., Raman Optical Activity on Solid Sample: Identification of Atropisomers of Perfluoroalkyl Chains Having a Helical Conformation and No Chiral Center, *J. Phys. Chem. A*, **123**, 3985-3991 (2019).

Nakamura, T.; Shioya, N.; Hasegawa, T.; Murata, Y.; Murdey, R.; Wakamiya, A., Phthalimide-Based Transparent Electron-Transport Materials with Oriented-Amorphous Structures: Preparation from Solution-Processed Precursor Films, *ChemPlusChem*, **84**, 1396-1404 (2019).

Tomita, K.; Shioya, N.; Shimoaka, T.; Eda, K.; Hasegawa, T., Two-Dimensional Film Growth of Zinc Tetrphenylporphyrin with the Aid of Solvent Coordination, *Bull. Chem. Soc. Jpn.*, **92**, 1335-1340 (2019).

Morita, K.; Horikoshi, M.; Yanagi, T.; Takagi, T.; Takahashi, H.; Amii, H.; Hasegawa, T.; Sonoyama, M., Thermotropic Transition Behaviors of Novel Partially Fluorinated Dimyristoylphosphatidylcholines with Different Perfluoroalkyl Chain Lengths, *Chem. Lett.*, **48**, 1105-1108 (2019).

Shioya, N.; Tomita, K.; Shimoaka, T.; Hasegawa, T., Second Generation of Multiple-Angle Incidence Resolution Spectrometry, *J. Phys. Chem. A*, **123**, 7177-7183 (2019).

Wang, C.; Sharma, S. K.; Olaluwoye, O. S.; Alrashdi, S. A.; Hasegawa, T.; Leblanc, R. M., Conformation Change of α -Synuclein(61-95) at the Air-Water Interface and Quantitative Measurement of the Tilt Angle of the Axis of its α -Helix by Multiple Angle Incidence Resolution Spectroscopy, *Colloids Surf. B*, **183**, [110401-1]-[110401-6] (2019).

Shimada, T.; Tochinal, K.; Hasegawa, T., Determination of pH Dependent Structures of Thymol Blue Revealed by Cooperative Analytical Method of Quantum Chemistry and Multivariate Analysis of Electronic Absorption Spectra, *Bull. Chem. Soc. Jpn.*, **92**, 1759-1766 (2019).

Sakakibara, K.; Nishiumi, K.; Shimoaka, T.; Hasegawa, T.; Tsujii, Y., pMAIRS Analysis on Chain-End Functionalization of Densely Grafted, Concentrated Polymer Brushes, *Macromolecules*, **52**, 6673-6682 (2019).

Nagai, N.; Okada, H.; Hasegawa, T., Morphology-Sensitive Infrared Absorption Bands of Polymers Derived from Surface Polaritons, *AIP Adv.*, **9**, [105203-1]-[105203-12] (2019).

Kusaka, Y.; Hasegawa, T.; Kaji, H., Noise Reduction in Solid-State NMR Spectra Using Principal Component Analysis, *J. Phys. Chem. A*, **123**, 10333-10338 (2019).

— Molecular Microbial Science —

Kawai, S.; Kawamoto, J.; Ogawa, T.; Kurihara, T., Development of a Regulatable Low-temperature Protein Expression System Using the Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10, as the Host, *Biosci. Biotechnol. Biochem.*, **83**, 2153-2162 (2019).

Casillo, A.; Di Guida, R.; Carillo, S.; Chen, C.; Kamasaka, K.; Kawamoto, J.; Kurihara, T.; Corsaro, M. M., Structural Elucidation of a Novel Lipooligosaccharide from the Cold-Adapted Bacterium OMVs Producer *Shewanella* sp. HM13, *Mar. Drugs*, **17**, [E34-1]-[E34-13] (2019).

[Others]

Ogawa, T., The Valuable Bacteria Producing EPA and DHA, *Seibutsu-kogaku Kaishi 2019*, **97**, 619 (2019) (in Japanese).

DIVISION OF MULTIDISCIPLINARY CHEMISTRY — Polymer Materials Science —

Nishitsuji, S.; Takenaka, M., Viscoelastic Effects on Dynamics of Concentration Fluctuations in Semi-dilute Polymer Solution in the Good Solvent Regime, *Polymer*, **179**, [121622-1]-[121622-7] (2019).

Hashimoto, T.; Amino, N.; Nishitsuji, S.; Takenaka, M., Hierarchically Self-organized Filler Particles in Polymers: Cascade Evolution of Dissipative Structures to Ordered Structures, *Polym. J.*, **51**, 109-130 (2019).

Ono, K.; Masuda, S.; Ogawa, H., Polymer-brush-decorated Colloidal Platelets: Precision Synthesis and Self-Assembly, *Polym. Chem.*, **10**, 2686-2696 (2019).

— Molecular Rheology —

Morelly, S. L.; Palmese, L.; Watanabe, H.; Alvarez, N. J., Effect of Finite Extensibility on Nonlinear Extensional Rheology of Polymer Melts, *Macromolecules*, **52**, 915-922 (2019).

Kwon, Y.; Matsumiya, Y.; Watanabe, H., Dielectric Relaxation of Type-A Chains Undergoing Head-to-Tail Association/Dissociation: Difference from Head-to-Head Case and Correlation with Viscoelastic Relaxation, *Macromolecules*, **52**, 8484-8502 (2019).

—Molecular Aggregation Analysis —

Nakamura, T.; Shioya, N.; Shimoaka, T.; Nishikubo, R.; Hasegawa, T.; Saeki, A.; Murata, Y.; Murdey, R.; Wakamiya, A., Molecular Orientation Change in Naphthalene Diimide Thin Films Induced by Removal of Thermally Cleavable Substituents, *Chem. Mater.*, **31**, 1729-1737 (2019).

Koedtrud, A.; Goto, M.; Amano Patino, M.; Tan, Z.; Guo, H.; Nakamura, T.; Handa, T.; Chen, W.-T.; Chuang, Y.-C.; Sheu, H.-S.; Saito, T.; Kan, D.; Kanemitsu, Y.; Wakamiya, A.; Shimakawa, Y., Structure-Property Relations in Ag-Bi-I Compounds: Potential Pb-free Absorbers in Solar Cells, *J. Mater. Chem. A*, **7**, 5583-5588 (2019).

Truong, M. A.; Lee, J.; Nakamura, T.; Seo, J.-Y.; Jung, M.; Ozaki, M.; Shimazaki, A.; Shioya, N.; Hasegawa, T.; Murata, Y.; Zakeeruddin, S. M.; Gratzel, M.; Murdey, R.; Wakamiya, A., Influence of Alkoxy Chain Length on the Properties of Two-Dimensionally Expanded Azulene Core-Based Hole-Transporting Materials for Efficient Perovskite Solar Cells, *Chem. Eur. J.*, **25**, 6741-6752 (2019).

Nakamura, T.; Ishikura, Y.; Arakawa, N.; Hori, M.; Satou, M.; Endo, M.; Masui, H.; Fuse, S.; Takahashi, T.; Murata, Y.; Murdey, R.; Wakamiya, A., Donor-Acceptor Polymers Containing Thiazole-Fused Benzothiadiazole Acceptor Units for Organic Solar Cells, *RSC Adv.*, **9**, 7107-7114 (2019).

Ozaki, M.; Shimazaki, A.; Jung, M.; Nakaike, Y.; Maruyama, N.; Yakumaru, S.; Rafieh, A. I.; Sasamori, T.; Tokitoh, N.; Ekanayake, P.; Murata, Y.; Murdey, R.; Wakamiya, A., A Purified, Solvent-Intercalated Precursor Complex for Wide Process Window Fabrication of Efficient Perovskite Solar Cells and Modules, *Angew. Chem. Int. Ed.*, **58**, 9389-9393 (2019).

Ozaki, M.; Ishikura, Y.; Truong, M. A.; Liu, J.; Okada, I.; Tanabe, T.; Sekimoto, S.; Ohtsuki, T.; Murata, Y.; Murdey, R.; Wakamiya, A., Iodine-rich Mixed Composition Perovskites Optimised for Tin(IV) Oxide Transport Layers: the Influence of Halide Ion Ratio, Annealing Time, and Ambient Air Aging on Solar Cell Performance, *J. Mater. Chem. A*, **7**, 16947-16953 (2019).

Nakamura, T.; Shioya, N.; Hasegawa, T.; Murata, Y.; Murdey, R.; Wakamiya, A., Phthalimide-Based Transparent Electron-Transport Materials with Oriented-Amorphous Structures: Preparation from Solution-Processed Precursor Films, *ChemPlusChem*, **84**, 1396-1404 (2019).

Tsukao, M.; Hashikawa, Y.; Toyama, N.; Muraoka, M.; Murata, M.; Sasamori, T.; Wakamiya, A.; Murata, Y., Propeller-Shaped Aluminum Complexes with an Azaperylene Core in the Ligands, *Inorganics*, **7**, 109 (2019).

Jung, H.; Kang, S.; Sim, Y.; Jung, M.; Wakamiya, A.; Leed, J.-H.; Park, J., Single Crystal Structure and Electroluminescence Efficiency of Blue Fluorescence OLED Emitters Using Triple Core Chromophores, *Organic Electronics*, **73**, 261-265 (2019).

Shigemori, K.; Watanabe, M.; Kong, J.; Mitsudo, K.; Wakamiya, A.; Mandai, H.; Suga, S., Iodide-Mediated or Iodide-Catalyzed Demethylation and Friedel-Crafts C-H Borylative Cyclization Leading to Thiophene-Fused 1,2-Oxaborine Derivatives, *Org. Lett.*, **21**, 2171-2175 (2019).

Yang, F.; Liu, J.; Wang, X.; Tanaka, K.; Shinokita, K.; Miyauchi, Y.; Wakamiya, A.; Matsuda, K., Planar Perovskite Solar Cells with High Efficiency and Fill Factor Obtained Using Two-Step Growth Process, *ACS Appl. Mater. Interfaces*, **11**, 15680-15687 (2019).

Ozaki, M.; Nakaike, Y.; Shimazaki, A.; Jung, M.; Maruyama, N.; Yakumaru, S.; Rafieh, A. I.; Ekanayake, P.; Saito, T.; Shimakawa, Y.; Sasamori, T.; Murata, Y.; Murdey, R.; Wakamiya, A., How to Make Dense and Flat Perovskite Layers for >20% Efficient Solar Cells: Oriented, Crystalline Perovskite Intermediates and Their Thermal Conversion, *Bull. Chem. Soc. Jpn.*, **92**, 1972-1979 (2019).

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE — Particle Beam Science —

Kitahara, R.; Hirota, K.; Ieki, S.; Ino, T.; Iwashita, Y.; Kitaguchi, M.; Koga, J.; Mishima, K.; Morishita, A.; Nagakura, N.; Oide, H.; Otono, H.; Seki, Y.; Sekiba, D.; Shima, T.; Shimizu, H. M.; Sumi, N.; Sumino, H.; Taketani, K.; Tomita, T.; Yamada, T.; Yamashita, S.; Yokohashi, M.; Yoshioka, T., Improved Accuracy in the Determination of the Thermal Cross Section of $^{14}\text{N}(n,p)^{14}\text{C}$ for Neutron Lifetime Measurement, *Prog. Theor. Exp. Phys.*, **2019**(9), 093C01 (2019).

Antoine, C. Z.; Aburas, M.; Four, A.; Weiss, F.; Iwashita, Y.; Hayano, H.; Kato, S.; Kubo, T.; Saeki, T., Optimization of Tailored Multilayer Superconductors for RF Application and Protection against Premature Vortex Penetration, *Supercond. Sci. Technol.*, **32**(8), [085005-1]-[085005-9] (2019).

Abe, M.; Bae, S.; Beer, G.; Bunce, G.; Choi, H.; Choi, S.; Chung, M.; da Silva, W.; Eidelman, S.; Finger, M.; Fukao, Y.; Fukuyama, T.; Haciomeroglu, S.; Hasegawa, K.; Hayasaka, K.; Hayashizaki, N.; Hisamatsu, H.; Iijima, T.; Iinuma, H.; Ikeda, H.; Ikeno, M.; Inami, K.; Ishida, K.; Itahashi, T.; Iwasaki, M.; Iwashita, Y.; Iwata, Y.; Kadono, R.; Kamal, S.; Kamitani, T.; Kanda, S.; Kapusta, F.; Kawagoe, K.; Kawamura, N.; Kim, B.; Kim, Y.; Kishishita, T.; Kitamura, R.; Ko, H.; Kohriki, T.; Kondo, Y.; Kume, T.; Lee, M. J.; Lee, S.; Lee, W.; Marshall, G. M.; Matsuda, Y.; Mibe, T.; Miyake, Y.; Murakami, T.; Nagamine, K.; Nakayama, H.; Nishimura, S.; Nomura, D.; Ogitsu, T.; Ohsawa, S.; Oide, K.; Oishi, Y.; Okada, S.; Olin, A.; Omarov, Z.; Otani, M.; Razuvaev, G.; Rehman, A.; Saito, N.; Saito, N. F.; Sasaki, K.; Sasaki, O.; Sato, N.; Sato, Y.; Semertzidis, Y. K.; Sendai, H.; Shatunov, Y.; Shimomura, K.; Shoji, M.; Shwartz, B.; Strasser, P.; Sue, Y.; Suehara, T.; Sung, C.; Suzuki, K.; Takatomi, T.; Tanaka, M.; Tojo, J.; Tsutsumi, Y.; Uchida, T.; Ueno, K.; Wada, S.; Won, E.; Yamaguchi, H.; Yamanaka, T.; Yamamoto, A.; Yamazaki, T.; Yasuda, H.; Yoshida, M.; Yoshioka, T., A New Approach for Measuring the Muon Anomalous Magnetic Moment and Electric Dipole Moment, *Prog. Theor. Exp. Phys.*, **2019**, [053C02-1]-[053C02-22] (2019).

Adeva, B.; Afanasyev, L.; Anania, A.; Aogaki, S.; Benelli, A.; Brekhovskikh, V.; Cechak, T.; Chiba, M.; Chliapnikov, P. V.; Doskarova, P.; Drijard, D.; Dudarev, A.; Dumitriu, D.; Fluerau, D.; Gorin, A.; Gorchakov, O.; Gritsay, K.; Guaraldo, C.; Gugiu, M.; Hansroul, M.; Hons, Z.; Horikawa, S.; Iwashita, Y.; Karpukhin, V.; Kluson, J.; Kobayashi, M.; Kruglov, V.; Kruglova, L.; Kulikov, A.; Kulish, E.; Lamberto, A.; Lanaro, A.; Lednický, R.; Mariñas, C.; Martincik, J.; Nemenov, L.; Nikitin, M.; Okada, K.; Olchevskii, V.; Ovsianikov, V.; Pentia, M.; Penzo, A.; Plo, M.; Prusa, P.; Rappazzo, G. F.; Romero Vidal, A.; Ryazantsev, A.; Rykalin, V.; Saborido, J.; Schacher, J.; Sidorov, A.; Smolik, J.; Takeuchi, F.; Trojek, T.; Trusov, S.; Urban, T.; Vrba, T.; Yazkov, V.; Yoshimura, Y.; Zrelov, P., First Measurement of a Long-Lived $\pi^+ \pi^-$ Atom Lifetime, *Phys. Rev. Lett.*, **122**, [082003-1]-[082003-7] (2019).

