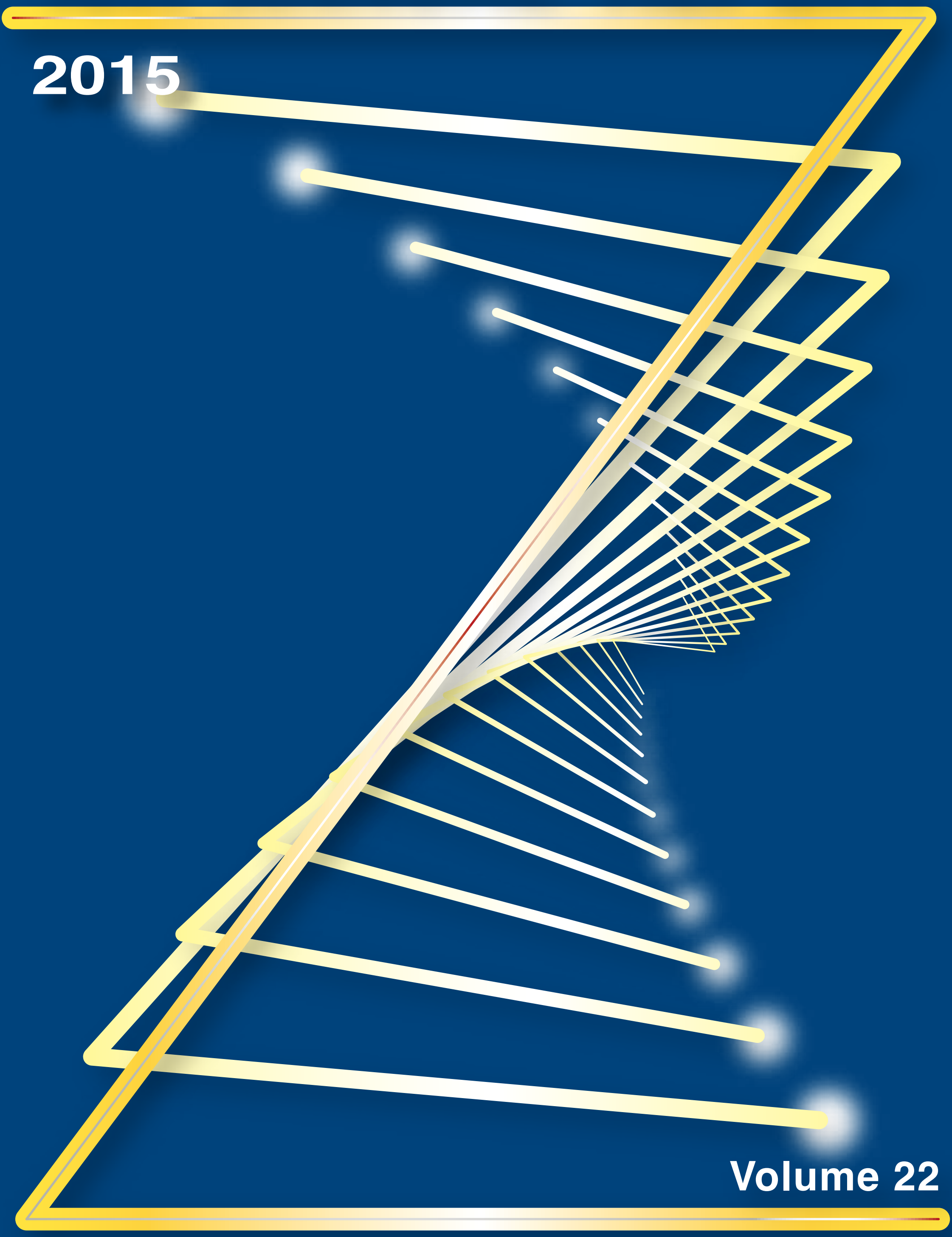
ISSN 1342-0321
IAREFM

ICR ANNUAL REPORT

2015



Volume 22

Institute for Chemical Research
Kyoto University

ICR ANNUAL REPORT 2015 (Volume 22) - ISSN 1342-0321 -

This Annual Report covers from 1 January to 31 December 2015

Editors:

Professor: KURIHARA, Tatsuo
Professor: TERANISHI, Toshiharu
Associate Professor: IWASHITA, Yoshihisa
Professor: OGATA, Hiroyuki

Editorial Staff:

Public Relations Section: HAMAOKA, Meri
TANIMURA, Michiko
INOUE, Junko
TAKEHIRA, Tokiyo
NAKAMURA, Kaori

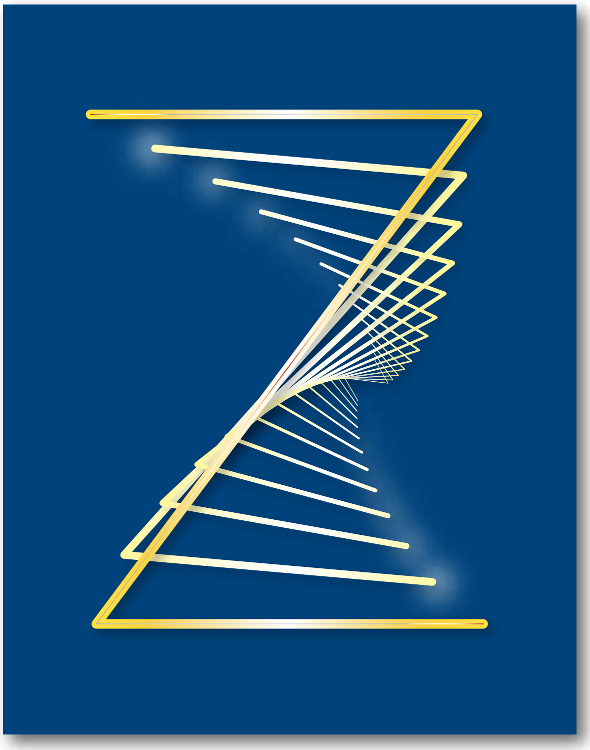
Published and distributed by:
Institute for Chemical Research (*ICR*), Kyoto University

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

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

Printed by
Zenis Co., Ltd.
67-10 Karahashi-Akakanecho, Minami-Ku, Kyoto 601-8463, Japan
TEL: +81-(0)75-671-7100 FAX: +81-(0)75-671-7107

ICR ANNUAL REPORT 2015



Institute for Chemical Research
Kyoto University
Volume 22

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 outstanding 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, informatics, and human/environmental studies. These laboratories are spearheading leading-edge research, and yielding outstanding results in their own and related research areas with publications such as: *1) Tara Oceans: Exploring the Plankton Forest under the Sea Surface, 2) Edge Mixing Dynamics in Graphene p–n Junctions in the Quantum Hall Regime, 3) Highly Efficient Perovskite Solar Cells using Sheet-shaped Molecule: Increasing Power Conversion Efficiency by 1.2 Times Compared with Conventional Material, and 4) A Mid-sized Agent Capable of Disrupting Intracellular Protein–Protein Interactions is Now Generated in Cells*, 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.

The ICR also collaborates with domestic and international universities and research organizations (with 66 official international collaboration agreements as of January 1, 2016) and functions as a Joint Usage/Research Center proclaiming the Frontier/Interdisciplinary Research Core for Deeping Investigation and Promoting Cooperation in Chemistry-Oriented Fields supported by MEXT (2010-2016); its activity received high commendation on the interim assessment in 2013. 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 Research on Chemical Synthesis (2010–2016), 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 2016

N. Tokitoh

TOKITOH, Norihiro
Director

ICR News 2015

ICR Joint Usage / Research Center: from first to second term

■ Prof WATANABE, Hiroshi (Head of Joint Research Station in the first term)

