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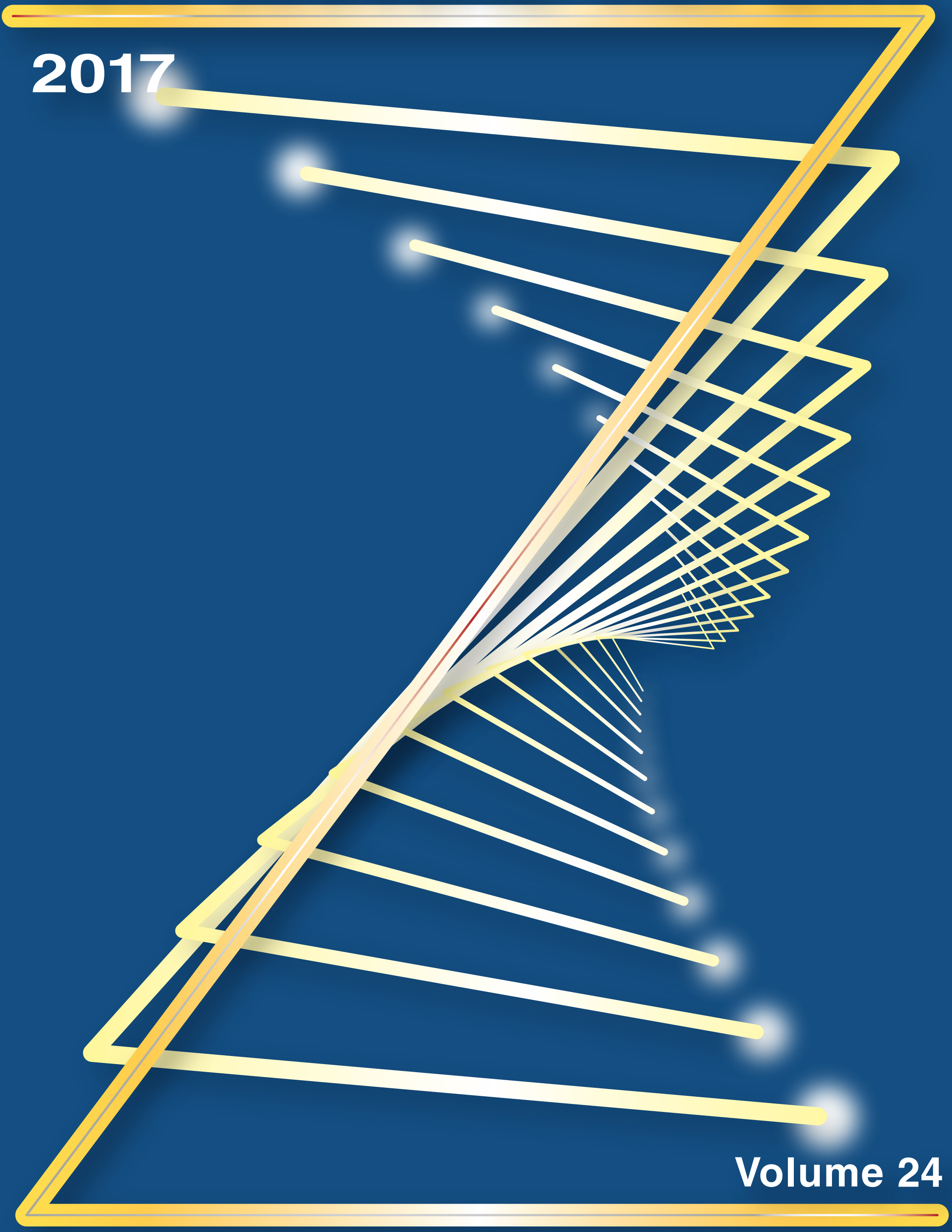

Volume 24

Institute for Chemical Research
Kyoto University

ICR ANNUAL REPORT 2017 (Volume 24) - ISSN 1342-0321 -

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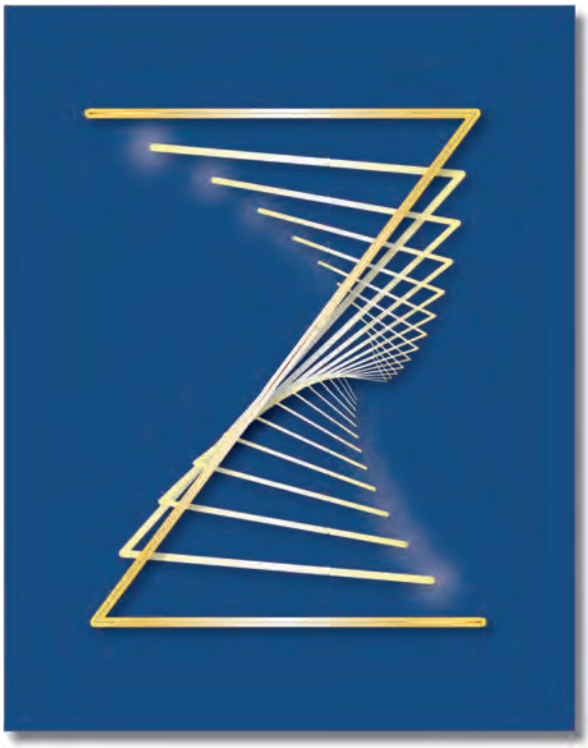


Institute for Chemical Research
Kyoto University
Volume 24

Preface

The Institute for Chemical Research (ICR) was launched in 1926 as the first research institute at Kyoto University, and celebrates its 90th Anniversary in 2016. The philosophy at the time of its foundation was to "Excel in the Investigation of Basic Principles of Chemistry and Their Applications," and studies on special medicinal substances, organometallic chemistry, incendiary reagents, and other topics were undertaken at nine research laboratories. Over its lifetime, the ICR has continuously produced out standing research achievements. Today, the organization is in five research divisions: Synthetic Chemistry, Materials Chemistry, Biochemistry, Environmental Chemistry, and Multidisciplinary Chemistry and three research centers on Beam Science, Elements Science (IRCELS), and Bioinformatics. About 120 faculty members, 210 graduate students and 60 researchers are engaged in research activities in 30 laboratories in total supervised by full-time professors. Further, five laboratories are supervised by visiting professors.

The research within the ICR encompasses the fields of chemistry, physics, biology, and informatics. The chemical studies core covers fields including physical chemistry, inorganic chemistry, organic chemistry, materials chemistry, and biochemistry. The graduate schools encompassing the laboratories accept students in diverse fields of science, engineering, agriculture, pharmaceutical sciences, medicine, and informatics. These laboratories are spearheading leading-edge research, and yielding outstanding results in their own and related research areas with publications such as: *1) Synthesis and Isolation of a Stable Germabenzenylpotassium, the First Heavier Congener of Phenyl Anion, 2) Isolation of the Simplest Hydrated Acid in Endohedral Fullerene, 3) Blue Organic Light-emitting Diodes Realizing External Quantum Efficiency over 25% Using Thermally Activated Delayed Fluorescence Emitters, 4) Cytosolic Antibody Delivery by Lipid-sensitive Endosomolytic Peptide, 5) Loosening of Lipid Packing Promotes Oligoarginine Entry into Cells, and 6) Fast Domain Wall Motion in the Vicinity of the Angular Momentum Compensation Temperature of Ferrimagnets*, all achieved last year. The legacy of our founding philosophy continues to the present day and describes the essence of our research activities. The ICR has entrusted its members, with this vision in mind, to choose and pursue research topics at the forefront of advanced chemistry with bottom-up paradigms. Sustainable and sustained growth of the human race is a key issue of this century, and we must reform our country from various perspectives. Hence, the ICR encourages its members to be actively involved in research projects and to value the development of unique interdisciplinary research projects, in order to contribute to the future of our society from materials-related fields.

Inside of the university, the ICR collaborates with other research institutes and centers as a key member of Kyoto University Research Coordination Alliance (KURCA), which was launched in 2015. Outside of the university, the ICR collaborates with domestic and international universities and research organizations (with 70 official international collaboration agreements as of January 1, 2018) and functions as a Joint Usage/Research Center proclaiming the Frontier and Interdisciplinary Research Core for Deepening Investigation and Promoting Collaboration in Chemistry-oriented Fields supported by MEXT (2016–2021); its activity during the former term received high commendation on the term-end assessment in 2016. In addition, the ICR collaborates with the Research Institute for Sustainable Humanosphere and the Institute of Advanced Energy at Kyoto University to start another MEXT-supported joint research project on bio-inspired smart materials as of April 1, 2015. Furthermore, the ICR—IRCELS in particular—is making a significant contribution to the MEXT Project of Integrated Consortium on Chemical Synthesis (2016–2021), in collaboration with the Catalysis Research Center at Hokkaido University, the Research Center for Materials Science at Nagoya University, and the Institute for Materials Chemistry and Engineering at Kyushu University. We also fully strive to foster and secure young researchers through these activities. For instance, we provide an in-house annual grant system named "ICR Grant for Encouraging Promoting Integrated Research." The strong collaboration basis so far constructed in-house and with outside researchers ensures that the Institute will continue to serve as a core of global research propellers in chemistry-oriented fields. With this consideration, we would appreciate your continued encouragement and support.

January 2018

N. Tokitoh

TOKITOH, Norihiro
Director

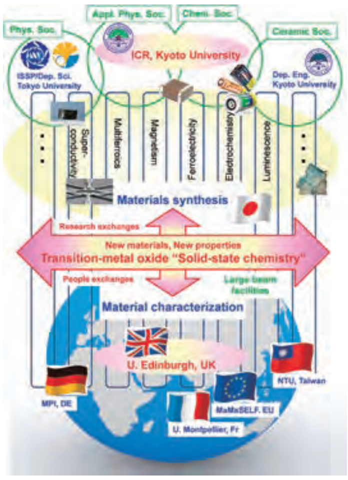
ICR News 2017

JSPS Core-to-Core Program Advanced Research Networks A. (2016-2021) Solid-State Chemistry for Transition-Metal Oxides: Exploring for New Materials with Novel Functionalities

■ Prof SHIMAKAWA, Yuichi

The discovery of new materials with outstanding properties motivates much of modern chemistry, physics and materials science. New materials with novel functionalities are also strongly demanded for developing future information and energy technologies. The general aim of this collaboration project is to discover new oxides having interesting and useful properties. Strong collaboration of materials synthesis teams and structure and property characterization teams will lead to development of advanced solid-state chemistry.

The consortium consists of materials chemists and physicists in Japan, UK, France, and Taiwan with common interests in materials science and solid-state chemistry and physics. The collaboration scheme encourages exchanges of scientific knowledge and people including young researchers and students. The program will also give many opportunities for young researchers in experiencing materials science research from synthesis to characterizations in large variety ways.



Institute for Chemical Research International Symposium of NMR 2017: DNP-NMR Workshop

■ Prof KAJI, Hironori

Nuclear magnetic resonance (NMR) is ever-growing, and developments of NMR based on novel concepts have been still ongoing. Among them, tremendous efforts have been made from various perspectives to solve the inherent NMR low sensitivity. Dynamic nuclear polarization-enhanced NMR (DNP-NMR) is one of the most successful technique for sensitivity enhancement, and thus commercially-available DNP-NMR systems have been introduced in Europe and the United States. Under such circumstances, we installed a DNP-NMR system at ICR, Kyoto University this year, which is the first commercial DNP-NMR product not only in Japan but also in Asia. On the occasion, we had an opportunity to hold the DNP-NMR workshop as an ICR International Symposium, "ICRIS-NMR '17: DNP-NMR Workshop". We had ten world-famous researchers as invited speakers and 131 attendees from all over the world in this workshop, showing the increasing interest for DNP-NMR as a novel analytical technique. We expect further developments of NMR and DNP-NMR community in near future.

This workshop was financially supported by Kyoto Convention Bereau (MICE support) and several companies. Travel and accommodation expenses were supported by JSPS KAKENHI (A) (No. 17H01231). We also acknowledge Kyoto University program (SPIRITS) and the Collaborative Research Program of ICR, Kyoto University (grant # 2015-90) for the introduction of DNP-NMR.

■ http://moma.kuicr.kyoto-u.ac.jp/icris2017/index-e.html

Materials Related with “Origin of Polyethylene Industry by the High-pressure Process in Japan” in the Institute for Chemical Research Were Added to the Registry of Essential Historical Materials for Science and Technology

■ Prof MURATA, Yasujiro

Engineering drawings, notebooks, and reports, industrial process of actual production of polyethylene in Japan conducted in Kyoto University, were added to the Registry of Essential Historical Materials for Science and Technology by the Center of the History of Japanese Industrial Technology, the National Museum of Nature and Science, Japan. These materials had been already certified last year as the Chemical Heritage by the Chemical Society of Japan.

The Registry includes one of the most important historical materials related to technology for the benefit of society in the future. The presentation ceremony of the Registry was held at the National Museum of Nature and Science, Tokyo, Japan on 12th September 2017. On behalf of the director of ICR, Prof. Murata, who succeeded the materials from the previous professors, attended the ceremony and received the certificate.

Renovation of the “Red Brick House” and Fresh Start as “Hekisui-sha”

■ Prof TSUJII, Yoshinobu

On the occasion of the 90th anniversary of the Institute for Chemical Research (ICR), the Ceramic Chemical Experiments Workshop “Red Brick House”, which had played an important role in Uji campus for a long time, was renovated and restarted freshly as “Hekisui-sha”. The building is installed not only with a multipurpose meeting space but also an exhibition space for the long history and splendid achievements of ICR. It will be effectively used as a common-use auditorium with unique and original atmosphere, contributing to research exchange among the faculties, researchers and students of ICR covering diverse fields.

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/

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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

Bioinformatics Center

Abbreviations used in the columns

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

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

ORGANIZATION

Institute for Chemical Research

5 Divisions and 3 Centers

Laboratories

Research Divisions

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

Research Centers

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

TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

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– Organoelement Chemistry –

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


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SUGAHARA, Tomohiro (D2)
YANAGISAWA, Tatsuya (D1)
HONJO, Kazuma (M2)
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JUN-I, Yuta (M1)
OSHIRO, Taku (M1)
TSUJI, Shingo (M1)

Guest Scholars

KUNZMANN, Robert	Universität Bonn, Germany, 2 August–2 October
JUNKER, Philip	Universität Bonn, Germany, 3 October–31 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 more extensive application of main group chemistry.

KEYWORDS

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

Selected Publications

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

Sugahara, T.; Sasamori, T.; Tokitoh, N., Highly Bent 1,3-Digerma-2-Silaallene, *Angew. Chem. Int. Ed.*, **56,** 9920-9923 (2017).

Majhi, P. K.; Ikeda, H.; Sasamori, T.; Tsurugi, H.; Mashima, K.; Tokitoh, N., Inorganic-Salt-Free Reduction in Main-Group Chemistry: Synthesis of a Dibismuthene and a Distibene, *Organometallics*, **36,** 1224-1226 (2017).

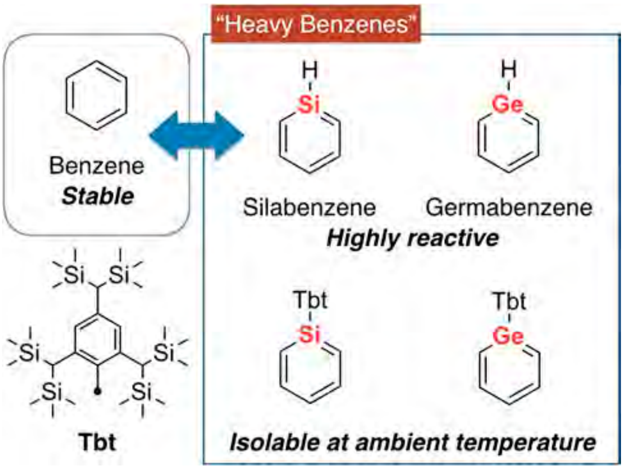
Tsunoyama, H.; Akatsuka, H.; Shibuta, M.; Iwasa, T.; Mizuhata, Y.; Tokitoh, N.; Nakajima, A., Development of Integrated Dry–Wet Synthesis Method for Metal Encapsulating Silicon Cage Superatoms of $M@Si_{16}$ (M = Ti and Ta), *J. Phys. Chem. C*, **121,** 20507-20516 (2017).

Kawasaki, K.; Sugiyama, R.; Tsuji, T.; Iwasa, T.; Tsunoyama, H.; Mizuhata, Y.; Tokitoh, N.; Nakajima, A., A Designer Ligand Field for Blue-Green Luminescence of Organoeuropium(II) Sandwich Complexes with Cyclononatetraenyl Ligands, *Chem. Commun.*, **53,** 6557-6560 (2017).

Heavy Phenyl Anion

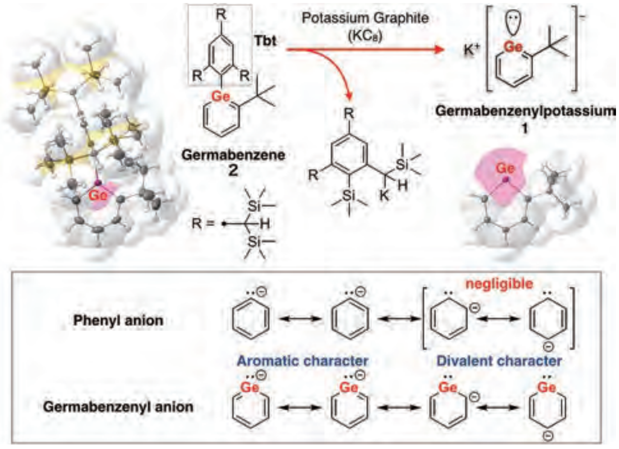
Benzene is the simplest aromatic compound and known as the basic skeleton in many organic compounds. It has been extensively studied not only from the industrial aspect such as petroleum chemistry but also the fundamental one as the most basic skeleton showing "aromaticity" since the beginning of organic chemistry.

"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 –200ºC. We have already succeeded in the synthesis and isolation of a series of "heavy benzenes" as stable compounds even at room temperature by taking advantage of kinetic stabilization afforded by a very bulky substituent, Tbt group (see the figure), to prevent the self-oligomerization. Although these compounds are found to have "aromaticity" and unique electronic state, the existence of the bulky substituent necessary for stabilization makes it difficult to develop their further applications.



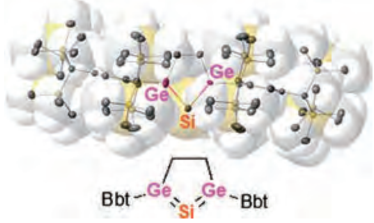
In this study, we have reported the formation of germabenzenylpotassium **1** as an isolable compound together with the elimination of the Tbt group during the reduction of the stable germabenzene **2** having a Tbt group on the germanium atom and a *t*-butyl group on the adjacent carbon atom with potassium graphite (KC_8). Compound **1** can be regarded as the anion retaining the germabenzene skeleton, *i.e.*, a germanium analog of a phenyl anion ($\ominus C_6H_5$). From both experimental and theoretical points of view, compound **1** shows not only the aromatic character but also the contribution of the canonical structure of divalent species (germylene), which is negligible in the case of phenyl anion, clearly showing the effect of substitution with germanium (heavy element).

Compound **1** can be expected as a useful reagent to introduce a germabenzene skeleton, and we have already succeeded in the synthesis of several types of new germabenzenyl derivatives. The findings of this research are expected to contribute to the design and development of novel functional molecules incorporating a germabenzene ring.



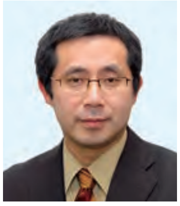
Highly Bent "Heavy Allene"

A 1,3-digerma-2-silacyclopenta-1,2-diene, *that is*, a 1,3-digerma-2-silaallene incorporated into a five-membered ring system, was synthesized and obtained as a stable orange solid, in which the Ge—Si—Ge moiety in the planar $SiGe_2C_2$ five-membered ring exhibited an acute angle with π-bonding character. On the basis of both experimental characterizations and theoretical calculations, 1,3-digerma-2-silaallene should be depicted as a $>Ge \rightarrow Si^0 \leftarrow Ge<$ species with a pronounced Si^0 character than as a $>Ge=Si=Ge<$ heterocumulene, because of the cyclic skeleton and the strong σ-donating properties of the germylene moieties. Further investigations into the physical and chemical properties of such 1,3-digerma-2-silaallenes are currently in progress.



Division of Synthetic Chemistry
– Structural Organic Chemistry –

http://www.scl.kyoto-u.ac.jp/~kouzou/en/index.html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WAKAMIYA, Atsushi
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Assist Prof
HASHIKAWA, Yoshifumi


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(Ph D)


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OKAMOTO, Shu (UG)
KAWASAKI, Hiroto (UG)
SHIMIZU, Yuma (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 semi-conducting 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
Perovskite-Based Solar Cells
Organic Solar Cells

Selected Publications

Shimogawa, H.; Yoshikawa, O.; Aramaki, Y.; Murata, M.; Wakamiya, A.; Murata, Y., 4,7-Bis[3-(dimesitylboryl)thien-2-yl]benzothiaziazole: Solvato-, Thermo-, and Mechanochromism Based on the Reversible Formation of an Intramolecular B-N Bond, *Chem. Eur. J.*, **23,** 3784-3791 (2017).

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Chaolumen; Murata, M.; Wakamiya, A.; Murata, Y., Unsymmetric Twofold Scholl Cyclization of 5,11-Dinaphthyltetracene: Selective Formation of Pentagonal and Hexagonal Rings via a Dication Pathway, *Angew. Chem. Int. Ed.*, **56,** 5082-5086 (2017).

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Ozaki, M.; Katsuki, Y.; Liu, J.; Handa, T.; Nishikubo, R.; Yakumaru, S.; Hashikawa, Y.; Murata, Y.; Saito, T.; Shimakawa, Y.; Kanemitsu, Y.; Saeki, A.; Wakamiya, A., Solvent-Coordinated Tin Halide Complexes as Purified Precursors for Tin-based Perovskites, *ACS Omega*, **2,** 7016-7021 (2017).

Hashikawa, Y.; Murata, M.; Wakamiya, A.; Murata, Y., Palladium-Catalyzed Cyclization: Regioselectivity and Structure of Arene-Fused C_{60} Derivatives, *J. Am. Chem. Soc.*, **139,** 16350-16358 (2017).

Palladium-Catalyzed Cyclization: Regioselectivity and Structure of Arene-Fused C_{60} Derivatives

The palladium-catalyzed cyclization on the fullerene C_{60} cage has been achieved using several aryl halides and C_{60}. This reaction was found to be accelerated by the addition of pivalic acid, which can be rationally explained by the computational study based on the concerted metalation-deprotonation mechanism. We have also demonstrated the regioselective π-functionalization using pre-functionalized molecules possessing the same substructure on the C_{60} cage. The single crystal X-ray analysis and electrostatic potential map revealed that the orientation of entrapped H_2O inside the naphthalene-fused open-cage C_{60} derivative is electrostatically demanded due to the naphthalene-fusion and construction of the opening.

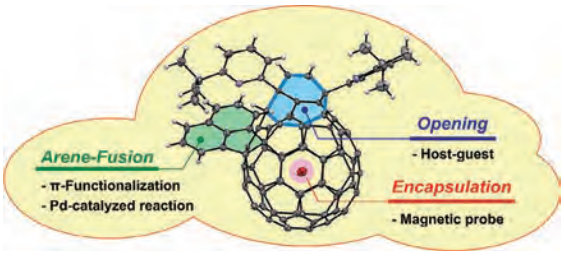

Figure 1. Regioselective naphthalene-fusion on the open-cage C_{60} derivative.

Synthesis of Azole-fused Benzothiadiazoles as Key Units for Functional π-Conjugated Compounds

2,1,3-Benzothiadiazole (BT) is a widely used electron-accepting unit in organic electronics including organic solar cells. As modifications of BT skeleton, two types of azole-fused BT units were designed and synthesized; thiazole-fused BT with an electron-withdrawing C=N bond and imidazole-fused BT with an electron-donating nitrogen atom as well as an electron-withdrawing C=N bond. Electrochemical measurements and theoretical calculations suggest that thiazole-fusion enhances the electron-accepting ability, whereas imidazole-fusion endows the BT skeleton with electron-donating ability while maintaining its electron-accepting ability. Moreover, in thiazole-fused BT units, the electronic structure could be further modulated by varying the oxidation state of the sulfur atom in methylthio group at the fused thiazole ring.

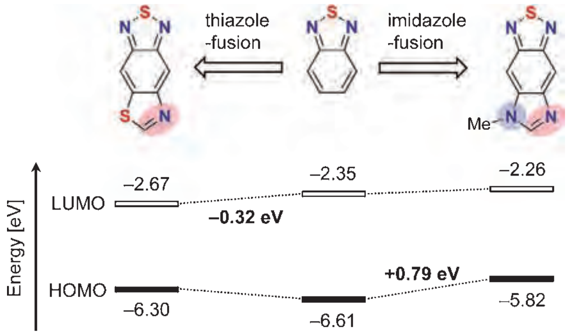

Figure 2. Effect of azole-fusion on the electronic structure of BT skeleton. Calculated at B3LYP/6-31G(d) level of theory.

Solvent-Coordinated Tin Halide Complexes as Purified Precursors for Tin-Based Perovskites

A series of solvent-coordinated tin halide complexes was prepared as impurity-free precursors for tin halide perovskites, and their structures were determined by single-crystal X-ray diffraction analysis. Using these precursors, the tin halide perovskites ($MASnI_3$ and $FASnI_3$) were prepared, and their electronic structures and photophysical properties were examined under inert conditions by means of photoelectron yield spectroscopy as well as absorption and fluorescence spectroscopies. Their valence bands ($MASnI_3$: −5.02 eV; $FASnI_3$: −5.16 eV) are significantly higher than those of $MAPbI_3$ or the typical hole-transporting materials 2,2',7,7'-tetrakis(*N*,*N*-di-*p*-methoxyphenylamino)-9,9'-spirobifluorene and poly(bis(4-phenyl)(2,4,6-trimethylphenyl) amine). These results suggest that to develop the solar cells using these tin halide perovskites with efficient hole-collection properties, hole-transporting materials should be chosen that have the highest occupied molecular orbital levels higher than −5.0 eV.

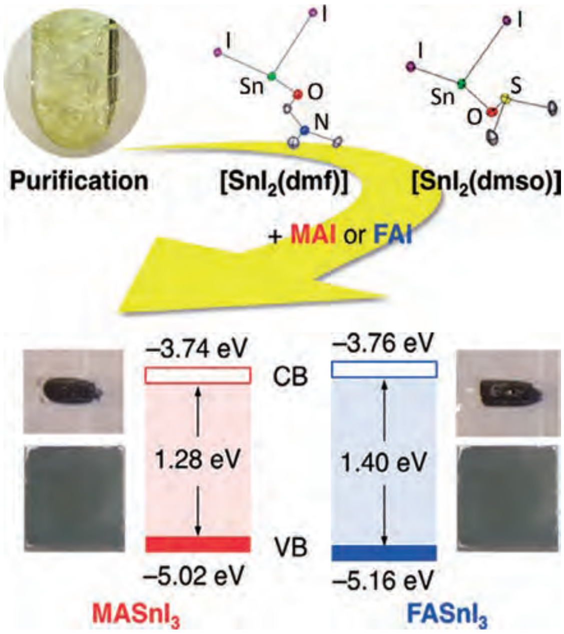

Figure 3. Valence and conduction bands of Sn-based perovskites prepared from purified precursor materials.

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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
Organocatalysis
Regioselective Functionalization
Dynamic Chirality
Unusual Amino Acid
Molecular Recognition

Selected Publications

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

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

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

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

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

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

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

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

Catalyst-Controlled Site-Selective Asymmetric Epoxidation of Dienylamine Derivatives

Epoxidation is one of the most fundamental and important transformations in organic synthesis. While catalytic asymmetric epoxidation of allylic alcohols has been extensively developed, site-selective epoxidation of polyene compounds has been relatively unexplored. Here, we report the first example of highly site- and enantioselective expoxidation of dienylamine derivatives. Novel catalyst **1** has been developed for this purpose. Whereas *m*CPBA oxidation of a nerylamine derivative took place selectively at the more electron-rich double bond to give the 6,7-epoxides, catalyst **1** provides the 2,3-epoxides in high site- and enantioselectivity by the oxidation of relatively electron-deficient double bond: *Chem. Commun.* **2017**, *53*, 9320-9323**.** Themed Collections: Site-Selctive Molecular Transformation, Kawabata T. & Taylor M, Eds.

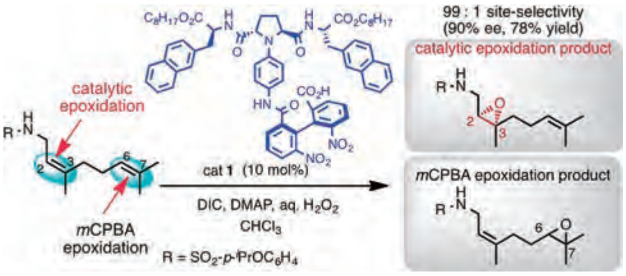

Figure 1.

Organocatalytic Site-Selective Acylation of Carbohydrates with a Low Catalyst Loading by an In-Situ Counter-Anion Exchange Method

Site-selective catalysis has attracted increasing attention because of its potential utility for direct diversification of bioactive natural products and medicinal candidates with multiple functional groups. Especially, development of catalysts that can promote the target reaction in a site-selective manner independent from the intrinsic reactivity of the substrates, *i.e., catalyst-controlled selectivity*, is a challenging objective in current organic synthesis. We reported site-selective acylation of a glucose derivative with organocatalyst **2**. Acylation of the intrinsically less reactive C(4)–OH in the presence of the otherwise more reactive primary C(6)–OH proceeds via precise molecular recognition between the catalytic intermediate and the substrate. However, relatively high catalyst loading (1 mol %) was indispensable for this transformation. We report here a new catalytic system that enables the catalyst loading to be reduced to 0.01 mol %. Acylpyridinium ions such as **A** and **B** have been known as catalytically-active species in acylation reactions catalyzed by 4-dimethylaminopyridine and its analogues. Acylpyridinium carboxylates **B** were found to be 800–1300 times more reactive than the corresponding acylpyridinium chlorides **A**. This catalytic system in which acylpyridinium carboxylates were generated by *in-situ* counter anion-exchange from the acylpyridinium chlorides made possible to the catalyst loading as low as 0.01 mol % and catalyst turnover number of up to 6700 for site-selective acylation, retaining the high site-selectivity of acylation of the carbohydrate: *Org. Lett.* **2017**, *19*, 3099-3102.

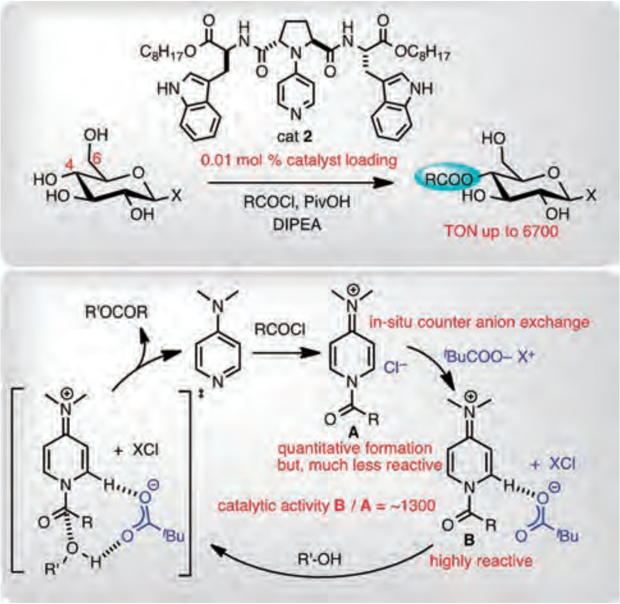

Figure 2.

Asymmetric Desymmetrization of Aliphatic *meso*-Dial via Intramolecular Aldol Reaction Catalyzed by Aniline-type Acid Base Catalyst

Multiple-substituted cyclopentanes have attracted much attention as a core structure of pharmaceuticals as well as natural products. Asymmetric desymmetrization of aliphatic *meso*-1,6-dial through intramolecular aldol reaction provides one of the attractive ways for accessing functionalized cyclopentanes. We found that aniline-type acid base catalyst **3** discriminated the enantiotopic formyl groups of *meso*-dial and controlled four contiguous stereogenic centers well to give *anti-anti*-aldol adduct as a sole product in high diastereo- and enantioselectivities.

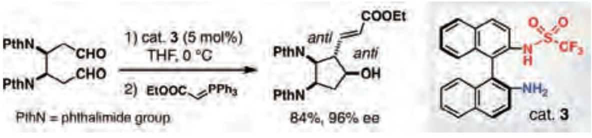

Figure 3.

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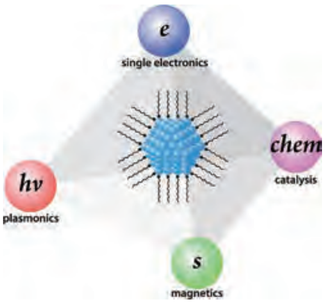
FARRAS, Pau (Ph D)
The National University of Ireland – Galway, Spain, 27 November–27 December

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
Nanocomposite Magnet
Single Electronics
Photocatalysts
Plasmonics

Selected Publications

Eguchi, D.; Sakamoto, M.; Tanaka, D.; Okamoto, Y.; Teranishi, T., Porphyrin Derivative-Protected Gold Cluster with a Pseudotetrahedral Shape, *J. Phys. Chem. C*, **121,** 10760-10766 (2017).

Kim, S.; Nishino, T.; Saruyama, M.; Sakamoto, M.; Kobayashi, H.; Akiyama, S.; Yamada, T.; Domen, K.; Teranishi, T., Formation of Layer-by-Layer Assembled Cocatalyst Films of S^{2-}-stabilized Ni_3S_4 Nanoparticles for Electrochemical Hydrogen Evolution Reaction, *ChemNanoMat*, **3,** 764-771 (2017).

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 Layer-by-Layer Assembled Cocatalyst Films of S^{2-}-Stabilized Ni_3S_4 Nanoparticles for Hydrogen Evolution Reaction

Production of hydrogen fuel by electrolysis of water is a promising and sustainable solution to energy problems. In recent years, a number of metal sulfide have been identified as promising candidates for hydrogen evolution reaction (HER) electrocatalysts. Nanoparticle (NP) materials have advantages for fabrication of HER electrodes based on their large surface-to-volume ratios, however, surface organic ligands can hinder electron transfer both from the electrode to the NPs and from the NPs to protons. Recently, ligand-exchange methods have been developed, in which small inorganic ligands are used to replace the original organic ligands. Here, we report the layer-by-layer (LbL) assembly of S^{2-}-stabilized Ni_3S_4 NPs (Ni_3S_4/S^{2-}) and metal cation modified Ni_3S_4/S^{2-} ($Ni_3S_4/S^{2-}/M^{2+}$ (M = Cd, Ni, Co, or Zn)) NPs to improve electron transfer and increase the electrochemically active surface area (Figure 1a). LbL film of Ni_3S_4/S^{2-} NPs showed much lower overpotential and higher stability than that of Ni_3S_4 NPs protected by organic ligands. Additionally, this LbL assembly technique could be applied as a HER cocatalyst on the cathodic photocatalyst electrode, CdS/Cu(In,Ga)Se_2. The photocurrent was enhanced compared with that of organic ligands-stabilized Ni_3S_4 NP-loaded and bare electrodes (Figure 1b). This LbL assembly process could be applicable to forming ligand-free and robust NP films for many types of photoelectrodes without deteriorating their intrinsic optical properties.