Tsukada, K.; Adachi, K.; Enokizono, A.; Fujita, T.; Hara, M.; Hori, T.; Hori, M.; Ichikawa, S.; Kasama, K.; Kurita, K.; Namba, K.; Ohnishi, T.; Suda, T.; Tamae, T.; Togasaki, M.; Wakasugi, M.; Watanabe, M.; Yamada, K., Electron Scattering from ^{208}Pb and ^{132}Xe Ions at the SCRIT Facility, *Hyperfine Interaction*, **240**, 102-109 (2019).

[Others]

Takeuchi, Y.; Iwashita, Y.; Tongu, H., Compact H^+ ECR Ion Source with Pulse Gas Valve, *Proc. of Linac2018*, 955-957 (2019).

Nakazawa, Y.; Iinuma, H.; Hasegawa, K.; Kondo, Y.; Morishita, T.; Hayashizaki, N.; Iwashita, Y.; Iwata, Y.; Kawamura, N.; Mibe, T.; Otani, M.; Yamazaki, T.; Yoshida, M.; Kitamura, R.; Yasuda, H. Y.; Saito, N.; Sue, Y., Prototype of an Inter-digital H-mode Drift-tube Linac for Muon Linac, *Proc. of Linac2018*, 180-183 (2019).

Iwashita, Y.; Abe, M.; Yako, T.; Fuwa, Y.; Terunuma, N., Steering Magnets with Permanent Magnets, *Proc. of Linac2018*, 264-266 (2019).

Katayama, R.; Iwashita, Y.; Tongu, H.; Four, A.; Antoine, C. Z.; Hayano, H.; Kubo, T.; Saeki, T.; Ito, H.; Ito, R.; Nagata, T.; Oikawa, H., Precise Evaluation of Characteristic of the Multilayer Thin-film Superconductor Consisting of NbN and Insulator on Pure Nb Substrate, *Proc. of Linac2018*, 391-394 (2019).

Ito, R.; Nagata, T.; Hayano, H.; Kubo, T.; Saeki, T.; Ito, H.; Iwashita, Y.; Katayama, R.; Oikawa, H., Construction of Thin-film Coating System Toward the Realization of Superconducting Multilayered Structure, *Proc. of Linac2018*, 445-447 (2019).

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 of Thin Film Superconductor, *Proc. of Linac2018*, 484-487 (2019).

Iwashita, Y.; Tongu, H.; Kuriyama, Y.; Hayano, H., Updates on the Inspection System for SRF Cavities, *Proc. 19th Int. Conf. on RF Superconductivity*, 1113-1115 (2019).

Katayama, R.; Hayano, H.; Kubo, T.; Saeki, T.; Antoine, C. Z.; Ito, H.; Ito, R.; Iwashita, Y.; Tongu, H.; Nagata, T., Evaluation of the Superconducting Characteristics of Multi-Layer Thin-Film Structures of NbN and SiO_2 on Pure Nb Substrate, *Proc. 19th Int. Conf. on RF Superconductivity*, 809-811 (2019).

Ito, H.; Antoine, C. Z.; Hayano, H.; Katayama, R.; Kubo, T.; Saeki, T.; Ito, R.; Nagata, T.; Iwashita, Y.; Tongu, H., Lower Critical Field Measurement of NbN Multilayer Thin Film Superconductor at KEK, *Proc. 19th Int. Conf. on RF Superconductivity*, 634-638 (2019).

Ito, R.; Nagata, T.; Hayano, H.; Katayama, R.; Kubo, T.; Saeki, T.; Ito, H.; Iwashita, Y., Nb₃Sn Thin Film Coating Method for Superconducting Multilayered Structure, *Proc. 19th Int. Conf. on RF Superconductivity*, 630-633 (2019).

Geng, R. L.; Fuwa, Y.; Iwashita, Y.; Hayano, H.; Ito, H.; Li, Z., Performance of First Prototype Multi-Cell Low-Surface-Field Shape Cavity, *Proc. 19th Int. Conf. on RF Superconductivity*, 222-226 (2019).

Saeki, T.; Hayano, H.; Inoue, H.; Katayama, R.; Kubo, T.; Hannon, F. E.; Rimmer, R. A.; Valente-Feliciano, A.-M.; Ito, H.; Iwashita, Y.; Tongu, H., Fabrication of 3.0-GHz Single-cell Cavities for Thin-film Study, *Proc. 19th Int. Conf. on RF Superconductivity*, 177-181 (2019).

Tongu, H.; Iwashita, Y.; Fuwa, Y.; Hayano, H.; Geng, R. L., High Density Mapping for Superconducting Cavities, *Proc. of IPAC2019*, 2860-2862 (2019).

Otani, M.; Futatsukawa, K.; Mibe, T.; Naito, F.; Hasegawa, K.; Ito, T.; Kitamura, R.; Kondo, Y.; Morishita, T.; Inuma, H.; Nakazawa, Y.; Iwashita, Y.; Saito, N., Disk and Washer Coupled Cavity Linac Design and Cold-Model for Muon Linac, *Proc. of IPAC2019*, 1924-1927 (2019).

Nakazawa, Y.; Inuma, H.; Iwata, Y.; Iwashita, Y.; Otani, M.; Kawamura, N.; Mibe, T.; Yamazaki, T.; Yoshida, M.; Kitamura, R.; Kondo, Y.; Hasegawa, K.; Morishita, T.; Saito, N.; Sue, Y.; Hayashizaki, N.; Yasuda, H., Development of Inter-Digital H-Mode Drift-Tube Linac Prototype with Alternative Phase Focusing for a Muon Linac in the J-PARC Muon G-2/EDM Experiment, *Proc. of IPAC2019*, 606-609 (2019).

— Laser Matter Interaction Science —

Mori, K.; Hashida, M.; Nagashima, T.; Li, D.; Teramoto, K.; Nakamiya, Y.; Inoue, S.; Sakabe, S., Increased Energy of THz Waves from a Cluster Plasma by Optimizing Laser Pulse Duration, *AIP Advances*, **9**, [015134-1]-[015134-4] (2019).

Nishiura, Y.; Inoue, S.; Kojima, S.; Teramoto, K.; Furukawa, Y.; Hashida, M.; Sakabe, S., Detection of Alpha Particles from ⁷Li(p, α)⁴He and ¹⁹F(p, α)¹⁶O Reactions Induced by Laser-accelerated Protons Using CR-39 with Potassium Hydroxide-ethanol-water Etching Solution, *Rev. Sci. Instrum.*, **90**, 83307 (2019).

Takenaka, K.; Tsukamoto, M.; Hashida, M.; Masuno, S.; Sakagami, H.; Kusaba, M.; Sakabe, S.; Inoue, S.; Furukawa, Y.; Asai, S., Ablation Suppression of a Titanium Surface Interacting with a Two-color Double-pulse Femtosecond Laser Beam, *Appl. Surf. Sci.*, **478**, 882-886 (2019).

— Electron Microscopy and Crystal Chemistry —

Yoshimoto, D.; Saito, H.; Hata, S.; Fujiyoshi, Y.; Kurata, H., Characterization of Nonradiative Bloch Modes in a Plasmonic Triangular Lattice by Electron Energy-Loss Spectroscopy, *ACS Photonics*, **5**, 4476-4483 (2018).

Matsumoto, K.; Sato, R.; Trinh, T. T.; Sakuma, N.; Shoji, T.; Haruta, M.; Kurata, H.; Teranishi, T., Formation of Strong L1₀-FePd/α-Fe Nanocomposite Magnets by Visualizing Efficient Exchange Coupling, *Nanoscale Adv.*, **1**, 2598-2605 (2019).

Ono, K.; Miyamoto, M.; Kurata, H.; Haruta, M.; Yatomi, A., Dynamic Behavior of Helium Bubbles at High Temperature in Si Studied by *in-situ* TEM, STEM-EELS and TDS, *J. Appl. Phys.*, **126**, [135104-1]-[135104-11] (2019).

Haruta, M.; Fujiyoshi, Y.; Nemoto, T.; Ishizuka, A.; Ishizuka, K.; Kurata, H., Extremely Low Count Detection for EELS Spectrum Imaging by Reducing CCD Read-out Noise, *Ultramicroscopy*, **207**, [112827-1]-[112827-6] (2019).

Kim, D.-H.; Haruta, M.; Ko, H.-W.; Go, G.; Park, H.-J.; Nishimura, T.; Kim, D.-Y.; Okuno, T.; Hirata, Y.; Futakawa, Y.; Yoshikawa, H.; Ham, W.; Kim, S.; Kurata, H.; Tsukamoto, A.; Shiota, Y.; Moriyama, T.; Choe, S.-B.; Lee, K.-J.; Ono, T., Bulk Dzyaloshinskii-Moriya Interaction in Amorphous Ferrimagnetic Alloys, *Nat. Mater.*, **18**, 685-690 (2019).

Shoji, S.; Ogawa, T.; Matsubara, S.; Tamiaki, H., Bioinspired Supramolecular Nanosheets of Zinc Chlorophyll Assemblies, *Sci. Rep.*, **9**, [14006-1]-[14006-8] (2019).

Lian, Z. C.; Sakamoto, M.; Kobayashi, Y.; Tamai, N.; Ma, J.; Sakurai, T.; Seki, S.; Nakagawa, T.; Lai, M. W.; Haruta, M.; Kurata, H.; Teranishi, T., Anomalous Photoinduced Hole Transport in Type I Core/Mesoporous-Shell Nanocrystals for Efficient Photocatalytic H₂ Evolution, *ACS Nano*, **13**, 8356-8363 (2019).

[Others]

Haruta, M.; Kurata, H., High Spatial Resolution Analysis of Elemental and Electronic Structure Analysis Using Electron Energy-loss Spectroscopy, *Ceramics Japan*, **54**, 77-80 (2019) (in Japanese).

Haruta, M.; Kurata, H., Local Elemental and Electronic Structure Analysis Using STEM-EELS, *J. Cryst. Soc. Jpn.*, **61**, 7-14 (2019) (in Japanese).

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Synthetic Organotransformation —

Kimura, M.; Miyashita, J.; Miyagawa, S.; Kawasaki, T.; Takaya, H.; Tokunaga, Y., Recognition Behavior of a Porphyrin Heterodimer Self-Assembled through an Amidinium-Carboxylate Salt Bridge, *Asian J. Org. Chem.*, **7**, 2087-2093 (2018).

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

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

Agata, R.; Kawamura, S.; Isozaki, K.; Nakamura, M., Iron-catalyzed Alkyl-Alkyl Negishi Coupling of Organoaluminum Reagents, *Chem. Lett.*, **48**, 238-241 (2019).

Aoki, Y.; O'Brien, H. M.; Kawasaki, H.; Takaya, H.; Nakamura, M., Ligand-Free Iron-Catalyzed C-F Amination of Diarylamines: A One-Pot Regioselective Synthesis of Diaryl Dihydrophenazines, *Org. Lett.*, **21**, 461-464 (2019).

Mihara, N.; Yamada, Y.; Takaya, H.; Kitagawa, Y.; Igawa, K.; Tomooka, K.; Fujii, H.; Tanaka, K., Site-Selective Supramolecular Complexation Activates Catalytic Ethane-Oxidation of μ -Nitrido-Bridged Iron Porphyrinoid Dimer, *Chem. Eur. J.*, **25**, 3369-3375 (2019).

Okuma, Y.; Tsukamoto, T.; Inagaki, T.; Miyagawa, S.; Kimura, M.; Naito, M.; Takaya, H.; Kawasaki, T.; Tokunaga, Y., Rotational Isomerism of the Amide Units in Rotaxanes Based on a Cyclic Tetraamide and Secondary Ammonium Ions, *Org. Chem. Front.*, **6**, 1002-1009 (2019).

Ouay, B. L.; Takaya, H.; Uemura, T., Controlling the Packing of Metal–Organic Layers by Inclusion of Polymer Guests, *J. Am. Chem. Soc.*, **141**, 14549-14553 (2019).

Iwamoto, T.; Hosokawa, A.; Nakamura, M., Endergonic Addition of N-methylamines to Aromatic Ketones Driven by Photochemical Offset of the Entropic Cost, *Chem. Commun.*, **55**, 11683-11686 (2019).

Kondo, S.; Masuda, J.; Komiyama, T.; Yasuda, N.; Takaya, H.; Yamanaka, M., Amphoteric Homotropic Allosteric Association between a Hexakis-Urea Receptor and Dihydrogen Phosphate, *Chem. Eur. J.*, **25**, 16201-16206 (2019).

[Others]

Takaya, H.; Isozaki, K.; Yokoi, T.; Ogata, K.; Shanoh, T.; Yasuda, N.; Iwamoto, T.; Nakamura, M., Metalated Amino Acids and Peptides: A Key Functional Platform for Applications to Controlled Metal Array Fabrication and Supramolecular Catalysts, *Journal of Synthetic Organic Chemistry Japan*, **76**, 1010-1023 (2019) (in Japanese).

— Advanced Solid State Chemistry —

Kan, D.; Sugano, S.; Kosugi, Y.; Kobayashi, K.; Uebayashi, N.; Koganezawa, T.; Shimakawa, Y., Selective Growth of α -Fe₂O₃, γ -Fe₂O₃ and Fe₃O₄ at Low-temperatures and Under Ambient Pressure, *Jpn. J. Appl. Phys.*, **58**, 95504 (2019).

de Irujo-Labalde, X. M.; Goto, M.; Urones-Garrote, E.; Amador, U.; Ritter, C.; Amano Patino, M. E.; Koedtrud, A.; Tan, Z.; Shimakawa, Y.; Garcia-Martin, S., Multiferroism Induced by Spontaneous Structural Ordering in Antiferromagnetic Iron Perovskites, *Chem. Mater.*, **31**, 5993-6000 (2019).

Kan, D.; Shimakawa, Y., Strain Effect on Thermoelectric Properties of SrRuO₃ Epitaxial Thin Films, *Appl. Phys. Lett.*, **115**, 22403 (2019).

Kobayashi, K.; Kan, D.; Matsumoto, S.; Mizumaki, M.; Shimakawa, Y., Orbital Magnetic Moments in Strained SrRuO₃ Thin Films, *J. Phys. Soc. Jpn.*, **88**, 84708 (2019).

Heo, Y.; Kan, D.; Anada, M.; Wakabayashi, Y.; Tajiri, H.; Shimakawa, Y., Correlations Between Oxygen Octahedral Distortions and Magnetic and Transport Properties in Strained La_{0.5}Sr_{0.5}CoO₃ Thin Films, *Phys. Rev. B*, **99**, 174420 (2019).

Chin, Y.-Y.; Lin, H.-J.; Hu, Z.; Shimakawa, Y.; Chen, C.-T., Direct Observation of the Partial Valence Transition of Cu in the A-site Ordered LaCu₃Fe₄O_{12.8} by Soft X-ray Absorption Spectroscopy, *Phys. B: Cond. Matter.*, **568**, 92-95 (2019).

Chen, W.-T.; Ablitt, C.; Bristowe, N. C.; Mostofi, A. A.; Saito, T.; Shimakawa, Y.; Senn, M. S., Negative Thermal Expansion in High Pressure Layered Perovskite Ca₂GeO₄, *Chem. Comm.*, **55**, 2984-2987 (2019).

Denis Romero, F.; Shimakawa, Y., Charge Transitions in Perovskite Oxides Containing Unusually High-valent Fe, *Chem. Comm.*, **55**, 3690-3696 (2019).