In 2010, the Institute for Chemical Research (ICR) began to serve as the Joint Usage/Research Center (JURC) approved by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. Since then, ICR-JURC has been offering its facilities, equipment, and international hub functionality as a base for joint research with out-of-ICR researchers working in chemistry-related fields, aiming at construction of a dense, interdisciplinary network of Japanese and overseas researchers, and at deepening the basic understanding in those fields. The joint research, backed up with frontier knowledge and hospitality of the ICR faculty members, has resulted in fruitful achievements, with over 400 joint papers published in internationally prestigious journals. These activities of ICR-JURC are highly appreciated by the participating researchers (as reported in *http://www.kuicr.kyoto-u.ac.jp/kyodo/tenkenhokoku24.pdf* and *http://www.kuicr.kyoto-u.ac.jp/kyodo/H27q.pdf*).

In 2015, MEXT evaluated the activities of ICR-JURC favorably to approve ICR as the JURC in the second term as of April 2016. In the second term (covering six years), ICR-JURC will conduct advanced joint research in chemistry-related fields, with the emphasis being placed on global cooperation and basic research that could also help development of a sustainable human society. The Joint Research Station, headed by Professor Toshiharu Teranishi in the second term, serves as the headquarter of ICR-JURC, and all ICR faculty members will make significant efforts to advance the joint research, ensuring us of further achievements by ICR-JURC in the second term.

Joint Research Project “Smart-Materials” (2015–2020)

■ Prof TSUJII, Yoshinobu (Vice-Director of ICR)

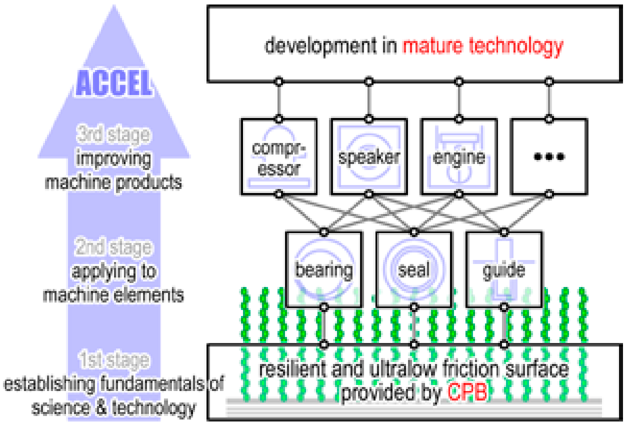
Since April of 2015, the Institute for Chemical Research (ICR), the Institute of Advanced Energy (IAE), and the Research Institute for Sustainable Humanosphere (RISH) have been working in cooperation on the “Smart-Materials” project, supported by the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan. The ever-increasing demand for materials and energy by the present social system has almost reached its limit, and the environment is heavily burdened by harmful byproducts and surplus heat from mass production. In order to overcome these issues, this project aims to fabricate smart materials and develop a joint research organization, achieving green innovation through “zero loss” at the production/transportation/usage of materials/energy. The model for the target materials is a biological system with molecular recognition ability, autonomy, and activity. The key to success is interdisciplinary research with flexibility and rapidity. Taking advantage of the three institutes being located at the same campus (Uji campus of Kyoto University), the under-one-roof scheme is expected to deliver internationally excellent results, contributing significantly to this research field.

ACCEL Project (2015–2020) : Development of Novel “SRT” System

■ Prof TSUJII, Yoshinobu

Japan Science and Technology Agency (JST), Strategic Basic Research Program, ACCEL, “Reinforcement of Resiliency of Concentrated Polymer Brushes and Its Tribological Applications — Development of Novel ‘Soft and Resilient Tribology (SRT)’ System”

Previously, we demonstrated that the concentrated polymer brushes (CPBs) newly synthesized by living radical polymerizations inherently possess unique structures and properties, such as high modulus, ultra-low friction and good lubrication, and excellent biocompatibility. On the basis of such breakthroughs, not only in polymer synthesis but also in polymer physics, this ACCEL project aims to reinforce such soft and resilient properties derived from the CPBs and hence apply them to various sliding mechanical elements, e.g., sliding bearings and seals, for prolonged life and energy saving. Our final goal is to develop a novel soft and resilient tribology (SRT) system for practical use through industry–academia collaboration. Eight universities and six companies are involved.