Ligand Effect on the Catalytic Activity of Porphyrin Protected Gold Clusters in the Electrochemical Hydrogen Evolution Reaction

Metal clusters (MCs) are promising catalysts due to their unique quantized electronic structures and large surface-to-volume ratios. Because of their large surface-to-volume ratios, the electronic structures of MCs should be perturbed by organic ligands. Recently, it was found that the face-on coordination of porphyrin derivatives (SC_nP, n = 1 or 2) with AuCs caused a dramatic perturbation in the electronic structure of the SC_nP. Therefore, face-coordination of SC_nP with AuCs could strongly influence their catalytic activity. Here, we systematically studied the ligand effect of SC_nP on AuCs in the electrochemical hydrogen evolution reaction (Figure 2a), which is a key catalytic reaction for producing clean energy from inexhaustible water. AuCs with face-coordinated SC_1P show a 460% higher current density at overpotential of 0.4 V compared with phenylethanethiol (PET)-protected AuCs (Figure 2b). The dramatic catalytic enhancement is attributed to charge migration from the porphyrin to the Au core. This ligand effect provides a novel strategy for enhancing the catalytic activity of MCs.

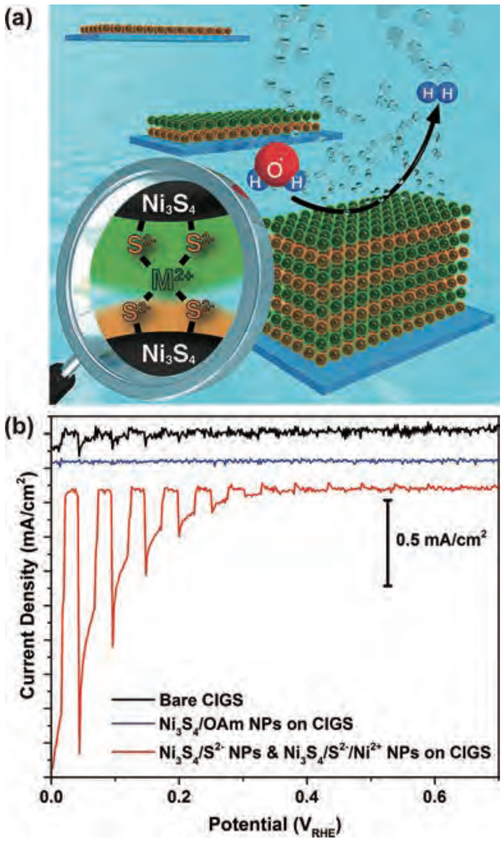


Figure 1. (a) Illustration of LbL assembly of Ni_3S_4/S^{2-} NPs on an electrode substrate. (b) Photocurrent density vs potential plots of bare, organic ligand-protected Ni_3S_4 NPs, and Ni_3S_4/S^{2-} NPs modified CdS/Cu(In,Ga)Se_2 photoelectrodes.

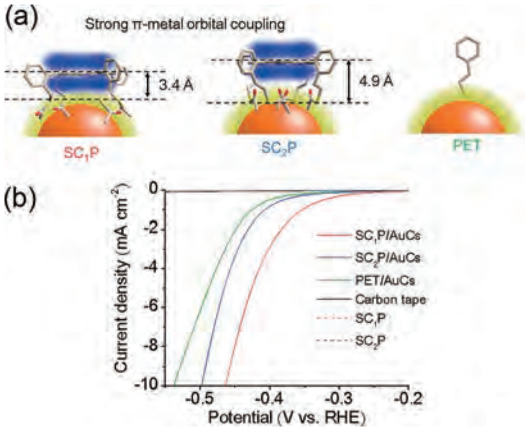


Figure 2. (a) Illustration of coordination fashions of SC_nP and PET on Au surface. (b) HER polarization curves of each AuCs, SC_nP, and bare carbon paper in 0.5 M phosphate buffer solution (pH 6.7).

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PIETRASIK, Joanna (Ph D)	Lodz University of Technology, Poland, 5 June–5 July

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
Hybrid Materials
Living Radical Polymerization
Biointerface
Polymer Brush

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).

Soft and Resilient Tribology (SRT) Systems Using Concentrated Polymer Brushes

Concentrated polymer brushes (CPBs) have received much attention because of their super-lubrication property in good solvents, exhibiting ultra-low frictional coefficient (μ) on the order of 10^{-4} revealed by AFM. We have revealed the lubrication mechanisms of CPBs, i.e., hydrodynamic and boundary lubrication, from the results of the swelling behavior as well as the solvent viscosity used for the microtribological measurements. Furthermore, the macroscopic super-lubrication property has recently been confirmed using extraordinarily thick CPBs synthesized under high-pressure surface-initiated atom transfer radical polymerization. Toward industrial applications, the issue of improving the durability/wearability/resiliency should be addressed. Here we demonstrate the tribological properties of thick poly(methyl methacrylate) (PMMA)-CPBs with an improved resilience in an ionic liquid, *N*-(2-methoxyethyl)-*N*-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide (MEMP-TFSI). Figure 1 shows the Stribeck curves (friction profiles) of PMMA-CPBs using a macroscopic ball-on-disk setup at rt, where η, υ, F_n represent viscosity of the solvent, sliding speed, and normal force, respectively. The low μ as 10^{-3} order under low sliding speeds was obtained in an extremely high normal force up to 50 N. Compared to the other soft-lubricating systems including the previously-reported CPBs, the resilient CPBs exhibited unique normal force-induced frictional increments over a wide range of sliding speeds. Such a deviation from the master Stribeck curve could be attributed to non-hydrodynamic effects owing to their viscoelastic properties of the swollen CPBs, which is a new mechanism to control the sliding surfaces upon high normal loads. The resilient CPBs have now been tested for various sliding surfaces including seals, bearings, and so on, with collaborations between chemical, rheological, informative, and machine engineering research groups.

Strain Hardening of Highly Stretchable Elastomeric Composites Reinforced with Well-Defined Nanofiber Network of Bacterial Cellulose

Highly stretchable poly(ethyl acrylate) (PEA) composites reinforced with a well-defined nanofiber network of bacterial cellulose (BC) were prepared via stepwise solvent exchange followed by *in situ* photo-initiated free radical polymerization. Despite the small volume fraction of BC (approximately 0.4 vol%), the BC/PEA composite showed significant increases in Young's modulus (26 times larger than that of the neat PEA), tensile strength (3.5 times larger), and fracture energy (3.8 times larger), with its fracture strain (1520 %) almost the same as that of the neat PEA (1660 %). This composite was characterized by effective strain hardening. The changes in strain-hardening modulus and tensile strength were explained well by the rule of mixtures. Confocal laser scanning microscopic (CLSM) observations revealed the structure of the nanofibers embedded in the elastomeric matrix. The enhanced mechanical properties were based on the rigidity and flexibility of the BC nanofibers and their entangled network, and were ascribed to the well-defined BC nanofiber network produced by the bacterium.

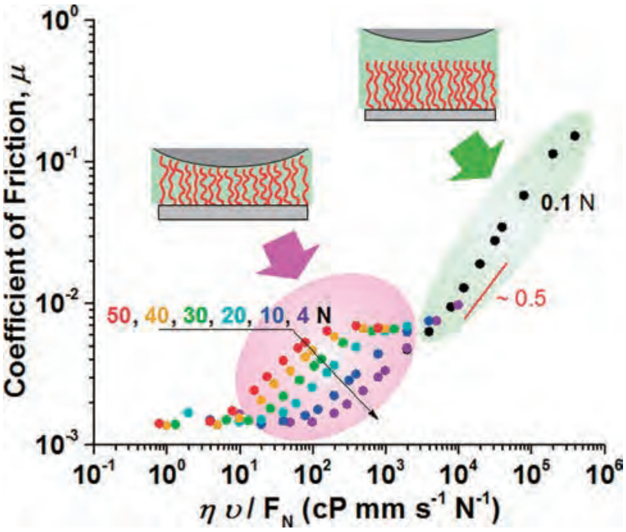

Figure 1. Plots of μ vs $\eta\upsilon/F_n$ for PMMA-CPB vs bare-glass measured in MEMP-TFSI at F_n = 0.1, 4, 10, 20, 30, 40, and 50 N.

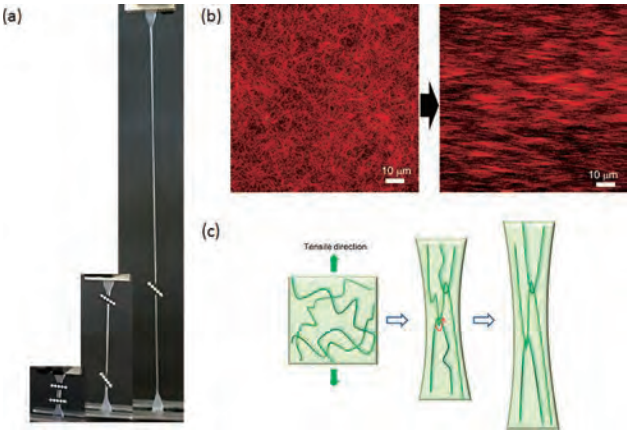

Figure 2. (a) Images of the BC/PEA composite in the tensile tests; the strains were 0, 400, and 1400 % from left to right. (b) CLSM images of the composites before (left) and during (right) stretching, indicating high alignment of bacterial cellulose nanofibers. (c) Schematic illustration of the proposed BC-reinforcement mechanism of the BC/PEA elastomer.

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Scope of Research

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

KEYWORDS

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

Selected Publications

Hashimoto, S.; Iwamoto, T.; Kurachi, D.; Kayahara, E.; Yamago, S., Shortest Double-Walled Carbon Nanotubes Composed of Cycloparaphenylenes, *Chempluschem*, **82,** 1015-1020 (2017).

Lu, Y.; Nemoto, T.; Tosaka, M.; Yamago, S., Synthesis of Structurally Controlled Hyperbranched Polymers Using a Monomer Having Hierarchical Reactivity, *Nat. Commun.*, **8,** 1863 (2017).

Shortest Double-Walled Carbon Nanotubes Composed of Cycloparaphenylenes

Multiwalled carbon nanotubes (CNTs) consist of multiple rolled layers of graphene. This type of materials have interesting electrical, optical, mechanical, and thermal properties. Because variety of applications are expected for these materials, it is important to better understand CNTs on the molecular level. Cycloparaphenylenes (CPPs) are good compounds as a model for the basic studies on CNTs because these nanorings are the smallest possible structures corresponding to the sidewalls of CNTs. It had been predicted that CPPs of different sizes would form host–guest complexes stabilized by attractive van der Waals interactions.

Our group did prove that CPPs form host–guest complexes (example pictured) selectively: when [6]CPP is mixed with equimolar amounts of [8]–[12]CPPs, the only complex that forms is that in which [6]CPP is nested inside [11]CPP, denoted as [11]CPP ⊃ [6]CPP (Figure 1, left). Our work indicated that in other favored combinations, the inner and outer rings differ in size by five phenylene units. The ternary complex [15]CPP ⊃ [10]CPP ⊃ C_{60} formed a “planetary orbit” structure (Figure 1, right). In all of these complexes, the difference in the diameters of the nesting aromatic hydrocarbons was found to be 0.035 nm which corresponds to the distance separating the curved graphene layers in CNTs.

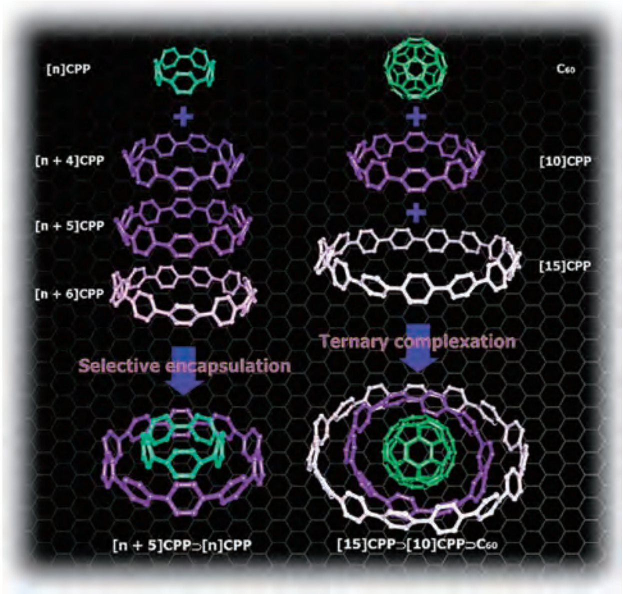

Figure 1. Selective encapsulation of CPPs and/or C_{60} into the larger CPP.

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

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

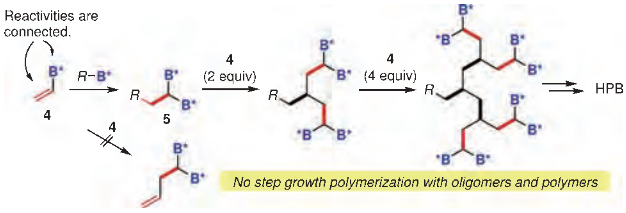

Figure 2. Scheme for the synthesis of structurally controlled hyperbranched polymer.

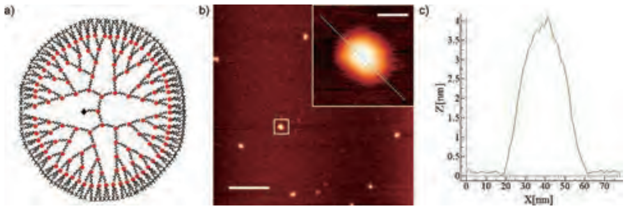

Figure 3. Structure and AFM image of the dendritic hyperbranched polymer.

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Scope of Research

NV center in diamond has been extensively interested because the single spin of it can be manipulated and detected at room temperature. Furthermore, spin coherence time of the NV center is very long. The coherence time is the time to retain coherence (superposition state) and directly relates to the sensitivity of sensor 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

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

Doi, Y.; Makino, T.; Kato, H.; Takeuchi, D.; Ogura, M.; Okushi, H.; Morishita, H.; Tashima, T.; Miwa, S.; Yamasaki, S.; Wrachtrup, J.; Suzuki, Y.; Mizuochi, N., Deterministic Electrical Charge State Initialization of Single Nitrogen-vacancy Center in Diamond, *Phys. Rev. X*, **4,** [11057-1]-[11057-11] (2014).

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

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

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Hybrid Quantum Magnetic-field Sensor with an Electron Spin and a Nuclear Spin in Diamond

Recently, magnetic-field sensors based on an electron spin of a nitrogen vacancy center in diamond have been studied both from an experimental and theoretical point of view. This system provides a nanoscale magnetometer, and it is possible to detect a precession of a single spin. In this research, we propose a sensor consisting of an electron spin and a nuclear spin in diamond as shown in Figure 1. Although the electron spin has a reasonable interaction strength with magnetic field, the coherence time of the spin is relatively short. On the other hand, the nuclear spin has a longer lifetime while the spin has a negligible interaction with magnetic fields. We show that, through the combination of such two different spins via the hyperfine interaction, it is possible to construct a magnetic-field sensor with the sensitivity far beyond that of previous sensors using just a single electron spin. We revealed that if the gate error is below 0.1%, the sensitivity of our sensor is one order of magnitude better than the conventional one.

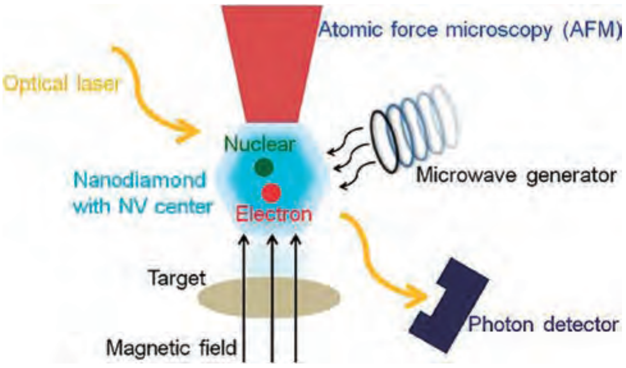

Figure 1. The structure of our hybrid NV center sensor: a diamond containing an NV center with an electron spin and a nuclear spin is attached to an AFM tip. Single qubit rotations and a C-NOT gate can be performed by directing a microwave into the diamond.

Perfect Selective Alignment of Nitrogen-vacancy Center in Diamond

Nitrogen-vacancy (NV) centers in diamond have attracted significant interest because of their excellent spin and optical characteristics for quantum information and metrology. In the diamond crystal structure, the orientations of NV centers are classified according to the alignment along one of four possible crystallographic axes: [111], $[1\bar{1}\bar{1}]$, $[\bar{1}1\bar{1}]$ or $[\bar{1}\bar{1}1]$ as shown in Figure 2. In most diamond samples, NV centers equally occupy these four orientations. To take advantage of the characteristics, the precise control of the orientation of the N–V axis in the lattice is essential. It is because improvement in readout contrast and a magnetic field sensitivity can be expected when compared to with those of standard samples with equal population of all NV orientations. Furthermore, spin and optical characteristics strongly depend on this orientation. In cases where photoluminescence (PL) is detected from the [111] direction, the PL intensity from N–V centers in which the N–V axis is parallel to [111] (NV ∥ [111]) is higher than others because electric dipole transitions are allowed for dipoles in the plane perpendicular to the N–V axis. With respect to spin, it is expected to play a key role at the quantum interface with photon and superconducting flux qubits.

We experimentally showed that the orientation of more than 99 % of the NV centers can be aligned along the [111]-axis by CVD homoepitaxial growth on (111)-substrates. We also discuss about mechanisms of the alignment. We examined the atomistic generation mechanism for the NV defect aligned in the [111] direction of C(111) substrates with first-principles electronic structure calculations. Our result enables a fourfold improvement in magnetic-field sensitivity and opens new avenues to the optimum design of NV center devices.

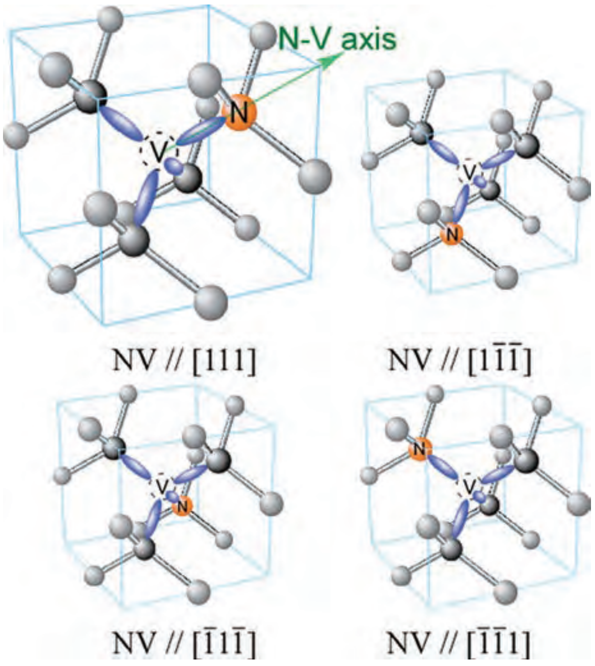

Figure 2. Four possible orientations of NV centers in diamond crystal.

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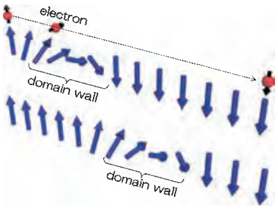
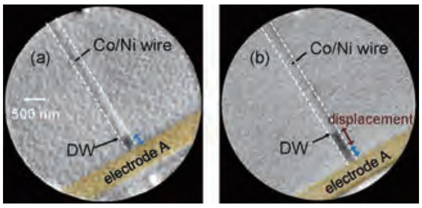
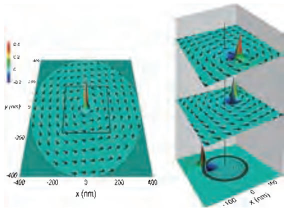
KEYWORDS
Spintronics
Magnetism
Magnetic Materials

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.







Selected Publications

Kim, K.-J.; Kim, S. K.; Hirata, Y.; Oh, S.-H.; Tono, T.; Kim, D.-H.; Okuno, T.; Ham, W.; Kim, S.; Go, G.; Tserkovnyak, Y.; Tsukamoto, A.; Moriyama, T.; Lee, K.-J.; Ono, T., Fast Domain Wall Motion in the Vicinity of the Angular Momentum Compensation Temperature of, *Nat. Mater.*, doi: 10.1038/nmat4990 (2017).
Kim, S.; Jang, P.; Kim, D.; Ishibashi, M.; Taniguchi, T.; Moriyama, T.; Kim, K.; Lee, K.; Ono, T., Magnetic Droplet Nucleation with a Homochiral Neel Domain Wall, *Phys. Rev. B*, **95,** 220402 (2017).
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Kim, K.; Yoshimura, Y.; Ham, W.; Ernst, R.; Hirata, Y.; Li, T.; Kim, S.; Moriyama, T.; Nakatani, Y.; Ono, T., Energy-efficient Writing Scheme for Magnetic Domain-wall Motion Memory, *Applied Physics Express*, **10,** 043002 (2017).

Modulation of the Magnetic Domain Size Induced by an Electric Field

The electric field (EF) control of magnetism has intensively investigated because of its potential importance for the reduction of power consumption in magnetic storage devices. In the past few years, we have been focusing on the electric field modulation of the magnetic anisotropy and the Curie temperature in magnetic thin films. However, the microscopic mechanism of why those magnetic properties change with an electric field were not clear in spite of several theoretical suggestions. In this work, we particularly focused on the configuration of the magnetic domains upon the application of the electric field (see Figure 1a for the detail measurement setup). With the electric field of ±10V, we observed the significant change in the domain size (Figure 1b). Detail analyses on the modification of the magnetic domain size revealed that it is the exchange interaction that is modulated with the electric field and is changing about 50% with ±10V. Our results suggest that the EF control of the magnetism is mainly driven by the modification of the exchange interaction which is a fundamental measure determining the magnetic interaction between microscopic spins.

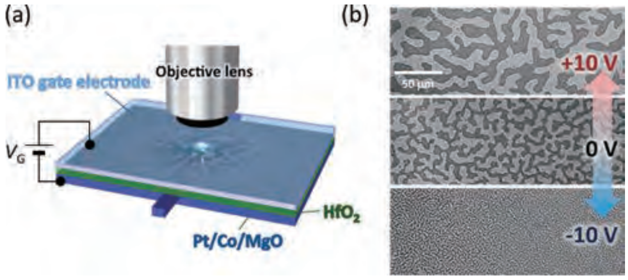

Figure 1. (a) Schematic illustration of the experimental setup (b) Modulation of the magnetic domain size with the electric field of ±10V.

Ultrafast Domain Wall Motion in Ferrimagnetic Materials

Antiferromagnetic spintronics is an emerging research field which aims to utilize antiferromagnets as core elements in spintronic devices. A central motivation towards this direction is that antiferromagnetic spin dynamics is expected to be much faster than its ferromagnetic counterpart. Recent theories indeed predicted faster dynamics of antiferromagnetic domain walls (DWs) than ferromagnetic DWs. However, experimental investigations of antiferromagnetic spin dynamics have remained unexplored, mainly because of the magnetic field immunity of antiferromagnets. Here we show that fast field-driven antiferromagnetic spin dynamics is realized in ferrimagnets at the angular momentum compensation point T_A. Using rare earth–3d-transition metal ferrimagnetic compounds where net magnetic moment is nonzero at T_A, the field-driven DW mobility is remarkably enhanced up to 20 km s^{-1} T^{-1}. The collective coordinate approach generalized for ferrimagnets and atomistic spin model simulations show that this remarkable enhancement is a consequence of antiferromagnetic spin dynamics at T_A. Our finding allows us to investigate the physics of antiferromagnetic spin dynamics and highlights the importance of tuning of the angular momentum compensation point of ferrimagnets, which could be a key towards ferrimagnetic spintronics.

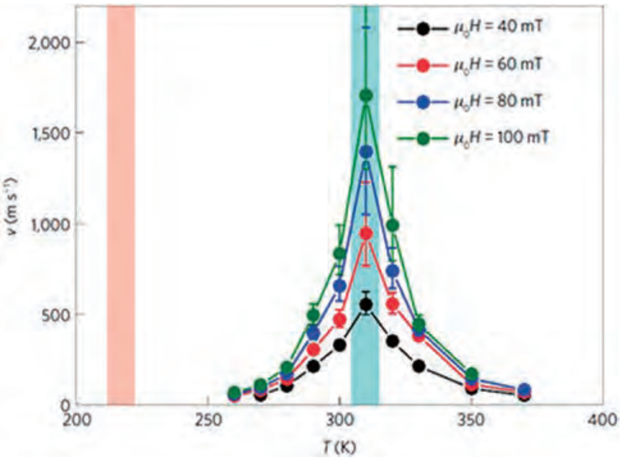

Figure 2. DW speed v as a function of temperature T for several driving fields. v diverges at T_A.

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NOMURA, Yohei (UG)
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Guest Res Assoc

ZSUZSA, Baranyai	MTA-ELTE, Hungary, 2–8 July

Scope of Research

The ultimate goal of our research is the regulation of cellular functions using designed peptides and proteins. Current research subjects include 1) development of novel intracellular delivery systems aiming at elucidation and control of cellular functions using designed membrane-permeable peptide vectors, 2) elucidation of the DNA binding modes of zinc finger proteins and TALEs, and design of artificial transcription factors with various DNA binding specificities, 3) elucidation and control of membrane curvature, and 4) design of stimulation-responsible artificial peptides and proteins.

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

Selected Publications

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

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

Futaki, S.; Nakase, I., Cell-Surface Interactions on Arginine-Rich Cell-Penetrating Peptides Allow for Multiplex Modes of Internalization, *Acc. Chem. Res.*, **50,** 2449-2456 (2017).

Tsuji, S.; Futaki, S.; Imanishi, M., Sequence-Specific Recognition of Methylated DNA by an Engineered Transcription Activator-Like Effector Protein, *Chem. Commun.*, **52,** 14238-14241 (2016).

Loosening of Lipid Packing Promotes Oligoarginine Entry into Cells

The mechanisms for internalization of arginine-rich cell-penetrating peptides (CPPs), including the HIV-1 TAT peptide and oligoarginines, are still under debate although many factors that promote direct translocation of CPPs across the cell plasma membrane were reported (Figure 1A). These days, amphipathic helices are found in the common motif for membrane active peptides / proteins, including curvature inducing proteins. We previously reported that the N-terminal segment of epsin-1 possesses positive membrane curvature inducibility and that this peptide promotes membrane translocation of R8, which is known as a representative CPP. We this time used differential scanning calorimetry (DSC) to assess the curvature inducibility of amphipathic peptides, which are derived from proteins to induce tabulation/fusion of liposomal membranes. As the result, cytosolic distribution of FITC-R8 was observed in the presence of EpN18 and Sar1p(1-23) with positive membrane curvature inducibility at about 80 % and 100 % of the cell population, respectively. Furthermore, the sites of R8 influx were found to have looser lipid packing than surrounding areas, revealed by using environment-sensitive probe (di-4-ANEPPDHQ). Taken together, the importance of lipid packing was demonstrated as a key factor, which underlies the various conditions to promote the direct membrane translocation of arginine-rich CPPs (Figure 1B).

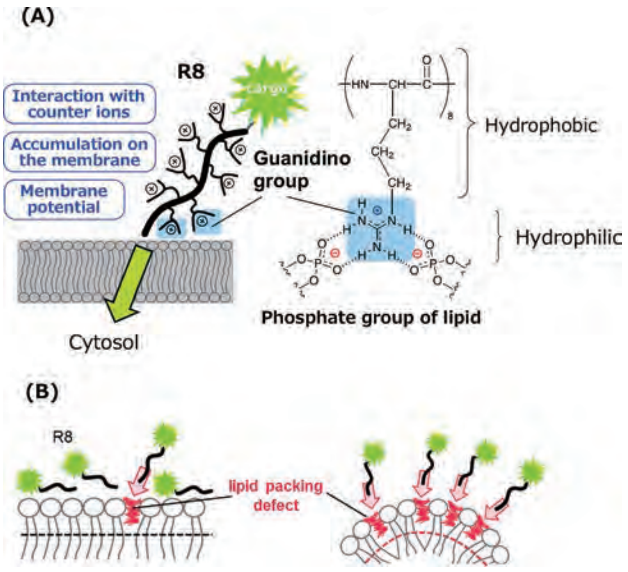

Figure 1. The mechanism underlying the membrane penetration of R8.

Cytosolic Antibody Delivery by Lipid-sensitive Endosomolytic Peptide

Antibodies have high abilities in molecular recognition and targeting. Intracellular antibody delivery could thus achieve controlling cellular events, such as protein-protein interaction and post-translational modification. This suggests the potential applicability of antibodies to attack intracellular therapeutic targets. Many approaches for intracellular delivery of biomacromolecules have been reported up to the present time. However, few of them are efficient enough to deliver high-molecular-weight proteins such as antibodies into cytosol to effectively modulate cell functions.

In order to deliver various membrane-impermeable molecules into the cytosol effectively and efficiently, we developed a novel endosome-destabilizing peptide, L17E by engineering the structure of a hemolytic peptide derived from a spider toxin. This peptide showed significant stimulation of cytosolic release of endocytosed molecules, including polydextran (10kDa), Cre recombinase and antibodies (IgG). Successful recognition of intracellular targets by the intracellularly delivered antibodies was confirmed by confocal microscopic analysis and the effect on signal transduction. These results suggested that this peptide holds the promise of modifying cell functions.

Unlike previously reported intracellular delivery peptides and polymers, the mechanism of action of L17E was found to be its preferential perturbation of negatively charged endosomal membranes. Additionally, we found that L17E also has a property to stimulate cellular uptake amount of biomacromolecues. These are unique features equipped with our peptide which have not been reported for other delivery peptides and polymers. We serendipitously found these features after we obtained this peptide.

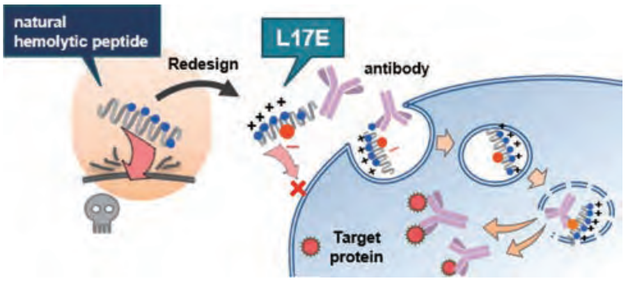

Figure 2. A simple redesign of spider venom peptide ‘M-lycotoxin’ into L17E enables the efficient release of antibodies from their endosome cages.

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Scope of Research

Life is the integration of numerous chemical interactions conducted by low molecular weight compounds and proteins. Our interest is understanding the mechanisms of these interactions from the viewpoint of organic chemistry. Our current research focuses on the following: a) Design and synthesis of a series of chemical probes in order to reveal not only ligand–protein and protein–protein interactions, but also behavior of low molecular weight compounds *per se*. b) Unraveling biosynthetic pathways of bioactive natural products at enzyme level. c) Application of our chemical probes in development of novel practical bioactive compounds.

KEYWORDS

Enzyme Inhibitors
γ-Glutamyl Transpeptidase
Fructosyl Peptide Oxidase
Diabetes Diagnosis
Protein–Protein Interaction Inhibitors

Selected Publications

Watanabe, B.; Tabuchi, Y.; Wada, K.; Hiratake, J., Synthesis and Evaluation of the Inhibitory Activity of the Four Stereoisomers of the Potent and Selective Human γ-Glutamyl Transpeptidase Inhibitor GGsTop, *Bioorg. Med. Chem. Lett.*, **27,** 4920-4924 (2017).

Watanabe, B.; Morikita, T.; Tabuchi, Y.; Kobayashi, R.; Li, C.; Yamamoto, M.; Koeduka, T.; Hiratake, J., An Improved Synthesis of the Potent and Selective γ-Glutamyl Transpeptidase Inhibitor GGsTop together with an Inhibitory Activity Evaluation of Its Potential Hydrolysis Products, *Tetrahedron Lett.*, **58,** 3700-3703 (2017).

Kamiyama, A.; Nakajima, M.; Han, L.; Wada, K.; Mizutani, M.; Tabuchi, Y.; Kojima-Yuasa, A.; Matsui-Yuasa, I.; Suzuki, H.; Fukuyama, K.; Watanabe, B.; Hiratake, J., Phosphonate-Based Irreversible Inhibitors of Human γ-Glutamyl Transpeptidase (GGT). GGsTop is a Non-Toxic and Highly Selective Inhibitor with Critical Electrostatic Interaction with an Active-Site Residue Lys562 for Enhanced Inhibitory Activity, *Bioorg. Med. Chem.*, **24,** 5340-5352 (2016).

Watanabe, B.; Ichiyanagi, A.; Hirokawa, K.; Gomi, K.; Nakatsu, T.; Kato, H.; Kajiyama, N., Synthesis and Inhibitory Activity of Substrate-Analog Fructosyl Peptide Oxidase Inhibitors., *Bioorg. Med. Chem. Lett.*, **25,** 3910-3913 (2015).

Watanabe, B.; Minami, S.; Ishida, H.; Yoshioka, R.; Nakagawa, Y.; Morita, T.; Hayashi, K., Stereospecific Inhibitory Effects of CCG-1423 on the Cellular Events Mediated by Myocardin-Related Transcription Factor A., *PLoS One*, **10,** [e0136242-1]-[e0136242-16] (2015).

Topics

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

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

Substrate-Analog Fructosyl Peptide Oxidase Inhibitors

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

Molecular Mechanism of Myocardin-Related Transcription Factor A Inhibitors

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

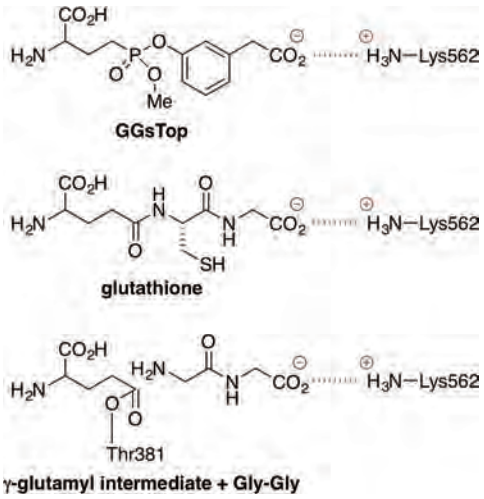

Figure 1. Proposed binding mode of GGsTop, glutathione, and acceptor substrate (Gly-Gly) to Lys562.

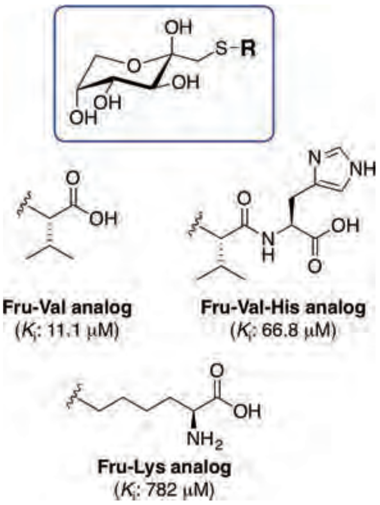

Figure 2. Chemical structures and inhibitory activity of FPOX inhibitors.