Koedtrud, A.; Goto, M.; Amano Patino, M.; Tan, Z.; Guo, H.; Nakamura, T.; Handa, T.; Chen, W.-T.; Chuang, Y.-C.; Sheu, H.-S.; Saito, T.; Kan, D.; Kanemitsu, Y.; Wakamiya, A.; Shimakawa, Y., Structure-property Relations in Ag-Bi-I Compounds: Potential Pb-free Absorbers in Solar Cells, *J. Mater. Chem. A*, **7**, 5583-5588 (2019).

— Nanophotonics —

Umanodan, T.; Kaneshima, K.; Takeuchi, K.; Ishii, N.; Itatani, J.; Hirori, H.; Sanari, Y.; Tanaka, K.; Kanemitsu, Y.; Ishikawa, T.; Koshihara, S.; Horiuchi, S.; Okimoto, Y., Ultrafast Control of Ferroelectricity with Dynamical Repositioning of Protons in a Supramolecular Cocrystal Studied by Femtosecond Nonlinear Spectroscopy, *J. Phys. Soc. Jpn.*, **88**, 013705 (2019).

Zhu, L.; Lee, K.-H.; Yamaguchi, M.; Akiyama, H.; Kanemitsu, Y.; Araki, K.; Kojima, N., Analysis of Nonradiative Recombination in Quantum Dot Solar Cells and Materials, *Prog. Photovolt. Res. Appl.*, **27**, 971-977 (2019).

Koedtrud, A.; Goto, M.; Amano Patino, M.; Tan, Z.; Guo, H.; Nakamura, T.; Handa, T.; Chen, W.-T.; Chuang, Y.-C.; Sheu, H.-S.; Saito, T.; Kan, D.; Kanemitsu, Y.; Wakamiya, A.; Shimakawa, Y., Structure-property Relations in Ag-Bi-I Compounds: Potential Pb-free Absorbers in Solar Cells, *J. Mater. Chem. A*, **7**, 5583-5588 (2019).

Yamada, T.; Aharen, T.; Kanemitsu, Y., Up-converted Photoluminescence from CH₃NH₃PbI₃ Perovskite Semiconductors: Implications for Laser Cooling, *Phys. Rev. Mater.*, **3**, 024601 (2019).

Hirori, H.; Xia, P.; Shinohara, Y.; Otobe, T.; Sanari, Y.; Tahara, H.; Ishii, N.; Itatani, J.; Ishikawa, K. L.; Aharen, T.; Ozaki, M.; Wakamiya, A.; Kanemitsu, Y., High-order Harmonic Generation from Hybrid Organic–inorganic Perovskite Thin Films, *APL Mater.*, **7**, 041107 (2019).

Yamada, Y.; Hoyano, M.; Oto, K.; Kanemitsu, Y., Effects of Impurity Doping on Photoluminescence Properties of APbX₃ Lead Halide Perovskites, *Phys. Status Solidi B*, **256**, 1800545 (2019).

Yoshida, S.; Hirori, H.; Tachizaki, T.; Yoshioka, K.; Arashida, Y.; Wang, Z.-H.; Sanari, Y.; Takeuchi, O.; Kanemitsu, Y.; Shigekawa, H., Subcycle Transient Scanning Tunneling Spectroscopy with Visualization of Enhanced Terahertz Near Field, *ACS Photonics*, **6**, 1356-1364 (2019).

Tahara, H.; Kanemitsu, Y., Coherent Spectroscopy of Multiple Excitons in Colloidal Nanocrystal Quantum Dots, *ChemNanoMat*, **5**, 977-984 (2019).

Sakamoto, M.; Hyeon-Deuk, K.; Eguchi, D.; Chang, I.-Y.; Tanaka, D.; Tahara, H.; Furube, A.; Minagawa, Y.; Majima, Y.; Kanemitsu, Y.; Teranishi, T., Impact of Orbital Hybridization at Molecule–Metal Interface on Carrier Dynamics, *J. Phys. Chem. C*, **123**, 25877-25882 (2019).

Handa, T.; Tahara, H.; Aharen, T.; Kanemitsu, Y., Large Negative Thermo-optic Coefficients of a Lead Halide Perovskite, *Sci. Adv.*, **5**, [eaax0786-1]-[eaax0786-8] (2019).

Nakahara, S.; Ohara, K.; Tahara, H.; Yumoto, G.; Kawawaki, T.; Saruyama, M.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Ionization and Neutralization Dynamics of CsPbBr₃ Perovskite Nanocrystals Revealed by Double-Pump Transient Absorption Spectroscopy, *J. Phys. Chem. Lett.*, **10**, 4731-4736 (2019).

Kojima, K.; Ikemura, K.; Matsumori, K.; Yamada, Y.; Kanemitsu, Y.; Chichibu, S. F., Internal Quantum Efficiency of Radiation in a Bulk CH₃NH₃PbBr₃ Perovskite Crystal Quantified by Using the Omnidirectional Photoluminescence Spectroscopy, *APL Mater.*, **7**, 71116 (2019).

Handa, T.; Wakamiya, A.; Kanemitsu, Y., Photophysics of Lead-free Tin halide Perovskite Films and Solar Cells, *APL Mater.*, **7**, 80903 (2019).

Kanemitsu, Y., Trion Dynamics in Lead Halide Perovskite Nanocrystals, *J. Chem. Phys.*, **151**, 170902 (2019).

Ohara, K.; Yamada, T.; Tahara, H.; Aharen, T.; Hirori, H.; Suzuura, H.; Kanemitsu, Y., Excitonic Enhancement of Optical Nonlinearities in Perovskite CH₃NH₃PbCl₃ Single Crystals, *Phys. Rev. Materials*, **3**, 111601 (2019).

BIOINFORMATICS CENTER

— Chemical Life Science —

Aramaki, T.; Blanc-Mathieu, R.; Endo, H.; Ohkubo, K.; Kanehisa, M.; Goto, S.; Ogata, H., KofamKOALA: KEGG Ortholog Assignment Based on Profile HMM and Adaptive Score Threshold, *Bioinformatics*, **btz859**, doi10.1093/bioinformatics/btz859 (2019).

Ibarbalz, F. M.; Henry, N.; Brandão, M. C.; Martini, S.; Busseni, G.; Byrne, H.; Coelho, L. P.; Endo, H.; Gasol, J. M.; Gregory, A. C.; Mahé, F.; Rigonato, J.; Royo-Llonch, M.; Salazar, G.; Sanz-Sáez, I.; Scalco, E.; Soviadan, D.; Zayed, A. A.; Zingone, A.; Labadie, K.; Ferland, J.; Marec, C.; Kandels, S.; Picheral, M.; Dimier, C.; Poulain, J.; Pisarev, S.; Carmichael, M.; Pesant, S.; Tara Oceans Coordinators; Babin, M.; Boss, E.; Iudicone, D.; Jaillon, O.; Acinas, S. G.; Ogata, H.; Pelletier, E.; Stemmann, L.; Sullivan, M. B.; Sunagawa, S.; Bopp, L.; de Vargas, C.; Karp-Boss, L.; Wincker, P.; Lombard, F.; Bowler, C.; Zinger, L., Global Trends in Marine Plankton Diversity Across Kingdoms of Life, *Cell*, **179**, 1084-1097 (2019).

Salazar, G.; Paoli, L.; Alberti, A.; Huerta-Cepas, J.; Ruscheweyh, H.-J.; Cuenca, M.; Field, C. M.; Coelho, L. P.; Cruaud, C.; Engelen, S.; Gregory, A. C.; Labadie, K.; Marec, C.; Pelletier, E.; Royo-Llonch, M.; Roux, S.; Sánchez, P.; Uehara, H.; Zayed, A. A.; Zeller, G.; Carmichael, M.; Dimier, C.; Ferland, J.; Kandels, S.; Picheral, M.; Pisarev, S.; Poulain, J.; Tara Oceans Coordinators; Acinas, S. G.; Babin, M.; Bork, P.; Bowler, C.; de Vargas, C.; Guidi, L.; Hingamp, P.; Iudicone, D.; Karp-Boss, L.; Karsenti, E.; Ogata, H.; Pesant, S.; Speich, S.; Sullivan, M. B.; Wincker, P.; Sunagawa, S., Gene Expression Changes and Community Turnover Differentially Shape the Global Ocean Metatranscriptome, *Cell*, **179**, 1068-1083 (2019).

Inoue, M.; Nakamoto, I.; Omae, K.; Oguro, T.; Ogata, H.; Yoshida, T.; Sako, Y., Structural and Phylogenetic Diversity of Anaerobic Carbon-monoxide Dehydrogenases, *Front. Microbiol.*, **9**, 3353 (2019).

Roux, S.; Adriaenssens, E. M.; Dutilh, B. E.; Koonin, E. V.; Kropinski, A. M.; Krupovic, M.; Kuhn, J. H.; Lavigne, R.; Brister, J. R.; Varsani, A.; Amid, C.; Aziz, R. K.; Bordenstein, S. R.; Bork, P.; Breitbart, M.; Cochrane, G. R.; Daly, R. A.; Desnues, C.; Duhaime, M. B.; Emerson, J. B.; Enault, F.; Fuhrman, J. A.; Hingamp, P.; Hugenholtz, P.; Hurwitz, B. L.; Ivanova, N. N.; Labonte, J. M.; Lee, K.-B.; Malmstrom, R. R.; Martinez-Garcia, M.; Mizrachi, I.; Ogata, H.; Paez-Espino, D.; Petit, M.-A.; Putonti, C.; Rattei, T.; Reyes, A.; Rodriguez-Valera, F.; Rosario, K.; Schriml, L.; Schulz, F.; Steward, G. F.; Sullivan, M. B.; Sunagawa, S.; Suttle, C. A.; Temperton, B.; Tringe, S. G.; Vega Thurber, R.; Webster, N. S.; Whiteson, K. L.; Wilhelm, S. W.; Wommack, K. E.; Woyke, T.; Wrighton, K.; Yilmaz, P.; Yoshida, T.; Young, M. J.; Yutin, N.; Allen, L. Z.; Kyrpides, N. C.; Eloe-Fadrosh, E. A., Minimum Information about Uncultivated Virus Genomes (MIUViG): a Community Consensus on Standards and Best Practices for Describing Genome Sequences from Uncultivated Viruses, *Nat. Biotechnol.*, **37**, 29-37 (2019).

Caputi, L.; Carradec, Q.; Eveillard, D.; Kirilovsky, A.; Pelletier, E.; Karlusich, J. J. P.; Vieira, F. R. J.; Villar, E.; Chaffron, S.; Malviya, S.; Scalco, E.; Acinas, S. G.; Alberti, A.; Aury, J.-M.; Benoiston, A.-S.; Bertrand, A.; Biard, T.; Bittner, L.; Boccara, M.; Brum, J. R.; Brunet, C.; Busseni, G.; Carratala, A.; Claustre, H.; Coelho, L. P.; Colin, S.; D'Aniello, S.; Da Silva, C.; Del Core, M.; Dore, H.; Gasparini, S.; Kokoszka, F.; Jamet, J.-L.; Lejeune, C.; Lepoivre, C.; Lescot, M.; Lima-Mendez, G.; Lombard, F.; Lukes, J.; Maillet, N.; Madoui, M.-A.; Martinez, E.; Mazzocchi, M. G.; Neou, M. B.; Paz-Yepes, J.; Poulain, J.; Ramondenc, S.; Romagnan, J.-B.; Roux, S.; Manta, D. S.; Sanges, R.; Speich, S.; Sprovieri, M.; Sunagawa, S.; Taillander, V.; Tanaka, A.; Tirichine, L.; Trottier, C.; Uitz, J.; Veluchamy, A.; Vesela, J.; Vincent, F.; Yau, S.; Kandels-Lewis, S.; Searson, S.; Dimier, C.; Picheral, M.; Tara Oceans Coordinators; Bork, P.; Boss, E.; de Vargas, C.; Follows, M. J.; Grimsley, N.; Guidi, L.; Hingamp, P.; Karsenti, E.; Sordino, P.; Stemmann, L.; Sullivan, M. B.; Tagliabue, A.; Zingone, A.; Garczarek, L.; d'Ortenzio, F.; Testor, P.; Not, F.; Ribera d'Alcala, M.; Wincker, P.; Bowler, C.; Iudicone, D., Community-level Responses to Iron Availability in Open Ocean Planktonic Ecosystems, *Global Biogeochem. Cycles*, **33**, 391-419 (2019).

Gregory, A. C.; Zayed, A. A.; Conceicao-Neto, N.; Temperton, B.; Bolduc, B.; Alberti, A.; Ardyna, M.; Arkhipova, K.; Carmichael, M.; Cruaud, C.; Dimier, C.; Dominguez-Huerta, G.; Ferland, J.; Kandels, S.; Liu, Y.; Marec, C.; Pesant, S.; Picheral, M.; Pisarev, S.; Poulain, J.; Tremblay, J. E.; Vik, D.; Tara Oceans Coordinators; Babin, M.; Bowler, C.; Culley, A. I.; de Vargas, C.; Dutilh, B. E.; Iudicone, D.; Karp-Boss, L.; Roux, S.; Sunagawa, S.; Wincker, P.; Sullivan, M. B., Marine DNA Viral Macro- and Microdiversity from Pole to Pole, *Cell*, **177**, 1109-1123 (2019).

Aoki, K.; Hagiwara, R.; Akashi, M.; Murata, K.; Ogata, H.; Takemura, M., Fifteen Marseilleviruses Newly Isolated from Three Water Samples in Japan Reveal a Local Diversity of Marseilleviridae, *Front. Microbiol.*, **24**, 1152 (2019).

Castillo, Y. M.; Mangot, J.-F.; Benites, F.; Logares, R.; Kuronishi, M.; Ogata, H.; Jaillon, O.; Massana, R.; Sebastián, M.; Vaqué, D., Assessing the Viral Content of Uncultured Picoeukaryotes in the Global-ocean by Single Cell Genomics, *Mol Ecol.*, **28**, 4272-4289 (2019).

Li, Y.; Endo, H.; Gotoh, Y.; Watai, H.; Ogata, N.; Blanc-Mathieu, R.; Yoshida, T.; Ogata, H., The Earth Is Small for "Leviathans": Long Distance Dispersal of Giant Viruses Across Aquatic Environments, *Microbes Environ.*, **34**, 334-339 (2019).