Mini History Exhibition Corner Was Opened

■ Prof TSUJII, Yoshinobu (Vice-Director of ICR)

The Institute for Chemical Research (ICR), Kyoto University has been working on archiving its research results in order to widely announce their history of contributions to science and technology. As part of this attempt, a mini history exhibition corner was opened in March 2015 for an attractive outreach activity by ICR, with financial support from Kyoto University. It was designed especially for middle and high school students who visit the ICR. There are materials displayed (historical documents and photographs) related to scientists and projects previously enrolled and associated with the ICR, including “Vinylon” and “Synthetic Oil” (approved as Chemical Heritages by the Chemical Society of Japan). The collection of “Vinylon” is also registered in the Kyoto University Digital Archive System (KUDAS).

CONTENTS

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
M1〜2	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
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
  - Solution and Interface Chemistry
  - 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
  - Structural Molecular Biology
- **International Research Center for Elements Science**
  - Organic Main Group Chemisry
  - Advanced Solid State Chemistry
  - Organotransition Metal Chemistry
  - Photonic Elements Science
- **Bioinformatics Center**
  - Chemical Life Science
  - Mathematical Bioinformatics
  - Bio-knowledge Engineering
  - GenomeNet Project Management Office
- Visiting Divisions
- Joint Usage / Research Center
- Supercomputer System
- Low Temperature Laboratory

TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

Division of Synthetic Chemistry
– Organoelement Chemistry –

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


Prof
TOKITOH, Norihiro
(D Sc)


Assoc Prof
SASAMORI, Takahiro
(D Sc)


Assist Prof
MIZUHATA, Yoshiyuki
(D Sc)


Assist Prof
AGOU, Tomohiro
(D Sc)


Techn Staff
HIRANO, Toshiko


PD
GUO, Jing-Dong
(Ph D)


PD
MAJHI, Paresh Kumar
(Ph D)

Students

MIYAMOTO, Hisashi (D3)
NAGATA, Koichi (D3)
AWANE, Hiroyuki (D2)
HIRANO, Koki (D2)
SUZUKI, Yuko (D1)
FUJIMORI, Shiori (M2)
SUGAHARA, Tomohiro (M2)
HONJO, Kazuma (M1)
NAKANO, Tomohiro (M1)
YANAGISAWA, Tatsuya (M1)

Guest Scholars

KYRI, Andreas	University of Bonn, Germany, 30 April-31 August
FAßBENDER, Jan	University of Bonn, Germany, 23 August-4 September

Guest Res Assoc

STREUBEL, Rainer	University of Bonn, Germany, 6 June-11 June
MAYER, Ulrich F. J.	Mayer Scientific Editing, Germany, 19 May-13 June

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

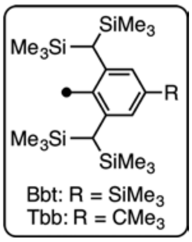
Selected Publications

Sasamori, T.; Sugahara, T.; Agou, T.; Sugamata, K.; Guo, J.-D.; Nagase, S.; Tokitoh, N., Reaction of a Diaryldigermyne with Ethylene, *Chem. Sci.*, **6,** 5526-5530 (2015).

Agou, T.; Wasano, T.; Sasamori, T.; Guo, J.-D.; Nagase, S.; Tokitoh, N., Ring Expansion to 1-Bromo-1-alumacyclonona-2,4,6,8-tetraene by Insertion of Two Alkyne Molecules into the Al–C Bonds, *Angew. Chem. Int. Ed.*, **54,** 9568-9571 (2015).