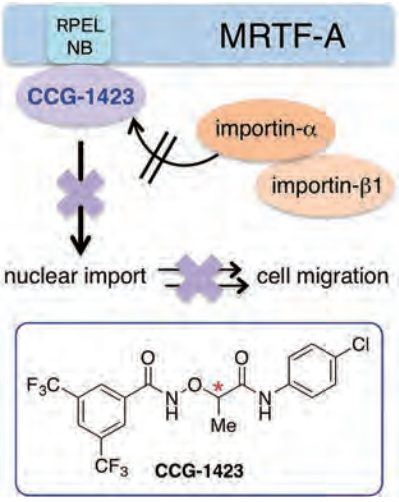

Figure 3. Molecular mechanism of MRTF-A inhibitor CCG-1423.

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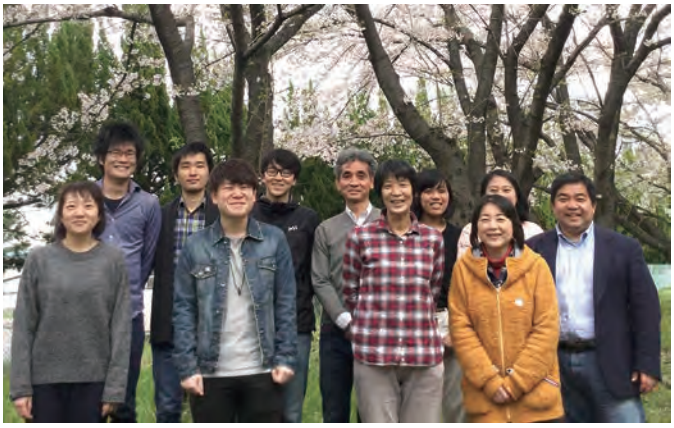
Scope of Research

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

KEYWORDS
Morphogenesis
Signal Transduction
Phospholipid Signaling
COP9 Signalosome
RNA



Selected Publications

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

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

Biological Functions of Phosphoinsitide Signaling in Plant Cells

Phosphatidylinositol 4,5-bisphosphate [PtdIns(4,5)P_2] regulates signal transduction for not only total cellular responses but also intracellular localizing events. It modulates the functions of a variety of actin regulatory proteins and regulators of exocytotic machinery on the plasma membrane by directly interacting with its effector proteins. In many cases, PtdIns(4,5)P_2 signaling pathways are tightly connected to those of small GTPases belonging to the Rho and Arf families in their upstream and downstream cascades. PtdIns(4,5)P_2 is also expected to play a pivotal regulatory role in the polarized expansion of plant cells. Indeed, PtdIns(4,5)P_2 localizes to the apical plasma membrane and cytoplasmic space of not only root hairs but also pollen tubes. We are studying on signaling functions of PtdIns(4,5)P_2 and its producing enzymes, PIP5Ks, in *Arabidopsis thaliana*. Recently, fluorescent molecular probes for phosphoinositides were drastically improved. Taking advantage of those probes, we are observing specific and dynamic localization patterns of PtdIns(4,5)P_2 in various types of *Arabidopsis* cells (Figure 1).

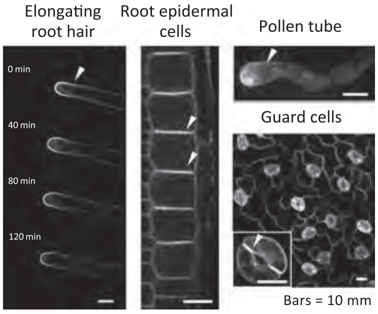

Figure 1. Dynamic localization patterns of PtdIns(4,5)P_2 markers (*UBQ10* promoter-driven fluorescence protein-fused 2xPH$^{PLC\delta}$). Arrowheads indicate loci where PtdIns(4,5)P_2 markers are preferentially localized.

Function of an *Arabidopsis thaliana* Brix Family Protein Gene in Female Gametogenesis

Male and female gametophytes, also called pollen grains and embryo sacs, respectively, include a few haploid cells embedded in the sexual reproductive organs of angiosperms. During gametogenesis of the female gametophyte in *Arabidopsis*, first, a hypodermal archesporial cell differentiates into a megaspore mother cell, which undergoes meiosis to produce four haploid megaspores. Three of these megaspores at the micropylar pole go through programmed cell death, while the chalazal-most one survives and then undergoes three consecutive rounds of nuclear division to give rise to an eight-nucleate, cenocytic embryo sac. Next, nuclear migration and cellularization occur, resulting in a seven-celled embryo sac: three antipodal cells at the chalazal pole, one diploid central cell, an egg cell and two synergid cells at the micropylar end (Figure 2).

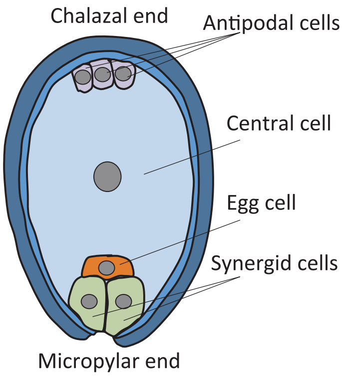

Figure 2. Schematic illustration of a seven-celled embryo sac.

AtSNAIL1 shares high sequence identity with yeast Ssf1 and Ssf2 proteins. The yeast strain *ssf1*-Δ *ssf2*-Δ was lethal. Reduction of the SSF gene products resulted in arrested cell division cycles and a decrease in the cell-mating efficiency. Further investigation showed that Ssf1 was required for synthesis of 5.8S and 25S rRNA and, thus, essential for the synthesis of the large ribosomal subunit. We found that the disruption of the *AtSNAIL1* gene caused retarded progression of mitotic division cycles during female gametophyte development *in vivo*, and thus led to severe reduction of female transmission efficiency in *snail1* (Figure 3). Furthermore, we found that the mutation in *SNAIL1* caused delay and failure in protein synthesis in the synergid cell. These indicate that functionally conserved *AtSNAIL1* is essential for reproductive development in *Arabidopsis*, possibly by affecting ribosome biogenesis.

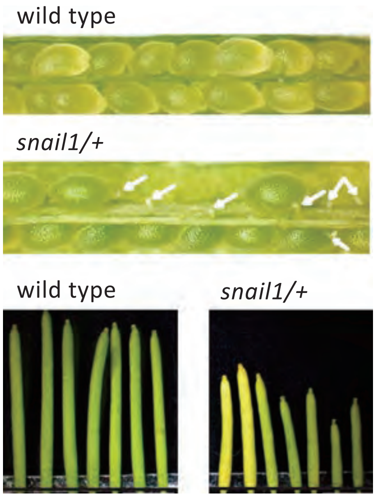

Figure 3. Seed sets (upper panels) and siliques (lower panels) of wild-type and *snail1/+* heterozygous plants. Arrows indicate unfertilized ovules in the *snail1/+* seed set.

Division of Biochemistry
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Scope of Research

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

KEYWORDS

Cell Therapy
Chemical Library
Chemical Biology
Chemical Genetics
Small Molecules

Selected Publications

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

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

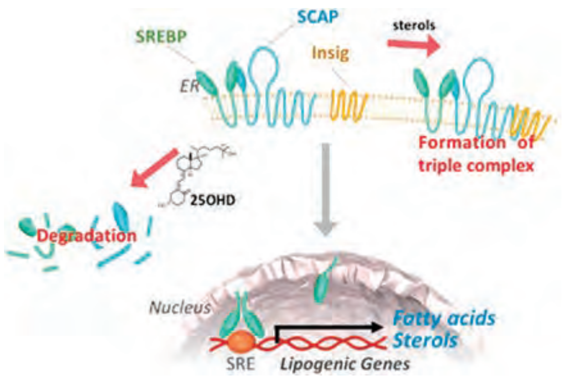
Katsuda, Y.; Sato, S.; Asano, L.; Morimura, Y.; Furuta, T.; Sugiyama, H.; Hagihara, M.; Uesugi, M., A Small Molecule that Represses Translation of G-quadruplex-containing mRNA, *J. Am. Chem. Soc.*, **138,** 9037-9040 (2016).

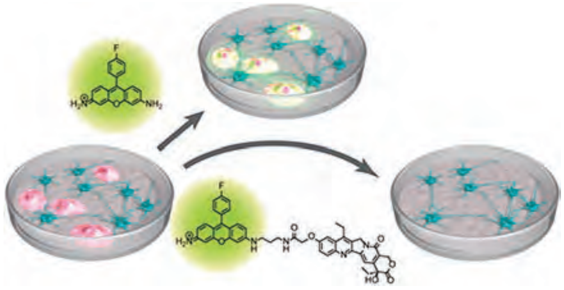
Vitamin D Metabolite, 25-Hydroxyvitamin D, Regulates Lipid Metabolism by Inducing Degradation of SREBP/SCAP

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

A Synthetic Hybrid Molecule for the Selective Removal of Human Pluripotent Stem Cells from Cell Mixtures

A major hurdle in stem cell therapy is the tumorigenic risk of residual undifferentiated stem cells. In this, we carried out the design and evaluation of synthetic hybrid molecules that efficiently reduce the number of human induced pluripotent stem cells (hiPSCs) in cell mixtures. The design takes advantage of Kyoto probe 1 (KP-1), a fluorescent chemical probe for hiPSCs, and clinically used anticancer drugs. Among the KP-1–drug conjugates we synthesized, we found an exceptionally selective, chemically tractable molecule that induced the death of hiPSCs. Mechanistic analysis suggested that the high selectivity originates from the synergistic combination of transporter-mediated efflux and the cytotoxicity mode of action. Our study offers a chemical and mechanistic rationale for designing selective, safe, and simple reagents for the preparation of non-tumorigenic clinical samples.





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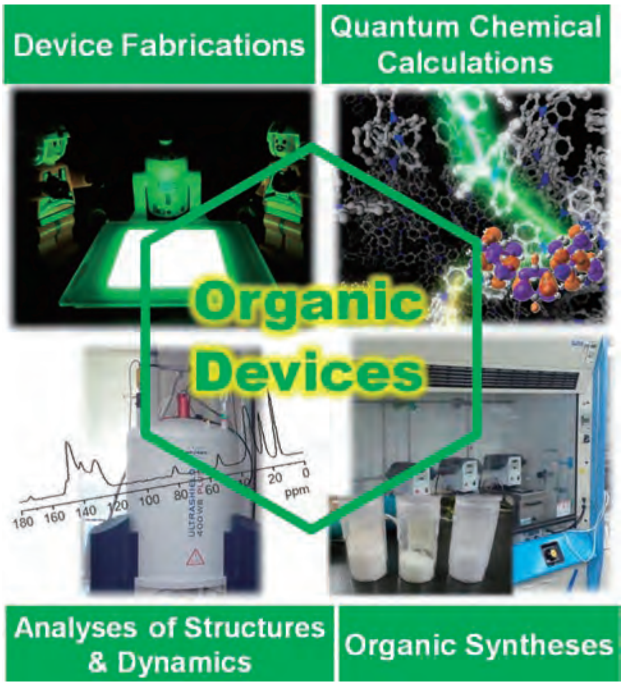
Scope of Research

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



KEYWORDS

Organic Light-Emitting Diodes
Organic Solar Cell
Solid-State NMR
Quantum Chemical Calculation
Amorphous Materials

Selected Publications

Suzuki, K.; Kubo, S.; Aussenac, F.; Engelke, F.; Fukushima, T.; Kaji, H., Analysis of Molecular Orientation in Organic Semiconducting Thin Films Using Static Dynamic Nuclear Polarization Enhanced Solid-State NMR Spectroscopy, *Angew. Chem. Int. Ed.*, **56,** 14842 (2017).

Miwa, T.; Kubo, S.; Shizu, K.; Komino, T.; Adachi, C.; Kaji, H., Blue Organic Light-Emitting Diodes Realizing External Quantum Efficiency Over 25% Using Thermally Activated Delayed Fluorescence Emitters, *Sci. Rep.*, **7,** 284 (2017).

Moon, C.; Suzuki, K.; Shizu, K.; Adachi, C.; Kaji, H.; Kim, J.-J., Combined Inter- and Intramolecular Charge-Transfer Processes for Highly Efficient Fluorescent Organic Light-Emitting Diodes with Reduced Triplet Exciton Quenching, *Adv. Mater.*, **29,** 1606448 (2017).

Deep-blue Organic Light-emitting Diodes Realizing External Quantum Efficiency Over 25% Using Horizontally Oriented Thermally Activated Delayed Fluorescence Emitters

Organic light-emitting diodes (OLEDs) have attracted great interest as a promising technique for developing solid-state lighting source and flexible flat-panel displays. To date, much improvements to the electroluminescence efficiency of OLEDs have been done employing thermally activated delayed fluorescence (TADF). However, it remains challenging to realize highly efficient deep-blue OLEDs. We develop deep blue TADF emitters, 3-(9H-[3,9′-bicarbazol]-9-yl)-9H-xanthen-9-one (CCX-I) and 3-(9′H-[9,3′:6′,9″-tercarbazol]-9′-yl)-9H-xanthen-9-one (CCX-II). They exhibit highly efficient deep-blue emission and high triplet-to-singlet conversion efficiency. In addition, CCX-I and CCX-II orient parallel to the glass substrate, which leads to increasing light-outcoupling efficiency and improving electroluminescence efficiency. A CCX-II-based OLED shows a maximum external quantum efficiency (EQE) of 25.9% with International de L'Eclairage (CIE) coordinates of (0.15, 0.22). With an out-coupling sheet, the maximum EQE further increased to 33.3%.

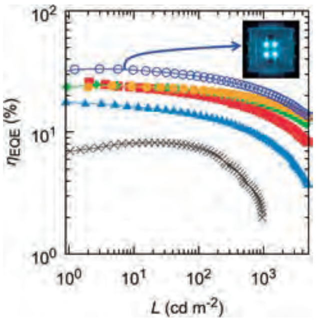


Figure 1. Luminance–EQE characteristics of the OLEDs containing CCX-II as an emitting dopant.

Charge Transport Simulations in Amorphous Thin Films for OLEDs

A fundamental understanding of charge transport properties of organic thin films is essential to improve OLED performance. Charge transport properties of organic molecules have been discussed in terms of their HOMO and LUMO energy levels and electronic couplings between molecules. The HOMO and LUMO can be calculated using quantum chemical calculations for isolated molecules, while the electronic couplings are considered to depend largely on an aggregated structure. We performed multiscale charge transport simulations for amorphous structures of *N*,*N*′-dicarbazole-3,5-benzene (mCP) and 4,4′-bis(*N*-carbazolyl)-1,1′-biphenyl (CBP), which have been used as a host material for OLEDs. By explicitly considering organic molecules, we investigated the contribution of respective molecular pairs to the charge transport in amorphous thin films. The molecular-level analysis of the charge transport simulations showed that molecular pairs with large electronic couplings are not most important in charge transport processes. Charges were found to be transported effectively in the forward direction via other molecular pairs that do not have substantially large electronic couplings.

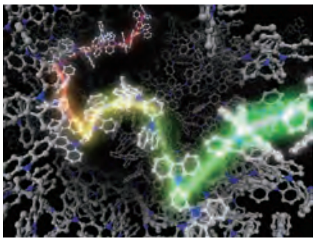


Figure 2. Image of charge transport in amorphous organic thin films.

Analysis of Molecular Orientation in Organic Semiconducting Thin Films Using Dynamic Nuclear Polarization Enhanced Solid-state NMR Spectroscopy

Molecular orientation in amorphous organic semiconducting thin-film devices is an important issue affecting device performance. However, to date it has not been possible to analyze the "distribution" of the orientations. Although solid-state NMR (ssNMR) spectroscopy can provide information on the "distribution" of molecular orientations, the technique is limited because of the small amount of sample in the device and the low sensitivity of ssNMR. Here, we report the first application of dynamic nuclear polarization enhanced ssNMR (DNP-ssNMR) spectroscopy for the orientational analysis of amorphous phenyldi(pyren-1-yl)phosphine oxide (POPy$_2$). The ^{31}P DNP-ssNMR spectra exhibited a sufficient signal-to-noise ratio to quantify the distribution of molecular orientations in amorphous films: the P=O axis of the vacuum-deposited and drop-cast POPy$_2$ shows anisotropic and iso-tropic distribution, respectively. The different molecular orientations reflect the molecular origin of the different charge transport behaviors.

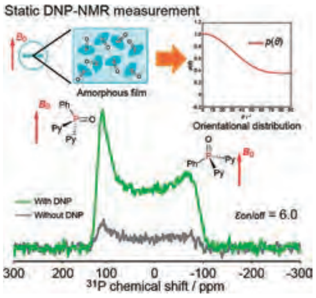


Figure 3. Analysis of molecular orientation using DNP-NMR.

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Scope of Research

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

KEYWORDS
Marine Chemistry
Trace Elements
Metal Ion Recognition
Analytical Chemistry
Stable Isotopes

Selected Publications

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

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

Nakashima, Y.; Shimizu, A.; Maruo, M.; Sohrin, Y., Trace Elements Influenced by Environmental Changes in Lake Biwa: (I) Seasonal Variations under Suboxic Hypolimnion Conditions during 2007 and 2009, *Limnol.*, **17,** 151-162 (2016).

Sohrin, Y.; Nakashima, Y.; Maruo, M., Trace Elements Influenced by Environmental Changes in Lake Biwa: (II) Chemical Variations in the Hypolimnion over the Last Half-century, *Limnol.*, **17,** 163-173 (2016).

Minami, T.; Konagaya, W.; Zheng, L.; Takano, S.; Sasaki, M.; Murata, R.; Nakaguchi, Y.; Sohrin, Y., An Off-line Automated Preconcentration System with Ethylenediaminetriacetate Chelating Resin for the Determination of Trace Metals in Seawater by High-resolution Inductively Coupled Plasma Mass Spectrometry, *Anal. Chim. Acta*, **854,** 183-190 (2015).

Takano, S.; Tanimizu, M.; Hirata, T.; Sohrin, Y., Isotopic Constraints on Biogeochemical Cycling of Copper in the Ocean, *Nat. Commun.*, **5,** [5663-1]-[5663-7] (2014).

Estimation of the Paleoenvironment Based on the Concentration and Isotope Ratio of Molybdenum and Tungsten in the Japan Sea Sediment

Molybdenum (Mo) and tungsten (W) are group 6 elements and exist as hexavalent oxoacid anion (MoO_4^{2-}, WO_4^{2-}) in the oxidative ocean. While Mo has concentration of about 107 mmol/kg in the modern ocean (Nakagawa *et al*. 2012), it is easily precipitated as thiomolybdate in the euxinic environment. On the other hand, W has concentration of about 49 pmol/kg in the modern ocean. Although W is not precipitated in the euxinic environment (Mohajerin *et al*. 2016), it is highly enriched in hydrothermal fluids (Kishida *et al*. 2004). Therefore, we expect that the Mo/W concentration ratio and the stable isotope ratio of Mo and W in marine sediments would be powerful ploxies in paleoceanography. Recently, we have developed a new method of stable isotope ratio analysis for Mo and W in marine sediments on the basis of microwave digestion, chelating column extraction, anion exchange separation, and determination by multicollector inductively coupled mass spectrometry (MC-ICP-MS). Using this method, we have analyzed a sediment core collected off Iwanai, Hokkaido in the Japan Sea (43°22'36.0"N, 140°04'10.0"E, 900 m depth) and estimated environmental changes at the bottom of the Japan Sea middle depth in the past 46,530 years. The high peaks of Mo concentration and Mo/W ratio suggested euxinic precipitation of Mo 10,000, 15,000, 30,000, and 46,000 years ago. However, $\delta^{98/95}$Mo neither exceed 0.9‰ nor correlate with the Mo/W ratio. Tungsten concentration was relatively uniform similarly to Al, and $\delta^{186/184}$W was about 0‰ throughout the core, suggesting that chemical supply from land was fairly constant.

Kishida K, Sohrin Y, Okamura K, Ishibashi J (2004) Tungsten enriched in submarine hydrothermal fluids. Earth Planet Sci Lett 222 (3-4):819-827. doi:10.1016/j.epsl.2004.03.034
Mohajerin TJ, Helz GR, Johannesson KH (2016) Tungsten–molybdenum fractionation in estuarine environments. Geochim Cosmochim Acta 177:105-119. doi:10.1016/j.gca.2015.12.030
Nakagawa Y, Takano S, Firdaus ML, Norisuye K, Hirata T, Vance D, Sohrin Y (2012) The molybdenum isotopic composition of the modern ocean. Geochem J 46 (2):131-141. doi:10.2343/geochemj.1.0158

Distributions of Dissolved and Labile Particulate Trace Metals (Al, Mn, Fe, Co, Ni, Cu, Cd, and Pb) in Seawater on 160°W in the North Pacific

The North Pacific Ocean is at the end of general ocean circulation, characterized by influx of North Pacific Intermediate Water and by aeolian supply of dust and aerosol through westerly wind. GEOTRACES ocean section studies of trace metals in seawater have covered the Atlantic Ocean but still limited in the Pacific Ocean. Recently, we have reported the distributions of trace metals around the Juan de Fuca Ridge (Zheng *et al*. 2017). In this study, we report the distributions of Al, Mn, Fe, Co, Ni, Cu, Cd, and Pb in dissolved (d) and labile particulate (lp) fractions on 160°W in the North Pacific, where seawater samples were collected during the R/V Hakuho-Maru KH-05-2 cruise in August-September 2005. The dAl concentrations were low at high latitude stations and the bottom maximum extended from south to north. DFe and lpFe concentrations took maxima at station ST14 that is ~190 km off the Aleutian Islands and decreased sharply when leaving from the continent. Both d and lp Mn and Co showed a maximum in surface water (~20 m) at ST14 and nearly constant concentrations in deep water. DNi and dCd showed nutrient-type distributions. LpNi and lpCd were not detected. DCu increased almost linearly from surface to a depth of 4,000 m. There was a strong correlation between dCu and Si down to a depth of 2000 m ($r^2 = 0.747$), but dCu substantially increased in deep water due to supply from the sediment. For Pb, the lp fraction was hardly detectable and d fraction showed a subsurface maximum centered at a depth of ~200 m, ~35°N. It is likely that anthropogenic Pb in aerosol particles caused by coal burning in the Asian continent falls to the Pacific Ocean, is subducted with surface seawater, and then spreads throughout the North Pacific Ocean by ocean currents.

Zheng L, Minami T, Takano S, Minami H, Sohrin Y (2017) Distribution and stoichiometry of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in seawater around the Juan de Fuca Ridge. J Oceanogr 73 (5):669-685. doi:10.1007/s10872-017-0424-2

Figure 1. A snapshot at seawater sampling during the R/V Hakuho Maru KH-17-3 cruise.

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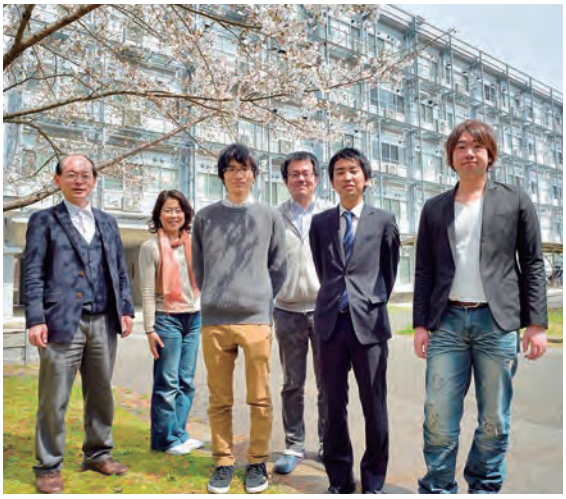
Scope of Research

To understand the chemical structure and properties of a molecular aggregated system, the keywords of molecular interactions and orientation are focused on, and the molecular aggregates are investigated by using originally developed spectroscopic techniques. The current major topics are: (1) Vibrational spectroscopy on fluorine chemistry; (2) controlling factors of a molecular packing and orientation in a thin film of an organic semiconductor compound; (3) the optimal experimental condition and the correlation factor of pMAIRS based on electrodynamics for estimating an accurate quantitative molecular orientation in a thin film.

KEYWORDS

Infrared and Raman Spectroscopy
Perfluoroalkyl Compounds
pMAIRS
Surface and Interface Chemistry
Organic Semiconductor



Selected Publications

Shioya, N.; Shimoaka, T.; Eda, K.; Hasegawa, T., Controlling Mechanism of Molecular Orientation of Poly(3-alkylthiophene) in a Thin Film Revealed by Using pMAIRS, *Macromol.*, **50(13),** 5090-5097 (2017).

Hasegawa, T., Physicochemical Nature of Perfluoroalkyl Compounds Induced by Fluorine, *Chem. Rec.*, **17,** 903-917 (2017).

Shimoaka, T.; Sonoyama, M.; Amii, H.; Takagi, T.; Kanamori, T.; Hasegawa, T., Study of Perfluoroalkyl Chain-Specific Band Shift in Infrared Spectra on the Chain Length, *J. Phys. Chem. A*, **121,** 8425-8431 (2017).

Shioya, N.; Norimoto, S.; Izumi, N.; Hada, M.; Shimoaka, T.; Hasegawa, T., Optimal Experimental Condition of IR pMAIRS Calibrated by Using an Optically Isotropic Thin Film Exhibiting the Berreman Effect, *Appl. Spectrosc.*, **71(5),** 901-910 (2017).

Shioya, N.; Shimoaka, T.; Murdey, R.; Hasegawa, T., Accurate Molecular Orientation Analysis Using Infrared pMAIRS Considering the Refractive Index of the Thin Film Sample, *Appl. Spectrosc.*, **71(6),** 1242-1248 (2017).

Controlling Mechanism of Molecular Orientation of Poly(3-alkylthiophene) in a Thin Film Revealed by Using pMAIRS

A face-on oriented thin film of poly(3-hexylthiophene) (P3HT) is suitable for an organic semiconductor layer in a photovoltaic device, and thus analysis of the film structure in terms of molecular orientation is crucial. Although the face-on film often has a poor crystallinity, diffraction techniques have long been employed for the structural analysis, and only very minor crystal parts have been discussed. In our previous study, P3HT was revealed to have a uniquely oriented structure even in an amorphous film by using p-polarized multiple-angle incidence resolution spectrometry (pMAIRS), which is powerful to analyze the molecular orientation, crystallinity, and the conjugation length of P3HT. With the best use of the potential of pMAIRS, in the present study, the controlling mechanism of the molecular orientation of P3HT correlated with the crystallinity in a spin-coated thin film is revealed. As a result, by employing a high-spin speed at 8,000 rpm, a highly face-on oriented thin film having a very low crystallinity is obtained, which readily reveals that the face-on component has a strong correlation with the amorphous aggregates.

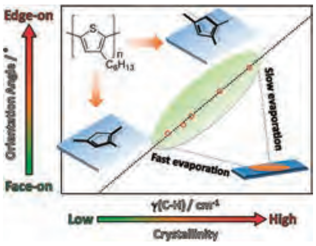


Figure 1. Beautiful correlation between the orientation angle of the thiophene ring and the crystallinity of P3HT thin films.

Study of Perfluoroalkyl Chain-Specific Band Shift in Infrared Spectra on the Chain Length

The CF_2 symmetric stretching vibration ($\nu_s(CF_2)$) band of a perfluoroalkyl (Rf) group in an infrared (IR) spectrum exhibits a unique character, that is, an apparent high wavenumber shift with increasing the chain length, which is an opposite character to that of the CH stretching vibration band of a normal alkyl chain. To reveal the mechanism of the unusual IR band shift, two vibrational characters of an Rf chain are focused: (1) a helical conformation of an Rf chain, (2) the carbon (C) atoms having a smaller mass than the fluorine (F) atom dominantly vibrate as a coupled oscillator leaving F atoms stay relatively unmoved. These indicate that a "coupled oscillation of the skeletal C atoms" of an Rf chain should be investigated considering the helical structure. In the present study, therefore, the coupled oscillation of the Rf chain dependent on the chain length is investigated by Raman spectroscopy, which is suitable for investigating a skeletal vibration. The Raman-active $\nu_s(CF_2)$ band is found to be split into two bands, the splitting is readily explained by considering the helical structure and length with respect to group theory, and the unusual peak shift is concluded to be explained by the helical length.

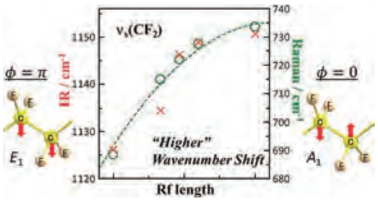


Figure 2. Higher wavenumber shift of the $\nu_s(CF_2)$ band with increasing the chain length is induced by the conformational change of the Rf skeleton.

Optimal Experimental Condition of IR pMAIRS Calibrated by Using an Optically Isotropic Thin Film Exhibiting the Berreman Effect

Infrared (IR) p-polarized multiple-angle incidence resolution spectrometry (pMAIRS) is a useful spectroscopic tool for revealing the molecular anisotropic structure in a thin film, which is used for the molecular orientation analysis of many functionalized organic thin films. Infrared pMAIRS provides both in-plane (IP) and out-of-plane (OP) vibrational mode spectra, which are influenced by the choice of the angles of incidence, i.e., angle set. To obtain quantitatively reliable pMAIRS spectra, therefore, the optimal angle set must be revealed. In a former study, an optimization study was carried out on a silicon substrate by using the band intensity ratio of the IP and OP spectra of highly oriented molecules in a thin film, which has a problem that the optimized results cannot be used for another substrate. In the present study, a totally new idea using an optically isotropic thin film as a standard sample is proposed to comprehensively explore the optimal angle set on various substrates: the band shift due to the Berreman effect of a strongly absorbing compound is used, instead of the band intensity. This new approach makes the pMAIRS calibration for various substrates a much easier task. With the optimal angle set, the molecular orientation angle in the film calculated by the pMAIRS spectra is also found to be reliable quantitatively. This technique opens a user-friendly way to a reliable molecular orientation analysis in an ultrathin film using IR pMAIRS.

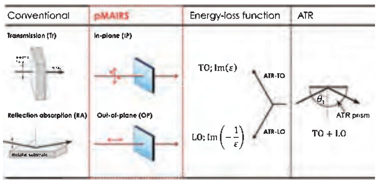


Figure 3. Interrelationship between pMAIRS and the representative infrared spectroscopic techniques via energy-loss functions.

Division of Environmental Chemistry
– Molecular Microbial Science –

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

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

KEYWORDS

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

Selected Publications

Yokoyama, F.; Kawamoto, J.; Imai, T.; Kurihara, T., Characterization of Extracellular Membrane Vesicles of an Antarctic Bacterium, *Shewanella livingstonensis* Ac10, and Their Enhanced Production by Alteration of Phospholipid Composition, *Extremophiles*, **21,** 723-731 (2017).
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, *Bioconjug. Chem.*, **28,** 2077-2085 (2017).
Kurihara, T.; Kawamoto, J.; Ogawa, T., Biosynthesis and Physiological Functions of ω-3 Long Chain Polyunsaturated Fatty Acids in Bacteria, *Vitamins*, **91,** 555-562 (2017).
Kurihara, T., Diversity of Bacterial Membrane Phospholipids: Their Biosynthesis and Functions, *Membrane*, **42,** 175-180 (2017).
Kawamoto, J.; Kurihara, T.; Esaki, N., Proteomic Insights of Psychrophiles, *Psychrophiles: From Biodiversity to Biotechnology*, 423-435 (2017).

Isolation and Characterization of a Membrane-Vesicle-Producing Bacterium, *Shewanella* sp. HM13

Protein expression at low temperatures is expected to alleviate the heat denaturation of proteins and would be suitable for the production of thermolabile proteins. To develop an efficient protein-production system, we isolated a cold-adapted Gram-negative bacterium, *Shewanella* sp. HM13, from fish intestine. This strain can produce about 5 mg/L culture of a secretory protein (P49), which was co-purified with the extracellular membrane vesicles (EMV) at the temperature range of 4~18°C. To determine the localization of P49, we prepared the EMV-containing fraction by ultracentrifugation and analyzed proteins co-purified with the EMVs, demonstrating that P49 is a major cargo protein of the EMVs, and more than 80% of P49 was recovered with the EMVs. These results suggested that specific cargo selection mechanism is operating for EMV proteins. Whole genome sequencing of *Shewanella* sp. HM13 demonstrated that the gene coding for P49 was located in a gene cluster containing *pulD* encoding a component of a general secretory pathway. The secretion of P49 within the EMVs was decreased in the *pulD*-disrupted mutant, suggesting that PulD is involved in the association of P49 with EMVs.

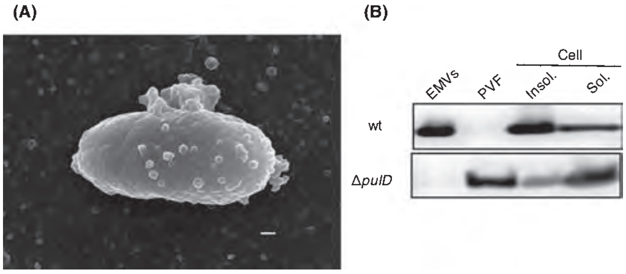

Figure 1. EMV-producing bacterium, *Shewanella* sp. HM13.
(A) SEM image of *Shewanella* sp. HM13. This strain can secrete EMVs from its cell surfaces to the extracellular milieu. Bar indicates 100 nm. (B) Localization of a cargo protein, P49. In the wild type strain, P49 was observed from the EMVs and the insoluble fraction of the cells. Gene deletion of *pulD* alters the localization of P49 from the EMVs to the post-vesicle fraction (PVF) and the soluble fraction of the cells, indicating that PulD is involved in the membrane association of P49.

Analysis of Protein-Protein Interaction between Polyunsaturated Fatty Acid-producing Enzymes

Some marine bacteria produce ω-3 long-chain polyunsaturated fatty acids (PUFAs) such as eicosapentaenoic acid (EPA) and docosahexaenoic acid. They exist mainly as an acyl chain of membrane phospholipids and are inferred to play important physiological roles in extreme environments. Bacterial PUFA biosynthesis requires five enzymes, *i.e.* Orf2, Orf5, Orf6, Orf7, and Orf8, that catalyze a cycle of acyl chain elongation and C=C bond formation. Because each of the enzymes has different catalytic domains, it is proposed that they work cooperatively to accomplish PUFA biosynthesis. However, it has been uncertain whether and how the five enzymes interact with each other. To reveal it, we developed monoclonal antibodies and performed pull-down assays for the enzymes from an Antarctic EPA-producing bacterium *Shewanella livingstonensis* Ac10. As a result, we found that Orf5, Orf6, Orf7, and Orf8 tightly interact with each other, whereas Orf2 transiently. We also found their interaction with a lysophosphatidic acid acyltransferase, namely PlsC, from *S. livingstonensis* Ac10, an enzyme that incorporates EPA into membrane phospholipids *in vivo*. These results suggested that the protein-protein interactions enable the efficient production of EPA and EPA-containing phospholipids, which may contribute to the survival in hostile environments.