- Okazaki, Y.; Nishimura, Y.; Yoshida, T.; Ogata, H.; Nakano, S., Genome-resolved Viral and Cellular Metagenomes Revealed Potential Key Virus-host Interactions in a Deep Freshwater Lake, *Environ. Microbiol.*, **21**, 4740-4754(2019).
- Yoshikawa, G.; Blanc-Mathieu, R.; Song, C.; Kayama, Y.; Mochizuki, T.; Murata, K.; Ogata, H.; Takemura, M., Medusavirus, a Novel Large DNA Virus Discovered from Hot Spring Water, *J. Virol.*, **93**, e02130-18(2019).
- Xia, X.; Cheung, S.; Endo, H.; Suzuki, K.; Liu, H., Latitudinal and Vertical Variation of Synechococcus Assemblage Composition Along 170° W Transect From the South Pacific to the Arctic Ocean, *Microb. Ecol.*, **77**, 333-342 (2019).
- Yan, D.; Endo, H.; Suzuki, K., Increased Temperature Benefits Growth and Photosynthetic Performance of the Sea Ice Diatom *Nitzschia cf. Neglecta* (Bacillariophyceae) Isolated from Saroma Lagoon, Hokkaido, Japan, *J. Phycol.*, **55**, 700-713 (2019).
- Endo, H.; Suzuki, K., Spatial Variations in Community Structure of Haptophytes Across the Kuroshio front in the Tokara Strait, *Nagai, T., Saito, H., Suzuki, K., Takahashi, M.(eds.), Kuroshio Current: Physical, Biogeochemical and Ecosystem Dynamics, AGU Geophysical Monograph Series, AGU-Wiley*, 207-221 (2019).
- **Mathematical Bioinformatics** —
- Koyano, H.; Hayashida, M.; Akutsu, T., Optimal String Clustering Based on a Laplace-like Mixture and EM Algorithm on a Set of Strings, *J. Comput. Syst. Sci.*, **106**, 94-128 (2019).
- Itami-Matsumoto, S.; Hayakawa, M.; Uchida-Kobayashi, S.; Enomoto, M.; Tamori, A.; Mizuno, K.; Toyoda, H.; Tamura, T.; Akutsu, T.; Ochiya, T.; Kawada, N.; Murakami, Y., Circulating Exosomal miRNA Profiles Predict the Occurrence and Recurrence of Hepatocellular Carcinoma in Patients with Direct-Acting Antiviral-Induced Sustained Viral Response, *Biomedicines*, **7**, [87-1]-[87-14] (2019).
- Wang, J.; Yang, B.; An, Y.; Marquez-Lago, T.; Leier, A.; Wilksch, J.; Hong, Q.; Zhang, Y.; Hayashida, M.; Akutsu, T.; Webb, G. I.; Strugnell, R. A.; Song, J.; Lithgow, T., Systematic Analysis and Prediction of Type IV Secreted Effector Proteins by Machine Learning Approaches, *Brief. Bioinform.*, **20**, 931-951 (2019).
- Song, J.; Wang, Y.; Li, F.; Akutsu, T.; Rawlings, N. D.; Webb, G. I.; Chou, K. C., iProt-Sub: a Comprehensive Package for Accurately Mapping and Predicting Protease-specific Substrates and Cleavage Sites, *Brief. Bioinform.*, **20**, 638-658 (2019).
- Nishiyama, Y.; Shurbevski, A.; Nagamochi, H.; Akutsu, T., Resource Cut, a New Bounding Procedure to Algorithms for Enumerating Tree-Like Chemical Graphs, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **16**, 77-90 (2019).
- Nacher, J. C.; Ishitsuka, M.; Miyazaki, S.; Akutsu, T., Finding and Analysing the Minimum Set of Driver Nodes Required to Control Multilayer Networks, *Sci. Rep.*, **9**, [576-1]-[576-12] (2019).
- Hou, W.; Ruan, P.; Ching, W. K.; Akutsu, T., On the Number of Driver Nodes for Controlling a Boolean Network when the Targets are Restricted to Attractors, *J. Theor. Biol.*, **463**, 1-11 (2019).
- Ravindran, V.; Nacher, J. C.; Akutsu, T.; Ishitsuka, M.; Osadccenco, A.; Sunitha, V.; Bagler, G.; Schwartz, J. M.; Robertson, D. L., Network Controllability Analysis of Intracellular Signalling Reveals Viruses are Actively Controlling Molecular Systems, *Sci. Rep.*, **9**, [2066-1]-[2066-11] (2019).
- Marini, S.; Vitali, F.; Rampazzi, S.; Demartini, A.; Akutsu, T., Protease Target Prediction via Matrix Factorization, *Bioinformatics*, **35**, 923-929 (2019).
- Wang, J.; Li, J.; Yang, B.; Xie, R.; Marquez-Lago, T. T.; Leier, A.; Hayashida, M.; Akutsu, T.; Zhang, Y.; Chou, K. C.; Selkrig, J.; Zhou, T.; Song, J.; Lithgow, T., Bastion3: a Two-layer Ensemble Predictor of Type III Secreted Effectors, *Bioinformatics*, **35**, 2017-2028 (2019).
- Matsubara, T.; Ochiai, T.; Hayashida, M.; Akutsu, T.; Nacher, J. C., Convolutional Neural Network Approach to Lung Cancer Classification Integrating Protein Interaction Network and Gene Expression Profiles, *J. Bioinform. Comput. Biol.*, **17**, [1940007-1]-[1940007-11] (2019).
- Lin, C. Y.; Ruan, P.; Li, R.; Yang, J. M.; See, S.; Song, J.; Akutsu, T., Deep Learning with Evolutionary and Genomic Profiles for Identifying Cancer Subtypes, *J. Bioinform. Comput. Biol.*, **17**, [1940005-1]-[1940005-15] (2019).
- Schwartz, J. M.; Otokuni, H.; Akutsu, T.; Nacher, J. C., Probabilistic Controllability Approach to Metabolic Fluxes in Normal and Cancer Tissues, *Nat. Commun.*, **10**, [2725-1]-[2725-9] (2019).
- Akutsu, T.; Melkman, A. A., Identification of the Structure of a Probabilistic Boolean Network from Samples Including Frequencies of Outcomes, *IEEE Transactions on Neural Networks and Learning Systems*, **30**, 2383-2396 (2019).
- Akutsu, T.; Nagamochi, H., A mixed Integer Linear Programming Formulation to Artificial Neural Networks, *Proc. 2nd International Conference on Information Science and System*, 215-220 (2019).
- Mori, T.; Takaoka, H.; Yamane, J.; Alev, C.; Fujibuchi, W., Novel Computational Model of Gastrula Morphogenesis to Identify Spatial Discriminator Genes by Self-organizing Map (SOM) Clustering, *Sci. Rep.*, **9**, 12597 (2019).
- Bao, Y.; Marini, S.; Tamura, T.; Kamada, M.; Maegawa, S.; Hosokawa, H.; Song, J.; Akutsu, T., Toward More Accurate Prediction of Caspase Cleavage Sites: A Comprehensive Review of Current Methods, Tools and Features, *Brief. Bioinform.*, **20**, 1669-1684 (2019).
- Nacher, J. C.; Akutsu, T., Controllability Methods for Identifying Associations Between Critical Control ncRNAs and Human Diseases, *Methods Mol. Biol.*, **1912**, 289-300 (2019).
- Zhang, Y.; Xie, R.; Wang, J.; Leier, A.; Marquez-Lago, T. T.; Akutsu, T.; Webb, G. I.; Chou, K. C.; Song, J., Computational Analysis and Prediction of Lysine Malonylation Sites by Exploiting Informative Features in an Integrative Machine-Learning Framework, *Brief. Bioinform.*, **20**, 2185-2199 (2019).
- Chen, Z.; Liu, X.; Li, F.; Li, C.; Marquez-Lago, T. T.; Leier, A.; Akutsu, T.; Webb, G. I.; Xu, D.; Smith, A. I.; Li, L.; Chou, K. C.; Song, J., Large-Scale Comparative Assessment of Computational Predictors for Lysine Post-Translational Modification Sites, *Brief. Bioinform.*, **20**, 2267-2290 (2019).

Li, F.; Wang, Y.; Li, C.; Marquez-Lago, T. T.; Leier, A.; Rawlings, N. D.; Haffari, G.; Revote, J.; Akutsu, T.; Chou, K. C.; Purcell, A. W.; Pike, R. N.; Webb, G. I.; Smith, A. I.; Lithgow, A.; Daly, R. J.; Whisstock, J. C.; Song, J., Twenty Years of Bioinformatics Research for Protease-Specific Substrate and Cleavage Site Prediction: A Comprehensive Revisit and Benchmarking of Existing Methods, *Brief. Bioinform.*, **20**, 2150-2166 (2019).

[Others]

Akutsu, T., Analysis of Boolean Networks and Boolean Models of Metabolic Networks, *Application of Omics, AI and Blockchain in Bioinformatics Research (J. J-P. Tsai and K-L. Ng, eds.)*, *World Scientific*, 141-158 (2019).

— Bio-knowledge Engineering —

duVerle, D. A.; Mamitsuka, H., CalCleaveMKL: a Tool for Calpain Cleavage Prediction, *Methods Mol. Biol. (Clifton, N.J.)*, **1915**, 121-147 (2019).

Eid, A. M.; Mamitsuka, H.; Wicker, N., A Metropolis-Hastings Sampling of Subtrees in Graphs, *Austrian Journal of Statistics*, **48**, 17-33 (2019).

Wicker, N.; Nguyen, C. H.; Mamitsuka, H., A p-Laplacian Random Walk: Application to Video Games, *Austrian Journal of Statistics*, **48**, 11-16 (2019).

You, R.; Yao, S.; Xiong, Y.; Huang, X.; Sun, F.; Mamitsuka, H.; Zhu, S., NetGO: Improving Large-scale Protein Function Prediction with Massive Network Information, *Nucleic Acids Res.*, **47**, W379-W387 (2019).

Nguyen, D. H.; Nguyen, C. H.; Mamitsuka, H., ADAPTIVE: leArning DATA-dePendenT, ConcIse Molecular VEctors for Fast, Accurate Metabolite Identification from Tandem Mass Spectra, *Bioinformatics (Proceedings of the 27th International Conference on Intelligent Systems for Molecular Biology (ISMB/ECCB 2019))*, **35**, i164-i172 (2019).

Sun, L.; Nguyen, C. H.; Mamitsuka, H., Multiplicative Sparse Feature Decomposition for Efficient Multi-View Multi-Task Learning, *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence*, 3506-3512 (2019).

Sun, L.; Nguyen, C. H.; Mamitsuka, H., Fast and Robust Multi-View Multi-Task Learning via Group Sparsity, *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence*, 3499-3505 (2019).

Gillberg, J.; Marttinen, P.; Mamitsuka, H.; Kaski, S., Modelling G×E with Historical Weather Information Improves Genomic Prediction in New Environments, *Bioinformatics*, **35**, 4045-4052 (2019).

Seki, H.; Nguyen, C. H.; Huynh, V.-N.; Inuiguchi, M., Integrated Uncertainty in Knowledge Modelling and Decision Making, *LNCS*, **11471**, (2019).

[Others]

Zhou, S.; Chen, Y.-P. P.; Mamitsuka, H., Editorial, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **16**, 350 (2019).

Mamitsuka, H., Machine Learning for Marketing, *Global Data Science Publishing, Kyoto* (2019).

HAKUBI PROJECT

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

Denis Romero, F.; Shimakawa, Y., Charge Transitions in Perovskite Oxides Containing Unusually High-valent Fe, *Chem. Comm.*, **55**, 3690-3696 (2019).

INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]

La Trobe University, Department of Computer Science and Information Technology

Monash University, Biomedicine Discovery Institute

RMIT University, School of Engineering

University of Sydney, Sydney Medical School

[Canada]

University of Toronto, Department of Cell & Systems Biology

[China, P.R.]

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

Fudan University, Key Laboratory of Computational Neuroscience and Brain-Inspired Intelligence

Fudan University, School of Computer Science and Shanghai Key Lab of Intelligent Information Processing

Fudan University, School of Pharmacy

Peking University, College of Life Science

Peking University, Department of Chemical Biology

Shanghai Jiao Tong University, Department of Bioinformatics and Biostatistics

The Chinese Academy of Sciences, Institute of Botany

The University of Hong Kong, Department of Mathematics

Tsinghua University, Department of Chemistry

[Finland]

Aalto University, Department of Computer Science

Helsinki Institute for Information Technology HIIT

Luke Natural Resources Institute Finland, Production Systems

University of Helsinki, Institute of Biotechnology and Viikki Plant Science Centre

[France]

Centre National de la Recherche Scientifique

Ecole Centrale de Nantes, Institut de Recherche en Génie Civil et Mécanique (GeM)

Institute Charles Gerhardt Montpellier

Université de Lille, Département de Mathématiques

[Germany]

European Molecular Biology Laboratory

Helmholtz Center Munich, Plant Genome and Systems Biology

University of Bonn, Institute for Inorganic Chemistry

University of Hohenheim, Institute of Plant Physiology and Biochemistry

[Greece]

University of Crete, FORTH-IESL and Department of Materials Science and Technology

[Ireland]

National Institute for Bioprocessing Research and Training, Characterisation and Comparability Laboratory

[Israel]

Ben-Gurion University of the Negev, Department of Computer Science

[Italy]

University of Naples "Federico II", Department of Chemical Sciences

[Kenya]

Biosciences Eastern and Central Africa-International Livestock Research Institute (BecA-ILRI) Hub

[Korea, R.]

Institute for Basic Science, Center for Genomic Integrity

Korea Institute of Science and Technology, Center for Spintronics

Korea Research Institute of Bioscience and Biotechnology, Korean Bioinformation Center

Korea University, Department of Materials Science & Engineering

Korea University, KU-KIST Graduate School of Converging Science and Technology

Seoul National University, Department of Agricultural Biotechnology

Seoul National University, Department of Physics

Seoul National University, Institute of Applied Physics

Seoul National University, Interdisciplinary Program in Agricultural Genomics

Seoul National University, Plant Genomics and Breeding Institute

Sungkyunkwan University, School of Chemical Engineering

University of Ulsan, Department of Physics

[Norway]

University of Bergen, Department of Biology

[Spain]

Universidad Complutense, Departamento de Química Inorgánica,
Facultad de C.C. Químicas

University of Castilla-La Mancha, Physical Chemistry

[Switzerland]

Department of Earth Sciences, Institute of Geochemistry and Petrology

[Taiwan]

National Chiao Tung University, Institute of Bioinformatics and Systems Biology

National Taiwan University, Center for Condensed Matter Sciences

[U.K.]

University of Bristol, School of Chemistry

University of Manchester, School of Biological Sciences

[U.S.A.]