Sasamori, T.; Sugahara, T.; Agou, T.; Guo, J.-D.; Nagase, S.; Streubel, R.; Tokitoh, N., Synthesis and Characterization of a 1,2-Digermabenzene, *Organometallics*, **34,** 2106-2109 (2015).

Reactions of Diaryldigermynes with Ethylene and Acetylene



Recently, divalent or multiple-bonded compounds of heavier group 14 elements have received much attention as potential transition metal–free catalysts. We have investigated the reactivity of stable Ge–Ge triple-bond compounds, digermynes, with small molecules and reported their unique and transition metal–free transformations with ethylene and acetylene.

Reaction of the digermyne BbtGe≡GeBbt (**1a**, Bbt = 2,6-[$CH(SiMe_3)_2$]$_2$-4-[$C(SiMe_3)_3$]-C_6H_2) with ethylene initially afforded the corresponding 1,2-digermacyclobutene **2**. Depending on the reaction conditions applied, further reaction of **2** with ethylene furnished two different reaction products: 1,4-digermabicyclo[2.2.0]hexane **3** or a bis(germiranyl)ethane **4**. Combined experimental and theoretical results suggested that **3** and **4** are the thermodynamic and kinetic reaction products, respectively.

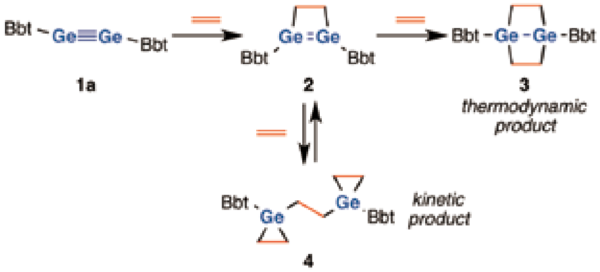


Figure 1. Reactions of digermyne **1a** with ethylene.

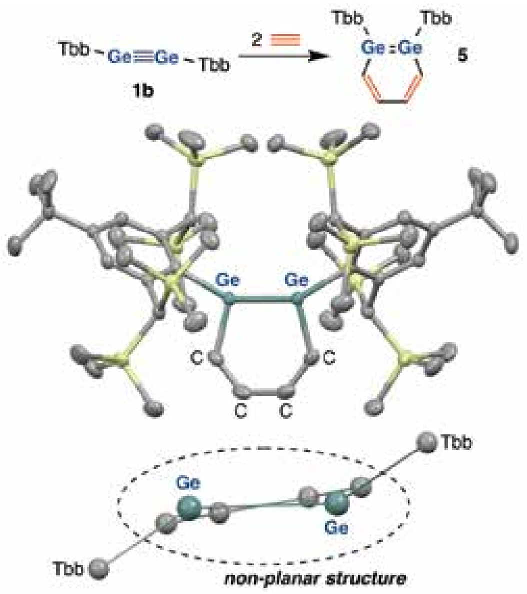


Figure 2. Reaction of digermyne **1b** with acetylene and the structure of **5** (overhead and side views).

The reaction of the digermyne TbbGe≡GeTbb (**1b**, Tbb = 4-*t*-Bu-2,6-[$CH(SiMe_3)_2$]$_2$-C_6H_2) with two equivalents of acetylene gave the 1,2-digermabenzene **5** as a stable, crystalline compound via a formal [2 + 2 + 2] reaction. The [Ge_2C_4] ring of **5** exhibited a nonplanar structure, wherein six π electrons are partially delocalized. Despite its non-planar structure, theoretical calculations suggested aromaticity for **5**, comparable to that of 1,2-disilabenzenes.