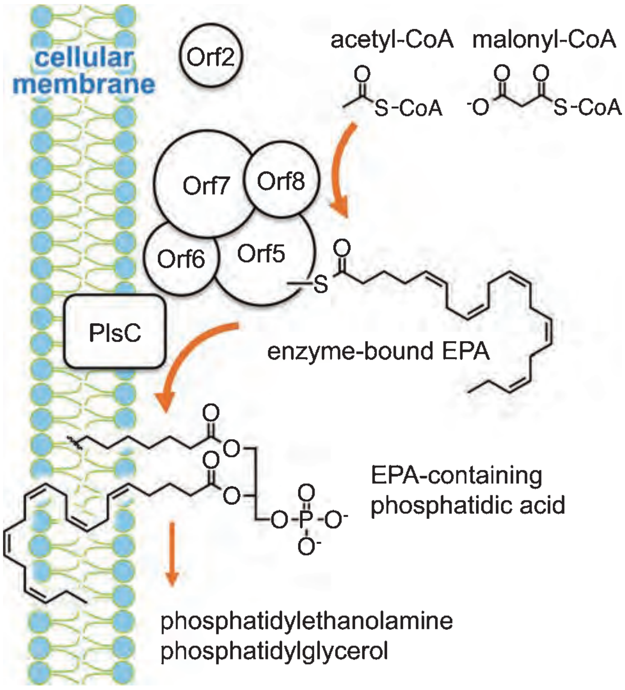

Figure 2. Schematic view of EPA and EPA-containing phospholipid biosynthesis.

Division of Multidisciplinary Chemistry
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Scope of Research

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

KEYWORDS

Polymer Physics
Self Assembly
Hierarchical Structure
Polymer Properties
Softmatter

Selected Publications

Wang, Y.-C.; Wakabayashi, M.; Hasegawa, H.; Takenaka, M., 3D-TEM Study on the Novel Bicontinuous Microdomain Structure, *Soft Matter*, **13**, 8824-8828 (2017).

Wang, Y.-C.; Inoue, A.; Hasegawa, H.; Takenaka, M., The Formation of OTDD Network Structure in PS-b-PI-b-PDMS Triblock Terpolymer Authors, *Macromol. Chem. Phys.*, **218,** 1700008(1-7) (2017).

Ogawa, H.; Nishikawa, Y.; Takenaka, M.; Fujiwara, A.; Nakanishi, Y.; Tsujii, Y.; Takata, M.; Kanaya, T., Visualization of Individual Images in Patterned Organic-inorganic Multilayers Using GISAXS-CT, *Langmuir*, **33,** 4675-4681 (2017).

3D-TEM Study on the Novel Bicontinuous Microdomain Structure

An ordered bicontinuous double-diamond (OBDD) morphology was found in Polystyrene-*block*-(poly-4-vinylphenyldimethylvinylsilane-*graft*-polyisoprene), PS-*b*-(PVS-*g*-PI), block-graft copolymer. We obtained 3D image of the microdomain structure formed in PS-*b*-(PVS-*g*-PI) by using 3D-TEM method. The 3D image shows the polystyrene (PS) phase consists of two independent and interwoven networks. The structures of two networks are identical and tetrapod units form a planar six-membered ring in the networks. The features of the networks agree with those in OBDD, indicating the morphology of PS-*b*-(PVS-*g*-PI) is an ordered three-dimensional OBDD networks of PS phase in polyisoprene (PI) matrix phase. The grafted PI chains induce the frustration of PS chains and thus the effects of specific interface are more dominant that those of the packing frustration in the formation of the morphology and OBDD phase is thus stabilized.

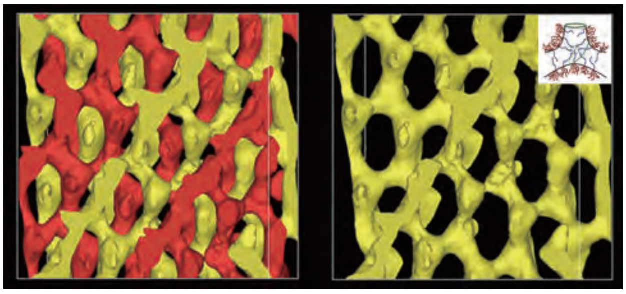

Figure 1. 3D TEM image of OBDD in PS-*b*-(PVS-*g*-PI).

Visualization of Individual Images in Patterned Organic-inorganic Multilayers Using GISAXS-CT

Grazing-incidence small-angle X-ray scattering (GISAXS) have been used for nanometer level structural analysis of thin organic and in-organic films. Two-dimensional (2D) patterns of GISAXS enable quantitative morphological analysis on the length scales ranging from 1 nm to 100 nm. In the case of GISAXS coupled with CT, owing to the reconstruction based on the scattering intensities, it is possible to obtain spatial distribution images of nanostructures in thin film samples on the substrate. GISAXS-CT was employed for characterizing Au and PS-*b*-P2VP multilayers. Owing to the difference between total reflection angles of Au and PS-*b*-P2VP, the scattering profiles for Au nanoparticles and self-assembled nanostructures of PS-*b*-P2VP could be independently obtained by changing the X-ray angle of incidence. Reconstruction of scattering profiles allows to separately characterize spatial distributions in Au and PS-*b*-P2VP nanostructures.

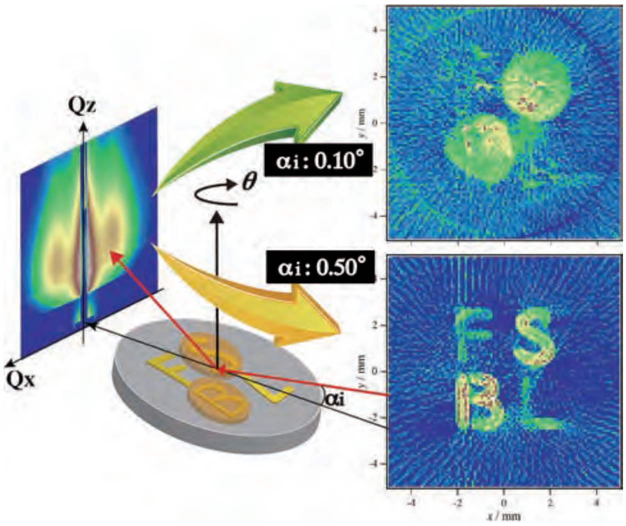

Figure 2. Reconstruction images from Au layer buried under a thin PS-*b*-P2VP layer.

Division of Multidisciplinary Chemistry
– Molecular Rheology –

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

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Guest Res Assoc

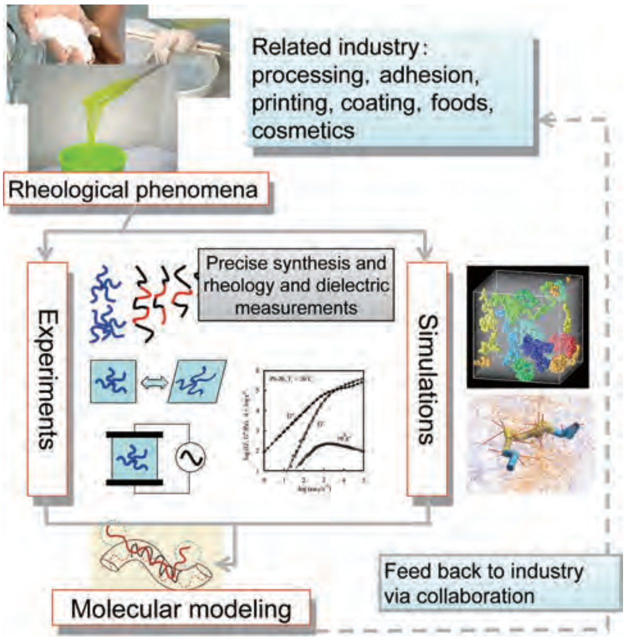
BHATTACHARYYA, Arup R. (Ph D)	Indian Institute of Technology Bombay, India, 5 May–7 July
KWON, Oh Min	Seoul National University, Korea, R., 2–29 July

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 new aspect of softmatter physics.

KEYWORDS

Rheology　　Dielectric Spectroscopy　　Softmatter



Selected Publications

Watanabe, H.; Matsumiya, Y.; Kwon, Y., Dynamics of Rouse Chains undergoing Head-to-Head Association and Dissociation: Difference between Dielectric and Viscoelastic Relaxation, *J. Rheol.*, **61,** 1151-1170 (2017).

Kwon, O. M.; Watanabe, H.; Ahn, K. H.; Lee, S. J., Growths of Mechanical Elasticity and Electrical Conductance of Graphene Nanoplatelets/Poly(lactic acid) Composites Under Strong Electric Field: Correlation with Time Evolution of Higher Order Structure of Graphene Nanoplatelets, *Rheol. Acta*, **56,** 871-885 (2017).

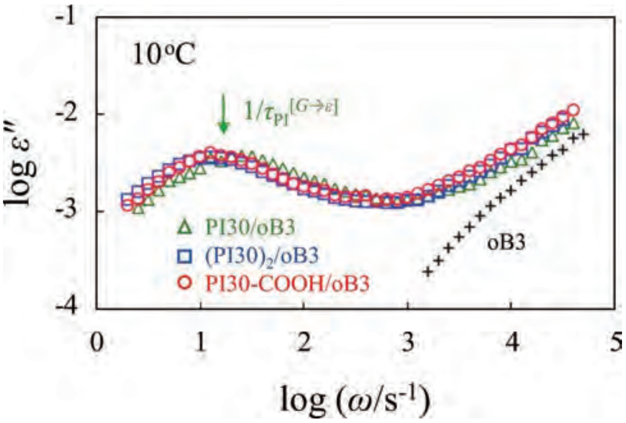
Watanabe, H.; Matsumiya, Y., Revisit the Elongational Viscosity of FENE Dumbbell Model, *J. Soc. Rheol. Jpn.*, **45,** 185-190 (2017).

Doi, Y.; Matsumoto, A.; Inoue, T.; Iwamoto, T.; Takano, A.; Matsushita, Y.; Takahashi, Y.; Watanabe, H., Re-Examination of Terminal Relaxation Behavior of High-Molecular-Weight Ring Polystyrene Melts, *Rheol. Acta*, **56,** 567-581 (2017).

Kwon, O. M.; Watanabe, H.; Ahn, K. H.; Lee, S. J., Interplay between Structure and Property of Graphene Nanoplatelet Networks Formed by an Electric Field in a Poly(lactic acid) Matrix, *J. Rheol.*, **61,** 291-303 (2017).

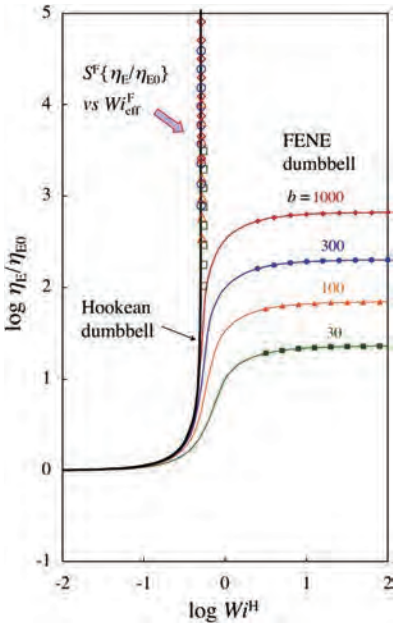
Dynamics of Rouse Chains undergoing Head-to-Head Association and Dissociation: Difference between Dielectric and Viscoelastic Relaxation

For monofunctionally head-associative Rouse chains having type-A dipoles, the Rouse equation of motion was combined with the association/dissociation kinetics to calculate the dielectric relaxation function, $\Phi_j(t)$ with $j = 1$ and 2 for unimer and dimer. $\Phi_1(t)$ reflects the orientation of the end-to-end vector of the unimer, whereas $\Phi_2(t)$ detects the orientation of two end-to-center vectors of the dimer (having symmetrical dipole inversion), both being in the direction of the applied electric field. The calculation was made by mapping the conformation of dissociating dimer onto the created unimer and vice versa with the aid of the Rouse eigenmode expansion of the bond vector of segments (Gaussian subchains). It turned out that $\Phi_j(t)$ is not influenced by the association/dissociation reaction. This result makes a striking contrast to the behavior of the viscoelastic relaxation function $g_j(t)$: $g_j(t)$ is strongly affected by the motional coupling between the unimer and dimer due to the reaction. This difference emerged because the dielectric $\Phi_j(t)$ corresponds to the vectorial first-moment average of the segmental bond vector at time t, $\mathbf{u}(n,t)$ with n being the segment index, whereas the viscoelastic $g_j(t)$ corresponds to the tensorial second-moment average. Because of this difference in the averaging moment, $\Phi_j(t)$ is subjected to cancelation in the conformational mapping but $g_j(t)$ is not, so that the reaction effect emerges only for $g_j(t)$. The experimental data of head-carboxylated high-*cis* polyisoprene chains (having the type-A dipoles) confirms this difference; see Figure.



Revisit the Elongational Viscosity of FENE Dumbbell Model

The dumbbell model with a finite extensibility was developed almost a half century ago as a model for those chains under strong flow. This model exhibits the finite extensible nonlinear elasticity (FENE) effect under strong flow to provide the elongational viscosity η_E with the strain-hardening feature but without any divergence. This study focuses on the effective relaxation time $\tau_{\rm eff}^{\rm F}$ of the FENE dumbbell under steady elongational flow by taking into account stiffening of the FENE dumbbell. It turned out that the stiffening of the FENE dumbbell leads to a decrease of $\tau_{\rm eff}^{\rm F}$ in proportion to $\dot{\varepsilon}^{-1}$ at $\dot{\varepsilon} > 1/2\tau_{\rm eq}^{\rm H}$, where $\dot{\varepsilon}$ is the elongational strain rate. This decrease of $\tau_{\rm eff}$ allows the effective Weissenberg number of the FENE dumbbell under flow, $Wi_{\rm eff}^{\rm F} = \dot{\varepsilon}\tau_{\rm eff}^{\rm F}$, to stay below a critical value of ~1/2 even for $\dot{\varepsilon}\to\infty$. This limited increase of $Wi_{\rm eff}^{\rm F}$ allows the FENE dumbbell to change its conformation just slightly even for a large increase of $\dot{\varepsilon}$ from $1/2\tau_{\rm eq}^{\rm H}$ to any higher value, which naturally leads to the lack of divergence of η_E.



Division of Multidisciplinary Chemistry
– Molecular Aggregation Analysis –

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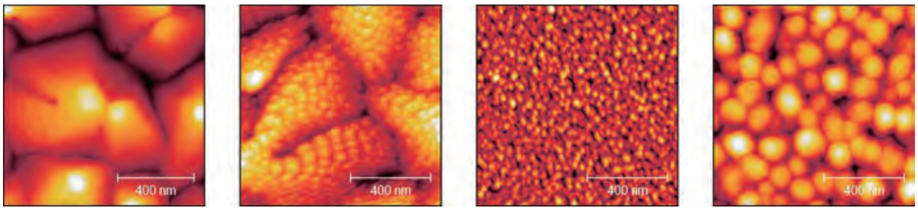
Scope of Research

The laboratory explores the electronic and photo-electronic properties of organic semiconductor thin films, examining how the physics of charge generation and transport reflects the precise and intricate way molecules assemble, orient, and order in the solid state. Characterization of film growth and studies on the influence of environmental variables on the film structure are combined with *in situ* electrical conductance and photoconductivity measurements. The experimental conditions are carefully controlled to discover new details about charge injection and transport, charge generation, and intermolecular electronic interactions.

KEYWORDS

Organic Semiconductor
Molecular Electronics
Thin Films
Electrical Conductivity and Photoconductivity
Charge Generation and Transport

1 µm ×1 µm AFM images of thin organic films grown on silicon wafers.



10 nm pentacene

10 nm pentacene
+ 10 nm C_{60}

10 nm C_{60}

10 nm C_{60}
+ 10 nm pentacene

Selected Publications

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

Murdey, R.; Sato, N., Photocurrent Action Spectra of Organic Semiconductors, *Advances in Organic Crystal Chemistry Comprehensive Reviews 2015*, 627-652 (2015).

Murdey, R.; Sato, N., Interpretation of the Thermal Activation Energy of Conduction for Molecular Semiconductor Thin Films with Blocking Contacts, *Jpn. J. Appl. Phys.*, **53,** 05FY04 (2014).

Murdey, R.; Sato, N., Voltage Stress Induced Reversible Diode Behavior in Pentacene Thin Films, *J. Chem. Phys.*, **137,** 234703 (2012).

Murdey, R.; Sato, N., *In Situ* Conductance Measurements of Copper Phthalocyanine Thin Film Growth on Sapphire [0001], *J. Chem. Phys.*, **134,** 234702 (2011).

Nonlinear Photocurrent Spectroscopy

As photocurrent is proportional to the quantity of absorbed radiation it is possible in principle to extract an optical absorption spectrum using the photocurrent recorded at different wavelengths. Photocurrent in this instance can be considered as a measure of the absorbed light. If the relationship between photocurrent, I, and the absorbed light intensity, F, is not linear, however, the incident light intensity for each data point must be attenuated such that the photocurrent remains constant – unless a mathematical function can be found to transform the photocurrent into a linear function of absorbance. We have determined that this linearization function, called the current response function, can be expressed as,

$$A = -\log\left(1 - \frac{1}{Y}\frac{I}{eF}\left(\frac{I}{I_\mathrm{d}} + 1\right)^{\frac{1-\gamma}{\gamma}}\right).$$

Y is a scaling parameter, while I_d and γ may be determined by a simple fitting procedure. The expression appears to be generally valid for most organic semiconductor films.

This new technique is called Nonlinear Photocurrent Spectroscopy (NPS). Absorption spectra can be quickly and easily obtained for thin and irregular shaped films, even on nontransparent substrates. There is no need to adjust the incident light intensity for each wavelength. Since NPS has very high sensitivity, the method is well-suited for examining gap states and impurity states in organic semiconductors, as well as for studying very thin films down to a single monolayer. A demonstration of this sensitivity is shown in Figure 1.

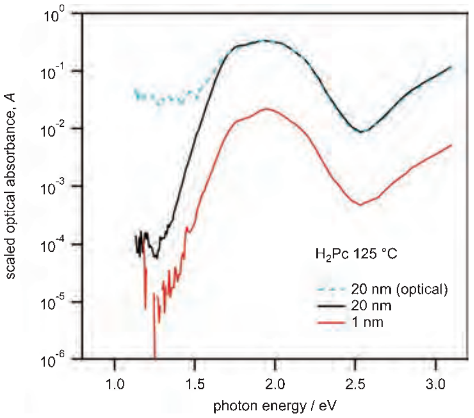


Figure 1. Absorbance spectra of 20 nm and 1 nm free base phthalocyanine thin films derived from photocurrent measurements after application of the nonlinear current response function and scaled to an optical reference. The reference optical spectra for the 20 nm film measured with the transmitted beam intensity (dotted blue line) is also shown.

Conductance in Organic Radical Solids

Organic radical molecules are distinctive for their singly occupied molecular orbital (SOMO) which causes them to behave as narrow gap intrinsic semiconductors in the solid state.

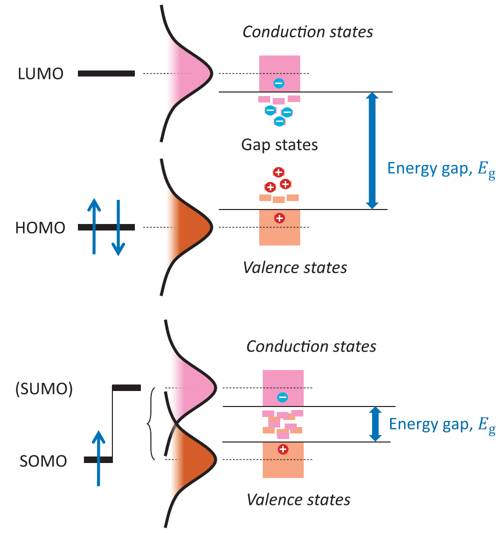


Figure 2. The relation between the molecular orbitals and the solid state energy gap E_g in a) typical closed shell organic semiconductors, and b) open shell organic radicals. Charge held in gap states is said to be “trapped”.

Radical bisphthalocyaninato complexes are open shell organic radical compounds which combine high electrical conductivity with chemical and thermal stability, making them promising materials for studying the charge transport of organic semiconductors. The small energy gap effectively removes the influence of deep traps, greatly enhancing the response time and facilitating reliable measurements.

In recent work we have shown that the conductance equation of $TbPc_2$ thin films may be separated into exponential and linear terms in temperature. The energy gap is found by this method to be 0.316 eV.

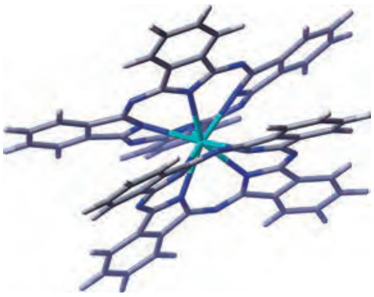


Figure 3. Molecular structure of the phthalocyanine sandwich complex bis(phthalocyanininato)terbium(III) ($TbPc_2$). A single unpaired electron is shared between the two phthalocyanine ligands.

Advanced Research Center for Beam Science
– Particle Beam Science –

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

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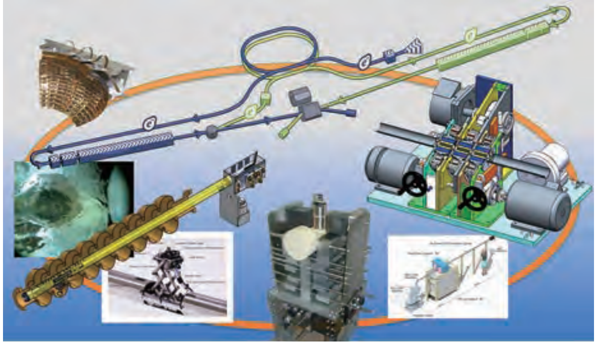
YAMAZAKI, Yuki (M1)

Guest Scholar

JAMESON, Robert A. (Ph D)	Goethe University, Frankfurt Germany, 2–15 October

Scope of Research

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



KEYWORDS

Beam Physics
Accelerator Physics
Neutron Optics
Phase Rotation
International Linear Collider

Selected Publications

Conway, Z. A.; Ge, M.; Iwashita, Y., Instrumentation for Localized Superconducting Cavity Diagnostics, *Supercond. Sci. Technol.*, **30,** 034002 (2017).

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

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Iwashita, Y.; Tongu, H.; Fuwa, Y.; Ichikawa, M., Compact Permanent Magnet H^+ ECR Ion Source with Pulse Gas Valve, *Rev. Sci. Instrum.*, **87-2,** 02A718-1-02A718-3 (2016).

Yamada, M.; Iwashita, Y.; Ichikawa, M.; Fuwa, Y.; Tongu, H.; Shimizu, H. M.; Mishima, K.; Yamada, N. L.; Hirota, K.; Otake, Y.; Seki, Y.; Yamagata, Y.; Hino, M.; Kitaguchi, M.; Kennedy, S. J.; Lee, W. T.; Andersen, K. H.; Guerard, B.; Manzin, G.; Geltenbort, P., Pulsed Neutron-beam Focusing by Modulating a Permanent-magnet Sextupole Lens, *Prog. Theor. Exp. Phys.*, **2015,** 043G01 (2015).

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

Evaluating the Multi-Layer Thin-Film Superconductor Using the Third Harmonic Voltage Method

The superconducting accelerating cavity has an advantage of storing electromagnetic energy efficiently and achieving a high gradient accelerating electric field for charged particles easily. In general, the maximum accelerating gradient is limited by the critical magnetic field because the superconductive state cannot be maintained when the magnetic field induced by the accelerating electric field becomes larger than it. Today, niobium is generally widely used as the de-facto standard for the base material of the superconducting acceleration cavity, and the critical magnetic field is 200 mT. However, in recent years, it is pointed out that the critical magnetic field can be increased more by coating inner surfaces with multilayer-thin film superconductor and insulator.

As an example, Figures 1 and 2 show contour plots of the maximum permissible magnetic field that can maintain the superconducting state in the case that NbN or Nb3Sn is assumed for the superconducting single layer. The vertical axis represents the film thickness of the superconducting layer, the horizontal axis represents the film thickness of the insulating layer, and the numerals in the figure represent the maximum permissible magnetic field [mT]. If it is possible to realize the technology to optimize the performance as shown in Figures 1 and 2, the acceleration gradient can be increased up to several times higher than the conventional gradient. Thereby, we can aim at the physics of multi TeV, which is impossible at the present for the next generation electron-positron collider experiments. Hence, it is desirable to study the feasibility of this technique in detail.

In order to prove the above prediction, we constructed a dedicated system in Uji, Kyoto University, to measure the lower critical magnetic field H_{c1}, which is the indicator that can maintain the superconducting state. The third harmonic voltage induction method was adopted to determine H_{c1}. In this method, the AC magnetic field is applied while changing the temperature of the sample, and the temperature dependence of H_{c1} can be clarified from the rise of the inductance nonlinear component generated in the coil. In this study, the inductance of the coil is derived by dividing the third harmonic voltage by the current. Figure 3 shows the schematic diagram of the third harmonic system. The sample and a coil and a heater can be set in a stage, and the stage is installed inside the cryostat filled with the liquid helium. The stage is actually suspended from above and is partially immersed in liquid helium. A coil is fixed on the stage at a distance from the sample, and the magnetic field can be controlled by applying a current.

The temperature of the sample is adjusted by using the heater and the liquid helium. Applying voltage and current to the coil are read out by the four-terminal method, and the third harmonic component of the voltage induced in the coil extracted by using a high-pass filter. Finally, after conversion from the analog value to the digital value, the voltage and the current are recorded in the PC.

Figure 4 shows the preliminary result of the H_{c1} dependence on the temperature for a sample consisting of one insulating layer and one superconducting thin NbN film layer and a silicon substrate. The vertical axis is H_{c1} of the sample, and the horizontal axis is the temperature of the sample of the superconducting thin film. From this measurement, it is found that H_{c1} at 0 K becomes 7.2 mT. This is the temperature dependence of H_{c1} clarified by this measurement, which is expected to provide a solid basis for comparison of the above mentioned theoretical model.

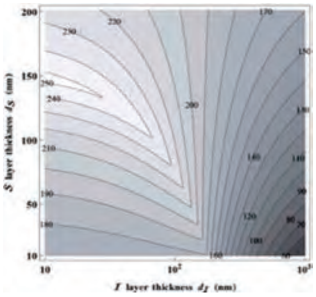

Figure 1.

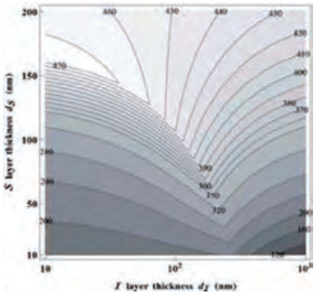

Figure 2.

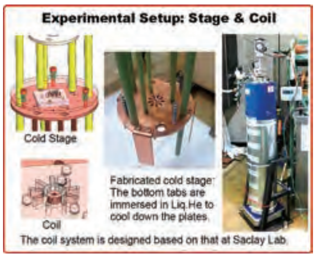

Figure 3.

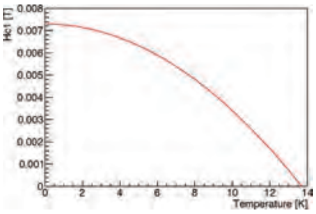

Figure 4.

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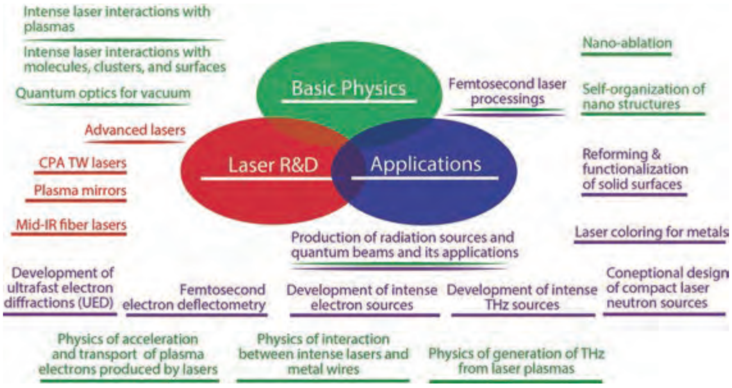
Scope of Research

The interaction of femtosecond laser pulses with matter involves interesting physics not seen with nanosecond laser pulses. Through investigation 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., Directional Linearly Polarized Terahertz Emission from Argon Clusters Irradiated by Noncollinear Double-pulse Beams, *Appl. Phys. Lett.*, **111,** 241107 (2017).

Furukawa, Y.; Sakata, R.; Konishi, K.; Ono, K.; Matsuoka, S.; Watanabe, K.; Inoue, S.; Hashida, M.; Sakabe, S., Demonstration of Periodic Nanostructure Formation with Less Ablation by Double-pulse Laser Irradiation on Titanium, *Appl. Phys. Lett.*, **108,** 264101 (2016).

Hashida, M.; Nishii, T.; Miyasaka, Y.; Sakagami, H.; Shimizu, M.; Inoue, S.; Sakabe, S., Threshold Fluence for Femtosecond Laser Nanoablation for Metals, *Electron Commun. Jpn.*, **99,** 88-95 (2016).

Inoue, S.; Maeda, K.; Tokita, S.; Mori, K.; Teramoto, K.; Hashida, M.; Sakabe, S., Single Plasma Mirror Providing 104 Contrast Enhacement and 70% Reflectivity for Intense Femtosecond Lasers, *Appl. Opt.*, **55,** 5647-5651 (2016).

Induction of Sub-terahertz Surface Wave on a Metal-wire by Intense Laser Interaction with a Foil

In recent years, the generation of terahertz-frequency electromagnetic waves (hereinafter simply THz waves) has been made possible by advances in femtosecond laser technology. A high peak-power THz wave is required for many applications. Because plasma does not suffer damage when used as a source element, even for intense laser pulses, laser plasma has been the subject of considerable study for the generation of intense THz waves.

We have demonstrated that a pulsed electromagnetic wave (surface wave) of sub-terahertz frequency and an 11-MV m^{-1} field strength is induced on a metal wire by the interaction of an intense femtosecond laser interaction with an adjacent metal foil at a laser intensity of 8.5×10^{18} W/cm^2. A tungsten wire is placed normal to an aluminum foil with a gap so that the wire is not irradiated and damaged by the laser pulse, making it possible to generate surface waves on the wire repeatedly (Figure 1 (a)). Figure 1(b) shows typical waveforms of the sub-THz surface wave induced by the irradiation of the intense laser pulse on the foil target for various foil-wire gaps (d = 0.5, 1, 2, 4 mm) with a resolution of 500 fs. The electric field has a rapid (sub-picosecond) rise time for each distance. A half-cycle surface wave is observed over ~10 ps and low frequency fluctuations follow the peak for tens of picoseconds. We also performed a three-dimensional electromagnetic field numerical simulation for understanding the process of surface wave induction. Figure 1 (c) shows the dependence of the peak electric field at the wire surface on the foil-wire gap *d*. Open and closed circles represent the peak electric field of the surface wave which obtained by the experiment and the calculation for various foil-wire gaps d respectively. The experimental data are well reproduced by the simulation. Numerical simulation suggests that electromagnetic wave associated with electron emission from the foil induces the surface wave.

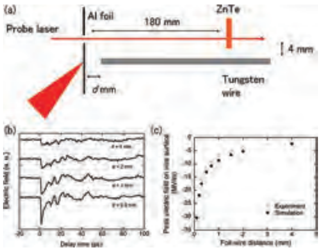


Figure 1. (a) Experimental setup for the generation and measurement of the surface wave. (b) Typical waveform of the surface wave at various distances (d = 0.5, 1, 2, 4 mm) between the foil and the wire. (c) Peak electric field of the surface wave on the wire for various distances between the foil and the wire.

Linearly Polarized Terahertz Wave Generation from Argon Cluster Plasma Produced by Double-Pulse Laser

The distinguishing properties have been observed in the THz wave emission from argon clusters irradiated by double intense femtosecond laser pulses with appropriate intervals in time and space: high directivity, power enhancement, and linear polarization, which is variable by changing the pointing of the second pulse relative to that of the first pulse. All are useful for applications because of high use efficiency, higher power, and variability of polarization, respectively. To understand the mechanism of THz emission from clusters under the irradiation of double pulses, we have proposed that the ions emitted from clusters Coulomb-exploded by the first pulse work as a bias. After the ions are emitted by Coulomb explosion, they form a positively charged ion cloud that works as a DC field (Figure 2).

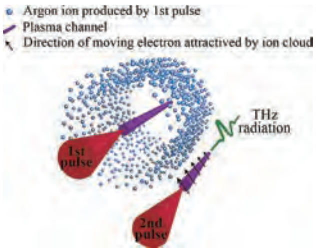


Figure 2. Diagram of THz generation from cluster plasma under irradiation by a double-pulse beam.

Reduction of Ablation Rate on Silicon Surface Irradiated by Double-Pulse Beam

To achieve laser nano-fabrication much smaller size than that of diffraction limit, the knowledge of the laser-matter interaction is important, especially for reducing the ablation rate of materials. To discuss the ablation rate dependence on materials, the ablation threshold for objective material has been measured precisely for single laser beam irradiation. We found that the nonlinear absorption on metal surface irradiated by femtoseocnd laser pulses is important role. Recently, ablation rate reduction has been clearly observed by using double pulsed beam with single color. The mechansim of reduction is under debated and we need further investigation. The characteristics of laser processing (ablation threshold, ablation rate, and interspace of grationg structures depended on laser fluence) were also measured for discussing the optimum laser condition for double laser beam irradiation. In this study we have demonstarted the reduction of ablation rate on a silicon surface irradiated by a double-pulse beam cross-polarized in time delays of Δt = –1000–1000 ps. We find that ablation rate of silicon is clearly decreased at delay times of 600 ps.

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Scope of Research

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

KEYWORDS
EELS
STEM
Surface Plasmon
Nanoparticle
Substrate Effect

Selected Publications

Haruta, M.; Kurata, H., Direct Observation of Crystal Defects in an Organic Molecular Crystals of Copper Hexachlorophthalocyanine by STEM-EELS, *Sci. Rep.*, **2,** [252-1]-[252-4] (2012).

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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).

Studying Substrate Effects on Localized Surface Plasmons in an Individual Silver Nanoparticle Using Electron Energy-Loss Spectroscopy

Localized surface plasmons (LSPs) in metallic nanoparticles (NPs) are accompanied by enhanced electromagnetic fields confined within regions smaller than the optical diffraction limit. LSPs in metallic NPs have found applications in biological sensing, solar light harvesting, photocatalysis, optical waveguides and so on. Since LSPs are sensitive to the environment surrounding the NPs as well as to the NP structure, it is important to investigate LSPs in individual NPs supported on substrates with high spatial resolution. In this study, electron energy-loss spectroscopy (EELS) in conjunction with scanning transmission electron microscopy (STEM) was used to investigate LSPs in a single silver NP on a magnesium oxide (MgO) substrate, employing an incident electron trajectory parallel to the substrate surface.