Baylor College of Medicine, Department of Biochemistry & Molecular Biology

California State University, Department of Biological Science

DOE Joint Genome Institute

Drexel University, Chemical and Biological Engineering

Joint BioEnergy Institute

Lawrence Berkeley National Laboratory, Environmental Genomics and Systems Biology Division

Middle Tennessee State University, Department of Chemistry

Pennsylvania State University, Department of Biology

Salk Institute for Biological Studies

Sandia National Laboratories

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

United States Department of Agriculture

University of California, Riverside, Department of Botany and Plant Sciences

University of California, San Diego, Section of Cell and Developmental Biology

University of Georgia, Department of Genetics

University of Pennsylvania, Department of Materials Science

University of South Florida, College of Marine Science and School of Geosciences

University of Southern California, Department of Earth Sciences

University of Southern California, Quantitative and Computational Biology, Department of Biological Sciences

University of Virginia, Department of Biology

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

SELECTED GRANTS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Tokitoh, N.
Synthesis and Properties of Group 14 Analogues of Phenyl Anion
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2019

Mizuhata, Y.
Creation of Novel Conjugated Molecules with Heavy Phenyl Anions as Building Blocks
Grant-in-Aid for Scientific Research (B)
1 April 2018–31 March 2021

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

Tokitoh, N.
Synthesis of Hexasilabenzene
Grant-in-Aid for Challenging Research (Pioneering)
28 June 2019–31 March 2022

Yukimoto, M.
Creation of Tautomerizable Heavy Group 14–16 Double Bonded Compounds
Grant-in-Aid for Early-Career Scientists
1 April 2018–31 March 2022

— Structural Organic Chemistry —

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

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

Hashikawa, Y.
Nanostructure Control and Creation of Novel Functions on Three-Dimensional π -Conjugated Molecules Using Weak Interactions
Grant-in-Aid for Early-Career Scientists
1 April 2018–31 March 2020

— Synthetic Organic Chemistry —

Kawabata, T.
Glycosylation of Unprotected Sugars and Its Application to Short-Step Total Synthesis
The 6th Research Grant from Kobayashi Foundation
14 February 2018–20 February 2021

Ueda, Y.
Silyl-Group-Directed Site-Selective C-H Functionalization
Grant-in-Aid for Early-Career Scientists
1 April 2018–31 March 2020

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

Morisaki, K.
Site-Selective C-H Functionalization
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2022

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 (Accelerated Innovation Research Initiative Turning Top Science and Ideas into High-Impact Values), JST
1 September 2015–31 March 2020

— 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

— Nanospintronics —

Ono, T.
Spin-orbitronics and Device Application
New Research Projects under Specially Promoted Research
1 April 2015–31 March 2020

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

DIVISION OF BIOCHEMISTRY
— **Biofunctional Design-Chemistry** —

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

Futaki, S.
Development of New Methods for Cytosolic Delivery of Bioactive Proteins
Grant-in-Aid for Scientific Research (A)
1 April 2018–31 March 2020

Imanishi, M.
Control of RNA Modification for Antivirus Activities
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2021

Kawano, K.
Elucidation of the Mechanism at the Influx Point Occurrence of Membrane Penetrating Peptide Using Artificial Lipid Raft
Grant-in-Aid for Early-Career Scientists
1 April 2018–31 March 2020

— **Chemistry of Molecular Biocatalysts** —

Yamaguchi, S.
Molecular Mechanisms for the Timing of the Production of Stem Cells in Plants
Grant-in-Aid for Scientific Research on Innovative Area “Principles of Pluripotent Stem Cells Underlying Plant Vitality”
1 April 2018–31 March 2019

— **Molecular Biology** —

Aoyama, T.
Plant Epidermal Cell Differentiation Regulated by the Transcription Factor GL2
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2020

— **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 Molecules
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

Uesugi, M.
Exploration of Self-Assembling Bioactive Small Molecules
Grant-in-Aid for Scientific Research (A)
1 April 2019–31 March 2022

Uesugi, M.
Asian Chemical Biology Initiative
Core-to-Core Program, JSPS
1 April 2016–31 March 2019

Uesugi, M.
Asian Chemical Biology Initiative
Core-to-Core Program, JSPS
1 April 2019–31 March 2022

DIVISION OF ENVIRONMENTAL CHEMISTRY
— **Molecular Materials Chemistry** —

Kaji, H.
Construction of Basic Science of Organic Devices by Precise Structural Analysis and Theoretical Chemical Calculation
Grant-in-Aid for Scientific Research (A)
1 April 2017–31 March 2020

— **Hydrospheric Environment Analytical Chemistry** —

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

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 Early-Career Scientists
1 April 2018–31 March 2020

Zheng, L.
Stoichiometry and Sectional Distributions of Bioactive Trace Metals in the North Pacific Ocean and the Southern Ocean
Mitsumasa Ito Memorial Research Grant, Research Institute for Ocean Chemistry Foundation
1 April 2019–31 March 2020

Zheng, L.
Sectional Distribution of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, Pb in the Southern North Pacific Ocean
The Sasakawa Scientific Research Grant, The Japan Science Society
1 April 2019–31 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) “Analytical Chemistry”
1 April 2015–31 March 2020

Shimoaka, T.
Molecular Interaction Analysis for Understanding Perfluoroalkyl Compound-Specific Properties
Grant-in-Aid for Young Scientists (B) “Analytical Chemistry”
1 April 2017–31 March 2020

Shioya, N.
Development of Multiple-Angle Incidence Resolution Reflection Spectrometry and Its Application to Organic Thin-Film Devices
Grant-in-Aid for Early-Career Scientists “Analytical Chemistry”
1 April 2019–31 March 2022

— **Molecular Microbial Science** —

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.
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.
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

Kurihara, T.
Elucidation of the Mechanism of Selective Protein Transport to Bacterial Extracellular Membrane Vesicles and Their Application for Construction of an Extracellular Platform for Protein Production
A Large Research Grant from the Institute for Fermentation, Osaka
1 April 2019–31 March 2021

Ogawa, T.
Exploration and Functional Elucidation of a Novel Protein Involved in the Metabolism of ω -3 Polyunsaturated Fatty Acids in Bacteria
Grant-in-Aid for Early-Career Scientists
1 April 2019–31 March 2021

Ogawa, T.
Research on Bacterial Conversion of ω -3 Polyunsaturated Fatty Acids and its Application
A General Research Grant from the Institute for Fermentation, Osaka
1 April 2019–31 March 2021

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

— **Polymer Materials Science** —

Takenaka, M.
Study on Adhesion Processes by Using 4D Analyses of GI-SAXS Innovative Adhesion Technology Based on 4-Dimensional Multi-Scale Analysis of Interface
1 October 2018–31 March 2027

Ogawa, H.
Development of Visualizing Method through Cooperative Small Angle x-Ray Scattering Coupled with Computed Tomography (SAXS-CT) and Information Science
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 September 2016–31 March 2020

— **Molecular Rheology** —

Watanabe, H.
Unified Understanding of the Polymer Dynamics under Elongational and Shear Flows
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

— **Molecular Aggregation Analysis** —

Wakamiya, A.
Development of High Performance and Environmentally Friendly Perovskite Type Solar Cells
ALCA (Advanced Low Carbon Technology Research and Development Program), JST
16 November 2016–31 March 2021

Wakamiya, A.
Development of Film-type Solar Cells
COI STREAM (Center of Innovation Science and Technology Based Radical Innovation and Entrepreneurship Program), JST
1 October 2013–31 March 2022

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

— **Laser Matter Interaction Science** —

Hashida, M.
Surface Structures on Solar Cells by Advanced 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 (Quantum 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

Inoue, S.
Development of Ultrafast Transient Electric Field Observation Method for Elucidation of Femtosecond Laser Ablation Mechanism
The Amada Foundation AF-2019236-C2
1 April 2018–31 March 2022

— **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.
Electronic Structure Analysis by Aloof Beam EELS
Grant-in-Aid for Challenging Research
1 April 2019–31 March 2022

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

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Synthetic Organotransformation —

Nakamura, M.
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
Core-to-Core Program, JSPS
1 April 2016–31 March 2020

— Nanophotonics —

Kanemitsu, Y.
Fusing Nanomaterials and Strong Electric Field Nonlinear Optics for New Advances in Photonics
Grant-in-Aid for Specially Promoted Research
23 April 2019–31 March 2024

Kanemitsu, Y.
Design of Next-Generation Flexible Photonic Devices Based on Metal Halide Perovskites
CREST (Core Research for Evolutionary Science and Technology), JST
1 October 2016–31 March 2022

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 “Neo-virology, the Raison d’Etre of Viruses”
30 June 2016–31 March 2021

Ogata, H.
The Biosphere of Aggregated Particles: Elucidating the Regulatory Mechanisms of Marine Carbon Cycles
Grant-in-Aid for Scientific Research (S)
3 July 2019–31 March 2023

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.
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 Carboxydrotrophic Bacteria through Spatio-Temporal Search
Grant-in-Aid for Scientific Research (S)
1 April 2016–31 March 2021

Endo, H.
Integrative Understanding of Marine Nitrogen Fixation Based on Global Observations from Tropics to Polar Regions
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

Endo, H.
Experimental Investigation of the Effects of Phytoplankton Diversity on Ecosystem Functioning in the Ocean
Grant-in-Aid for for Early-Career Scientists
1 April 2019–31 March 2022

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 —

Akutsu, T.
Analysis and Application of Discrete Preimage Problems
Grant-in-Aid for Scientific Research (A)
1 April 2016–31 March 2023

Mori, T.
Development of Cell Trajectory Inference and Comparison Algorithm Based on Single-cell Omics Data
Grant-in-aid for Early-Career Scientists
1 April 2019–31 March 2021

— **Bio-knowledge Engineering** —

Mamitsuka, H.
Reinforcement of Resiliency of Concentrated Polymer Brushes and
Its Tribological Applications Strategic Basic Research Program
ACCEL (Accelerated Innovation Research Initiative Turning Top
Science and Ideas into High-Impact Values), JST
1 September 2015–31 March 2020

Mamitsuka, H.
Efficient Estimation of Data Structure from Multiple Tensors
Grant-in-Aid for Scientific Research (B)
1 April 2019–31 March 2022

Nguyen, C. H.
Machine Learning on Large Graphs
Grant-in-Aid for Scientific Research (C)
1 April 2018–31 March 2021

THESES

- AGATA, Ryosuke
D Eng, Kyoto University
“Development of Iron-Catalyzed Selective Cross-Coupling Reactions toward Natural Product Synthesis”
Supervisor: Prof NAKAMURA, Masaharu
25 March 2019
- AKISHIBA, Misao
D Pharm Sc, Kyoto University
“Cytosolic Delivery of Proteins by Endosomolytic Peptide Analogues”
Supervisor: Prof FUTAKI, Shiroh
25 March 2019
- AOKI, Yuma
D Eng, Kyoto University
“Development of Iron-Catalyzed C-N and C-C Bond Forming Reactions toward Functional Arylamine Synthesis”
Supervisor: Prof NAKAMURA, Masaharu
25 March 2019
- FAN, Weijia
D Eng, Kyoto University
“Design and Utilization of New Organotellurium Chain Transfer Agents for Advanced Polymer Synthesis”
Supervisor: Prof YAMAGO, Shigeru
23 May 2019
- FUJIMORI, Shiori
D Sc, Kyoto University
“Synthetic Studies on the Heavier Group 14 Element Analogues of Aryl Anions and Elucidation of Their Properties”
Supervisor: Prof TOKITOH, Norihiro
25 March 2019
- HAM, Wooseung
D Sc, Kyoto University
“Spin-orbit Phenomena in Non-centrosymmetric Magnetic Multilayers”
Supervisor: Prof ONO, Teruo
18 January 2019
- HASHIKAWA, Yoshifumi
D Eng, Kyoto University
“Synthesis of Endohedral Fullerenes and Dynamic Behavior of Encapsulated Water Molecules”
Supervisor: Prof MURATA, Yasujiro
23 July 2019
- LU, Yangtian
D Eng, Kyoto University
“Synthesis of Structurally Controlled hyperbranched Polymers Through the Design of New Monomers with Hierarchical”
Supervisor: Prof YAMAGO, Shigeru
23 July 2019
- MATSUMOTO, Kenshi
D Sc, Kyoto University
“Crystal Structural Control of Nanomaterials toward High-Performance Permanent Magnets”
Supervisor: Prof TERANISHI, Toshiharu
25 November 2019
- MIZUNO, Hayato
D Sc, Kyoto University
“Electric Field Effect on a Magnetic Ultra Thin Films”
Supervisor: Prof ONO, Teruo
18 January 2019
- NAKAMURA, Tomoya
D Eng, Kyoto University
“Molecular Orientation Control of Organic Semiconducting Materials for Thin Film Electronics”
Supervisor: Prof MURATA, Yasujiro
25 March 2019
- OZAKI, Masashi
D Eng, Kyoto University
“High Performance Solar Cells Based on Perovskite Layers Prepared from Purified Precursor Materials”
Supervisor: Prof MURATA, Yasujiro
25 March 2019
- SHIMIZU, Yoshihiko
D Eng, Kyoto University
“Systematic Studies on Novel Polymeric Nanocomposites Embedded with a Well-Defined Fine Network”
Supervisor: Prof TSUJII, Yoshinobu
25 March 2019
- SHINODA, Koki
D Pharm Sc, Kyoto University
“Design of Functional RNA Binding Proteins Based on PUFs”
Supervisor: Prof FUTAKI, Shiroh
25 March 2019
- SUGAHARA, Tomohiro
D Sc, Kyoto University
“Studies on the Small-molecule-activation Reactions by Utilizing Low-coordinated Germanium Species”
Supervisor: Prof TOKITOH, Norihiro
25 March 2019
- TOYOTAKE, Yosuke
D Agr, Kyoto University
“Studies of Lysophosphatidic Acid Acyltransferases Generating Membrane Lipid Diversity in Bacteria”
Supervisor: Prof KURIHARA, Tatsuo
25 March 2019
- YAMADA, Takumi
D Sc, Kyoto University
“Photoluminescence Dynamics of Lead-Halide Perovskite Single Crystals”
Supervisor: Prof KANEMITSU, Yoshihiko
25 March 2019
- YATSUZUKA, Kenji
D Med Sc, Kyoto University
“Live-Cell Imaging of Multiple Endogenous mRNAs Permits the Direct Observation of RNA Granule Dynamics”
Supervisor: Prof UESUGI, Motonari
25 March 2019



**THE 119TH
ICR ANNUAL
SYMPOSIUM**

SEMINARS

**MEETINGS AND
SYMPOSIA**



THE 119TH ICR ANNUAL SYMPOSIUM

(13 December 2019)

ORAL PRESENTATION

KAWANO, Kenichi (Biofunctional Design-Chemistry)
“Development of a Membrane Curvature-sensing Peptide Based on a Structure–activity Study”

HARUTA, Mitsutaka (Electron Microscopy and Crystal Chemistry)
“High Spatial Resolution Elemental and Electronic Structure Analysis by Electron Microscopy”

SATO, Shinichi (Chemical Biology)
“Live-Cell Imaging of Endogenous Bioorganic Molecules with Short RNAs and Fluorescent Probes”

MURDEY, Richard (Molecular Aggregation Analysis)
“Performance Evaluation of Perovskite Solar Cells for Ambient Light Environments”

TAKENAKA, Mikihito (Polymer Materials Science)
“Strain-induced Density Fluctuations in Glassy Materials”

— ICR Award for Young Scientists —
HERBSCHLEB, Ernst David (Inorganic Photonics Materials)
“Ultra-long Coherence Times Amongst Room-temperature Solid-state Spins”

— ICR Award for Graduate Students —
OKUNO, Takaya (Nanospintronics)
“Spin-transfer Torques for Domain Wall Motion in Antiferromagnetically-coupled Ferrimagnets”

YOSHIKAWA, Genki (Chemical Life Science)
“Medusavirus, a Novel Large DNA Virus Discovered from Hot Spring Water”

— ICR Grants for Promoting Integrated Research —
SARUYAMA, Masaki (Advanced Inorganic Synthesis)
“Synthesis and Carrier Dynamics of Nanoparticle Heterostructure with Narrow Band Gap Semiconductor Toward Effective Usage of Sunlight”

UEDA, Yoshihiro (Synthetic Organic Chemistry)
“Catalytic Kinetic Resolution of Racemic Open-Caged Fullerene Possessing Inherent Chirality”

MORISHITA, Hiroki (Inorganic Photonics Materials)
“Fundamental Study Toward the Realization of Diamond Quantum-spintronics Devices”

PINCELLA, Francesca (Synthetic Organotransformation)
“Development of Peptide Based Catalysts for Oxidative Lignin Depolymerization”

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 JUN-I, Yuta; MIZUHATA, Yoshiyuki; TOKITOH, Norihiro
“Stereoselective Synthesis of Silicon-containing Reactive Species Having Convertible Aryl Groups”