Formation of an Alumacyclononatetraene by Insertion of Two Alkyne Molecules into the Al–C Bonds of an Alumacyclopentadiene

The reaction of heteroles with compounds containing carbon–carbon multiple bonds, such as alkynes, is a useful method to construct new heterocyclic skeletons with specific structures and properties. Treatment of 1-bromo-2,3,4,5-tetraethylalumole (**6**) with 3-hexyne afforded the corresponding ring-expansion product 1-bromo-1-alumacyclonona-2,4,6,8-tetraene (**7**), accompanied by the formation of hexaethylbenzene. Compound **6** is, to our knowledge, the first example of structurally characterized, stable group 13 element–containing cyclononatetraene derivative. The AlC_8 nine-membered ring of **6** exhibited a highly twisted, nearly C_2-symmetric structure both in the crystalline state and in solution. Deuterium-labeling experiments and DFT calculations on the reaction of **6** with 3-hexyne suggested that 1-bromo-1-alumacyclohepta-2,4,6-triene (**8**), which is formed by the insertion of one molecule of 1-hexyne into the Al–C bond of alumole **6**, is the key intermediate for the generation of **7** as well as hexaethylbenzene.

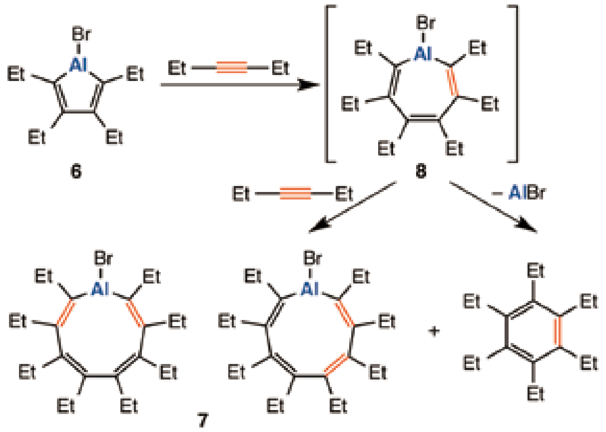


Figure 3. Reaction of bromoalumole **6** with 3-hexyne.

Division of Synthetic Chemistry
– Structural Organic Chemistry –

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


Prof
MURATA, Yasujiro
(D Eng)


Assoc Prof
WAKAMIYA, Atsushi
(D Eng)


Assist Prof
MURATA, Michihisa
(D Eng)


PD
ARAMAKI, Yoshitaka
(D Eng)


PD
GOPAL, Anesh
(Ph D)


PD
AHAREN, Tomoko
(Ph D)

Researchers(pt)
HORI, Megumi
ARAKAWA, Noriko

Assist Techn Staffs
NAKAIKE, Yumi (D Eng)
SHIMAZAKI, Ai

Students
NISHIMURA, Hidetaka (D3)
CHAOLUMEN (D3)
FUTAGOISHI, Tsukasa (D2)
SHIMOGAWA, Hiroyuki (D2)
ZHANG, Rui (D2)
HASHIKAWA, Yoshifumi (D1)
MARUYAMA, Naoki (M2)
KAJI, Shoji (M1)
OKAZAKI, Shuhei (UG)
TSUKAO, Masahiro (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
Functional Materials
Organic Solar Cells
Endohedral Fullerenes
Perovskite-Based Solar Cells

Selected Publications

Futagoishi, T.; Murata, M.; Wakamiya, A.; Murata, Y., Trapping N_2 and CO_2 on the Sub-Nano Scale in the Confined Internal Spaces of Open-Cage C_{60} Derivatives: Isolation and Structural Characterization of the Host–Guest Complexes, *Angew. Chem. Int. Ed.*, **54,** 14791-14794 (2015).

Nishimura, H.; Eliseeva, M. N.; Wakamiya, A.; Scott, L. T., 1,3,5,7-Tetra(Bpin)azulene by Exhaustive Direct Borylation of Azulene and 5,7-Di(Bpin)azulene by Selective Subsequent Deborylation, *Synlett*, **26,** 1578-1580 (2015).

Wakamiya, A.; Yamaguchi, S., Designs of Functional π-Electron Materials based on the Characteristic Features of Boron, *Bull. Chem. Soc. Jpn.*, **88,** 1357-1377 (2015).