Figure 1 shows the experimental results obtained by high angle annular dark field (HAADF) and spectrum imaging (SI) methods. The substrate effects are clearly evident in the EEL spectra and in the map, and appear as a slight peak shift in the spectra and as the asymmetrical intensity distribution in the map. To understand the substrate effects, we performed the discrete dipoles approximation (DDA) simulations. Figure 2a presents the EEL spectra calculated for three different electron trajectories. The LSP dipole modes for which the polarization is perpendicular or parallel to the substrate are excited by electrons having trajectories A and B, respectively. Polarization perpendicular to the substrate localizes the charges near the substrate surface, resulting in a stronger interaction between the NP and the substrate compared to parallel polarization. Therefore, the resonance energy of the LSP with polarization perpendicular to the substrate is lower than that of the LSP having parallel polarization. The intensity of the LSP peak associated with trajectory A is strong compared to that for an isolated NP, while that for trajectory C is considerably weaker. This characteristic intensity distribution is also noticeable in the LSP map shown in Figure 2b. When the incident electron is located at the top surface of the NP, the polarization field due to the image charge in the substrate enhances the applied field experienced by the NP compared to that which would be generated only by the incident electron, meaning that many dipoles are excited in the NP and leading to the high LSP peak intensity at the top surface of the NP compared to that of an isolated NP, as shown in Figure 2a. In contrast, when the electron is incident in the vicinity of the interface between the NP and the substrate, the applied field in the NP is weak and its distribution is limited to the region near the interface. This is attributed to the strong cancellation in the NP region resulting from the polarization field of the substrate, because the NP is located in the opposite direction to the image charge with respect to the position of the incident electron. Therefore, the energy-loss probability is low in the vicinity of the interface. In the case of an electron travelling near the side of the NP, the applied field distribution in the NP is similar to that in an isolated NP. Therefore, the substrate effect is weak and limited to the region between the incident electron and the interface, leading to a similar LSP peak intensity (Figure 2a).

The resonance energies of LSPs were dependent on the polarization direction relative to the substrate surface. This result is similar to those obtained previously from optical studies using polarized light. However, the LSP maps obtained by STEM-EELS analysis show an asymmetric intensity distribution with the highest intensity at the top surface of the NP (that is, far from the substrate), a result that is not predicted by optical simulations. We show that modifications of the applied electric field by the substrate cause this asymmetric intensity distribution in the LSP maps.

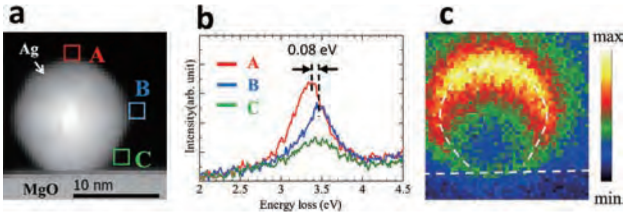

Figure 1. Experimental EELS results obtained from a silver NP placed on an MgO substrate, applying electron irradiation in the direction of the cross-section. (a) HAADF image, in which three 2 nm squares are indicated, each 1 nm from the NP surface. (b) EELS spectra obtained from the top, side and gap regions indicated in (a) as A (red), B (blue) and C (green). (c) EELS map generated using an energy window from 3.20 to 3.60 eV.

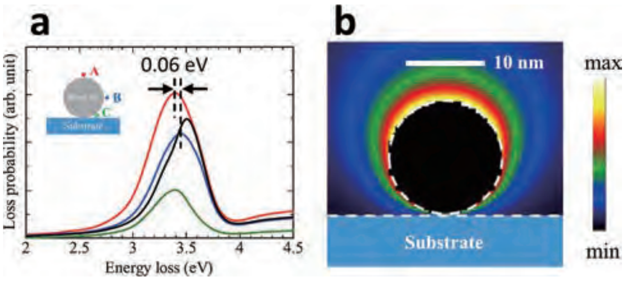

Figure 2. The EELS spectra and map calculated for a silver nano-sphere placed on an MgO substrate. (a) EELS spectra calculated for electron trajectories at the top, side and gap regions marked as A (red), B (blue) and C (green) in the inset, and that calculated for an isolated NP in a vacuum (black). These spectra were broadened by the instrumental energy resolution. (b) EELS map calculated at an energy of 3.40 eV.

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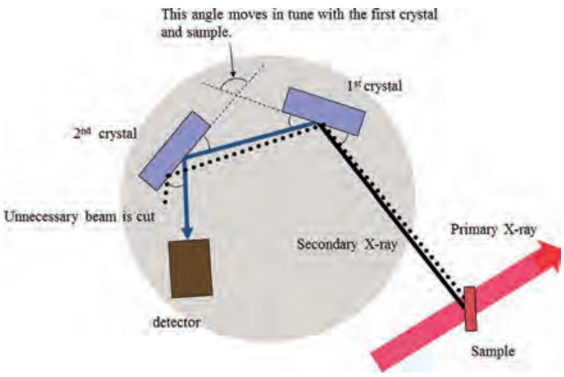
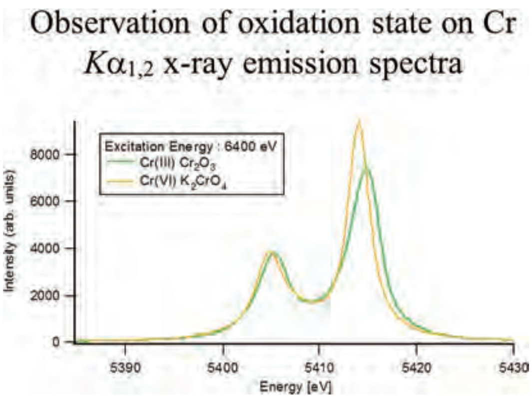
Scope of Research

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

KEYWORDS

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





Selected Publications

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

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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).

$K\alpha_{1,2}$ X-ray Linewidths, Asymmetry Indices, and [*KM*] Shake Probabilities in Elements Ca to Ge

The content described below is the result of our research on the asymmetry of the $K\alpha_{1,2}$ x-ray spectra in the 3*d* transition metals that have been unknown in the history of about 100 years in atomic physics.

Research on the width and shape of the asymmetric *K*α x-ray doublet of 3d elements ($21 \leq Z \leq 30$) has been the object of interest for a long time, both from the theoretical and experimental points of view. Although several causes have been proposed to explain this asymmetry such as, for example, shake processes, conduction-band collective excitations, exchange, and final-state interactions, the origin of the asymmetric shape is still under investigation and debate.

In order to obtain a simple description of the Cu $K\alpha_{1,2}$ spectrum, Berger assumed a doublet model for each of the $K\alpha_1$ and $K\alpha_2$ peaks and used two pairs of Lorentzian functions, determined $K\alpha_{11}$ and $K\alpha_{12}$, and $K\alpha_{21}$ and $K\alpha_{22}$, respectively, to fit them. A physical meaning for this simple model was given by Deutsch et al., based on the theoretical reasoning that the asymmetry in Cu *K*α spectra is due to the existence of shake processes leading to a 3*d* spectator hole. When a hole is created in the 1*s* shell, there is a probability that a second hole is created also in the 3*d* subshell. This shake-off process leaves the system with two holes and will be referred to subsequently as [1*s*3*d*] shake. Thus, the $K\alpha_{11}$ and $K\alpha_{21}$ Lorentzian peaks would correspond to the $K\alpha_1$ and $K\alpha_2$ diagram lines, respectively, and the $K\alpha_{21}$ and $K\alpha_{22}$ peaks to the corresponding satellite lines.

In a similar way, Ito et al. attributed the asymmetry in Zn $K\alpha_{1,2}$ spectra to the [1*s*3*d*] shake processes. Using the two-Lorentzian model, Ito et al. and Polasik et al. investigated the emission line shape in elements Ti to Zn and concluded that the full width at half maximum (FWHM) of the $K\alpha_{11}$ line is larger in these elements than the semi-empirical values reported by Krause and Oliver.

As it was considered that a simple description of the peak profiles by two Lorentzian functions was acceptable for the Cu *K*α lines, we measured and analyzed systematically the *K*α emission spectra in elements from Ca to Ge using a high-resolution double-crystal x-ray spectrometer and the same model, in order to elucidate the physical meaning of the asymmetry index of the lines, and the contribution of the [*KM*] shake processes (Figure 1). The overall tendency of the corrected full width at half maximum of the $K\alpha_1$ and $K\alpha_2$ lines as a function of Z, as well as the linewidths, are in good agreement with the data reported in the literature (Figures 2 and 3). The asymmetry index of $K\alpha_1$ in 3d elements from Sc to Zn is ascribed to the existence of a 3*d* spectator hole (Figure 1).

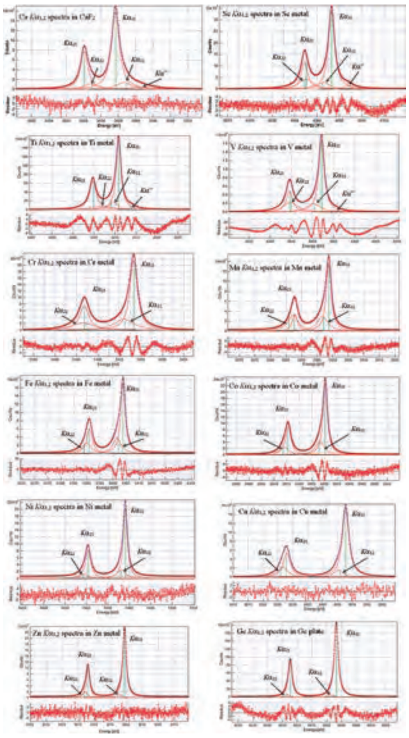

Figure 1. The observed $K\alpha_{1,2}$ spectra in elements Ca to Ge are shown with the Lorentzian functions used in the fitting process. These spectra were measured using the antiparallel double-crystal x-ray spectrometer. $K\alpha_{11}$ is the $K\alpha_1$ diagram line, and $K\alpha_{21}$ is the $K\alpha_2$ line. $K\alpha_{12}$ and $K\alpha_{22}$ satellite lines are due to 2*p* -> 1*s* electron transitions in the presence of an extra 3d hole resulting from shake processes. The *K*α" line is a satellite line ascribed to a 3*p* spectator hole.

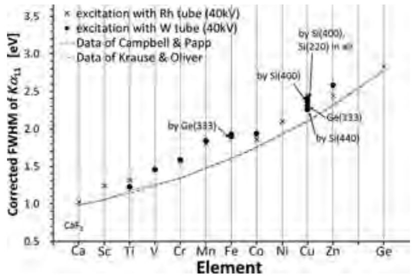

Figure 2. The corrected FWHM (CF) of the $K\alpha_{11}$ line of elements Ca to Ge together with the semi-empirical and recommended values. The widths of Krause and Oliver are semi-empirical values and those reported by Campbell and Papp are recommended values. The CF values for both the $K\alpha_{11}$ and $K\alpha_{21}$ diagram lines were obtained from the observed FWHM through Tochio's method.

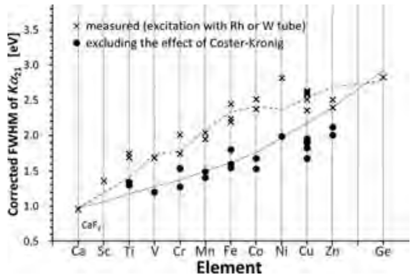

Figure 3. The CF of the $K\alpha_{21}$ line of elements Ca to Ge is shown together with the recommended values. Solid circles are the values subtracting the Coster-Kronig broadening effects reported by Nyholm *et al.*.

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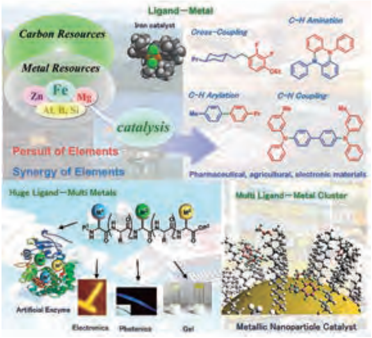
Scope of Research

Our research activity focuses on the development of new molecular transformations, which can contribute to better or ideal synthesis of functional molecules as well as to exploitation of new chemical (metal and carbon) resources. The present research subjects are (1) metal-catalyzed carbon–carbon and carbon–heteroatom bond forming reactions by using universal metals such as iron (2) development of smart materials based on synergistic effect of various metals on artificial peptides (3) development of smart metallic nanoparticle catalysts based on supramolecular approaches (4) understanding of reaction mechanism of these catalytic reactions with the help of quantum chemical methods and synchrotron X-ray absorption spectroscopy.



KEYWORDS

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

Selected Publications

Sharma, A. K.; Sameera, W. M. C.; Adak, L.; Jin, M.; Okuzono, C.; Iwamoto, T.; Nakamura, M.; Morokuma, K., DFT and AFIR Study on the Mechanism and the Origin of Enantioselectivity in Iron-Catalyzed Cross-Coupling Reactions, *J. Am. Chem. Soc.*, **139,** 16117-16125 (2017).

Iwamoto, T.; Nishikori, T.; Nakagawa, N.; Takaya, H.; Nakamura, M., Iron-Catalyzed anti-Selective Carbosilylation of Internal Alkynes, *Angew. Chem. Int. Ed.*, **56,** 13298-13301 (2017).

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

Nakajima, S.; Takaya, H.; Nakamura, M., Iron-catalyzed Methylation of Arylboron Compounds with Iodomethane, *Chem. Lett.*, **46,** 711-714 (2017).

Takaya, H.; Yokoi, T.; Yoshida, R.; Isozaki, K.; Kawakami, T.; Takenaka, T.; Nakamura, M., Synthesis and Structural Analysis of Ruthenium-Bound Norvaline Peptides, *Chem. Lett.*, **46,** 665-668 (2017).

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 a representative example, we developed the first example of iron-catalyzed enantioselective cross-coupling reaction, which enable facile acsess to optically active α-aryl esters from racemic α-chloroesters and aryl Grignard reagents. However, the reaction mechanism and the origin of enantioselectivity remained unclear. Here we performed DFT and AFIR calculations to reveal that the reaction proceeds via a novel $\mathrm{Fe}^{\mathrm{I–II–III}}$ mechanism, where iron (I) species **A** homolytically cleaves the C–Cl bond of α-chloropropionate substrates and the resulting alkyl radical recombines to the iron center of organoiron (II) intermediates **C** to generate organoiron (III) intermediates **D** (Figure 1). Finally, the iron (III) intermediate undergoes reductive elimination in a stereoselective manner to furnish optically active α-arylpropionates as the corresponding coupling product.

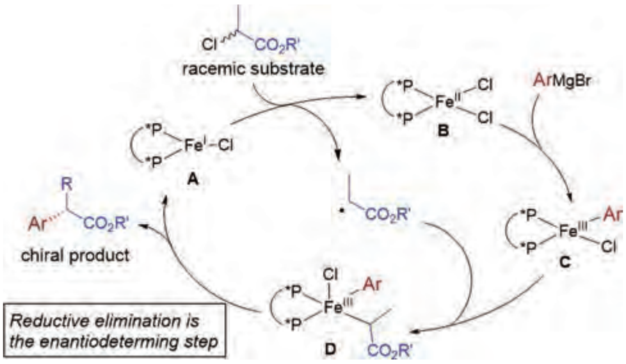


Figure 1. Mechanism of iron-catalyzed enantioselective coupling reaction.

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

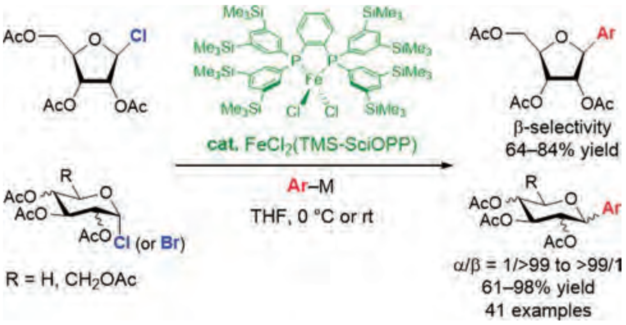


Figure 2. Synthesis of Aryl *C*-Glycosides via Iron-Catalyzed Cross-Coupling of Halosugars.

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

This project focuses on 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 methoxy-benzene 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.

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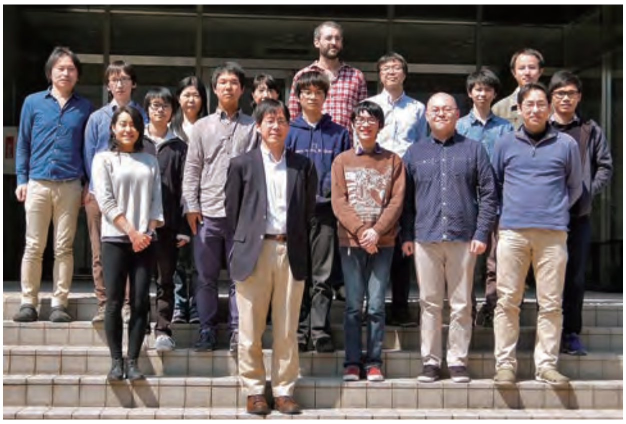
KEYWORDS
Solid State Chemistry
Functional Transition Metal Oxides
Epitaxial Thin Film Growth
High Pressure Synthesis

Scope of Research

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



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

Chen, W.-T.; Mizumaki, M.; Seki, H.; Senn, M.; Saito, T.; Kan, D.; Attfield, J. P.; Shimakawa, Y., A Half-metallic A- and B-site-ordered Quadruple Perovskite Oxide $CaCu_3Fe_2Re_2O_{12}$ with Large Magnetization and a High Transition Temperature, *Nat. Comm.*, **5,** 3909/1-7 (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,** 27/1-4 (2011).

Inoue, S.; Kawai, M.; Ichikawa, N.; Kageyama, H.; Paulus, W.; Shimakawa, Y., Anisotropic Oxygen Diffusion at Low Temperature in Perovskite-structure Iron Oxides, *Nat. Chem.*, **2,** 213-217 (2010).

Long, Y. W.; Hayashi, N.; Saito, T.; Azuma, M.; Muranaka, S.; Shimakawa, Y., Temperature-induced A-B Intersite Charge Transfer in an A-site-ordered $LaCu_3Fe_4O_{12}$ Perovskite, *Nature*, **458,** 60-63 (2009).

Charge and Spin Order in $Ca_{0.5}Bi_{0.5}FeO_3$

Unusually high-valent transition-metal ions in ABO_3 perovskite-related oxides have been the subject of significant attention due to the rich variety of physical properties they can display. These materials are of particular interest as their inherent electronic instabilities are often relieved via charge disproportionation (CD). The perovskite $Ca_{0.5}Bi_{0.5}FeO_3$ has recently been reported to contain unusually high-valent $Fe^{3.5+}$ and to undergo sequential charge transitions on cooling. Magnetic and transport properties show significant anomalies associated with the charge transitions. In this study we present detailed analysis of the crystal and magnetic structures of this material with neutron powder diffraction data and reveal that $Ca_{0.5}Bi_{0.5}FeO_3$ undergoes a remarkable sequence of CD and charge-transfer (CT) transitions on cooling due to competing electronic instabilities: $Ca_{0.5}Bi^{3+}_{0.5}Fe^{3.5+}O_3$ $\rightarrow Ca_{0.5}Bi^{3+}_{0.5}Fe^{3+}_{0.67}Fe^{4.5+}_{0.33}O_3$ (CD phase) → $Ca_{0.5}Bi^{3+}_{0.25}Bi^{5+}_{0.25}Fe^{3+}O_3$ (CT phase). As shown in Figure 1, the CT phase adopts a simple G-type antiferromagnetic structure of Fe^{3+} spins but the CD phase adopts an unusual charge and magnetic arrangement in which Fe^{3+} spins are antiferromagnetically ordered but the $Fe^{4.5+}$ moments have no long-range order due to magnetic frustration and form a spin glass at low temperatures.

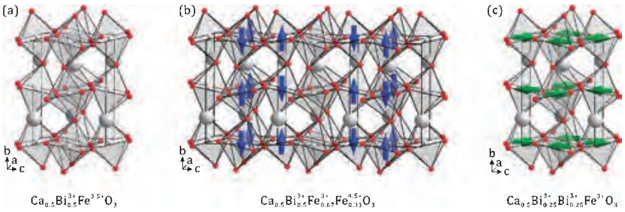

Figure 1. Refined structures of the three phases of $Ca_{0.5}Bi_{0.5}FeO_3$ showing the Fe spin orders in the low-temperature CD (middle) and CT phases (right).

Melting of Oxygen Vacancy Order at Oxide−Heterostructure Interface

Modifications in oxygen coordination environments in heterostructures consisting of dissimilar oxides often emerge and lead to unusual properties of the constituent materials. Engineering the oxygen coordination environments at the heterostructure interfaces is thus considered a new way of tailoring functional properties. Although lots of attention has been paid to slight modifications in the rigid oxygen octahedra of perovskite-based heterointerfaces, revealing the modification behaviors of the oxygen coordination environments in the heterostructures containing oxides with oxygen vacancies have been challenging. Here, we performed cross-sectional HAADF- and ABF-STEM observations for heterointerface between $SrFeO_{2.5}$ (SFO) and $DyScO_3$ (DSO), and found that a significant modification in the oxygen coordination environments -melting of oxygen vacancy order- is induced at the SFO/DSO heterointerface. When an oxygen-deficient perovskite (brownmillerite structure) $SrFeO_{2.5}$ film grows epitaxially on a perovskite $DyScO_3$ substrate, both FeO_6 octahedra and FeO_4 tetrahedra in the (101)-oriented $SrFeO_{2.5}$ thin film connect to ScO_6 octahedra in $DyScO_3$. As a consequence of accommodating a structural mismatch, the alternately ordered arrangement of oxygen vacancies is significantly disturbed and reconstructed in the 2 nm thick heterointerface region (Figure 2). The stabilized heterointerface structure consists of Fe^{3+} octahedra with an oxygen vacancy disorder. The melting of the oxygen vacancy order, which in bulk $SrFeO_{2.5}$ occurs at 1103 K, is induced at the present heterointerface at ambient temperatures.

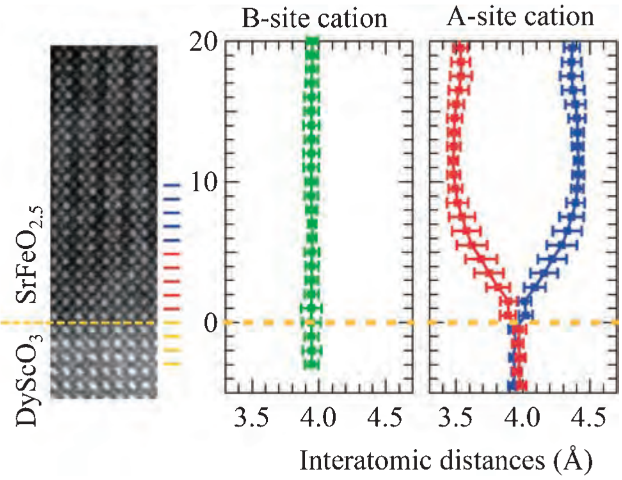

Figure 2. Cross-sectional HAADF-STEM image of the SFO/DSO heterostructure. In-plane interatomic distances of B-site (Fe or Sc) cations and A-site (Sr or Dy) cations across the interface as a function of the atomic position along the out-of-plane direction of the film. The topmost ScO_2 layer in $DyScO_3$ is defined as the zeroth atomic row (dashed yellow lines)

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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 Publication

Wakioka, M.; Takahashi, R.; Ichihara, N.; 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).

A Square Planar Complex of Platinum(0)

The Pt(0) complex [Pt(PPh_3)($Eind_2$-BPEP)] with a pyridine-based PNP-pincer-type phosphaalkene ligand ($Eind_2$-BPEP) has a highly planar geometry around Pt with Σ(Pt) = 358.6°. This coordination geometry is very uncommon for formal d^{10} complexes, and the Pd and Ni homologues with the same ligands adopt distorted tetrahedral geometries. DFT calculations reveal that both the Pt and Pd complexes are M(0) species with nearly ten valence electrons on the metals whereas their atomic orbital occupancies are evidently different from one another. The Pt complex has a higher occupancy of the atomic 6s orbital because of strong s–d hybridization due to relativistic effects, thereby adopting a highly planar geometry reflecting the shape and orientation of the partially unoccupied d_{x2-y2} orbital.

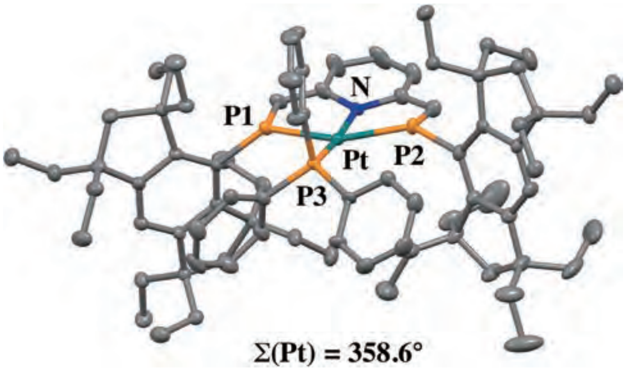


Figure 1. Molecular Structure of [Pt(PPh_3)($Eind_2$-BPEP)].

Square Planar Pt(0) Phosphaalkene Complexes

Recently, we found that the platinum(0) complex [Pt(PPh_3)($Eind_2$-BPEP)] (**1**) coordinated with a pyridine-based PNP-pincer type phosphaalkene ligand ($Eind_2$-BPEP) adopts a highly planar structure around the platinum; this coordination geometry is very uncommon for four-coordinate complexes of formal d^{10} metals. In this study, we synthesized [Pt(L)($Eind_2$-BPEP)] type derivatives of **1** having a series of L [DMAP (**2**), 3,5-lutidine (**3**), PMe_3 (**4**), *t*BuNC (**5**), CO (**6**)], and examined the effects of L on the coordination geometry and spectroscopic properties. The X-ray analysis of **3**, **4**, and **6** demonstrated highly planar coordination geometry comparable to **1**. Complexes **2**–**6** displayed strong absorption in a near infrared region, exhibiting a very deep color in solution as well as in the solid. These absorption bands due to the HOMO–LUMO transitions tended to shift to a shorter wavelength as the π-accepting ability of L increased.

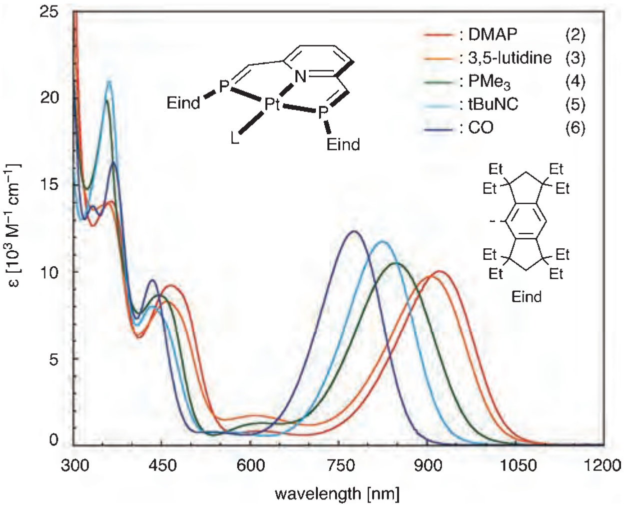
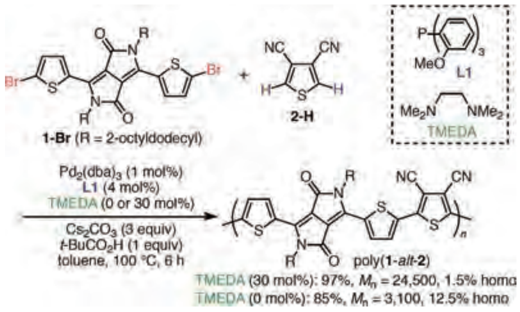


Figure 2. UV-vis-NIR spectra of [Pt(L)($Eind_2$-BPEP)] complexes in THF at room temperature.

Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Highly Selective Synthesis of π-Conjugated Polymers with Diketopyrrolopyrrole Units

We found that the combined use of P(2-$MeOC_6H_4$)$_3$ (**L1**) and TMEDA as ligands effectively prevents defect formation in palladium-catalyzed direct arylation polymerization (DArP) to give donor-acceptor polymers (DA polymers) with diketopyrrolopyrrole (DPP) units. The reaction of 3,6-bis(5-bromo-2-thienyl)diketopyrrolopyrrole (**1-Br**) and 3,4-dicyanothiophene (**2-H**) in the presence of **L1** as the only ligand formed a notable amount of insoluble materials via branching and cross-linking, and the soluble part (M_n = 3100) contained a large quantity of homocoupling defects (12.5%). In contrast, in the presence of **L1** and TMEDA, the formation of insoluble materials was completely suppressed, and homocoupling defects decreased to 1.6%. Moreover, the molecular weight of poly(**1**-*alt*-**2**) remarkably increased (M_n = 24500, 97% yield).



Scheme 1.

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Scope of Research

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

KEYWORDS

Femtosecond Laser Spectroscopy
Semiconductor Nanoparticles
Perovskites
Single Photon Spectroscopy
Solar Cells

Selected Publications

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

Yamada, T.; Yamada, Y.; Nishimura, H.; Nakaike, Y.; Wakamiya, A.; Murata, Y.; Kanemitsu, Y., Fast Free-Carrier Diffusion in $CH_3NH_3PbBr_3$ Single Crystals Revealed by Time-Resolved One- and Two-Photon Excitation Photoluminescence Spectroscopy, *Adv. Electron. Mater.*, **2,** [1500290-1]-[1500290-5] (2016).

Ihara, T.; Kanemitsu, Y., Absorption Cross-section Spectrum of Single CdSe/ZnS Nanocrystals Revealed Through Photoluminescence Excitation Spectroscopy, *Phys. Rev. B*, **92,** [155311-1]-[155311-5] (2015).

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

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

Observation of Ultrafast Multiexciton Coherence in PbS Nanocrystals Probed by Using a Phase-locked Interference Detection Technique

Generation and recombination dynamics of multiexcitons in nanocrystals have been investigated to understand fundamental physics and use them for device applications. However, their initial generation processes have not yet been clarified. To directly observe ultrafast generation processes of multiexcitons, we developed a new pump-probe system using a phase-locked interference detection technique. Using this system, we successfully observed dipole oscillations of multiexcitons. Furthermore, we found that high-frequency dipoles, i.e., harmonic dipole oscillations, are generated by multiexcitons, even though excitation photon energy is set to the low-frequency exciton resonance. These results provide important insight into multiexciton generation mechanisms.

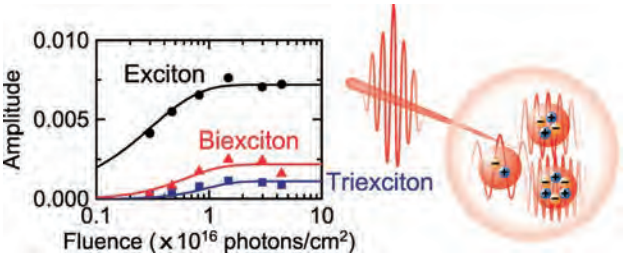

Figure 1. Amplitudes of multiexciton dipole oscillations.

Charged Exciton and Biexciton Dynamics in $CsPbBr_3$ Perovskite Nanocrystals

Lead halide perovskite nanocrystals are attracting much attention owing to their highly luminescent properties. However, nonradiative recombination processes such as Auger recombination of charged excitons (trions) and biexcitons have not yet been understood sufficiently. In this study, we clarified that relaxation dynamics of photoexcited carriers in $CsPbBr_3$ nanocrystals is dominated by three components of exciton, charged exciton, and biexciton, using femtosecond transient-absorption (TA) and single-dot second-order photon correlation spectroscopy. The relaxation lifetimes of charged excitons and biexcitons are determined to be ~40 ps and ~200 ps, respectively. Furthermore, we confirmed the existence of charged excitons even under weak photoexcitation based on the second-order photon correlation measurements.

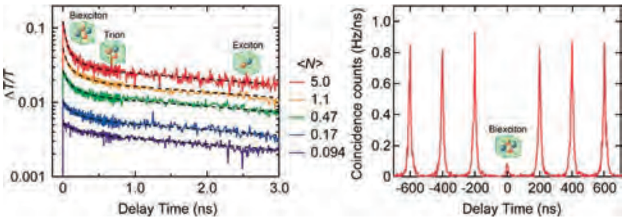

Figure 2. Transient absorption dynamics and second-order photon correlation of $CsPbBr_3$ nanocrystals.

Charge Extraction Processes in $CH_3NH_3PbI_3$ Perovskite Solar Cells

Lead halide perovskites are promising candidates for cost-effective electronic devices including solar cells and light-emitting diodes. In this work, we investigated the photocarrier extraction dynamics in high-efficiency $CH_3NH_3PbI_3$ perovskite solar cells by means of time-resolved photoluminescence (PL) and photocurrent (PC) measurements. We found a peculiar slowdown in the PL lifetime of the perovskite layer for high laser excitation powers, followed by a decrease in the external quantum efficiency of PC. This result indicates that the carrier-extraction process experienced a bottleneck under strong light illumination, limiting the device performance. We conclude that the carrier-extraction rate is sensitive to the photocarrier density, and consequently, the carrier-extraction bottleneck strongly enhances photocarrier recombination losses in the perovskite layer.

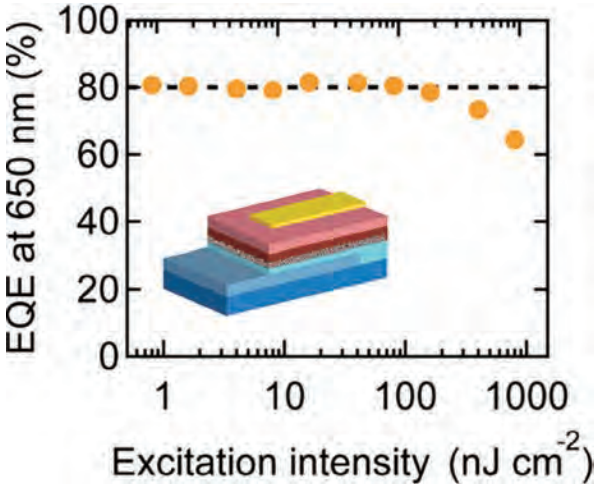

Figure 3. Excitation intensity dependence of external quantum efficiency of perovskite solar cells.

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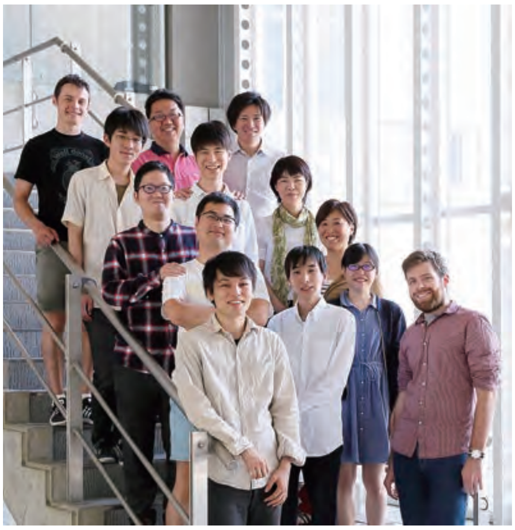
Scope of Research

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

Matsui, T.; Yoshikawa, G.; Mihara, T.; Chatchawankanphanich, O.; Kawasaki, T.; Nakano, M.; Fujie, M.; Ogata, H.; Yamada, T., Replications of Two Closely Related Groups of Jumbo Phages Show Different Level of Dependence on Host-encoded RNA Polymerase, *Front. Microbiol.*, **8,** 1010 (2017).