GE TSUJI, Shingo; MIZUHATA, Yoshiyuki; TOKITOH, Norihiro
“Synthetic Studies on Heavy Aryl Anions”

GE OSHIRO, Taku; MIZUHATA, Yoshiyuki; TOKITOH, Norihiro
“Synthetic Studies on 1-Germaazulene”

— Structural Organic Chemistry —

LW “Recent Studies of Structural Organic Chemistry”

GE IDE, Yuki; HASEGAWA, Shota; ADACHI, Ayumi; HASHIKAWA, Yoshifumi; HIROSE, Takashi; MURATA, Yasujiro
“Syntheses of Open-Cage Fullerene C₆₀ Derivatives Containing Hydrogen Peroxide and Acetonitrile”

— Synthetic Organic Chemistry —

LW “Recent Research of Laboratory of Synthetic Organic Chemistry”

GE NINOMIYA, Ryo; ARAI, Kenta; MORISAKI, Kazuhiro; UEDA, Yoshihiro; KAWABATA, Takeo
“Dirhodium-catalyzed β -position-selective C(sp³)-H Amination of Alkylsilanes”

— Advanced Inorganic Synthesis —

LW “Recent Progress of Advanced Inorganic Synthesis”

GE KIM, Jungryang; TRINH, Thang Thuy; SATO, Ryota; TERANISHI, Toshiharu
“Nanoparticle Approach to the Formation of Sm(Fe_{1-x}Co_x)₁₁Ti Particles”

GE MATSUMOTO, Kenshi; SATO, Ryota; TATETSU, Yasutomi; TERANISHI, Toshiharu
“Creation of Mille-Feuille FePd₃ Framework Induced by Inter-Element Miscibility”

— **Chemistry of Polymer Materials** —

[LW] “Recent Activities in Chemistry of Polymer Materials Laboratory”

[GE] TORIBUCHI, Taito; SAKAIBARA, Keita; INOUE, Shunsuke; HASHIDA, Masaki; SAKABE, Shuji; TSUJII, Yoshinobu
“Tribological Properties of Concentrated Polymer Brushes on the Surface of Femtosecond Laser Processed Substrates”

— **Polymer Controlled Synthesis** —

[LW] “Research Activities in Laboratory of Polymer Controlled Synthesis”

[GE] JIANG, Yuhan; FAN, Weijia; YAMAGO, Shigeru
“Synthesis of High-molecular-weight Polystyrene and Polyacrylate by Ab-initio Emulsion Controlled Radical Polymerization”

[GE] IMAMURA, Yuji; YAMAGO, Shigeru
“Dual Control Over Molecular Weight and Stereoregularity of Poly(*N,N*-diethylacrylamide) Using TERP in the Presence of Lewis Acid”

[GE] ONOZUKA, Kota; HASHIMOTO, Sigma; KAYAHARA, Eiichi; KATO, Tatsuhisa; YAMAGO, Shigeru
“Characterization of Twisted-Cycloparaphenylene Derivatives and Their Oxidized Species”

[GE] SUN, Liansheng; KAYAHARA, Eiichi; YAMAGO, Shigeru
“Synthesis and Characterization of a Doubly Annulated Cycloparaphenylene and Its Dication”

— **Inorganic Photonics Materials** —

[LW] “Research Progress at Inorganic Photonic Lab”

— **Nanospintronics** —

[GE] ISHIBASHI, Mio
“Large Nonreciprocal Frequency Shift of Propagating Spin Waves in Synthetic Antiferromagnets”

[GE] LI, Tian
“Snell’s Law for Isotropically Propagating Spin Wave”

[GE] HIRATA, Yushou
“Magnetoresistance in α -RuCl₃”

— **Biofunctional Design-Chemistry** —

[LT] HSU, Wei-Yuan; MASUDA, Toshihiro; SAKAI, Takayuki; FUTAKI, Shiroh
“Interaction with Plasma Membrane and Curvature Inducibility of Branched Oligomeric EpN18”

[GE] NISHIMURA, Motoki; MASUDA, Toshihiro; AFONIN, Sergii; KAWANO, Kenichi; ULRICH, Anne S.; FUTAKI, Shiroh
“Structural Parameters Contributing to the Ability of Amphipathic Peptides to Induce Membrane Curvature”

— **Chemistry of Molecular Biocatalysts** —

[LW] “Research Activities in Laboratory of Chemistry of Molecular Biocatalysts”

— **Molecular Biology** —

[LW] “Latest Research Topics in Molecular Biology Laboratory”

— **Chemical Biology** —

[LW] “Create New World of Bioactive Synthetic Molecules”

— **Molecular Materials Chemistry** —

[LW] “Molecular Materials Chemistry”

[GE] WADA, Hiromasa; SUZUKI, Katsuaki; KAJI, Hironori
“Development of Blue Thermally Activated Fluorescence Emitters with Benzimidazole Moiety”

[GE] SAWADA, Ayaka; KAJI, Hironori
“Analysis of Aggregated Structure and Charge Transport Properties for Amorphous Cycloparaphenylene Systems Based on Multiscale Simulation”

— **Hydrospheric Environment Analytical Chemistry** —

[LT] TSUCHIYA, Mao; TAKANO, Shotaro; TSUJISAKA, Makoto; IMAI, Shoji; YAMAMOTO, Yuhei; SOHRIN, Yoshiki
“Improved Isotopic Analysis for Ni, Cu, and Zn and Its Application to Natural Water Samples”

[GE] FUJIWARA, Yuta; TSUJISAKA, Makoto; TAKANO, Shotaro; SOHRIN, Yoshiki
“Determination of Stable Isotope Ratio of Tungsten in Seawater Using TSK-8HQ Resin Column”

— **Chemistry for Functionalized Surfaces** —

[GE] YAMAGUCHI, Yuta; SHIMOAKA, Takafumi; SHIOYA, Nobutaka; HASEGAWA, Takeshi
“In-Situ Molecular Orientation Analysis of a π -Gelator at Air–Water Interface by Using Infrared Spectroscopy”

[GE] FUJII, Masamichi; SHIOYA, Nobutaka; FUJIWARA, Ryoji; TOMITA, Kazutaka; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
“Analysis of Thermal Conversion of a DNTT Precursor Thin Film Using pMAIRS”

— **Molecular Microbial Science** —

[LW] “Research Activities in Molecular Microbial Science Laboratory”

[GE] YUSUF, Yustina; HIROSE, Kazuki; OGAWA, Takuya; KAWAMOTO, Jun; KURIHARA, Tatsuo
“Mechanism of Docosahexaenoic Acid Conversion in Eicosapentaenoic Acid-Producing Bacterium”

— **Polymer Materials Science** —

[LW] “Polymer Materials Science”

[LT] IKEDA, Yuta; TAKENAKA, Mikihiro
“A Study of Induced Density Fluctuations of Glassy Materials”

GE HIKAMI, Yuichi; OGAWA, Hiroki; TAKENAKA, Mikihito; TAKAGI, Hideaki; SHIMIZU, Nobutaka; IGARASHI, Noriyuki
“Analyses of Depth Dependence of Order-order Transition in PS-b-P2VP Thin Films by Grazing Incidence Small Angle Scattering with Tender X-ray”

— **Molecular Rheology** —

LT MATSUMIYA, Yumi; WATANABE, Hiroshi
“Viscoelastic and Dielectric Relaxation of Mono-functionally End-associative Polymers”

— **Molecular Aggregation Analysis** —

LW “Research Progress in Molecular Aggregation Analysis Laboratory”

— **Particle Beam Science** —

LW “Research in Particle Beam Science Laboratory”

— **Laser Matter Interaction Science** —

LW “Research Activities in Laboratory of Laser Matter Science”

GE HOSOKAWA, Chikai; HASHIDA, Masaki; NAGASHIMA, Takeshi; INOUE, Shunsuke; SAKABE, Shuji
“Development of Intense Terahertz Light Source Aiming at Forming Periodic Surface Structures on Material Surface”

GE FURUKAWA, Yuki; HASHIDA, Masaki; INOUE, Shunsuke; SAKABE, Shuji
“Change in the Optical Properties of Titanium Plate Induced by Below-ablation-threshold Femtosecond Laser Irradiation”

GE INOUE, Shunsuke; HIRAHARA, Yusuke; OZAKI, Takaya; NOBUHIRO, Akihide; HOMMA, Kensuke; SAKABE, Shuji; HASHIDA, Masaki; NAKAMIYA, Yoshihide; NEAGU, Liviu; TESILEANU, Ovidiu
“Extension of the Search for Resonance Fields at Sub-eV with Femtosecond Inducing Laser Produced OPA”

GE TANAKA, Yohei; HOSOKAWA, Chikai; HASHIDA, Masaki; ZEN, Heishun; NAGASHIMA, Takeshi; OZAKI, Norimasa; INOUE, Shunsuke; SAKABE, Shuji
“Comparison of Ultrafine LIPSS Formation Thresholds of Various Semiconductors Irradiated by Mid-infrared Free Electron Laser”

— **Electron Microscopy and Crystal Chemistry** —

LW “Research Activities in Division of Electron Microscopy and Crystal Chemistry”

GE YAMAGUCHI, Atsushi; NEMOTO, Takashi; KURATA, Hiroki
“Analysis of Core-hole Effect on Carbon K-edge ELNES of Copper Phthalocyanine”

— **Atomic and Molecular Structures** —

LW “Introduction of Atomic and Molecular Structures Laboratory”

— **Synthetic Organotransformation** —

GE LU, Siming
“Regio- and Stereoselective Synthesis of 1,4-Enynes by Iron-Catalyzed Suzuki–Miyaura Coupling”

GE NAKATANI, Yuya; TAKAYA, Hikaru; HAYASHI, Kazuhiro; NAKATA, Eiji; MORII, Takashi; NAKAMURA, Masaharu
“Development of Lignin-binding Peptide for Selective Depolymerization of Wood Biomass”

GE KAWASAKI, Hiroto
“Nickel-catalyzed C–H Arylation of Arylamines”

— **Advanced Solid State Chemistry** —

LW “Research Introduction in Advanced Solid State Chemistry Laboratory”

— **Organometallic Chemistry** —

LW “Activity Report: Organometallic Chemistry Laboratory”

GE ISHIZUKA, Risa; WAKIOKA, Masayuki; OZAWA, Fumiyuki
“Synthesis of Alternating Copolymers of Thiophene Substituted Diketopyrrolopyrrole and Dithienylethene via Highly Selective Direct Arylation Polymerization”

— **Nanophotonics** —

LW “Recent Research Topics of Nanophotonics Group”

— **Chemical Life Science** —

LW “Introduction to Research in Chemical Life Science”

— **Mathematical Bioinformatics** —

LT LIU, Pengyu
“Extracting Boolean Rules from Trained Neural Networks”

— **Bio-knowledge Engineering** —

LT NGUYEN, Dai Hai; NGUYEN, Hao Canh; MAMITSUKA, Hiroshi
“Adaptive: Learning Data-dependent, Concise Molecular Vectors for Fast, Accurate Metabolite Identification from Mass Spectra”

SEMINARS

Assoc Prof ADACHI, Shunsuke
Graduate School of Science, Kyoto University, Kyoto, Japan
“Probing Ultrafast Dynamics during and After Passing Through Conical Intersections with Vacuum Ultraviolet Laser”
1 November 2019

Prof AFONIN, Sergii
Karlsruher Institut für Technologie, Germany
“Using Unnatural Amino Acids for Structural Studies and Functional Modulation of Membrane-Active Peptides”
29 October 2019

Dr AKASHI, Motohiro
Tokyo University of Science, Tokyo, Japan
“To Understand the Evolutionary Mechanisms of Giant Viruses”
2 July 2019

Prof ANDERSON, Harry L.
Department of Chemistry, University of Oxford, U.K.
“Chemistry of Giant Porphyrin Rings”
8 April 2019

Prof ARMIDO, Studer
Institute of Organic Chemistry, University of Munster, Germany
“Applications of Nitroxides in Materials Science and Novel On-surface Chemistry”
5 February 2019

Prof and Director BAGDY, Gyorgy
Department of Pharmacodynamics, Semmelweis University, Hungary
“Gene-environment and Gene-gene Interactions: Clues to the ‘Missing Heritability’ Enigma in Major Depression?”
24 July 2019

Prof CAI, Hongmin
School of Computer Science & Engineering South China University of Technology, China, P.R.
“Identification of Gene-drug and Multi-omics Regulatory Modules Through Integrative Analysis”
5 September 2019

Prof CANN, Isaac
Carl R. Woese Institute for Genomic Biology, University of Illinois at Urbana-Champaign, U.S.A.
“Initiation of DNA Replication in *Methanosarcina acetivorans* is Coupled to Cell Division”
12 July 2019

Prof CHAIRUANGSRI, Torranin
Faculty of Science, Chiang Mai University, Thailand
“Micro- and Nano-structural Characterization by Advanced Transmission Electron Microscopy of Novel Functional Materials for Battery Development”
7 October 2019

Dr CHAKRABARTY, Arindam
Graduate School of Agriculture, Kyoto University, Kyoto, Japan
“Functional Copolymers via Controlled Radical Polymerization in Emulsion”
29 November 2019

Prof CHEN, Luonan
Key Laboratory of Systems Biology, Chinese Academy of Sciences, China, P.R.
“Network Biomarker for Disease Diagnosis and Dynamic Network Biomarker for Disease Prediction”
8 February 2019

Dr CHEN, Yu-Chen
University of Stuttgart, Germany
“Laser Writing of Scalable Single Colour Centres in Wide Bandgap Materials”
3 October 2019

Dr CHRISTOPH, Nebel
Fraunhofer Institute for Applied Solid State Physics, Germany
“Diamond, a Great Material for Future Applications”
22 August 2019

Prof CHURCHILL, David G.
Korea Advanced Institute of Science and Technology, Korea, R.
“Derivatization of Immunomodulatory Targets with Organoselenide Substituents to Achieve Reversible ROS Fluorescence Detection”
28 August 2019

Dr CLOUTET, Eric
Laboratoire de Chimie des Polymères Organiques CNRS-Université de Bordeaux, France
“‘Green’ Synthesis Routes to Semiconducting (Co)polymers”
23 May 2019

Dr COWLEY, Michael J.
University of Edinburgh, U.K.
“Phosphorus-Boron Double Bonds: Synthesis, Structure and Reactivity”
27 June 2019

Dr DELMONT, Tom
Pasteur Institute, France
“Genome-resolved Metagenomics and Comparative Genomics Applied to TARA Oceans”
2 September 2019

Dr FABIEN, Durola
CNRS, Université de Bordeaux, France
“Six Years of Glyoxylic Perkin Strategy: From Short Ribbons to Möbius Rings”
6 December 2019

Prof FONTAINE, Frédéric-Georges
Université Laval, Canada
“Ligand Design in Organometallic Chemistry Taken to the Extremes: When the Metal is no Longer Needed”
13 September 2019

Assoc Prof GOVINDARAJU, Thimmaiah
Jawaharlal Nehru Centre for Advanced Scientific Research, India
“Silk and Peptidomimetics Based Smart Biomaterials”
21 October 2019

Dr GRIMSLEY, Nigel
Center National de la Recherche Scientifique, France
“Prasinovirus Infection Is Firstly Furtive, Then Furious, but Phytoplankton Fight”
23 July 2019