Wang, S.; Yang, D.-T.; Lu, J.; Shimogawa, H.; Gong, S.; Wang, X.; Mellerup, S. K.; Wakamiya, A.; Chang, Y.-L.; Yang, C.; Lu, Z.-H., In Situ Solid-State Generation of $(BN)_2$-Pyrenes and Electroluminescent Devices, *Angew. Chem. Int. Ed.*, **54,** 15074-15078 (2015).

Chaolumen; Murata, M.; Sugano, Y.; Wakamiya, A.; Murata, Y., Electron Deficient Tetrabenzo-Fused Pyracylene and Conversions into Curved and Planar π-Systems with Distinct Emission Behaviors, *Angew. Chem. Int. Ed.*, **54,** 9308-9312 (2015).

Trapping N_2 and CO_2 on the Sub-nano Scale in the Confined Internal Spaces of Open-cage C_{60} Derivatives: Isolation and Structural Characterization of the Host–Guest Complexes

We have previously reported the synthesis of open-cage C_{60} **1** with a 17-membered-ring opening and one sulfur atom on the rim. It was found that **1** was able to encapsulate molecular nitrogen and carbon dioxide after its exposure to high pressures of N_2 and CO_2 gas. A subsequent reduction of one of the four carbonyl groups on the rim of the opening induced a contraction of the opening (→**2**) and trapped the guest molecules inside. The molecular structures of $N_2@$**2** and $CO_2@$**2** were determined by single-crystal X-ray diffraction analyses, which revealed a short N≡N triple bond for the encapsulated N_2 and an non-symmetric molecular structure for the encapsulated molecule of CO_2.

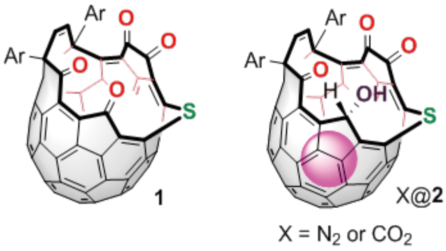


Figure 1. The structures of open-cage C_{60} derivative **1** and host–guest complexes $N_2@$**2** and $CO_2@$**2**.

Hole-transporting Materials with a Two-dimensionally Expanded π-System around an Azulene Core for Efficient Perovskite Solar Cells

Two-dimensionally expanded π-systems, consisting of partially oxygen-bridged triarylamine skeletons that are connected to an azulene (**1**–**3**) or biphenyl core (**4**), were synthesized. When tetra-substituted azulene **1** was used as a hole-transporting material (HTM) in perovskite solar cells, the observed performance (power conversion efficiency = 16.5%) was found to be superior to that of the current HTM standard Spiro-OMeTAD. Based on a comparison of the optoelectronic and electrochemical properties of **1**–**4** and Spiro-OMeTAD, we were able to elucidate the factors that are required for HTMs to act efficiently in perovskite solar cells.

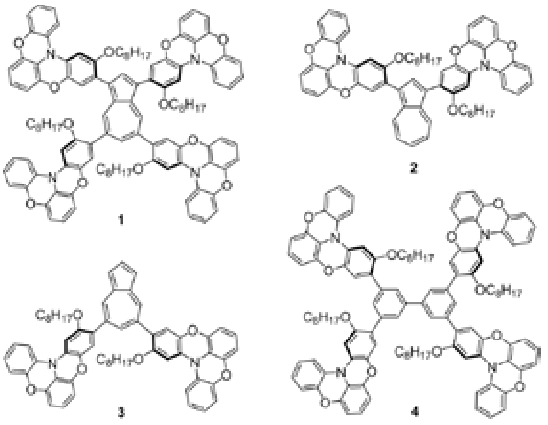


Figure 2. The structures of **1**–**4** with two-dimensionally expanded π-systems.