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Shimizu, Y.; Ogata, H.; Goto, S., Discriminating the Reaction Types of Plant Type III Polyketide Synthases, *Bioinformatics*, **33,** 1937-1943 (2017).

Nishimura, Y.; Watai, H.; Honda, T.; Mihara, T.; Omae, K.; Roux, S.; Blanc-Mathieu, R.; Yamamoto, K.; Hingamp, P.; Sako, Y.; Sullivan, M. B.; Goto, S.; Ogata, H.; Yoshida, T., Environmental Viral Genomes Shed New Light on Virus-host Interactions in the Ocean, *mSphere*, **2,** e00459-16 (2017).

Shimizu, Y.; Ogata, H.; Goto, S., Type III Polyketide Synthases: Functional Classification and Phylogenomics, *ChemBioChem*, **18,** 50-65 (2017).

Diversity and Biogeography of Diatoms and Haptophytes in the Pacific Ocean

Diatoms and haptophytes are two major phytoplankton groups, playing pivotal roles in global biogeochemical cycles and marine ecosystems. Previous studies suggest that diatoms and haptophytes are *r*- and *K*-selected species, respectively, but precise linkages between their ecological traits and geographical distributions remain poorly understood. We recently examined the basin-scale variability of the abundance and taxonomic composition of these two phytoplankton groups across thirty-five sites in the Pacific Ocean using DNA metabarcoding targeting the 18S rRNA gene. The diatom community was generally dominated by a few genera at each sample site, whereas the haptophyte community consisted of a large number of genera in most of the sites, suggesting greater inter-genus competition among diatoms (Figure 1). Consequently, the diversity of diatoms was generally lower than that of haptophytes, with haptophyte diversity fairly stable within the study area. The diversity and composition of haptophyte community showed stronger correlations with environmental variables than diatom community, indicating that the diatom community is more affected by other factors such as physical forcing. Our data further supports that their distinct ecological strategies underlies the emergence of the contrasting diversity patterns of these phytoplankton groups in the central Pacific at a basin scale.

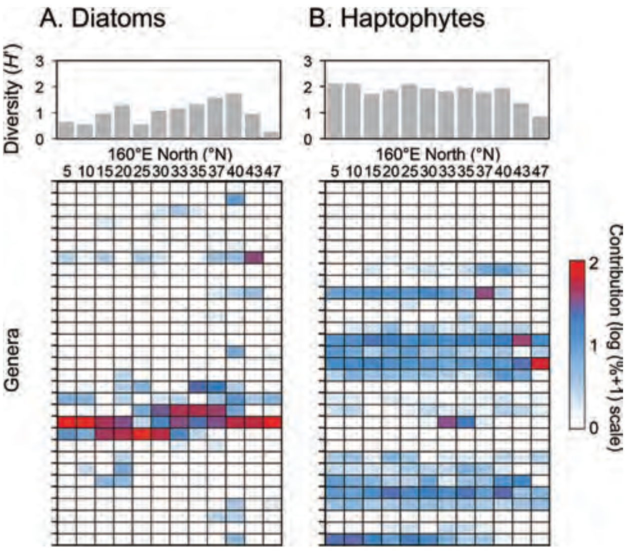

Figure 1. Genus-level diversity and distribution patterns of (A) diatoms and (B) haptophytes in the surface layer of the western North Pacific (5°N−47°N along the 160°E transect).

Two Closely Related Groups of Jumbo Phages Encoding RNA Polymerase Differ in Their Level of Dependence on Host Transcription Machinery

Ralstonia solanacearum phages ϕRP12 and ϕRP31 are jumbo phages presenting similar virion morphology, genome organization and host range. Phylogenetic and comparative analyses at both genomic and gene levels revealed ϕRP12 and ϕRP31 are closely related to previously recognized ϕKZ-related phages, and most closely related to *R. solanacearum* phages ϕRSL2 and ϕRSF1 (Figure 2). Compared with the ϕRSL2 group (ϕRSL2 and ϕRSF1), the ϕRP12 group (ϕRP12 and ϕRP31) possess larger genomes (ca. 280 kbp, 25% larger). The genomes of both groups encode many genes conserved in ϕKZ-related phages, including the β and β' subunits of the multisubunit RNA polymerase (RNAP). The replication of ϕRP12 and ϕRP31 was not affected by rifampicin treatment (20 μg/ml), suggesting that phage-encoded RNAPs function to start and complete the infection cycle of these phages without the need of host-encoded RNAPs. In contrast, ϕRSL2 and ϕRSF1 did not produce progeny phages in the presence of rifampicin (5 μg/ml). This observation suggests that some ϕRP12/ϕRP31 factors, that are absent in ϕRSL2 and ϕRSF1, are involved in their host-independent (or rifampicin-resistant) RNAP activity.

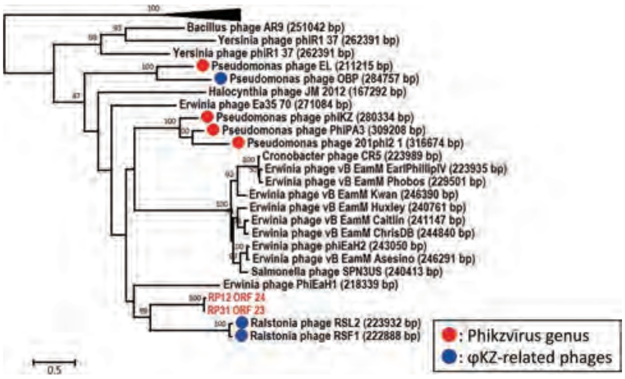

Figure 2. Maximum likelihood phylogenetic tree of the terminase proteins of ϕKZ-related phages. Bootstrap branch support is given for each branch. Number at scale bar indicates the number of substitutions per site.

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Assoc Prof
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LIN, Chun-Yu
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Students

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YU, Coleman (D1)
TAKAGI, Motoshige (D1)
LI, Ruiming (M2)
CAO, Yu (M1)
MARUTA, Kunpei (M1)
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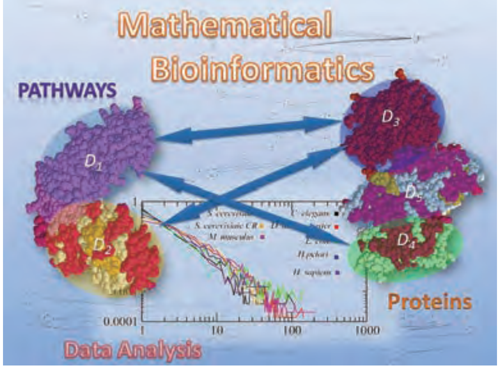
WANG, Feiqi (RS)

Scope of Research

Due to 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, 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.; Jansson, J.; Takasu, A.; Tamura, T., On the Parameterized Complexity of Associative and Commutative Unification, *Theor. Comput. Sci.*, **660,** 57-74 (2017).

Cheng, X.; Tamura, T.; Ching, W. K.; Akutsu, T., Discrimination of Singleton and Periodic Attractors in Boolean Networks, *Automatica*, **84,** 205-213 (2017).

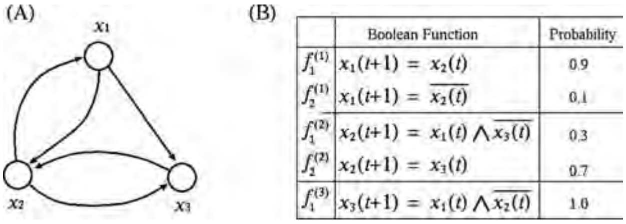
Kato, Y.; Mori, T.; Sato, S.; Maegawa, S.; Hosokawa, H.; Akutsu, T., An Accessibility-Incorporated Method for Accurate Prediction of RNA-RNA Interactions from Sequence Data, *Bioinformatics*, **33,** 202-209 (2017).

Ishitsuka, M.; Akutsu, T.; Nacher, J. C., Critical Controllability Analysis of Directed Biological Networks Using Efficient Graph Reduction, *Sci. Rep.*, **7,** [14361-1]-[14361-10] (2017).

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

Various kinds of mathematical models have been utilized for understanding dynamical behavior of biological systems. Among them, the Boolean network (BN) is a simple but well-studied discrete model, especially for modeling genetic regulatory networks. In a BN, each node takes a Boolean value, 0 or 1, at each time step, and the states of all nodes are updated synchronously according to Boolean functions assigned to nodes, where each node corresponds to a gene, and 1 and 0 mean that genes are active and inactive, respectively. Since a BN is a deterministic model and thus cannot cope with such effects as noise and uncertainty, several probabilistic extensions of a BN have been proposed and studied. Among them, the probabilistic Boolean network (PBN) has been well-studied. Different from a BN, multiple Boolean functions can be assigned to each node in a PBN and one function is randomly selected at each time step according to the prescribed probability distribution (Figure 1).

For both BNs and PBNs, it is important to infer the network model from such data as gene expression time series data and many methods have been proposed. However, almost no theoretical studies have been done on inference of a PBN from sample data. Since it is quite difficult to exactly determine the probabilities from samples, we focus on determining only the structure (graph structure + Boolean functions) of a PBN and study the number of samples required for uniquely determining the structure. We show via theoretical analysis and computer simulation that the structure of a PBN can be exactly identified with high probability from a relatively small number of samples for interesting classes of PBNs of bounded indegree (i.e., the number of edges per node is bounded by a constant). On the other hand, we also show that there exist classes of PBNs for which it is impossible to uniquely determine the structure of a PBN from samples. We are also performing detailed theoretical analyses with focusing on an important subclass of PBNs which consist of Boolean threshold functions.



	Boolean Function	Probability
$f_1^{(1)}$	$x_1(t+1) = x_2(t)$	0.9
$f_2^{(1)}$	$x_1(t+1) = \overline{x_2(t)}$	0.1
$f_1^{(2)}$	$x_2(t+1) = x_1(t) \wedge \overline{x_3(t)}$	0.3
$f_2^{(2)}$	$x_2(t+1) = x_3(t)$	0.7
$f_1^{(3)}$	$x_3(t+1) = x_1(t) \wedge \overline{x_2(t)}$	1.0

Figure 1. Example of a probabilistic Boolean network (PBN). (A) Graph structure of PBN. (B) Boolean functions and corresponding probabilities assigned to each node.

Observability of Singleton and Periodic Attractors in Boolean Networks

Knowing internal states of complex systems is important for diagnosing various kinds of biological, artificial, and social systems. Especially, it is important to identify a small set of variables so that we can reconstruct the system's complete internal state at any given time step from time-series data of these variables. In such a case, the system is called observable. This observability problem has been well-studied for linear systems. However, biological systems contain non-linear elements to which existing theory/methods cannot be effectively applied. Furthermore, existing studies suggest that a large number of variables/nodes are required to observe the whole state of certain kinds of non-linear biological systems.

In order to cope with this difficult situation, we do not intend to identify the whole state instead focus on identification of statically and periodically stable states (attractors) because attractors are often considered to correspond to cell types. In this study, we adopt a Boolean network (BN) as a non-linear model of biological systems and consider the problem of identifying a minimum set of sensor nodes to discriminate static and periodic attractors using the BN (Figure 2), which might be useful to identify cell types. We prove that one node is not necessarily enough but two nodes are always enough to discriminate two periodic attractors by making use of the Chinese remainder theorem. Based on this, we develop an algorithm to determine the minimum number of nodes to discriminate all given attractors. The results of computational experiments suggest that attractors (corresponding to cell types) in realistic BN models can be discriminated by observing the states of only a small number of nodes.

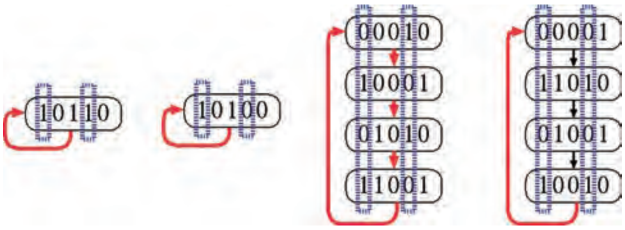


Figure 2. These four attractors (two statically stable and two periodically stable states) can be discriminated by observing time series data of two nodes (shown by blue dotted curves), where four attractors correspond to four different cell types.

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Program-Specific Res
WIMALAWARNE, Kishan
(D Eng)


Program-Specific Res
SUN, Lu
(D Eng)

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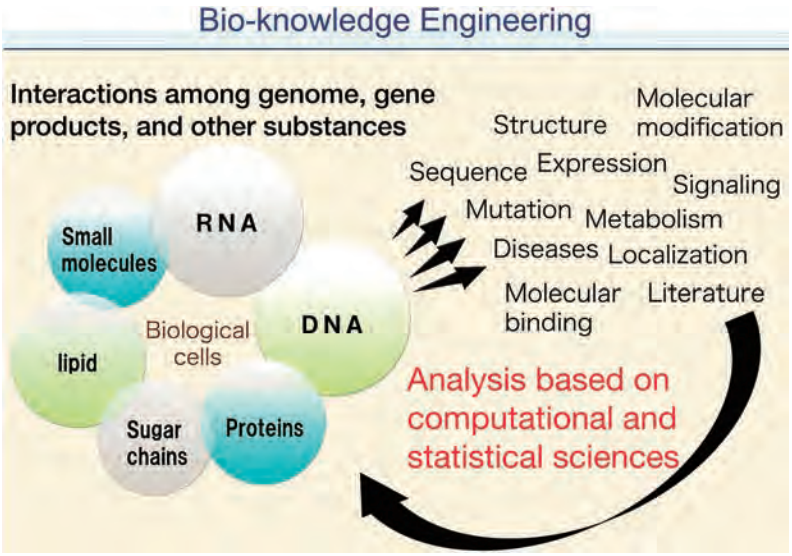
NGUYEN, Dai Hai (D1)
TOHZAKI, Yudai (M2)
KANEKO, Teruo (UG)

Guest Scholar

LI, Limin (Ph D) Xi'an Jiaotong University, China, P.R., 17 November–1 December

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

Yamada, M.; Lian, W.; Goyal, A.; Chen, J.; Wimalawarne, K.; Kahn, S.; Kaski, S.; Mamitsuka, H.; Chang, Y., Convex Factorization Machine for Toxicogenomics Prediction, *Proceedings of the Twenty-third ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD 2017)*, 1215-1224 (2017).

Karasuyama, M.; Mamitsuka, H., Adaptive Edge Weighting for Graph-Based Learning Algorithms, *Mach. Learn.*, **106(2),** 307-335 (2017).

Takigawa, I.; Mamitsuka, H., Generalized Sparse Learning of Linear Models over the Complete Subgraph Feature Set, *IEEE Trans. Pattern Anal. Mach. Intell.*, **39(3),** 617-624 (2017).

Yotsukura, S.; Karasuyama, M.; Takigawa, I.; Mamitsuka, H., Exploring Phenotype Patterns of Breast Cancer within Somatic Mutations, *Brief. Bioinform.*, **18(4),** 619-633 (2017).

Yotsukura, S.; duVerle, D.; Hancock, T.; Natsume-Kitatani, Y.; Mamitsuka, H., Computational Recognition for Long Non-coding RNA (lncRNA): Software and Databases, *Brief. Bioinform.*, **18(1),** 9-27 (2017).

Distances on Graph with Global Information

Graph is an important topic in Machine Learning for many reasons. Graph, as a model of networks, is frequently used for network analysis, which found many applications in biological, chemical and social networks. Moreover, graph has been used in many other situation in analyzing complicated data. In high dimensional data, one of the most difficult situation for statistical analysis, neighborhood graph can encode data distribution to avoid the curse of dimensionality in many usual statistical models. Data on manifolds, which are too complicated for parametric models, are usually converted into graphs. Graph has surprising properties on other problem such as in semi-supervised learning, regularization and spectral clustering. It offers a nice way to estimate the number of clusters of data, which is usually a very difficult problem. In short, graph is a flexible tool to model data in difficult situations.

A graph encodes distribution of data, the common problem is that one needs to learn a statistical model from the graphs. As a graph usually represents similarity relationship among data points, it is the objective to learn a model that is smooth on the graph. Graph Laplacian is used to score how smooth a function is on graph. For its computational efficiency, most methods extract information on graph Laplacians to construct learning models, such as graph kernels, commute time, hitting time distance, resistance distances and Laplacian graph embedding.

However, it was recently discovered that in large graphs, graph Laplacians usually do not give meaningful information for learning problem. This is known as the global information loss problem. That is, spectral clustering would have almost random results. Semi-supervised learning models, usually extract information from unlabeled data, cannot benefit from large graphs encoding the data. It was later proven that for large enough graphs, graph Laplacians only contain local information, not suitable for learning models. This is a key problem with large data where graph Laplacians have been usually used. This result shows why graph fail to fulfill its potential of a flexible tool to model difficult distributions.

The aim of our research is to make graph a versatile tool for learning statistical models even for large graphs. We wish to estimate pairwise distances on a graph that reflect global information so that it can be used for learning models. Our idea is to solve the problem of resistance distance that an electrical flow on the graph would spread out too much, resulting in its energy function to be concentrated around its sources. We designed new resistance distances that account for this problem with a new energy function on the electrical flow. We also proved that the new distances keep global information. Our new distances were then applied to various problem of learning on graphs and show its usefulness for large data.

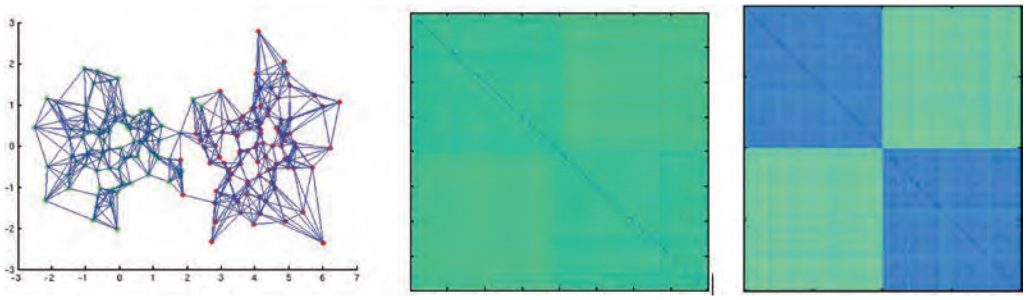


Figure 1. A graph (left) consists of two well-connected clusters. The distance based on graph Laplacian (heatmap in the middle heatmap) does not show cluster structure. Our new distance shows the two clusters by having two dark diagonal blocks on the heatmap (right).

HAKUBI RESEARCHERS' ACTIVITIES IN ICR

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

Research Topic

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

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

Host Laboratory Laboratory of Advanced Solid State Chemistry

Host Professor SHIMAKAWA, Yuichi

Outline of Research

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

ACTIVITIES OF JOINT USAGE/RESEARCH CENTER

JURC Cooperative Research Subjects 2017

(1 April 2017 ~ 31 March 2018)

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

Synthesis of Transition Metal Complexes with a Pincer-Type Phosphaalkene Ligand and Their Application to Catalytic Reactions
MATSUO, Tsukasa, Faculty of Science and Engineering / Graduate School of Science and Engineering Research, Kindai University
Host in JURC TAKEUCHI, Katsuhiko

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

Investigation of Carrier Transport Mechanism in Halide-perovskite-based Photodevices
YAMADA, Yasuhiro, Department of Physics, Graduate School of Science, Chiba University
Host in JURC KANEMITSU, Yoshihiko

Many Body Interactions between Excitons in Semiconductor Quantum Dots
OGAWA, Yoshihiro, Joetsu University of Education
Host in JURC KANEMITSU, Yoshihiko

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

Iron-Catalyzed Enantioselective C–C Bond Formation
ILIES, Laurean, Department of Chemistry, School of Science, The University of Tokyo
Host in JURC NAKAMURA, Masaharu

Study on First-raw Late Transition-metal Complexes Bearing Anionic Tridentate Ligand
YAMAGUCHI, Yoshitaka, Faculty of Engineering, Division of Materials Science and Chemical Engineering, Yokohama National University
Host in JURC NAKAMURA, Masaharu

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

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

Genome Analysis of New Giant DNA Virus Isolated from Hot Spring Water in Japan
TAKEMURA, Masaharu, Faculty of Science, Tokyo University of Science
Host in JURC OGATA, Hiroyuki

Establishment of a New Virus-evolution-hypothesis Through an Intensive Quest of Megaviruses in a Highly Enclosed Inlet, Uranouchi Bay, Where Various Algal Blooms Frequently Occur
NAGASAKI, Keizo, Faculty of Agriculture and Marine Science, Kochi University
Host in JURC OGATA, Hiroyuki

New Prediction Method for Metabolic Pathway from Genome and Metagenome by Combination of MAPLE and GENIES
TAKAMI, Hideto, Research and Development Center for Submarine Resources, Japan Agency for Marine-Earth Science and Technology
Host in JURC OGATA, Hiroyuki

Machine Learning Based on Sparsity Regularization with Auxiliary Genomic Information
SHIGA, Motoki, Informatics Course, Department of Electrical, Electronic and Computer Engineering, Faculty of Engineering, Gifu University
Host in JURC MAMITSUKA, Hiroshi I

Creation of Highly Active Polypodna Complexes and Their Intracellular Delivery
NISHIKAWA, Makiya, Faculty of Pharmaceutical Sciences, Tokyo University of Science
Host in JURC FUTAKI, Shiroh

Development of Novel Heteroazulene Oligomer Toward Organic Functional Dyes
KUROTOBI, Kei, National Institute of Technology, Kurume College
Host in JURC MURATA, Yasujiro

Synthesis of π-Extended Thienofuran Derivatives by Dehydrative Cyclization, and Their Properties
SUGA, Seiji, Graduate School of Natural Science and Technology, Okayama University
Host in JURC MURATA, Yasujiro

Synthesis of Metal Complexes with Three-dimensional π-Systems and their Performance as Organic Semiconductors
MURATA, Michihisa, Department of Applied Chemistry, Osaka Institute of Technology
Host in JURC MURATA, Yasujiro

Molecular Engineering of Highly Crystalline Organic Semiconductors via Precursor Approaches
SUZUKI, Mitsuharu, Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST)
Host in JURC MURATA, Yasujiro

Study on Highly Efficient Transportation of Metal Ions through a Membrane Containing Ionic Liquid
MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education
Host in JURC SOHRIN, Yoshiki

Elucidation of Hydrogen Distribution in Single-crystalline Pd Nanoparticles
YAMAUCHI, Miho, International Institute for Carbon-Neutral Energy Research, Kyushu University
Host in JURC TERANISHI, Toshiharu F

I : International Joint Research
F : Female PI

Design and Creation of New Functional Material Having Both Optical Diagnostic and Therapeutic Effects using Metal Nanoparticle
ISHIHARA, Miya, National Defense Medical College
Host in JURC TERANISHI, Toshiharu F

Test of Resonant Effect in Plasmon Heating of Periodic Lattice of Metal Domain
SHIMADA, Ryoko, Department of Mathematical and Physical Sciences, Faculty of Science, Japan Women's University
Host in JURC WATANABE, Hiroshi F

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

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

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

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

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

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

Diagnostics of Li-Ion Batteries with Laser-Accelerated Protons
KATO, Yoshiaki, The Graduate School for the Creation of New Photonics Industries
Host in JURC SAKABE, Shuji

Development on a Repetitive Laser-driven Neutron Source
ARIKAWA, Yasunobu, Institute of Laser Engineering, Osaka University
Host in JURC INOUE, Shunsuke

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

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

Research and Development on Future Accelerator Toward ILC Project
HAYANO, Hitoshi, Accelerator Laboratory, High Energy Accelerator Research Organization
Host in JURC IWASHITA, Yoshihisa

Research on the High-performance Superconducting Cavity with the Inner-surface Preparation
by Nitrogen-doping and Thin-film Creation Processes
SAEKI, Takayuki, Accelerator Laboratory, High Energy Accelerator Research Organization
Host in JURC IWASHITA, Yoshihisa

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

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

Activation of Small Molecules at the Reaction Sites Composed of Transition-metal and Heavier Typical Elements
OKAZAKI, Masaaki, Graduate School of Science and Technology, Hirosaki University
Host in JURC OZAWA, Fumiyuki

Development of Iron Polycarboxylate Complexes which Catalyze Oxidation Reactions
SUGIURA, Masaharu, Faculty of Life Sciences, Kumamoto University
Host in JURC NAKAMURA, Masaharu

Elucidation of Electronic Structures of Cycloparaphenylenes and Their Application to Materials Science
UCHIYAMA, Masanobu, Graduate School of Phamaceutical Science, The University of Tokyo
Host in JURC YAMAGO, Shigeru

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

Cell Penetrating Peptide-based Intracellular Delivery of Inhibitors of Protein-protein Interactions
OHKANDA, Junko, Academic Assembly School of Science and Technology Institute of Agriculture, Shinsyu University
Host in JURC FUTAKI, Shiroh F

A Study of Reactivity on Open-shell Molecules in Macrocyclic Systems
ABE, Manabu, Graduate School of Science, Hiroshima University
Host in JURC YAMAGO, Shigeru

Excited-state Dynamics of Cycloparaphenylene Dications
MAJIMA, Tetsuro, The Institute of Scientific and Industrial Research, Osaka University
Host in JURC YAMAGO, Shigeru

Host-guest Chemistry of Cycloparaphenylenes and Fullerene Derivatives
MATSUO, Yutaka, School of Chemistry and Materials Science, University of Science and Technology of China
Host in JURC YAMAGO, Shigeru I

Exploration of Non-lead Perovskite Solar Cell and Development of Novel Efficient Organic Hole Transfer Layer
SAEKI, Akinori, Graduate School of Engineering, Osaka University
Host in JURC WAKAMIYA, Atsushi

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

Flux Study of Bioactive Trace Metals in the East China Sea
NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kindai University
Host in JURC SOHRIN, Yoshiki

Structural Analyses for Adhesive Mechanism in Tri-block Polymer Thin Films Using Neutron Reflectivity and Grazing Incidence X-ray Scattering Measurement
MIYAZAKI, Tsukasa, Comprehensive Research Organization for Science and Society
Host in JURC TAKENAKA, Mikihito

Dynamics of Guest Chains in Polymer Networks with Different Crosslinking Types
KATASHIMA, Takuya, Graduate School of Science, Osaka University
Host in JURC MATSUMIYA, Yumi

Dynamical Correlations between Molecules in Polymeric Liquids
SUKUMARAN, Sathish Kumar, Graduate School of Organic Materials Science, Yamagata University
Host in JURC WATANABE, Hiroshi I

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

Study on the Regulatory Mechanism of Plant Epidermal Cell Differentiation
TOMINAGA, Rumi, Graduate School of Biosphere Science, Hiroshima University
Host in JURC AOYAMA, Takashi F

Study on Lipid Secretion Pathways of Plant Cells
YAZAKI, Kazufumi, Research Institute for Sustainable Humanosphere, Kyoto University
Host in JURC AOYAMA, Takashi

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

New Cellular Functions of Acyldopamine
ITO, Akihiro, RIKEN Center for Sustainable Resource Science, Chemical Genomics Research Group
Host in JURC UESUGI, Motonari

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

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

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

Selective Chemical Modification of Biomolecules in Membrane by Functionalized Catalysts
KUNISHIMA, Munetaka, Faculty of Pharmaceutical Sciences, Institute of Medical, Pharmaceutical, and Health Sciences, Kanazawa University
Host in JURC KAWABATA, Takeo

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

Structural Control and Functional Development of Alkali Silicate Glasses by High Pressure Synthesis
MASAI, Hirokazu, Department of Materials and Chemistry, National Institute of Advanced Industrial Science and Technology
Host in JURC SAITO, Takashi

Application of Surfactants for Separation of Boron Group Elements as Synergist
KURAHASHI, Kensuke, Environmental and Materials Chemistry Course, Osaka Prefecture University College of Technology
Host in JURC SOHRIN, Yoshiki

Development of Organic Reagents Highly Selective for the Extraction and Adsorption of Rare Metals
YAMAZAKI, Shoko, Department of Chemistry, Nara University of Education
Host in JURC UMETANI, Shigeo F

Precise Analyses of Hierarchical Structure of Polymer Composite Materials by Electron/X-ray/Neutron Beams
MURASE, Hiroki, Faculty of Home Economics, Kyoritsu Women’s University
Host in JURC TSUJII, Yoshinobu

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

Dielectric Relaxation of Linear Rouse Chains having Type-A Dipole and Undergoing Head-to-Head Association and Dissociation
KWON, Youngdon, School of Chemical Engineering, Sungkyunkwan University
Host in JURC MATSUMIYA, Yumi I

The Sequence Control of Two-component Multiblock Copolymers and the Investigation of Bulk and Surface Properties
TAKANO, Atsushi, Graduate School of Engineering, Nagoya University
Host in JURC WATANABE, Hiroshi

Mode of Action Study of Benzoylphenylurea Insecticides at the Molecular Level
NAKAGAWA, Yoshiaki, Graduate School of Agriculture, Kyoto University
Host in JURC WATANABE, Bunta

Synthesis and Application of Macrocyclic Compounds Incorporating Triphenylamine Units
IWANAGA, Tetsuo, Department of Chemistry, Faculty of Science, Okayama University of Science
Host in JURC MURATA, Yasujiro

Study of Surface Enhanced Infrared Absorption by Using Multiple-angle Incidence Resolution Spectrometry
SHIMADA, Toru, Faculty of Education, Hirosaki University
Host in JURC HASEGAWA, Takeshi

Even-odd Effects on Film Structures of Dicarboxylic Acids on Air/Water Interface and Their Atmospheric Implications
HAMA, Tetsuya, Institute of Low Temperature Science, Hokkaido University
Host in JURC HASEGAWA, Takeshi

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

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

Developments of Highly Functional Spinel Ferrite Thin Films as a Novel Spintornic Materials
NAGAHAMA, Taro, Laboratory of Advanced Materials Chemistry, Graduate School of Engineering, Hokkaido University
Host in JURC ONO, Teruo

Measurements of Giant Magnetoresistance Effect in Magnetic Nanowires with Multilayer Structure
YAMADA, Keisuke, Faculty of Engineering, Gifu University
Host in JURC ONO, Teruo

Magnetic Nanostructures Confined or Created by Electric Field
CHIBA, Daichi, School of Physical Science and Engineering, Nagoya Institute of Technology
Host in JURC ONO, Teruo

A Study on the Relationship between Structures and Functions for Organic Devices
FUKUSHIMA, Tatsuya, Department of Chemical Science and Engineering, Kobe University
Host in JURC KAJI, Hironori

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

Studies on the Function and Formation Mechanism of the Bound D-Amino Acids in Food Proteins
OMORI, Taketo, Faculty of Engineering, Osaka Institute of Technology
Host in JURC KURIHARA, Tatsuo

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

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

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

In-situ Measurements of Physical Properties and Crystallization Process of Glasses Under High Temperatures and High Pressures
MASUNO, Atsunobu, Graduate School of Science and Technology, Hirosaki University
Host in JURC SHIMAKAWA, Yuichi

Photochemical Control of Gel-gel Transitions in Polymer-brush-afforded Silica Particle/Photoresponsive Liquid Crystals
YAMAMOTO, Takahiro, Research Institute for Sustainable Chemistry, National Institute of Advanced Industrial Science and Technology (AIST)
Host in JURC OHNO, Kohji

Synthesis and Characterization of Novel Narrow Band Gap Semiconductor Nanocrystals
TACHIBANA, Yasuhiro, School of Aerospace, Mechanical and Manufacturing Engineering, RMIT University
Host in JURC TERANISHI, Toshiharu I

Identification of Proteins Interacting with Cell-penetrating Peptides for Cancer Targeting
KUWATA, Keiko, Institute of Transformative Bio-Molecules, Nagoya University
Host in JURC FUTAKI, Shiroh F

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

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

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

Study on the Biosynthetic Pathway of Steroidal Glycoalkaloids in *Solanaceae* Plants
MIZUTANI, Masaharu, Graduate School of Agricultural Science, Kobe University
Host in JURC WATANABE, Bunta

SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

Elucidation of a Mechanism of Crystalline-to-amorphous Framework Transformation in Coordination Polymers
INUKAI, Munehiro, Faculty of Science and Technology, Tokushima University
Host in JURC KAJI, Hironori

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

Fabrication of Helical Ultrathin Au Nanowires with Chiral Photonic-metamaterial Property
KAWAI, Takeshi, Faculty of Engineering, Tokyo University of Science
Host in JURC KURATA, Hiroki

Analysis of Local Magnetic Moment in Nd-Fe-B Magnet by Electron Energy-loss Spectroscopy
SAITO, Hikaru, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University
Host in JURC KURATA, Hiroki

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

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

Synthesis and Structural Elucidation of Unsaturated Compounds of Germanium
MATSUO, Tsukasa, Faculty of Science and Engineering, Kindai University
Host in JURC TOKITOH, Norihiro

Experimental Electron Density Distribution Analysis of Organosilicon Compounds
HASHIZUME, Daisuke, Center for Emergent Matter Science, RIKEN
Host in JURC TOKITOH, Norihiro

Synthesis and Emission Properties of Aromatic Compounds Containing a Phosphorus Atom
NAGAHORA, Noriyoshi, Department of Chemistry, Faculty of Science, Fukuoka University
Host in JURC TOKITOH, Norihiro

Synthesis and Structure of Kinetically Stabilized Main Group Element Compounds using 9-Triptycylmethyl Groups
MINOURA, Mao, Faculty of Science, Rikkyo University
Host in JURC TOKITOH, Norihiro

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

Isolation and Mass Spectrometry of Intermediate Clusters Synthesized by Ligand Exchange Reaction
NEGISHI, Yuichi, Faculty of Science, Department of Applied Chemistry, Tokyo University of Science
Host in JURC ISOZAKI, Katsuhiro

SUBJECTS ENCOURAGING JOINT PROGRAM

Exploring for Novel Functional Transition-metal Oxides by High-pressure Synthesis
CHEN, Wei-Tin, Center for Condensed Matter Sciences, National Taiwan University
Host in JURC SHIMAKAWA, Yuichi I

Elucidating the Cycle of Dissolved and Particulate Trace Metals in the Ocean Based on Stable Isotope Analysis
HO, Tung-Yuan, Research Center for Environmental Changes, Academia Sinica
Host in JURC TAKANO, Shotaro I

Precise Synthesis of Photo-functional Polymers Using Organocatalyzed Living Radical Polymerization
GOTO, Atsushi, School of Physical and Mathematical Sciences, Nanyang Technological University
Host in JURC TSUJII, Yoshinobu I

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

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

JURC Publications (Selected Examples)

(until 31 May 2017)

A Square-Planar Complex of Platinum(0)

Takeuchi, K.; Taguchi, H.; Tanigawa, I.; Tsujimoto, S.; Matsuo, T.; Tanaka, H.; Yoshizawa, K.; Ozawa, F., *Angew. Chem. Int. Ed.*, **55,** 15347-15350 (2016).