Prof HASEGAWA, Hiroshi
Faculty of Chemistry, Institute of Science and Engineering,
Kanazawa University, Ishikawa, Japan
“Development of New Chemical Separation Technique for Metallic Elements in Environmental Samples”
19 July 2019

Prof HIRAIISHI, Kunihiko
School of Information Science, Japan Advanced Institute of Science and Technology, Ishikawa, Japan
“Formal Modeling and Its Applications to Bioinformatics”
28 May 2019

Dr HO, Tung-Yuan
Research Center for Environmental Changes, Academia Sinica, Taiwan
“Ni: A Major Factor Affecting N₂ Fixation & H₂ Cycling in Some Marine Cyanobacteria”
9 December 2019

Prof HRISTOVA, Kalina
Whiting School of Engineering, Johns Hopkins University, U.S.A.
“Membrane Active pH-sensitive Peptides”
23 July 2019

Prof HUANG, Xueliang
Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, China, P.R.
“Palladium Carbene Enabled Acylation Reactions”
4 March 2019

Dr IGARASHI, Ryuji
National Institutes for Quantum and Radiological Science and Technology, Chiba, Japan
“Quantum Biology by Nano-diamond Quantum Sensor”
7 October 2019

Prof INOUE, Shigeyoshi
Technical University of Munich, Germany
“Multiply-bonded Aluminium Compounds in Bond Activations and Catalysis”
2 August 2019

Prof IWAMOTO, Satoshi
Research Center for Advanced Science and Technology, The University of Tokyo, Tokyo, Japan
“Cavity Polaritons: Fundamentals and Recent Development”
2 July 2019

Senior Fellow JITSUNO, Takahisa
ELI-NP, Horia Hulubei National Institute, Bucharest, Romania
“Current Status of ELI-NP Activities and Future Prospects”
23 December 2019

Assoc Prof JUHASZ, Gabriella
Semmelweis University, Hungary
“Environmental Causes of Depression”
24 July 2019

Prof JUNK, Peter C.
James Cook University, Australia
“Recent Developments in Redox Transmetallation Chemistry Involving Rare Earth Metals”
30 January 2019

Prof KAMITAKAHARA, Hiroshi
Graduate School of Agriculture, Kyoto University, Kyoto, Japan
“Precise Synthesis and Structure-Property Relationship of Cellulose-type Diblock Copolymers”
26 April 2019

Prof / Director KASKI, Samuel
Aalto University / Finnish Center for Artificial Intelligence (FCAI), Finland
“Probabilistic Modelling with the Experts”
24 May 2019

Prof KERTON, Francesca M.
Department of Chemistry, Memorial University of Newfoundland, Canada
“Reactions of Carbon Dioxide and Epoxides Catalysed by Homogeneous Iron- and Boron-centered Catalysts”
7 October 2019

Prof KNAPP, Ernst-Walter
Free University of Berlin, Germany
“Statistics: ANOVA and More”
9 July 2019

Prof KONO, Junichiro
William Marsh Rice University, U.S.A.
“Current Status and Future Prospects of Flexible Photonics”
4 October 2019

Assoc Prof KORENDOVYCH, V. Ivan
Syracuse University, U.S.A.
“De Novo Design of Protein and Peptide Catalysts”
17 June 2019

Proj Assoc Prof KOSONO, Saori
Biotechnology Research Center, The University of Tokyo, Tokyo, Japan
“Metabolic Regulation via Protein Acylation in Bacteria”
28 June 2019

Prof KOZAK, Christopher M.
Department of Chemistry, Memorial University of Newfoundland, Canada
“Transition Metal-catalyzed Copolymerization of Epoxides and Carbon Dioxide”
7 October 2019

Prof LEI, Aiwen
College of Chemistry and Molecular Sciences, Wuhan University, China, P.R.
“Oxidation Induced C-H Activation and Oxidative Cross-Coupling with Hydrogen Evolution”
22 July 2019

Prof MATILE, Stefan
University of Geneva, Switzerland
“Weekend Disulfide Magic”
31 August 2019

Dr MATTHIAS, Niethammer
University of Stuttgart, Germany
“Coherent Electrical Readout of Spin-Active Defects in 4H-SiC for Quantum Sensors Using Photo-Ionization at Ambient Conditions”
3 October 2019

Dr MICHAEL, Hanks
National Institute of Informatics, Tokyo, Japan
“Spin Measurement of Negatively-Charged Defects in Diamond”
29 March 2019

- Dr MORIOKA, Naoya
University of Stuttgart, Germany
“Very Stable Optical Transitions of Silicon Vacancy Centers in SiC towards Quantum Information Platform”
3 October 2019
- Prof MÜLLER, Thomas
Carl von Ossietzky University Oldenburg, Germany
“An Old Hat with New Feathers – Heterodianions as Precursors for Unusual Silicon and Germanium Compounds”
29 August 2019
- Prof NAGASAWA, Hideko
Gifu Pharmaceutical University, Gifu, Japan
“Structure-Activity Relationship of Bicyclic Octadepsipeptide”
21 February 2019
- Assist Prof NAKATO, Ryuichiro
Institute for Quantitative Biosciences, The University of Tokyo, Tokyo, Japan
“Comprehensive Epigenome Characterization Reveals the Diverse Transcriptional Heterogeneity across Human Vascular Endothelial Cells”
1 February 2019
- Prof NISHINA, Yuta
Graduate School of Natural Science and Technology, Okayama University, Okayama, Japan
“Materials Science toward Departure from Oil and Decreasing Carbon Dioxide”
26 April 2019
- Prof NJARDARSON, T. Jon
University of Arizona, U.S.A.
“No Strain No Gain”
15 March 2019
- Dr. OHASHI, Yohei
MRC Laboratory of Molecular Biology, U.K.
“In Vitro Studies on the Class III PI3K (VPS34) Complexes”
23 December 2019
- Prof OIWA, Akira
The Institute of Scientific and Industrial Research, Osaka University, Osaka, Japan
“A Poincaré Interface Based on Photon-electron Spin Quantum State Conversion”
11 November 2019
- Prof OTTOSSON, Henrik
Uppsala University, Sweden
“Is Time Ready to Put Baird’s Rule on Excited State Aromaticity and Antiaromaticity into Action?”
27 November 2019
- Prof OZAKI, Tsuneyuki
The Institut National de la Recherche Scientifique, Canada
“High Intensity Laser Science Research at INRS”
9 December 2019
- Prof PEZACHI, John
Department of Chemistry and Biomolecular Sciences, University of Ottawa, Canada
“Chemical Biology of Virus-Host Interactions and Beyond”
12 July 2019
- Dr PRAMONO, Ajeng
Tokyo Institute of Technology, Tokyo, Japan
“Terminite Gut Microorganisms and Viruses”
29 July 2019
- Prof QI, Yabin
Okinawa Institute of Science and Technology, Okinawa, Japan
“Perovskite Material and Solar Cell Research by Surface Science and Advanced Characterization”
3 July 2019
- Prof ROBB, Frank T.
Department of Microbiology and Immunology, University of Maryland School of Medicine, U.S.A.
“Adapting Extremophile Model Systems for Medical Applications”
14 February 2019
- Assoc Prof SAIGO, Hiroto
Graduate School and Faculty of Information Science and Electrical Engineering, Kyushu University, Fukuoka, Japan
“Prediction Models that Consider Variable Interactions”
19 September 2019
- Prof SAKAMOTO, Masami
Graduate School of Engineering, Chiba University, Chiba, Japan
“Development of Asymmetric Reactions Utilizing Chirality of Crystal”
31 January 2019
- Assoc Prof SANNO, Tomokazu
Graduate School of Engineering, Osaka University, Osaka, Japan
“Fundamentals and Applications of Material Modification by Femtosecond Laser Induced Shock Waves”
25 November 2019
- Chairman and Executive Director SHIMADA, Toyoshi
Sihreact K.K., Kyoto, Japan
“Surface Functionalization of Various Materials with Hydrosilanes”
17 September 2019
- Prof Em SHINOZUKA, Yuzo
Wakayama University, Wakayama, Japan
“Electron-Lattice Interactions in Nonmetallic Materials”
21 June 2019
- Prof SHIRAKAWA, Eiji
School of Science and Technology, Kwansai Gakuin University, Hyogo, Japan
“Electrocatalytic Cross-coupling Reaction”
1 November 2019
- Assoc Prof SONG, Jiangning
Monash Biomedicine Discovery Institute (BDI), Monash University, Australia
“DeepCleave: a Deep Learning-based Approach and Tool for more Accurate Prediction of Protease-specific Cleavage Sites”
18 September 2019
- Prof SONG, Kyungmee
Korea Institute for Science and Technology, Korea, R.
“Dynamics of Magnetic Skyrmions”
23 January 2019
- Prof SOUMYANARAYANAN, Anjan
National University of Singapore, Singapore
“Magnetic Skyrmions: Creation, Stability and Dynamics”
8 October 2019
- Prof STASEVICH, Tim
Department of Biochemistry and Molecular Biology, Colorado State University, U.S.A.
“Multi-Color Imaging of Non-Canonical Translation Dynamics with Single Molecule Resolution in Living Cells”
24 June 2019

Prof STEPIEŃ, Marcin
Department of Chemistry, University of Wrocław, Poland
“Carbon-Rich p-Aromatic Surfaces: Topology, Curvature, and Function”
11 November 2019

Prof STREUBEL, Rainer
University of Bonn, Germany
“Chemistry of 1,4-Diphosphinines and P-linked Bis-*N*-heterocyclic Carbenes”
27 November 2019

Prof SULLIVAN, Matthew B.
The Ohio State University, U.S.A
“Viruses of Microbes: Lessons from the Oceans, Soils, and Humans”
1 November 2019

Prof SUZUKI, Keisuke
Department of Chemistry, Tokyo Institute of Technology, Tokyo, Japan
“Lessons from Total Synthesis of Complex Natural Products”
22 November 2019

Assoc Prof TERAMOTO, Yoshikuni
Graduate School of Agriculture, Kyoto University, Kyoto, Japan
“Biomass Material Chemistry Based on Compounding and Simple Processing”
29 November 2019

Assoc Prof TOKITA, Masatoshi
Department of Chemical Science and Engineering, Tokyo Institute of Technology, Tokyo, Japan
“Microphase-Separated Morphology and Liquid Crystal Orientation in Block Copolymers with Liquid Crystalline Segments”
16 December 2019

Prof TOVAR, J. D.
Johns Hopkins University, U.S.A.
“Repurposing Aromaticity for Organic Electronics: Making, Breaking and Stacking pi-Circuits”
14 February 2019

Chief Scientist UESAKA, Tomohiro
RIKEN, Nishina Center for Accelerator Based Science, Saitama, Japan
“Diverseness of Nuclear Matter”
29 November 2019

Prof VAO-SOONGNERN, Visit
Suranaree University of Technology, Thailand
“Molecular Simulation of the Coarse-grained Models of Associating/dissociating Head-to-head Polymer”
14 November 2019

Prof WIMLEY, C. William
Tulane University School of Medicine, U.S.A.
“Synthetic Molecular Evolution of Peptide Antibiotics”
23 July 2019

Prof WIRTH, Thomas
Cardiff University, U.K.
“Iodin Reagents in Synthesis and Flow Chemistry”
28 August 2019

Dr YASUDA, Nobuhiro
NobuChem LLC, U.S.A.
“The Art of Process Chemistry -A Research Life in Industrial Settings-”
19 June 2019

MEETINGS AND SYMPOSIA

Asian Chemical Biology Initiative 2019 Yangon Meeting

Organized by UESUGI, Motonari
18–21 January 2019 (Myanmar)

The 14th International Workshop for East Asian Young Rheologists (IWEAYR-14)

Co-organized by WATANABE, Hiroshi
23–25 January 2019 (Nagoya, Japan)

Shanghai-Kyoto Chemistry Forum

Organized by UESUGI, Motonari
23 March 2019 (China, P.R.)

39th Anniversary Meeting of Prof. Masayoshi Ishibashi, Research Institute of Oceanchemistry Foundation

Organized by SOHRIN, Yoshiki
27 April 2019 (Kyoto, Japan)

Annual Meeting of the Spectroscopical Society of Japan 2019

Organized by HASEGAWA, Takeshi
14–16 May 2019 (Kyoto, Japan)

The 66th Annual Meeting of the Japanese Biochemical Society, Kinki Branch

Organized by FUTAKI, Shiroh
25 May 2019 (Kyoto, Japan)

International Workshop on Bioinformatics and Systems Biology 2019

Organized by MAMITSUKA, Hiroshi
14–17 July 2019 (Kyoto, Japan)

The 1st Germany–Japan–China Joint Workshop on Extremely Large π -Systems

Organized by MURATA, Yasujiro; HIROSE, Takashi
18 July 2019 (Kyoto, Japan)

457th Research Council on Vitamin B

Organized by KURIHARA, Tatsuo
30 August 2019 (Kyoto, Japan)

KAPLAT Talent-Spot 2019 Ulaanbaatar

Organized by UESUGI Motonari
1 September 2019 (Mongolia)

The 8th Japanese-Sino Symposium on Organic Chemistry for Young Scientists

Organized by KAWABATA, Takeo
17–20 September 2019 (Kyoto, Japan)

26th International Workshop on Oxide Electronics

Organized by SHIMAKAWA, Yuichi
29 September–2 October 2019 (Kyoto, Japan)

107th Meeting of Discussion Group for Plasma Spectrochemistry

Organized by SOHRIN, Yoshiki
4 October 2019 (Kyoto, Japan)

JST CREST International Workshop New Developments toward Wearable Photonics: From Materials to Devices

Organized by KANEMITSU, Yoshihiko
7 October 2019 (Tokyo, Japan)

Shanghai-Kyoto Chemistry Forum 2019

Organized by UESUGI, Motonari
14 October 2019 (China, P.R.)

Environmental Virus Meeting 2019

Organized by ENDO, Hisashi
2 November 2019 (Kyoto, Japan)

73rd Annual Autumn Meeting of Research Institute of Oceanchemistry Foundation

Organized by SOHRIN, Yoshiki
16 November 2019 (Kyoto, Japan)

Solid State NMR Forum

Organized by KAJI, Hironori
5 December 2019 (Kyoto, Japan)

The 4th MAIRS Workshop

Organized by HASEGAWA, Takeshi
5 December 2019 (Tokyo, Japan)

Joint GIW/ABACBS-2019 Bioinformatics Conference

Program Committee Co-Char by AKUTSU, Tatsuya
9–11 December 2019 (Australia)



INDEX

NAME INDEX

[A]		FUJIWARA, Masanori	16	[I]	
ABE, Masashi	42	FUJIWARA, Ryoji	32	ICHIHARA, Tomoe	8
ABO, Masahiro	26	FUJIWARA, Takashi	24	ICHIKAWA, Noriya	52
ADACHI, Ayumi	6	FUJIWARA, Yuta	30	IDE, Yuki	6
ADO, Genyir	26	FUJIWARA-KATO, Mariko	24	IKARI, Seiji	14
AGATA, Ryosuke	50, 85, 88	FUKUMI, Aki	32	IKEBUCHI, Tetsuya	18
AKAGI, Chika	24	FUNADA, Shinsaku	18	IKEDA, Yuta	36
AKUTSU, Tatsuya	60	FURUKAWA, Yuki	44	IMAMURA, Yuji	14
AMANO PATINO, Midori Estefani	52, 83	FUTAKI, Shiroh	20, 81	IMANISHI, Miki	20
ANDO, Fuyuki	18	[G]		INOUE, Shunsuke	44
AOKURA, Shuta	36	GARCIA, Julius	4	ISHIBASHI, Mio	18
AOYAMA, Takashi	24	GARCIA, Kimberly Gacayon	58	ISHIDA, Hisayuki	12
ARAFILES, Jan Vincent V.	20	GELDSTZER, Jan	28	ISHIDA, Kosuke	14
[B]		GLEIM, Florian	4	ISHIDA, Toshiaki	22
BAN, Hiroki	58	GONDOH, Naruhiro	8, 80	ISHIDA, Yasuhiro	76
BECKER, David	4	GOTO, Masato	52, 83	ISHIKURA, Yasushi	40
BLANC-MATHIEU, Romain	58	GOTOH, Kengo	8	ISHIWARI, Kenji	22
BOUAD, Vincent	12	GRIMSLEY, Nigel	58	ISHIZUKA, Risa	54
[C]		GUNDIGA PUTTOJIRAO, Gurumurthy	30	ISOZAKI, Katsuhiko	50
CAI, Hongmin	76	[H]		IWAI, Kento	4
CHAN, Cheuk-Yin	30	HAKARIYA, Hayase	26, 81	IWAKI, Hiroyuki	18
CHANDA, Tanmoy	8	HAN, Yutong	12	IWAMOTO, Takahiro	50, 85
CHEN, Chen	34	HANDA, Taketo	56, 85, 88	IWASAKI, Yasuko	40
CHEN, Dongyang	14	HARUTA, Mitsutaka	46	IWASE, Misato	30
CHEN, Gong	8	HASE, Kanako	22	IWASHIMIZU, Chisaki	46
CHEN, Mengyi	34	HASEGAWA, Takeshi	32	IWASHITA, Yoshihisa	42
CHEN, Yun-Ti	60	HASHIDA, Masaki	44, 85	IWATA, Takahiro	20
CHIGA, Yuuki	10	HASHIKAWA, Yoshifumi	6	[J]	
CHO, Kenichi	56	HASHIMOTO, Hisashi	8	JIANG, Yuhan	14
CRUZADO, Kevin Tan	26	HASHIMOTO, Kentaro	58	JIN, Shuyu	26
CUI, Changyi	26	HASHIMOTO, Ruito	40	JO, Minwoo	4
[D]		HAYASHI, Kan	16	JUNG, Yejin	26
DAO, Nhung Thi	26	HAYASHI, Kyosuke	34	JUN-I, Yuta	4
DELMONT, Tom	58	HE, Yu Zhong	14	[K]	
DENIS ROMERO, Fabio	66	HERBSCHLEB, Ernst David	16, 81, 87	KAJI, Hironori	28
[E]		HIKAMI, Yuichi	36	KAMASAKA, Kouhei	34, 82
EGUCHI, Hiroshi	12, 86	HIRAI, Yusuke	20	KAN, Daisuke	52
EMI, Ryota	8	HIRANO, Rena	22	KANAYA, Taku	6
ENDO, Hisashi	58	HIRANO, Toshiko	4	KANEHISA, Minoru	76
[F]		HIRATA, Yushou	18	KANEKO, Hiroto	58
FAN, Weijia	14	HIRORI, Hideki	56	KANEKO, Ryota	10
FANG, Yue	58	HIROSE, Hisaaki	20	KANEMITSU, Yoshihiko	56, 83, 85
FU, Haining	16	HIROSE, Kazuki	34	KASAHARA, Hiroyuki	76
FUJIE, Masahiro	16	HIROSE, Takashi	6, 79	KASKI, Samuel	62
FUJIHASHI, Akiko	8	HISATOMI, Ryusuke	18	KATAYAMA, Ken-ichi	89
FUJII, Masamichi	32	HONG, Yu Min	18	KATO, Tatsuhisa	14
FUJII, Tomomi	48	HONJO, Kazuma	4	KAWABATA, Takeo	8
FUJIMORI, Shiori	79	HOSOKAWA, Chikai	44	KAWAGUCHI, Tomoki	46
FUJIMURA, Kouki	8	HSU, Wei-Yuan	20	KAWAI, Soichiro	34
FUJITA, Takehiro	14	HU, Shuai Feng	40	KAWAMOTO, Jun	34
		HU, Weizhe	28	KAWANO, Kenichi	20
		HUANG, Guanglin	6	KAWASAKI, Hiroto	50
				KAYAHARA, Eiichi	14, 80
				KIM, Jungryang	10

KIM, Kyusun	40	MASHIGUCHI, Kiyoshi	22	NODA, Kaoru	18
KINOSE, Yuji	12	MASUDA, Toshihiro	20	NODA, Naotaka	26
KISHI, Keisuke	12	MATAYOSHI, Aki	8	NOMURA, Satsuki	50
KISHI, Shintaro	34	MATSUDA, Hiroshi	50, 85	NOMURA, Yohei	20
KISHIMOTO, Mizuki	36	MATSUKAWA, Kimihiro	12		
KITAYAMA, Kaori	34	MATSUMIYA, Yumi	38, 85		
KIYOMURA, Tsutomu	46	MATSUMOTO, Kenshi	10, 80	[O]	
KIZAKI, Kazuro	6	MATSUMOTO, Soma	28	ODA, Kento	18, 85
KOBAYASHI, Takahiro	22	MATSUMOTO, Yuko	40	ODA, Tappei	36
KOBAYASHI, Yuta	18	MENDOZA, Aileen de-Leon	26	OGATA, Hiroyuki	58
KOBIYAMA, Etsuki	56	MENG, Lingjie	58, 84	OGAWA, Hiroki	36
KOEDTRUAD, Anucha	52, 88	MICHIBATA, Junya	20	OGAWA, Takuya	34
KONGO, Ryota	44	MISONO, Tomoya	28	OGAWA, Tetsuya	46
KOSHI, Yuuki	10	MITANI, Kenta	36	OHARA, Keiichi	56, 88
KOSONO, Saori	76	MIYASAKA, Yuta	18	OHASHI, Noboru	40
KOSUGI, Yoshihisa	52, 83	MIYAZAKI, Urara	58	OHKI, Izuru	16
KOYAMA, Tomohisa	6	MIZUHATA, Yoshiyuki	4, 79	OHMINE, Kyoko	28
KUBOSHIMA, Misaki	34	MIZUOCHI, Norikazu	16	OHNO, Haruhisa	12
KUMAGAWA, Daiki	36	MORANDINI, Andrea	12	OHNO, Kohji	12
KUMANO, Sou	60	MORI, Takahiro	14	OHTOMO, Masahiro	60
KUNO, Taiki	14	MORI, Tomoya	60	OIWA, Akira	76
KURATA, Hiroki	46	MORIKI, Yoshihito	12	OKADA, Tasuku	12
KUREBAYASHI, Toshiki	34	MORISAKI, Kazuhiro	8	OKAMOTO, Shu	6
KURIHARA, Tatsuo	34	MORISHITA, Hiroki	16, 87	OKAMOTO, Yasuo	10
KURIYAMA, Masashi	20	MORITA, Kouki	16	OKAZAKI, Masato	52
KURODA, Ryo	24	MORIWAKI, Kazuki	28, 81	OKUBO, Ryo	12, 87
KUROKI, Kakeru	20	MORIYAMA, Takahiro	18, 85	OKUNO, Takaya	18, 81
KUSAKABE, Yu	28	MOTEKI, Wataru	38	OMATSU, Yamato	4, 86
KUWATA, Satoshi	36	MÜNZNER, Ulrike Tatjana Elisabeth	60, 88	ONCHI, Koshiro	14
				ONO, Teruo	18, 85
[L]		MURAI, Takuya	8, 80	ONOZUKA, Kota	14, 87
LAI, Ming Wei	46	MURAMATSU, Kanako	16	OSHIRO, Taku	4
LEE, Jung-Yu	60	MURAMATSU, Tomomi	28	OTONARI, Kenko	20
LI, Hui	6	MURATA, Yasujiro	6, 79	OTSUKA, Kento	40, 87
LI, Jiayue	6	MURDEY, Richard	40		
LI, Ruiming	60			[P]	
LI, Tian	18	[N]		PARK, Beomsu	14
LI, Wenjuan	14	NABETA, Tomoki	8	PELICANO, Christian	10
LI, Xiaopei	14	NAGAE, Ayumi	30	PERRON, Amelie	26
LI, Zhanzhao	10	NAGANO, Yuki	20	PINCELLA, Francesca	50, 83
LIAN, Zichao	10	NAKAGAWA, Fumiko	10	PINEDA ARISTA, Karla Mariel	26
LIN, Xiang-Yu	60	NAKAGAWA, Hiromichi	28	PRODINGER, Florian	58, 84
LIU, Jiewei	40	NAKAGAWA, Kotaro	56	PUNZALAN, Louvy Lynn Calvelo	26
LIU, Ming-Han	10	NAKAJIMA, Yuki	12		
LIU, Pengyu	60	NAKAMICHI, Kimiyo	12	[R]	
LIU, Xingyuan	28	NAKAMIYA, Yoshihide	44	RAFIEH, Alwani Imanah	40
LIU, Yuqing	34	NAKAMURA, Masaharu	50, 85	REN, Yongxia	28
LU, Siming	50	NAKAMURA, Masaya	16		
LU, Yangtian	14	NAKAMURA, Tomoya	40	[S]	
		NAKAMURA, Yuki	50	SAIGO, Hiroto	76
[M]		NAKASHIMA, Shogo	60	SAITO, Masahiro	12
MA, Yier	60	NAKATANI, Yuya	50	SAKABE, Shuji	44, 78
MAEDA, Junya	54	NARITA, Asuka	34	SAKAI, Kahori	28
MAENO, Ayaka	28	NEMOTO, Takashi	46	SAKAI, Takayuki	20
MAHAPATRA, Amarjyoti Das	26	NGUYEN, Dai Hai	62	SAKAKIBARA, Keita	12, 80, 86
MAMITSUKA, Hiroshi	62	NGUYEN, Duc Anh	62	SAKAMOTO, Kentarou	20, 81
MANABE, Kouhei	10	NGUYEN, Hao Canh	62	SAKAMOTO, Masanori	10
MANDAI, Yuji	36	NINOMIYA, Ryo	8, 80, 86	SANARI, Yasuyuki	56
MANDAL, Sathi	26	NISHIKAWA, Tetsuri	16	SANO, Tomokazu	76
MAO, Di	26	NISHIMURA, Motoki	20	SANTO, Jyunya	52
MARUOKA, Naruyuki	34	NISHIMURA, Tomoe	18	SARUYAMA, Masaki	10
MARUYAMA, Tatsuki	38	NISHIO, Kosuke	26	SASAYAMA, Ryuto	4
MASADA, Sojiro	56	NISHIYAMA, Hiroki	58	SATO, Ryota	10
				SATO, Shinichi	26

KEYWORD INDEX

[A]		[H]		[P]	
Accelerator Physics	42	Helical Structures	6	Peptide Design	20
Amorphous Materials	28	Heteroatom	4	Perfluoroalkyl Compounds	32
Analytical Chemistry	30	Hierarchical Structure	36	Perovskite Solar Cells	40
		High Pressure Synthesis	52	Perovskites	56
[B]		Homogeneous Catalyst	54	Phospholipid Acyltransferase	34
Bacterial Cold-adaptation Mechanism	34	Hybrid Materials	12	Phospholipid Signaling	24
Beam Physics	42			Photocatalysts	10
Bioinformatics	58, 62	[I]		Plant Hormone	22
Biointerface	12	Infrared and Raman Spectroscopy	32	Plasmonics	10
Biosynthesis	22	Inorganic Nanoparticles	10	pMAIRS and MAIRS2	32
Boolean Networks	60	Intense Laser Science	44	Polymer Brush	12
		Intracellular Delivery	20	Polymer Physics	36
[C]		Iron Catalyst	50	Polymer Properties	14, 36
Cell Therapy	26			Polymer Synthesis	14
Chemical Biology	26	[K]		Polyunsaturated Fatty Acid	34
Chemical Genetics	26	Kinetic Stabilization	4	Precision Polymerization	12
Chemical Graphs	60			Protein Crystallography	48
Chemical Library	26	[L]		Protein Informatics	60
Complex Networks	60	Laser Nano-ablation Physics	44		
Computational Genomics	62	Laser Plasma Radiations		[Q]	
π -Conjugated Polymer	54	(Electrons, Ions, and THz)	44	Quantum Chemical Calculation	28
π -Conjugated Systems	6	Living Radical Polymerization	12, 14	Quantum Information Science	16
COP9 Signalosome	24	Low-coordinate Phosphorus Ligand		Quantum Materials	16
Crystal	48		54	Quantum Sensing	16
Curved π -Conjugated Molecules	14	Low-coordinated Species	4		
Cytochrome P450	22			[R]	
		[M]		Radical Species	6
[D]		Machine Learning	62	Reaction Mechanism	54
Data Mining	62	Magnetic Materials	18	Read-out Noise	46
Diamond	16	Magnetism	18	Receptor	22
Dielectric Spectroscopy	38	Marine Chemistry	30	Rheology	38
DNA/RNA Binding Protein	20	Membrane Curvature	20	RNA	24
Dynamic Chirality	8	Membrane-Permeable Peptides	20		
Dynamic Nuclear Polarization		Metal Ion Recognition	30	[S]	
Enhanced NMR	28	Metalated Peptide	50	Selective Organic Reaction	50
		Metallic Nanoparticle Catalyst	50	Self Assembly	36
[E]		Molecular Aggregation	40	Semiconductor Nanoparticles	56
Endohedral Fullerenes	6	Molecular Design and Synthesis	40	Semiconductors	40
Environmental Genomics	58	Molecular Evolution	58	Signal Transduction	24
Epitaxial Thin Film Growth	52	Molecular Recognition	8	Single Electronics	10
Extracellular Membrane Vesicle	34	Morphogenesis	24	Single Photon Spectroscopy	56
Extremely Low Count Detection	46			Site-Selective Functionalization	8
Extremophiles	34	[N]		Small Molecules	26
		Nanocomposite Magnet	10	Softmatter	36, 38
[F]		Neural Networks	60	Solar Cells	56
Femtosecond Laser Processing	44	Neutron Optics	42	Solid State Chemistry	52
Femtosecond Laser Spectroscopy	56	NV Center	16	Solid-State NMR	28
Functional Materials	6, 40			Solution-Phase XAS Analysis	50
Functional Transition Metal Oxides	52	[O]		Spectrum Imaging	46
		Organic Light-Emitting Diodes	28	Spintronics	18
[G]		Organic Semiconductors	32	Stable Isotopes	30
Gain Normalized Spectrum	46	Organic Synthesis	14	STEM-EELS	46
GenomeNet	58	Organocatalysis	8	Steric Protection	4
				Storage Ring	42
				Strigolactone	22

Structural Biology	48
Structure and Function	48
Surface and Interface Chemistry	32
Systems Biology	62

[T]

Trace Elements	30
Transition Metal Complex	54
Transition Metal Complexes	4

[U]

Ultrafast Electron Diffraction (UED)	44
Unstable Nuclear Physics	42
Unusual Amino Acid	8

[V]

Virology	58
----------	----

[X]

X-ray Crystallographic Analysis	48
---------------------------------	----

Institute for
C_hemical
R_esearch

Kyoto University