Abstract

The Pt^0 complex $[Pt(PPh_3)(Eind_2\text{-}BPEP)]$ with a pyridine-based PNP-pincer-type phosphaalkene ligand ($Eind_2$-BPEP) has a highly planar geometry around Pt with $\sum(Pt)=358.6°$. This coordination geometry is very uncommon for formal d^{10} complexes, and the Pd and Ni homologues with the same ligands adopt distorted tetrahedral geometries. DFT calculations reveal that both the Pt and Pd complexes are M^0 species with nearly ten valence electrons on the metals whereas their atomic orbital occupancies are evidently different from one another. The Pt complex has a higher occupancy of the atomic 6s orbital because of strong s–d hybridization due to relativistic effects, thereby adopting a highly planar geometry reflecting the shape and orientation of the partially $d_{x^2-y^2}$ unoccupied orbital.

Interfacial Charge-Carrier Trapping in $CH_3NH_3PbI_3$-Based Heterolayered Structures Revealed by Time-Resolved Photoluminescence Spectroscopy

Yamada, Y.; Yamada, T.; Shimazaki, A.; Wakamiya, A.; Kanemitsu, Y., *J. Phys. Chem. Lett.*, **7,** 1972-1977 (2016).

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Abstract

The fast-decaying component of photoluminescence (PL) under very weak pulse photoexcitation is dominated by the rapid relaxation of the photoexcited carriers into a small number of carrier-trapping defect states. Here, we report the subnanosecond decay of the PL under excitation weaker than 1 nJ/cm^2 both in $CH_3NH_3PbI_3$-based heterostructures and bare thin films. The trap-site density at the interface was evaluated on the basis of the fluence-dependent PL decay profiles. It was found that high-density defects determining the PL decay dynamics are formed near the interface between $CH_3NH_3PbI_3$ and the hole-transporting Spiro-OMeTAD but not at the $CH_3NH_3PbI_3/TiO_2$ interface and the interior regions of $CH_3NH_3PbI_3$ films. This finding can aid the fabrication of high-quality heterointerfaces, which are required improving the photoconversion efficiency of perovskite-based solar cells.

Critical Controllability in Proteome-wide Protein Interaction Network Integrating Transcriptome

Ishitsuka, M.; Akutsu, T.; Nacher, J. C., *Sci. Rep.*, **6,** [23541-1]-[23541-13] (2016).

Abstract

Recently, the number of essential gene entries has considerably increased. However, little is known about the relationships between essential genes and their functional roles in critical network control at both the structural (protein interaction network) and dynamic (transcriptional) levels, in part because the large size of the network prevents extensive computational analysis. Here, we present an algorithm that identifies the critical control set of nodes by reducing the computational time by 180 times and by expanding the computable network size up to 25 times, from 1,000 to 25,000 nodes. The developed algorithm allows a critical controllability analysis of large integrated systems composed of a transcriptome- and proteome-wide protein interaction network for the first time. The data-driven analysis captures a direct triad association of the structural controllability of genes, lethality and dynamic synchronization of co-expression. We believe that the identified optimized critical network control subsets may be of interest as drug targets; thus, they may be useful for drug design and development.

Detailed Analysis of Charge Transport in Amorphous Organic Thin Layer by Multiscale Simulation without Any Adjustable Parameters

Uratani, H.; Kubo, S.; Shizu, K.; Suzuki, F.; Fukushima, T.; Kaji, H., *Sci. Rep.*, **6,** 39128, doi: 10.1038/srep39128 (2016).

Abstract

Hopping-type charge transport in an amorphous thin layer composed of organic molecules is simulated by the combined use of molecular dynamics, quantum chemical, and Monte Carlo calculations. By explicitly considering the molecular structure and the disordered intermolecular packing, we reasonably reproduce the experimental hole and electron mobilities and their applied electric field dependence (Poole–Frenkel behaviour) without using any adjustable parameters. We find that the distribution of the density-of-states originating from the amorphous nature has a significant impact on both the mobilities and Poole–Frenkel behaviour. Detailed analysis is also provided to reveal the molecular-level origin of the charge transport, including the origin of Poole–Frenkel behaviour.

Activation of Dihydrogen by Masked Doubly Bonded Aluminum Species

Nagata, K.; Murosaki, T.; Agou, T.; Sasamori, T.; Matsuo, T.; Tokitoh, N., *Angew. Chem. Int. Ed.*, **55,** 12877-12880 (2016).

Abstract

Activation of dihydrogen by masked dialumenes (Al=Al doubly bonded species) is reported. Reactions of barrelene-type dialumanes, which have the reactivity as masked equivalents of 1,2-diaryldialumenes ArAl=AlAr, with H_2 afforded dihydroalumanes $ArAlH_2$ at room temperature (Ar: bulky aryl groups). These dihydroalumanes form hydrogen-bridged dimers $[ArHAl(\mu\text{-}H)]_2$ in the crystalline state, while a monomer–dimer equilibrium was suggested in solution. The 1,2-diaryldialumenes generated from the barrelene-type dialumanes are the putative active species in the cleavage of H_2.

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
TANAKA, Kentaro
(D Eng)

Laboratory of Advanced Inorganic Synthesis

Professor, Graduate School of Science, Nagoya University
(Furo-cho, Chikusa-ku, Nagoya-shi, Aichi 464-8602)

Lecture at *ICR*
Chemistry of Soft Nanospace and Self-assembly

Vis Prof
FUKUYAMA, Tohru
(Ph D)

Laboratory of Chemical Biology

Specially-appointed Professor, Graduate School of Pharmaceutical Sciences, Nagoya University
(Furo-cho, Chikusa-ku, Nagoya-shi, Aichi 464-8601)

Lecture at *ICR*
Scientific English
Looking back at My Past

Vis Prof
SAKURAI, Shinichi
(D Eng)

Laboratory of Polymer Materials Science

Professor, Kyoto Institute of Technology
(Matsugasaki, Sakyo-ku, Kyoto 606-8585)

Lecture at *ICR*
In-situ SAXS Measurements of Block Copolymers during Deformation

Vis Prof
TANASE, Tomoaki
(D Eng)

Laboratory of Organometallic Chemistry

Professor, Faculty of Science, Nara Women's University
(Kitauoyanishimachi, Nara 630-8506)

Lecture at *ICR*
Structurally Constrained Transition Metal Clusters by Using Linear Multidentate Phosphines —Focusing on Molecular Metal Atom Chains—

Vis Prof
WICKER, Nicolas
(Ph D)

Laboratory of Bio-knowledge Engineering

Professor, Université Lille 1
(UFR de Mathématiques Cité Scientifique 59655, Villeneuve d'Ascq, France)

Lecture at *ICR*
Multidimensional Fitting and Projection under Pairwise Distance Control

Vis Prof
YANG, Jye-Shane
(Ph D)

Laboratory of Polymer Controlled Synthesis

Professor, National Taiwan University
(No. 1, Sec. 4, Roosevelt Rd., Taipei 10617, Taiwan (R.O.C.))

Lecture at *ICR*
Design and Synthesis of Novel π-Conjugated Molecules and Development of Their Functions

Vis Assoc Prof
MATSUZAKI, Yuichiro
(Ph D)

Laboratory of Inorganic Photonics Materials

Research Scientist, Hybrid Nano-Structure Physics Research Group, NTT Basic Research Laboratories
(3-1, Morinosato Wakamiya, Atsugi-shi, Kanagawa 243-0198)

Lecture at *ICR*
Quantum Measurement Theory

Vis Assoc Prof
ENAMI, Shinichi
(D Eng)

Laboratory of Chemistry for Functionalized Surfaces

Senior Researcher, National Institute for Environmental Studies
(16-2 Onogawa, Tsukuba-shi, Ibaraki 305-8506)

Lecture at *ICR*
Study of Interface Science Using Newly Developed Mass Spectrometry

Vis Assoc Prof
MIZOGUCHI, Teruyasu
(D Eng)

Laboratory of Electron Microscopy and Crystal Chemistry

Associate Professor, Institute of Industrial Science, The University of Tokyo
(4-6-1 Komaba, Meguro-ku, Tokyo 153-8505)

Lecture at *ICR*
Materials Research Using Atomic-resolution Analysis and Machine Learning

Vis Assoc Prof
SESE, Jun
(D Sc)

Laboratory of Bio-knowledge Engineering

Team Leader, AIST on Machine Learning
(2-3-26 Aomi, Koto-ku, Tokyo 135-0064)

Lecture at *ICR*
Statistical Significance of Marker Combinations: Theory and Applications

Prof Em KANEHISA, Minoru (D Sc)

Appointed as Res (pt) at ICR,
1 April 2012–31 March 2018

PERSONAL

Awards

TOKITOH, Norihiro

Award for the Best Reviewers of Grant-in-Aid for Scientific Research

Japan Society for the Promotion of Science

29 September 2017

FUJIMORI, Shiori

CSJ Student Presentation Award 2017

The 97th Annual Meeting of the Chemical Society Japan

"Synthesis and Structure of Heavier Group 14 Analogues of Phenyl Anion"

The Chemical Society of Japan

30 March 2017

ICR Award for Graduate Students

"Germabenzenylpotassium: A Germanium Analogue of a Phenyl Anion"

Institute for Chemical Research, Kyoto University

1 December 2017

SUGAHARA, Tomohiro

CSJ Student Presentation Award 2017

The 97th Annual Meeting of the Chemical Society Japan

"Cyclotrimerization of Arylacetylenes Using a Germanium Catalyst and the Reaction Mechanism"

The Chemical Society of Japan

30 March 2017

ICR Award for Graduate Students

"Highly Bent 1,3-Digerma-2-silaallene"

Institute for Chemical Research, Kyoto University

1 December 2017

Best Presentation Award

The 44th Symposium on Main Group Element Chemistry

"Synthesis, Structure and Property of the First Stable 1,4-Digermabenzene"

Organizing Committee of the 44th Symposium on Main Group Element Chemistry

9 December 2017

CHAOLUMEN

Reaxys PhD Prize

"Electron Deficient Tetrabenzo-Fused Pyracylene and Conversions into Curved and Planar π-Systems"

Reaxys

19 October 2017

KAWABATA, Takeo

The Pharmaceutical Society of Japan Award '17

"Novel Strategies for Enantio- and Site-Selective Molecular Transformations"

The Pharmaceutical Society of Japan

24 March 2017

MORISAKI, Kazuhiro

Best Presentation Award

The 137th Annual Meeting of the Pharmaceutical Society of Japan

"Direct Catalytic Alkynylation of *N*-Unprotected Trifluoromethyl Ketimines"

The Pharmaceutical Society of Japan

31 March 2017

SAKAMOTO, Masanori

Nanoscale Horizons Award

The 15th Annual Meeting of the Society of Nano Science and Technology

"Light Stimulated Carrier Dynamics of $CuInS_2$/CdS Heterostructured Nanocrystals"

The Society of Nano Science and Technology

11 May 2017

SATO, Ryota

Nanoscale Horizons Award

The 15th Annual Meeting of the Society of Nano Science and Technology

"Pseudomorphic Synthesis of Pd-based Alloy Nanoparticles by Element-selective Galvanic Replacement"

The Society of Nano Science and Technology

11 May 2017

KIMURA, Masato

CSJ Student Presentation Award 2017

The 97th Annual Meeting of the Chemical Society Japan

"Investigation on Long-lived Charge Separation in Visible Light-responsive Au_XS/ZnS Heterostructured Nanoparticles"

The Chemical Society of Japan

30 March 2017

FAN, Weijia

ICR Award for Graduate Students

"Synthesis of Multivalent Organotellurium Chain Transfer Agents by Post-modification and Their Applications in Living Radical Polymerization"

Institute for Chemical Research, Kyoto University

1 December 2017

MASUDA, Toshihiro

The Excellent Presentation Award

The 137th Annual Meeting of the Pharmaceutical Society of Japan

"Development of a New Tool Inducing Cell Movement by Changing Membrane Tension"

The Pharmaceutical Society of Japan

31 March 2017

The Excellent Presentation Award

The 64th Annual Meeting of The Japanese Biochemical Society, Kinki Branch

"Development of Amphipathic Peptide Inducing F-actin Morphological Change by Interaction with Membrane"

The Japanese Biochemical Society, Kinki Branch

27 May 2017

SAKAMOTO, Kentarou

Excellent Stone Award, Annual Meeting of JPS

The 54th Japanese Peptide Symposium

"Histidines in L17E Endosome-Destabilizing Peptide"

The Japanese Peptide Society

21 November 2017

UESUGI, Motonari

49th Ichimura Prize in Science for Distinguished Achievement

“Small Molecules for Cell Therapy”

The New Technology Develoment Foundation

26 April 2017

ASANO, Risa

Outstanding Student Presentation Award

The 137th Annual Meeting of the Pharmaceutical Society of Japan

“Inhibition of Lipid Synthesis by Vitamin D Metabolites”

The Pharmaceutical Society of Japan

31 March 2017

SOHRIN, Yoshiki

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

“Development of Highly Accurate Analytical Methods for Trace Metals and Its Application to Aquatic Chemistry”

Minister of Education, Culture, Sports, Science and Technology

19 April 2017

DOI, Yuya

The 33rd Inoue Research Award for Young Scientists

“Preparation and Viscoelasticity of Ring Polymers with Various Architectures”

Inoue Foundation for Science

3 February 2017

TERAMOTO, Kensuke

Award for the Presentation of an Excellent Paper

The 37th Annual Meeting of the Laser Society of Japan

“Surface Waves Generated on a Metal Wire by Intense Laser Plasma”

The Laser Society of Japan

31 May 2017

FURUKAWA, Yuki

Outstanding Student Presentation Award

The papers of Technical Meeting on “Light Application and visual Science”, IEE Japan

“Features of Double-pulse Laser Induced Nanostructure on Titanium with Time Intervals Up to Nanosecond”

The Institute of Electric Engineers of Japan

6 September 2017

NAKAMURA, Masaharu

CSJ Award for Creative Work

“A Study on Selective Synthetic Organic Reactions Catalyzed by Iron”

The Chemical Society of Japan

17 March 2017

IWAMOTO, Takahiro

Showa Denko Award in Synthetic Organic Chemistry, Japan

“Development of Novel synthetic Method of α-Amino Acid via Photocatalysis”

The Society of Synthetic Organic Chemistry, Japan

16 February 2017

ICR Award for Young Scientists

“Iron-Catalyzed *anti*-Selective Carbosilylation of Internal Alkyne”

Institute for Chemical Research, Kyoto University

1 December 2017

SHIMAKAWA, Yuichi

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

"Studies on Synthesis of Novel Functional Oxide Materials and Their Structure and Property Relationship"

Minister of Education, Culture, Sports, Science and Technology

19 April 2017

KAN, Daisuke

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

"Research on Explorations of Functional Properties of Transition Metal Oxides by Atomic Level Structural Engineering"

Minister of Education, Culture, Sports, Science and Technology

19 April 2017

KAN, Daisuke;
SHIMAKAWA, Yuichi

The 41st Japan Society of Powder and Powder Metallurgy Award for Innovatory Research

"Explorations of Functional Properties of Transition Metal Oxides by Atomic Level Structural Engineering"

Japan Society of Powder and Powder Metallurgy

31 May 2017

TAKEUCHI, Katsuhiko

ICR Award for Young Scientists

"A Square Planar Complex of Platinum(0)"

Institute for Chemical Research, Kyoto University

1 December 2017

IHARA, Toshiyuki

Young Scientist Award of the Physical Society of Japan

"One-Dimensional Band-Edge Absorption in a Doped Quantum Wire"

"Absorption Cross-section Spectrum of Single CdSe/ZnS Nanocrystals Revealed Through Photoluminescence Excitation Spectroscopy"

"Biexciton Cascade Emission Reveals Absolute Absorption Cross Section of Single Semiconductor Nanocrystals"

The Physical Society of Japan

18 March 2017

TAHARA, Hirokazu

The 33rd Inoue Research Award for Young Scientists

"Coherent Transients of Excitons Generated in Semiconductors"

Inoue Foundation for Science

3 February 2017

LE, Phuong Quang

ICR Award for Young Scientists (Foreign Researcher's Category)

"Free Excitons and Exciton–Phonon Coupling in $CH_3NH_3PbI_3$ Single Crystals Revealed by Photocurrent and Photoluminescence Measurements at Low Temperatures"

Institute for Chemical Research, Kyoto University

1 December 2017

AKUTSU, Tatsuya

Best Reviewer Award of 2016, JSPS's Screening Committee for Young Researcher Fellowships

Japan Society for the Promotion of Science

31 July 2017

Paper Awards

LU, Yangtian

Student Lecture Award

The 97th CSJ Annual Meeting

“One Pot Synthesis of Dendritic Hyperbranched Polymers by Using Vinyl Tellurides”

The Chemical Society of Japan

18 May 2017

SAKABE, Shuji;

KURATA, Hiroki;

HASHIDA, Masaki;

TOKITA, Shigeki[1];

INOUE, Shunsuke;

NEMOTO, Takashi;

WATANABE, Kota[2]

LSJ Award for Distinguished Achievements in Research

“Evolution of Electron-Microscopes and the Ultrafast Electron Diffraction with Laser Accelerated Electrons”

The Laser Society of Japan

31 May 2017

[1] Institute of Laser Engineering, Osaka University

[2] Nippon Steel & Sumitomo Metal Corporation

SAKABE, Shuji;

HASHIDA, Masaki;

TOKITA, Shigeki[1];

INOUE, Shunsuke;

TERAMOTO, Kensuke;

WATANABE, Kota[2]

Award of the Japanese Society of Microscopy

“Ultrafast Electron Diffraction and Deflectometry with Electron Sources Generated and Accelerated by Intense Femtosecond Lasers”

The Japanese Society of Micrscopy

31 May 2017

[1] Institute of Laser Engineering, Osaka University

[2] Nippon Steel & Sumitomo Metal Corporation

Poster Awards

GUO, Jing-Dong

Poster Prize

The 18th International Symposium on Silicon Chemistry (ISOS XVIII)/The 6th Asian Silicon Symposium (ASiS-6)

“Mechanistic Study on the Reaction of a Digermyne with Acetylene”

11 August 2017

SUGAHARA, Tomohiro

Best Poster Award

The 21st Symposium of the Society of Silicon Chemistry

“Selenization of the Stable 1,2-Digermacyclobutadiene: Synthesis and Structure of 2,5-Digermaselenophene”

The Society of Silicon Chemistry, Japan

27 October 2017

OMATSU, Yamato

Best Poster Award

The 21st Symposium of the Society of Silicon Chemistry

“Synthesis of Hexasilacyclohexane Derivatives”

The Society of Silicon Chemistry, Japan

27 October 2017

OKAZAKI, Shuhei

Poster Award

28th Symposium on Physical Organic Chemistry

“Development of Near-Infrared Dyes Using Imidazole-Fused Benzothiadiazole Skeleton”

The Society of Physical Organic Chemistry

9 September 2017

NINOMIYA, Ryo

Best Poster Award

The 137th Annual Meeting of the Pharmaceutical Society of Japan

“Organocatalytic Site-selective Cyanosilylation of Diketones”

The Pharmaceutical Society of Japan

31 March 2017

TAKASHIMA, Megumi

Chemistry Letters Young Poster Award

The 8th International Meeting on Halogen Chemistry

“Direct Asymmetric α-Fluorination of Amino Acids”

Organizing Committee of The 8th International Meeting on Halogen Chemistry

15 September 2017

HASHIMOTO, Hisashi

Chemical Pharmaceutical Bulletin Award

The 47th Congress of Heterocyclic Chemistry

“Asymmetric Desymmetrization of σ-Symmetric Diols by Catalytic Asymmetric Silylation”

Organizing Committee of 47th Congress of Heterocyclic Chemistry

28 October 2017

SAKAKIBARA, Keita

Soft Matter Poster Award

The 15th IUMRS-International Conference on Advanced Materials

“Preparation of High-Density Poyethylene Nanocomposites Well Reinforced by Cellulose Nanofiber Using Diblock Copolymer-type Dispersants”

The 15th IUMRS-International Conference on Advanced Materials

30 August 2017

MURAJI, Koichi

Poster Award

The 17th Symposium of Research Group on Polymer Surface and Interface

"Precise Synthesis and Tribological Property of Cross-Linked Thick Polymer Brush"

Research Group on Polymer Surface and Interface, The Society of Polymer Science, Japan

27 October 2017

NIWA, Ryota

Poster Award

The 17th Symposium of Research Group on Polymer Surface and Interface

"Synthesis of Concentrated Polymer Brushes with Large Thickness in Ionic Liquids Based on Kinetics"

Research Group on Polymer Surface and Interface, The Society of Polymer Science, Japan

27 October 2017

LU, Yangtian

Poster Award

254th ACS National Meeting & Exposition

"One Pot Synthesis of Structurally Controlled Hyper-branched Polymers by Using a Stimuli-responsive Monomer"

American Chemical Society

22 August 2017

Young Scientist Poster Award Silver Prize

2017 KIPS International Symposium

"Synthesis of Structurally Controlled Hyperbranched Poly(methyl methacrylate)s Through Living Radical Copolymerization of a Stimuli-responsive Monomer"

Kyoto Institute of Polymer Science

7 September 2017

FAN, Weijia

Young Scientist Poster Award Gold Prize

2017 KIPS International Symposium

"Aqueous Organotellurium Chain Transfer Agents and Tellurols for Living Radical Polymerization in Water and Recovery of Tellurium"

Kyoto Institute of Polymer Science

7 September 2017

AKISHIBA, Misao

Poster Award

The 11th Joint Symposium of Bio-related Divisions of the Chemical Society of Japan

"Development of Endosome Destabilizing Peptide for Intracellular Delivery of Biomacromolecules"

Division of Biofunctional Chemistry and Division of Biotechnology, The Chemical Society of Japan

8 September 2017

ARAFILES, Jan Vincent V.

Award for Excellence at Poster Presentation

The 54th Japanese Peptide Symposium

"Novel Macropinocytosis-Inducing Cell Penetrating Peptides"

The Japanese Peptide Society

21 November 2017

KUBO, Shosei

The Poster Award

The 64th Japan Society of Applied Physics, Spring Meeting

"Blue Organic Light-Emittng Diodes with External Quantum Efficiency over 25% Using Thermally Activated Delayed Fluorescence Emitters"

The Japan Society of Applied Physics

1 April 2017

SHIOYA, Nobutaka

Japan Symposium on Macromolecules Poster Award 2017

66th Symposium on Macromolecules

"Controlling Mechanism of Molecular Orientation in an Organic Semiconductor Thin Film Revealed by Using pMAIRS and GIXD"

The Society of Polymer Science

22 September 2017

TOMITA, Kazutaka

Excellent Poster Presentation Award

11th Bunseki Hicho

"Effect of Solvent Annealing on Porphyrin Derivative Molecules in Thin Films: Structural Analysis of Thin Films Using pMAIRS"

The Japan Society for Analytical Chemistry, The Kinki Branch

8 August 2017

KAMASAKA, Kohei

Best Poster Award

18th Annual Meeting of the Japanese Society for Extremophiles

"Analysis of Selective Protein Secretion Mechanism via Extracellular Membrane Vesicles in a Psychrotrophic Bacterium *Shewanella* sp. HM13"

The Japanese Society for Extremophiles

11 November 2017

TSUJIOKA, Kouta

Annual Meeting Poster Award 2017

66th SPSJ Annual Meeting

"Depth-dependent Structural Analyses in PS-b-P2VP Thin Films as Revealed by Grazing Incidence Small Angle Scattering with Tender Region Energy"

The Society of Polymer Science, Japan

21 June 2017

Young Scientist Poster Award Bronze Prize

2017 KIPS International Symposium

"Depth-dependent Structural Analyses in PS-b-P2VP Thin Films as Revealed by Grazing Incidence Small Angle Scattering with Tender Region Energy"

Kyoto Institute of Polymer Science

7 September 2017

HARUTA, Mitsutaka

The Best Poster Award

The 73rd Annual Meeting of the Japanese Society of Microscopy

"Dependence of Detection Angle on ADF-STEM Image Contrast"

The Japanese Society of Microscopy

31 May 2017

YARITA, Naoki

Region5 Poster Awards

The Physical Society of Japan 2017 Autumn Meeting

"Biexcitons and Charged Excitons in Lead Halide Perovskite Nanocrystals"

The Physical Society of Japan

23 September 2017

PUBLICATIONS
INTERNATIONAL RESEARCH COLLABORATIONS
SELECTED GRANTS
THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Nishino, K.; Shiro, M.; Okura, R.; Oizumi, K.; Fujita, T.; Sasamori, T.; Tokitoh, N.; Yamada, A.; Tanaka, C.; Yamaguchi, M.; Hiradate, S.; Hirai, N., The (Oxalato)aluminate Complex as an Antimicrobial Substance Protecting the "Shiro" of Tricholoma Matsutake from Soil Micro-Organisms, *Biosci. Biotechnol. Biochem.*, **81,** 102-111 (2017).

Yamaguchi, K.; Murai, T.; Tsuchiya, Y.; Miwa, Y.; Kutsumizu, S.; Sasamori, T.; Tokitoh, N., Pyridinium 5-Aminothiazoles: Specific Photophysical Properties and Vapochromism in Halogenated Solvents, *RSC Adv.*, **7,** 18132-18135 (2017).

Kawamura, M.; Kamo, S.; Azuma, S.; Kubo, K.; Sasamori, T.; Tokitoh, N.; Kuramochi, K.; Tsubaki, K., Skeletal Rearrangements of Polycyclic α-Ketols, *Org. Lett.*, **19,** 301-202 (2017).

Tsubomoto, Y.; Hayashi, S.; Nakanishi, W.; Sasamori, T.; Tokitoh, N., Nature of E_2X_2 σ(4*c* –6*e*) of the *X*---*E*—*E*---*X* Type at Naphthalene 1,8-Positions and Model, Elucidated by X-Ray Crystallographic Analysis and QC Calculations with the QTAIM Approach, *Acta Crystallogr. Sect. B Struct. Sci. Cryst. Eng. Mater.*, **73,** 265-275 (2017).

Yamaguchi, K.; Murai, T.; Kutsumizu, S.; Miwa, Y.; Ebihara, M.; Guo, J.-D.; Tokitoh, N., Experimental and Theoretical Examination of the Radical Cations Obtained from the Chemical and Electrochemical Oxidation of 5-Aminothiazoles, *ChemistryOpen*, **6,** 282-287 (2017).

Lu, W.-J.; Pei, X.; Murai, T.; Sasamori, T.; Tokitoh, N.; Kawabata, T.; Furuta, T., Asymmetric Intramolecular C–H Insertion Promoted by Dirhodium(II) Carboxylate Catalyst Bearing Axially Chiral Amino Acid Derivatives, *Synlett*, **28,** 679-683 (2017).

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

Majhi, P. K.; Ikeda, H.; Sasamori, T.; Tsurugi, H.; Mashima, K.; Tokitoh, N., Inorganic-Salt-Free Reduction in Main-Group Chemistry: Synthesis of a Dibismuthene and a Distibene, *Organometallics*, **36,** 1224-1226 (2017).

Mizuhata, Y.; Omatsu, Y.; Tokitoh, N., Dodecaallylhexasilacyclohexane, *IUCrData*, **2,** x170807 (2017).

Kawasaki, K.; Sugiyama, R.; Tsuji, T.; Iwasa, T.; Tsunoyama, H.; Mizuhata, Y.; Tokitoh, N.; Nakajima, A., A Designer Ligand Field for Blue-Green Luminescence of Organoeuropium(II) Sandwich Complexes with Cyclononatetraenyl Ligands, *Chem. Commun.*, **53,** 6557-6560 (2017).

Agou, T.; Tokitoh, N., Reactivity of Organoaluminum Compounds with Unique Coordination Modes, *J. Synth. Org. Chem. Japan*, **75,** 723-734 (2017) (in Japanese).

Shouda, T.; Nakanishi, K.; Sasamori, T.; Tokitoh, N.; Kuramochi, K.; Tsubaki, K., Synthesis and Structures of Zigzag Shaped [12] Cyclo-*p*-Phenylene Composed of Dinaphthofuran Units and Biphenyl Units, *J. Org. Chem.*, **82,** 7850-7855 (2017).

Sugahara, T.; Sasamori, T.; Tokitoh, N., Highly Bent 1,3-Digerma-2-Silaallene, *Angew. Chem. Int. Ed.*, **56,** 9920-9923 (2017).

Koyanagi, Y.; Kawaguchi, S.; Fujii, K.; Kimura, Y.; Sasamori, T.; Tokitoh, N.; Matano, Y., Effects of Counter Anions, P-Substituents, and Solvents on Optical and Photophysical Properties of 2-Phenylbenzo[b]phospholium Salts, *Dalton Trans.*, **46,** 9517-9527 (2017).

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Tsunoyama, H.; Akatsuka, H.; Shibuta, M.; Iwasa, T.; Mizuhata, Y.; Tokitoh, N.; Nakajima, A., Development of Integrated Dry–Wet Synthesis Method for Metal Encapsulating Silicon Cage Superatoms of M@Si$_{16}$ (M = Ti and Ta), *J. Phys. Chem. C*, **121,** 20507-20516 (2017).

Mizuhata, Y.; Tokitoh, N., New Development on the Chemistry of "Heavy Benzene Ring", *Chemistry*, **72,** 72-73 (2017) (in Japanese).

— Structural Organic Chemistry —

Kimura, Y.; Maeda, T.; Iuchi, S.; Koga, N.; Murata, Y.; Wakamiya, A.; Yoshida, K., Characterization of Dye-Sensitized Solar Cells Using Five Pure Anthocyanidin 3-O-Glucosides Possessing Different Chromophores, *J. Photochem. Photobiol. A*, **335,** 230-238 (2017).

Futagoishi, T.; Murata, M.; Wakamiya, A.; Murata, Y., Unprecedented Photochemical Rearrangement of an Open-Cage C$_{60}$ Derivative, *Chem. Commun.*, **53,** 1712-1714 (2017).

Kimura, Y.; Oyama, K.; Murata, Y.; Wakamiya, A.; Yoshida, K., Synthesis of 8-Aryl-O-Methylcyanidins and Their Usage for Dye-Sensitized Solar Cell Devices, *Int. J. Mol. Sci.*, **18,** 427 (2017).

Wang, F.; Shimazaki, A.; Yang, F.; Kanahashi, K.; Matsuki, K.; Miyauchi, Y.; Takenobu, T.; Wakamiya, A.; Murata, Y.; Matsuda, K., Highly Efficient and Stable Perovskite Solar Cells by Interfacial Engineering Using Solution-Processed Polymer Layer, *J. Phys. Chem. C*, **121,** 1562-1568 (2017).

Futagoishi, T.; Murata, M.; Wakamiya, A.; Murata, Y., Encapsulation and Dynamic Behavior of Methanol and Formaldehyde inside Open-Cage C$_{60}$ Derivatives, *Angew. Chem. Int. Ed.*, **56,** 2758-2762 (2017).

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Hashikawa, Y.; Murata, M.; Wakamiya, A.; Murata, Y., Structural Modification of Open-Cage Fullerene C_{60} Derivatives Having a Small Molecule inside Their Cavities, *Can. J. Chem.*, **95,** 320-328 (2017).

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Shimogawa, H.; Yoshikawa, O.; Aramaki, Y.; Murata, M.; Wakamiya, A.; Murata, Y., 4,7-Bis[3-(dimesitylboryl)thien-2-yl] benzothiaziazole: Solvato-, Thermo-, and Mechanochromism Based on the Reversible Formation of an Intramolecular B-N Bond, *Chem. Eur. J.*, **23,** 3784-3791 (2017).

Shimogawa, H.; Endo, M.; Nakaike, Y.; Murata, Y.; Wakamiya, A., D-π-A Dyes with Diketopyrrolopyrrole and Boryl-Substituted Thienylthiazole Units for Dye-sensitized Solar Cells with High J_{SC} Values, *Chem. Lett.*, **46,** 715-718 (2017).

Shimogawa, H.; Endo, M.; Taniguchi, T.; Nakaike, Y.; Kawaraya, M.; Segawa, H.; Murata, Y.; Wakamiya, A., D-π-A Dyes with an Intramolecular B-N Coordination Bond as a Key Scaffold for Electronic Structural Tuning and Their Application in Dye-Sensitized Solar Cells, *Bull. Chem. Soc. Jpn.*, **90,** 441-450 (2017).

Futagoishi, T.; Aharen, T.; Kato, T.; Kato, A.; Ihara, T.; Tada, T.; Murata, M.; Wakamiya, A.; Kageyama, H.; Kanemitsu, Y.; Murata, Y., A Stable, Soluble, and Crystalline Supramolecular System with a Triplet Ground State, *Angew. Chem. Int. Ed.*, **56,** 4261-4265 (2017).

Chaolumen; Murata, M.; Wakamiya, A.; Murata, Y., Unsymmetric Twofold Scholl Cyclization of 5,11-Dinaphthyltetracene: Selective Formation of Pentagonal and Hexagonal Rings via a Dication Pathway, *Angew. Chem. Int. Ed.*, **56,** 5082-5086 (2017).

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Zhang, R.; Murata, M.; Wakamiya, A.; Shimoaka, T.; Hasegawa, T.; Murata, Y., Isolation of the Simplest Hydrated Acid, *Sci. Adv.*, **3,** e1602833 (2017).

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

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Kaneko, S.; Hashikawa, Y.; Fujii, S.; Murata, Y.; Kuguchi, M., Single Molecular Junction Study on $H_2O@C_{60}$: H_2O is "Electrostatically Isolated", *Chem. Phys. Chem.*, **18,** 1229-1233 (2017).

Nishimura, H.; Tanaka, K.; Morisaki, Y.; Chujo, Y.; Wakamiya, A.; Murata, Y., Oxygen-Bridged Diphenylnaphthylamine as a Scaffold for Full-Color Circularly Polarized Luminescent Materials, *J. Org. Chem.*, **82,** 5242-5249 (2017).

Nishimura, H.; Hasegawa, Y.; Wakamiya, A.; Murata, Y., Development of Transparent Organic Hole-Transporting Materials Using Partially Oxygen-Bridged Triphenylamine Skeletons, *Chem. Lett.*, **46,** 817-820 (2017).

Nakamura, T.; Okazaki, S.; Arakawa, N.; Satou, M.; Endo, M.; Murata, Y.; Wakamiya, A., Synthesis of Azole-Fused Benzothiadiazoles as Key Units for Functional π-Conjugated Compounds, *J. Photopolym. Sci. Technol.*, **30,** 561-568 (2017).

Ozaki, M.; Katsuki, Y.; Liu, J.; Handa, T.; Nishikubo, R.; Yakumaru, S.; Hashikawa, Y.; Murata, Y.; Saito, T.; Shimakawa, Y.; Kanemitsu, Y.; Saeki, A.; Wakamiya, A., Solvent-Coordinated Tin Halide Complexes as Purified Precursors for Tin-Based Perovskites, *ACS Omega*, **2,** 7016-7021 (2017).

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Yamada, T.; Yamada, Y.; Nakaike, Y.; Wakamiya, A.; Kanemitsu, Y., Photon Emission and Reabsorption Processes in $CH_3NH_3PbBr_3$ Single Crystals Revealed by Time-Resolved Two-Photon-Excitation Photoluminescence Microscopy, *Phys. Rev. Applied*, **7,** 14001 (2017).

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Hashikawa, Y.; Murata, Y., Facile Access to Azafullerenyl Cation $C_{59}N^+$ and Specific Interaction with Entrapped Molecules, *J. Am. Chem. Soc.*, **139,** 18468-18471 (2017).

Zhu, G.-Z.; Hashikawa, Y.; Liu, Y.; Zhang, Q.-F.; Cheung, L. F.; Murata, Y.; Wang, L. S., High-Resolution Photoelectron Imaging of Cryogenically-Cooled $C_{59}N^-$ and $(C_{59}N)_2^{2-}$ Azafullerene Anions, *J. Phys. Chem. Lett.*, **8,** 6220-6225 (2017).

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— Synthetic Organic Chemistry —

Lu, W.; Pei, X.; Murai, T.; Sasamori, T.; Tokitoh, N.; Kawabata, T.; Furuta, T., Asymmetric Intramolecular C-H Insertion Promoted by Dirhodium(II) Carboxylate Catalyst Bearing Axially Chiral Amino Acid Derivatives, *Synlet*, **28,** 679-683 (2017).

Kasamatsu, K.; Yoshimura, T.; Mandi, A.; Taniguchi, T.; Monde, K.; Furuta, T.; Kawabata, T., α-Arylation of α-Amino Acid Derivatives with Arynes via Memory of Chirality: Asymmetric Synthesis of Benzocyclobutenones with Tetrasubstituted Carbon, *Org. Lett.*, **19,** 352-355 (2017).

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— Advanced Inorganic Synthesis —

Eguchi, D.; Sakamoto, M.; Tanaka, D.; Okamoto, Y.; Teranishi, T., Porphyrin Derivative-Protected Gold Cluster with a Pseudo-tetrahedral Shape, *J. Phys. Chem. C*, **121,** 10760-10766 (2017).

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Yamamoto, M.; Azuma, Y.; Sakamoto, M.; Teranishi, T.; Ishii, H.; Majima, Y.; Noguchi, Y., Molecular Floating-Gate Single-Electron Transistor, *Sci. Rep.*, **7,** 1589(1-8) (2017).

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DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

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Sakakibara, K.; Kagata, H.; Ishizuka, N.; Sato, T.; Tsujii, Y., Fabrication of Surface Skinless Membranes of Epoxy Resin-based Mesoporous Monoliths toward Advanced Separators for Lithium Ion Batteries, *J. Mater. Chem. A*, **5,** 6866-6873 (2017).

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Sakakibara, K.; Moriki, Y.; Yano, H.; Tsujii, Y., Strategy for the Improvement of the Mechanical Properties of Cellulose Nanofiber-Reinforced High-Density Polyethylene Nanocomposites Using Diblock Copolymer Dispersants, *ACS Appl. Mater. Interfaces*, **9,** 44079-44087 (2017).

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— Polymer Controlled Synthesis —

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INTERNATIONAL RESEARCH COLLABORATIONS

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Aalto University, Department of Computer Science

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Bruker BioSpin

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Centre National de la Recherche Scientifique

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Nicolaus Copernicus University, Faculty of Chemistry

Nicolaus Copernicus University, Faculty of Physics

[Portugal]
University Nova of Lisbon, Department of Physics

University of Lisbon, Department of Physics

[Singapore]
Nanyang Technological University, School of Physical and Mathematical Sciences

[Spain]
Universidad Complutense, Departamento de Química Inorgánica, Facultad de C.C. Químicas

[Sweden]
Stockholm University, Department of Biochemistry and Biophysics

[Switzerland]
University of Fribourg, Department of Physics

[U.K.]
The University of Edinburgh, Centre for Science at Extreme Conditions and School of Chemistry

[U.S.A.]
The Ohio State University, Department of Microbiology & Department of Civil, Environmental, and Geodetic Engineering

University of Pennsylvania, Department of Materials Science and Engineering

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

SELECTED GRANTS

DIVISION OF SYNTHETIC CHEMISTRY
— Organoelement Chemistry —

Tokitoh, N.
Creation of Novel Catalysts Centered on the Coordination Diversity of Heavy Typical Elements
Grant-in-Aid for Scientific Research on Innovative Areas “Stimuli-responsive Chemical Species for the Creation of Functional Molecules”
28 June 2012–31 March 2017

Tokitoh, N.
Synthesis of Heavier Group 14 Element Analogues of Phenyl Anion and Their Properties
Grant-in-Aid for Scientific Research on Innovative Areas “Stimuli-responsive Chemical Species for the Creation of Functional Molecules”
1 April 2016–31 March 2019

Sasamori, T.
Construction of [2]Ferrocenophanes Linked by π-Bond between Heavier Group 14 Elements and Control of Their Ring-opening Polymerization
Grant-in-Aid for Scientific Research on Innovative Areas “Emergent Chemistry of Nano-scale Molecular Systems” and “New Polymeric Materials Based on Element-Blocks”
1 April 2013–31 March 2017

Sasamori, T.
Development of Transformations of Small Molecules and Multicomponent Couplings Utilizing Low-valent Compounds of Heavier Group 14 Elements
Grant-in-Aid for Scientific Research (B)
1 April 2015–31 March 2018

Sasamori, T.
Construction of d-π Electron Systems Containing Heavier Group 14 Elements and Their Functionalization
Grant-in-Aid for Challenging Exploratory Research
1 April 2015–31 March 2017

Mizuhata, Y.
Construction of Silicon-containing Dehydroannulenes and Their Aromaticity and Antiaromaticity
Grant-in-Aid for Scientific Research (C)
1 April 2014–31 March 2017

— Structural Organic Chemistry —

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

Murata, Y.
Spherical π-Figuration Based on Functionalization of Sub-Nano Space
Grant-in-Aid for Scientific Research on Innovative Areas “π-System Figuration”
1 April 2017–31 March 2019

Wakamiya, A.
Development of High Performance and Environmentally Friendly Perovskite Type Solar Cells
Advanced Low Carbon Technology Research and Development Program (ALCA)
16 November 2016–31 March 2021

— Synthetic Organic Chemistry —

Kawabata, T.
Regioselective Molecular Transformation of Multifunctionalized Molecules
Grant-in Aid for Scientific Research (S)
1 April 2014–31 March 2018

Furuta, T.
Direct Intra and Intermolecular Aldol Reaction by Catalytic Discrimination of Aldehydes
Grant-in-Aid for Scientific Research (C)
1 April 2014–31 March 2017

Ueda, Y.
Site-Selective Molecular Transformation Promoted by Anion-Exchange of Cationic Intermediates in Nucleophilic Catalysis
Grant-in-Aid for Young Scientists (B)
1 April 2015–31 March 2017

Ueda, Y.
Synthesis of Carbohydrate-Related Middle Molecules Based on Sequential Site-Selective Functionalization
Grant-in-Aid for Scientific Research on Innovative Areas
1 April 2016–31 March 2018

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

— Advanced Inorganic Synthesis —

Teranishi, T.
Synthesis of Magnetic Nanoparticles for Creating Novel Nanocomposite Magnetic Materials
Elements Strategy Initiative, MEXT
1 July 2012–31 March 2022

Teranishi, T.
Development of Green Sustainable Chemical Process
Mirai Kaitaku Research Project, NEDO
1 November 2012–31 March 2022

Teranishi, T.
Novel Development of Asymmetry Chemistry in Inorganic Nanocrystals
Grant-in-Aid for Scientific Research on Innovative Areas
30 June 2016–31 March 2021

Teranishi, T.
Formation of Novel Metallic Phase Nanoparticles and Development of Their Catalytic Properties
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2019

Teranishi, T.
Enhancement of Tightly Bound Hydrogen Storage Property of Pd Nanodisks by Visible-to-Near Infrared Plasmons
Grant-in-Aid for Challenging Exploratory Research
1 April 2016–31 March 2018

Sakamoto, M.
Development of Transparent Energy Conversion System Using the Heavily-doped Semiconductors as a Light Harvesting Layer
Grant-in-Aid for Challenging Research (Exploratory)
1 April 2017–31 March 2019

Sakamoto, M.
Fabrication of Highly Efficient Up Conversion Nanocrystal Driven by IR Excitation
Grant-in-Aid for Scientific Research on Innovative Areas
1 April 2017–31 March 2019

Saruyama, M.
Synthesis and Structure Specific Function of Multi-hetrostructured Semiconductor Nanoparticles
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2019

Sato, R.
Coinage-Metal-Free Plasmonic Metal Alloys for Visible Spectrum
Grant-in-Aid for Challenging Research (Exploratory)
1 April 2017–31 March 2020

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

Tsujii, Y.
Reinforcement of Resiliency of Concentrated Polymer Brushes and Its Tribological Applications – Development of Novel “Soft and Resilient Tribology (SRT)” System
ACCEL Program, JST
1 September 2015–31 March 2019

Ohno, K.
Development of Ionic Liquid-Containing Blend Films
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2013–31 March 2017

— Polymer Controlled Synthesis —

Yamago, S.
New Organic Chemistry and Material Science of Curved π-Conjugated Molecules
Grant-in-Aid for Scientific Research (S)
1 April 2016–31 May 2020

— Inorganic Photonics Materials —

Mizuochi, N.
High Sensitive and High Resolution Quantum Nano-sensor by Diamond
Grant-in-Aid for Scientific Research (A)
1 April 2016–31 March 2021

Mizuochi, N.
Innovative Magnetic Sensor Based on Nano-electronics of Carbon Materials
Core Research for Evolutional Science and Technology (CREST), JST
1 April 2014–31 March 2019

Morishita, H.
Electrical Coherent Detection of Electron Spin of NV Centers in Diamond
Grant-in-Aid for Young Scientists (B)
1 April 2016–31 March 2018

— Nanospintronics —

Ono, T.
Spin-orbitronics and Device Application
New Research Projects under Specially Promoted Research
1 April 2015–31 March 2020

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

Futaki, S.
New Strategies for Intracellular Delivery of Biopharmaceuticals
Grant-in-Aid for Scientific Research (A)
1 April 2015–31 March 2018

Imanishi, M.
Construction of Strategies for Sequence Specific Epigenomic Manipulation
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2019

— Molecular Biology —

Aoyama, T.
Plant Epidermal Cell Differebtiation Regulated by the Transcription Factor GL2
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2020

Aoyama, T.
Mechanism for Establishment of Planar Polarity in Plant Cell Morphogenesis
Grant-in-Aid for Scientific Research (C), Special Field
1 April 2016–31 March 2019

Fujiwara-Kato, M.
Elucidation of Phospholipid Signaling for Root Hair Elongation in Plants
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2019

— Chemical Biology —

Uesugi, M.
Control and Analysis of Cells by Synthetic Small Molecules
Grant-in-Aid for Scientific Research (S)
30 May 2014–31 March 2019

Uesugi, M.
Chemical Biological Exploration of New Functions of Endogenous Lipid-related Morecules
AMED-CREST
1 October 2014–31 March 2020

Uesugi, M.
Chemical Signals of Synthetic Nutrient Conjugates
Grant-in-Aid for Scientific Research on Innovative Areas
1 July 2017–31 March 2022

DIVISION OF ENVIRONMENTAL CHEMISTRY

— Molecular Materials Chemistry —

Kaji, H.
Fundamental Science of Organic Devices Based on Detailed Structural Analysis and Theoretical Chemistry
Grant-in-Aid for Scientific Research (A)
1 April 2017–31 March 2020

Shizu, K.
Density Form of Electronic Transitions and Its Applications to Electroluminescent Materials
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2019

— Hydrospheric Environment Analytical Chemistry —

Sohrin, Y.
Development of Novel Proxies for Paleoceanography on the Precise Analysis of Stable Isotopes of Heavy Metals
Grant-in-Aid for Challenging Exploratory Research
1 April 2014–31 March 2017

Sohrin, Y.
Development of Heavy Metal Stable Isotope Marine Chemistry to Understand Marine Environment and Ecosystem
Grant-in-Aid for Scientific Research (A)
1 April 2015–31 March 2018

Minami, T.
Research on Vertical Distribution of Bioactive Trace Metals between the Pacific Sector of the Antarctic Ocean and the South Pacific
Mr. Mitsumasa Itou Commemorative Research Fund, Research Institute for Oceanochemistry
1 April 2017–31 March 2018

— Chemistry for Functionalized Surfaces —

Hasegawa, T.
Development of ROA Imaging and its Application to Visualization of Atropisomers for a Study of Fluoroorganic Chemistry
Grant-in-Aid for Scientific Research (A)
1 April 2015–31 March 2020

Hasegawa, T.
Development of a Novel Analytical Spectroscopy for Strategic Molecular Design of a Fluorine-containing Acryl Polymer Enabling Us to Overcome Environmental Regulations
Matching Planner Program: Cooperation Research with a Company
1 June 2016–31 March 2017

Shimoaka, T.
Development of Analytical Techniques for Studying the Structure and Property of a Polymer Influenced by Minute Water Molecules Involved in a Polymer Thin Film
Grant-in-Aid for Young Scientists (B)
1 April 2014–31 March 2017

Shimoaka, T.
Molecular Interaction Analysis for Understanding Perfluoroalkyl Compound-specific Properties
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2020

— Molecular Microbial Science —

Kurihara, T.
Mechanism of Biogenesis of Membrane Microdomain Containing Polyunsaturated Fatty Acids in Bacteria and Its Physiological Functions
Grant-in-Aid for Scientific Research (B)
1 April 2015−31 March 2018

Kurihara, T.
Exploration and Development of Cold-Adapted Microorganisms for Low-Temperature Biotechnology for Material Production and Environmental Conservation
Grant-in-Aid for Scientific Research (B)
1 April 2017−31 March 2020

Kurihara, T.
Analysis of Cold-Adaptation Mechanism of Food Spoilage Bacteria and Its Application to Food Industry
Grant-in-Aid for Challenging Exploratory Research
1 April 2015−31 March 2017

Kawamoto, J.
Development of a Membrane Protein Production System by Using Tailor-made Membrane Vesicles Synthesized by Extremophiles
Grant-in-Aid for Challenging Exploratory Research
1 April 2016−31 March 2018

Ogawa, T.
Enzymatic Analysis of Molecular Basis for *de novo* Synthesis of Phosphatidic Acid
Grant-in-Aid for Young Scientists (B)
1 April 2017−31 March 2019

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

— Polymer Materials Science —

Takenaka, M.
Nano-Control Technologies for DSA Nano-Patterning
Nano Defect Management Project
1 July 2016–31 March 2018

Ogawa, H.
Development of Visualizing Method Through Cooperative Small Angle X-ray Scattering Coupled with Computed Tomography (SAXS-CT) and Information Science
Strategic Basic Research Programs, PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 September 2016–31 March 2020

— Molecular Rheology —

Watanabe, H.
Relationship between Chemical Structure and Extensional Behavior of Entangled Polymer Chain
Grant-in-Aid for Scientific Research (B)
1 April 2015–31 March 2018

Matsumiya, Y.
Experimental Test on the Dynamics of Telechelic Polymers
Grant-in-Aid for Scientific Research (C)
1 April 2015–31 March 2018

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

— Particle Beam Science —

Iwashita, Y.
Fundamental Technology Development for High Brightness X-ray Source and the Imaging by Compact Accelerator
Photon and Quantum Basic Research Coordinated Development Program
1 April 2013–31 March 2017

— Laser Matter Interaction Science —

Sakabe, S.
Proof of Concept for Electron Optical System Using Intense Laser-driven Surface Wave
Grant-in-Aid for Scientific Research (A)
1 April 2016–31 March 2019

Hashida, M.
Stable Formation of Advanced Functionality on Metal Surface Produced by High Electric Field of Laser Pulse
Grant-in-Aid for Scientific Research (C)
1 April 2016–31 March 2019

Hashida, M.
Advanced Research Program for Energy and Environmental Technologies/Manufacturing Technologies Development of High Quality Laser Material Processing for Inducing New Functionalities
New Energy and Industrial Technology Development Organization
4 January 2016–4 January 2017

Inoue, S.
Demonstration of Laser-driven Ultrafast and Intense Electron Source with Solid-plasma Hybrid Cathode
Grant-in-Aid for Young Scientists (B)
1 April 2016–31 March 2018

— Electron Microscopy and Crystal Chemistry —

Kurata, H.
Advanced Characterization Nanotechnology Platform at Kyoto University
Nanotechnology Platform Project, MEXT
2 July 2012–31 March 2022

Kurata, H.
Development of Precise Spatially Resolved EELS and Analysis of Interfacial Electronic States
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Kurata, H.
State Analysis of Organic Nanomaterials by High-Resolution EELS
Grant-in-Aid for Challenging Exploratory Research
1 April 2016–31 March 2018

Haruta, M.
Electronic State Mapping Using Oxygen
Grant-in-Aid for Young Scientists (A)
1 April 2014–31 March 2018

Haruta, M.
Basic Research of Atomic Resolution Organic Crystal Image Using STEM
Grant-in-Aid for Challenging Exploratory Research
1 April 2014–31 March 2017

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Synthetic Organotransformation —

Takaya, H.
Artificial Enzymes based on Metalated Peptide
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2019

Iwamoto, T.
Development of Novel Enantioconvergent Transformation of Amino Acid
Research Encouragement Grants, The Asahi Glass Foundation
1 April 2017–31 March 2018

Iwamoto, T.
Development of Direct Chlorination with Sodim Chloride
Grant for Japan-related Research Projects, The Sumitomo Foundation
16 November 2017–30 November 2018

— Advanced Solid State Chemistry —

Shimakawa, Y.
Solid-state Chemistry for Transition-metal Oxides: Exploring for New Materials with Novel Functionalities
JSPS Core-to-Core Program
1 April 2016–31 March 2020

— Organometallic Chemistry —

Ozawa, F.
Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Wakioka, M.
Development of High Performance π-Conjugated Polymer Based on cis-trans Photoisomerization
Grant-in-Aid for Scientific Research (C)
1 April 2017–31 March 2020

Takeuchi, K.
Development of FLP Type Acid-Base Catalyst Using PNP-Pincer Type Phosphaalkene Complexes as Lewis Acid
Grant-in-Aid for Young Scientists (B)
1 April 2017–31 March 2020

— Nanophotonics —

Kanemitsu, Y.
Evealuation of Nonradiative Carrier Reconbination Loss in Concentrator Heterostructure Solar Cells
CREST(Core Research for Evolutional Science and Technology), JST
1 October 2011–31 March 2017

Kanemitsu, Y.
Design of Next-generation Flexible Photonic Devices Based on Metal-halide Perovskites
CREST(Core Research for Evolutional Science and Technology), JST
1 October 2016–31 March 2022

BIOINFORMATICS CENTER
— Chemical Life Science —

Ogata, H.
Neo-virology, the raison d'être of Viruses – Deciphering the Mechanisms of Virus-Host Co-Existence in Aquatic Environments
Grant-in-Aid for Scientific Research on Innovative Areas
30 June 2016–31 March 2021

Ogata, H.
Probabilistic and Statistical Theory on Non-Abelian Topological Semigroup A* and its Application to Environmental Microbiology and Bioengineering
Grant-in-Aid for Scientific Research (B)
19 July 2016–31 March 2019

Ogata, H.
A Holistic Ecosystemic Investigation on Marine Giruses, Virophages and their Eukaryotic Hosts
Grant-in-Aid for Scientific Research (C)
1 April 2014–31 March 2017

Ogata, H.
Are Viruses Elementary Particles that Generate and Maintain the Diversity of Marine Organisms?
Pursuit of Ideal, The Canon Foundation
1 April 2014–31 March 2017

Goto, S.
Development of Integrated Proteome Database jPOST
Database Integration Coordination Program, JST
1 April 2015–31 March 2018

Goto, S.
Bioinformatics for Marine Microbial Genomes and Environmental Data
CREST (Core Research for Evolutional Science and Technology), JST
1 October 2012–31 March 2017

Goto, S.
Elucidation on Evolutionary Mechanisms of Antigenic Variation Gene Families
Grant-in-Aid for Scientific Research (B)
1 April 2014–31 March 2018

Ogata, H.
Deep Understanding of the Diversity and Ecology of Giant Viruses in Aquatic Microbial Communities
The Kyoto University Foundation
1 July 2017–31 March 2018

Ogata, H.
Innovative Foundation of Viral Oceanography based on a Comprehensive Virome Study
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Ogata, H.
Elucidation of the Origin and Mechanism of Success of Diatoms through Comparative Biological Analyses between Ancient Centric Diatoms and Their Sister Paramales
Grant-in-Aid for Scientific Research (B)
1 April 2017–31 March 2020

Ogata, H.
Comprehensive Study and Establishment of Application Foundation of Carboxydotrophic Bacteria through Spatio-Temporal Search
Grant-in-Aid for Scientific Research (S)
1 April 2016–31 March 2021

— Mathematical Bioinformatics —

Akutsu, T.
An Approach to Novel Structure Design by Combining Discrete Methods and Statistical Methods
Grant-in-Aid for Scientific Research (A)
1 April 2014–31 March 2019

— Bio-knowledge Engineering —

Mamitsuka, H.
Reinforcement of Resiliency of Concentrated Polymer Brushes and Its Tribological Applications
Strategic Basic Research Program, ACCEL, JST
1 September 2015–31 March 2020

Mamitsuka, H.
Efficiently Inferring Factors Embedded in Multiple Data Matrices
Grant-in-Aid for Scientific Research (B)
1 April 2016–31 March 2019

Yotsukura, S.
Computational Breeding Design of Least Allergen Crops
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2017–31 March 2019

THESES

ASANO, Lisa
D Med Sc, Kyoto University
“Vitamin D Metabolite, 25-Hydroxyvitamin D, Regulates Lipid Metabolism by Inducing Degradation of SREBP/SCAP”
Supervisor: Prof UESUGI, Motonari
23 March 2017

CHAOLUMEN
D Eng, Kyoto University
“Synthesis and Properties of Electron-Deficient Polycyclic Aromatic Compounds”
Supervisor: Prof MURATA, Yasujiro
23 March 2017

EGUCHI, Daichi
D Eng, Kyoto University
“High Functionalization of Nanomaterials by Controlling Organic-Inorganic Interface”
Supervisor: Prof TERANISHI, Toshiharu
25 September 2017

FUTAGOISHI, Tsukasa
D Eng, Kyoto University
“Synthesis and Properties of Open-Cage Fullerene C_{60} Derivatives Encapsulating a Small Molecule”
Supervisor: Prof MURATA, Yasujiro
23 March 2017

HIRATA, Atsushi
D Pharm Sc, Kyoto University
“Organocatalytic Chemo- and Enantioselective Acylation of Polyamines”
Supervisor: Prof KAWABATA, Takeo
23 March 2017

HOSAKA, Yoshiteru
D Sc, Kyoto University
“Electronic Phase Transtions in Perovskite Oxides with Unusually High Valence State Fe”
Supervisor: Prof SHIMAKAWA, Yuichi
23 March 2017

IMAJO, Sohei
D Sc, Kyoto University
“Development of Neutron Doppler Shifter as a Pulsed Ultra-cold Neutron Source”
Supervisor: Assoc Prof IWASHITA, Yoshihisa
23 March 2017

KAKIZAKAI, Haruka
D Sc, Kyoto University
“Electric Field Control of Magnetic Domain Walls”
Supervisor: Prof ONO, Teruo
18 January 2017

KASAMATSU, Koji
D Pharm Sc, Kyoto University
“Asymmetric α-Arylation and α-Fluorination of Amino Acid Derivatives via Memory of Chirality, and Investigation on Elongation of Life-Time of Chiral Enolate Intermediates”
Supervisor: Prof KAWABATA, Takeo
23 March 2017

LU, Wenjie
D Pharm Sc, Kyoto University
“Synthesis and Evaluation of Functionalized Dirhodium(II) Carboxylate Catalysts Bearing Axially Chiral Amino Acid Derivatives”
Supervisor: Prof KAWABATA, Takeo
23 March 2017

MAO, Di
D Med Sc, Kyoto University
“A Synthetic Hybrid Molecule for the Selective Removal of Human Pluripotent Stem Cells from Cell Mixtures”
Supervisor: Prof UESUGI, Motonari
23 May 2017

MORIYA, Yuki
D Sc, Kyoto University
“Bioinformatics Analysis for Pathway Prediction Using Genomic Information”
Supervisor: Assoc Prof GOTO, Susumu
23 March 2017

MURAYAMA, Tomo
D Pharm Sc, Kyoto University
“Sensing and Remodeling of the Structure of Lipid Bilayers by Curvature Inducing Peptides”
Supervisor: Prof FUTAKI, Shiroh
23 March 2017

NAKAJIMA, Sho
D Eng, Kyoto University
“Mechanistic and Synthetic Studies on Iron–Bisphosphine-Catalyzed Cross-Coupling Reactions of Alkyl Halides”
Supervisor: Prof NAKAMURA, Masaharu
23 March 2017

NISHIMURA, Yosuke
D Sc, Kyoto University
“Classification of Marine Viruses Using Complete Genomes Derived from Metagenomes and Inference of Their Infection Strategies from Gene Function”
Supervisor: Assoc Prof GOTO, Susumu
23 May 2017

SHIMIZU, Yugo
D Sc, Kyoto University
“Development of a New Functional Classification of Type III Polyketide Synthases and its Application to Functional Prediction”
Supervisor: Assoc Prof GOTO, Susumu
23 May 2017

SHIMOGAWA, Hiroyuki
D Eng, Kyoto University
“Development of Functional Organic Materials with an Intramolecular B-N Coordination Bond as a Key Scaffold”
Supervisor: Prof MURATA, Yasujiro
23 March 2017

SUZUKI, Furitsu
D Agr, Kyoto University
“Structural Studies on Charge-Transport and Emission Properties of Materials for Organic Light-Emitting Diodes”
Supervisor: Prof KAJI, Hironori
24 September 2017

TSUJI, Shogo
D Pharm Sc, Kyoto University
“Directed Evolution of Transcriptional Activator-Like Effectors”
Supervisor: Prof FUTAKI, Shiroh
23 March 2017

YAMADA, Kihiro
D Sc, Kyoto University
“Electric Field Effect on Ferromagnetic Thin Films”
Supervisor: Prof ONO, Teruo
18 January 2017

YOSHIDA, Ryota
D Eng, Kyoto University
“Development of Metalated Amino Acids and Peptides as Oxidation Catalysts and Application of Those to Selective Lignin Degradation”
Supervisor: Prof NAKAMURA, Masaharu
23 March 2017

ZHANG, Rui
D Eng, Kyoto University
“Synthesis and Properties of Endohedral Fullerene C_{70} Encapsulating Two Chemical Species”
Supervisor: Prof MURATA, Yasujiro
23 March 2017

THE 117TH ICR ANNUAL SYMPOSIUM

SEMINARS MEETINGS AND SYMPOSIA

THE 117TH ICR ANNUAL SYMPOSIUM

(1 December 2017)

ORAL PRESENTATIONS

MORISHITA, Hiroki (Inorganic Photonics Materials)
"Electrically Detected Magnetic Resonance of NV Centers in Diamond"

MORIYAMA, Takahiro (Nanospintronics)
"Antiferromagnetic Spintronics"

KAWAMOTO, Jun (Molecular Microbial Science)
"Function of a Polyunsaturated Fatty Acid in an Antarctic Cold-adapted Bacterium"

TAMURA, Takeyuki (Mathematical Bioinformatics)
"Computational Design of Metabolic Networks for Production of Valuable Compounds"

SUZUKI, Katsuaki (Molecular Materials Chemistry)
"Development of Highly Efficient Thermally Activated Delayed Fluorescence Emitters and the Orientational Analysis of Organic Amorphous Thin Films Using DNP-NMR"

— ICR Award for Young Scientists —
IWAMOTO, Takahiro (Synthetic Organotransformation)
"Iron-Catalyzed anti-Selective Carbosilylation of Internal Alkynes"

TAKEUCHI, Katsuhiko (Organometallic Chemistry)
"A Square-Planar Complex of Platinum(0)"

— ICR Award for Young Scientists (Foreign Researcher's Category) —
LE, Phuong Quang (Nanophotonics)
"Free Excitons and Exciton-Phonon Coupling in $CH_3NH_3PbI_3$ Single Crystals Revealed by Photocurrent and Photoluminescence Measurements at Low Temperatures"

— ICR Award for Graduate Students —
SUGAHARA, Tomohiro (Organoelement Chemistry)
"Highly Bent 1,3-Digerma-2-silaallene"

FUJIMORI, Shiori (Organoelement Chemistry)
"Germabenzenylpotassium: A Germanium Analogue of a Phenyl Anion"

FAN, Weijia (Polymer Controlled Synthesis)
"Synthesis of Multivalent Organotellurium Chain Transfer Agents by Post-modification and Their Applications in Living Radical Polymerization"

— ICR Grants for Promoting Integrated Research —
SHIMOAKA, Takafumi (Chemistry for Functionalized Surfaces)
"pMAIRS Study of Swollen Functionalized Concentrated Polymer Brushes"

IWAMOTO, Takahiro (Synthetic Organotransformation)
"Study of Magnetic Field Effect in Iron-Catalyzed Reaction"

BLANC-MATHIEU, Romain (Chemical Life Science)
"The Evolutionary History of PIP5K Subfamily B Genes in Core Eudicots"

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"

— Structural Organic Chemistry —

LW "Research Activities in Structural Organic Chemistry Laboratory"

GE NAKAMURA, Tomoya; SHIOYA, Nobutaka; SHIMOAKA, Takafumi; HASEGAWA, Takeshi; MURATA, Yasujiro; WAKAMIYA, Atsushi
"Naphthalene Diimide-Based Electron-Transporting Layer for Perovskite Solar Cells"

— Synthetic Organic Chemistry —

LW "Current Topics of Fine Organic Synthesis"

GE SHIBAYAMA, Hiromitsu; TAKEUCHI, Hironori; UEDA, Yoshihiro; FURUTA, Takumi; KAWABATA, Takeo
"Synthetic Studies Towards Coriariin A"

— Advanced Inorganic Synthesis —

LW "Current Research Activities in Advanced Inorganic Synthesis"

— Chemistry of Polymer Materials —

LW "Research Activities in Laboratory of Chemistry of Polymer Materials"

GE EGUCHI, Hiroshi; SAKAKIBARA, Keita; TSUJII, Yoshinobu
"Synthesis of Bottle-Brush Polymers Containing Polyallene Skeleton in Their Main Chain"

— Polymer Controlled Synthesis —

LW "Research Activities in Laboratory of Polymer Controlled Synthesis"

GE SUN, Liansheng; KAYAHARA, Eiichi; YAMAGO, Shigeru
"Synthesis and Physical Properties of [10]Cycloparaphenylene Derivatives with Hydro- and Benzoquinone Units"

GE LI, Xiaopei; NAKAMURA, Yasuyuki; YAMAGO, Shigeru
"A Study on the Termination Mechanism of Radical Polymerization of Acrylonitrile"

— Inorganic Photonics Materials —

LW “Research Topics of Inorganic Photonics Lab”

LT ASHIDA, Takaki; HAYASHI, Kan; TANIGUCHI, Takashi; MORISHITA, Hiroki; FUJIWARA, Masanori; HATANO, Mutsuko; MIZUOCHI, Norikazu
“Nitrogen Doping Control for High Sensitivity of Diamond Quantum Sensor”

GE MARUYAMA, Yuuichi; DANJYO, Takuya; WATANABE, Akira; KATO, Hiromitsu; MAKINO, Toshiharu; YAMASAKI, Satoshi; MORISHITA, Hiroki; FUJIWARA, Masanori; MIZUOCHI, Norikazu
“Spin Coherence Time of NV Center in Phosphorus Doped Diamond”

— Nanospintronics —

LW “Recent Research in Nano-Spintronics Lab”

LT HAM, Wooseung
“Temperature Dependence of Spin-Orbit Effective Fields in Pt/GdFeCo”

— Biofunctional Design-Chemistry —

LT ARAFILES, Jan Vincent; KAWANO, Kenichi; FUTAKI, Shiroh
“Novel Macropinocytosis-Inducing Intracellular Delivery Peptides”

GE TAMEMOTO, Naoki; AKISHIBA, Misao; SAKAMOTO, Kentarou; KAWANO, Kenichi; FUTAKI, Shiroh
“Evaluation of Antimicrobial Activity of Endosomolytic Peptide L17E and Some Analogues”

— Chemistry of Molecular Biocatalysts —

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Graduate School of Science, Chiba University, Chiba, Japan
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Laser Physics Centre Research School of Physics and Engineering, Australian National University, Australia
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Department of Chemistry, Yonsei University, Korea, R.
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Universite Montpellier 2, France
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Xi’an Jiaotong University, China, P.R.
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RIKEN, National Cancer Center Japan, Tokyo, Japan
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Department of Chemical Engineering, The Pennsylvania State University, U.S.A.
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Graduate School of Science, Nagoya University, Aichi, Japan
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Organo Corporation, Tokyo, Japan
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Department of Physics, Chalmers University of Technology, Sweden
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Graduate School of Engineering, Osaka University, Osaka, Japan
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Dr PAËPE, Gaël De
CEA Grenoble, France
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Université de Toulouse, France
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Assoc Prof SAEKI, Takayuki
High Energy Accelerator Research Organization, Ibaraki, Japan
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AIST on machine learning (Visiting associate professor of Bioinformatics Center), Tokyo, Japan
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Institute of Physical and Chemical Research, Saitama, Japan
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Kyoto Municipal Institute of Industrial Technology and Culture, Kyoto, Japan
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Nara Women's University, Nara, Japan
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Data Science Laboratory, School of Information and Communication Technology, Hanoi University of Science and Technology, Vietnam
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Intelligent Bioinformatics Research Team, Artificial Intelligence Research Center, Advanced Industrial Science and Technology (AIST), Tokyo, Japan
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Royal Society of Chemistry, Tokyo, Japan
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Universität Frankfurt, Germany
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Helsinki Institute of Information Technology, Finland
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Merck Research Institute, MERCK&CO., INC., U.S.A.
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Asian Chemical Biology Initiative 2017 Ho Chi Minh Meeting
Organized by UESUGI, Motonari
20–23 January 2017 (Vietnam)

The 12th International Workshop for East Asian Young Rheologists (IWEAYR-12)
Co-organized by WATANABE, Hiroshi
8–10 February 2017 (Chonburi, Thailand)

The 97th CSJ Annual Meeting, Special Symposium on Advanced Technology Program, "Recent Advances in Synchrotron Radiation based SAXS"
Organized by TAKAYA, Hikaru
19 March 2017 (Tokyo, Japan)

Rheology Review Lecture Meeting
Organized by MATSUMIYA, Yumi
20 May 2017 (Kyoto, Japan)

The International Polymer Conference of Thailand: PCT-7
Organized by TAKENAKA, Mikihito
1–2 June 2017 (Thailand)

IUMRS-ICAM 2017
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28–30 August 2017 (Kyoto, Japan)

Asian Chemical Biology Initiative 2017 Ulaanbaatar Meeting
Organized by UESUGI, Motonari
1–4 September 2017 (Mongolia)

Meeting of 5th REXDAB Steering Committee
Organized by ITO, Yoshiaki
10–12 September 2017 (Kyoto, Japan)

New Trends in Enzyme and Microbial Science in the Translational Biology Era
Co-organized by KURIHARA, Tatsuo
18–20 October 2017 (Italy)

Institute for Chemical Research International Symposium of NMR 2017 (ICRS-NMR'17): DNP-NMR Workshop
Organized by KAJI, Hironori
9–11 November 2017 (Kyoto, Japan)

The 2nd pMAIRS Workshop: Molecular Orientation is the Key of Thin-film Chemistry
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22 November 2017 (Kyoto, Japan)

International Workshop on Microbes in Hostile Environments
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