Electron Deficient Tetrabenzo-fused Pyracylene and Conversions into Curved and Planar π-Systems with Distinct Emission Behaviors

Polycyclic aromatic compounds containing fully unsaturated five-membered ring(s) have been intensively studied because of their unique properties, which include high electron affinity and reactivity. We demonstrated an efficient route for the synthesis of electron-deficient tetrabenzo-fused pyracylene **1** by using intramolecular oxidative C–H coupling. Compound 1 was shown to possess high electron affinity and to undergo addition reactions with *n*-butyllithium or benzyne. These reactions led to either a 1,4-addition compound **2** or triptycene-type adduct **3** with a curved or planar π-system, respectively. These compounds showed distinct emissions in the solid state with high quantum yields. X-ray diffraction analyses demonstrated that the **2** forms dimers with effective π-overlap, which can cause a significant red-shift in the fluorescence by the stabilization of excimer.

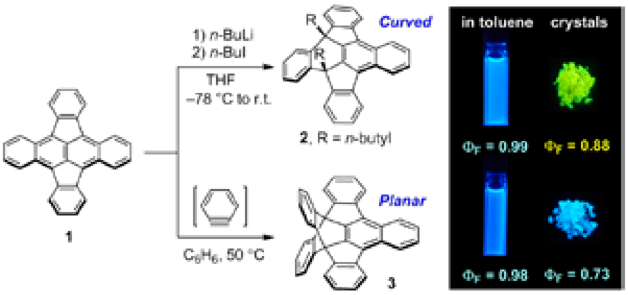


Figure 3. Conversions of electron deficient TBP **1** into curved and planar π-systems **2** and **3** having distinct emission behaviors.

Division of Synthetic Chemistry
– Synthetic Organic Chemistry –

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


Prof
KAWABATA, Takeo
(D Pharm Sc)


Assoc Prof
FURUTA, Takumi
(D Pharm Sc)


Assist Prof
YOSHIMURA, Tomoyuki
(D Pharm Sc)


Assist Prof
UEDA, Yoshihiro
(D Pharm Sc)


Techn Staff
FUJIHASHI, Akiko


PD
HARISADHAN, Ghosh
(Ph D)


PD
YELLA, Ramesh
(Ph D)

Researcher

NOBUTA, Tomoya (D Pharm Sc)

Students

BABA, Tomonori (D4)
YANAGI, Masanori (D4)
TAKEUCHI, Hironori (D3)
LU, Wenjie (D3)
TSUDA, Ayumi (D3)
HYAKUTAKE, Ryuichi (D3)
HIRATA, Atsushi (D3)
KASAMATSU, Koji (D2)
KURIBAYASHI, Toshifumi (D2)
NAKAGAWA, Akihiro (D2)
HAYASAKA, Manami (D2)
ARAI, Kenta (D1)
OTSUKI, Haruka (D1)
TANAKA, Yuya (M2)
FUJIMORI, Yusuke (M2)
NISHIJIMA, Hideyuki (M2)
ORITA, Takuya (M1)
GONDOH, Naruhiro (M1)
SHIBAYAMA, Hiromitsu (M1)
SHIMODA, Shotaro (M1)
MATAYOSHI, Aki (M1)
SHIMMIYA, Ruri (UG)
NAGAISHI, Masaru (UG)
NINOMIYA, Ryo (UG)
YAMAMOTO, Satoru (UG)

Scope of Research

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

KEYWORDS

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).

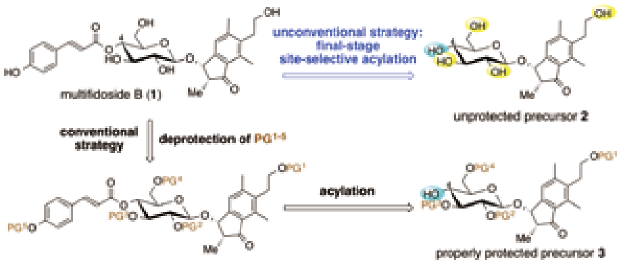
Yoshimura, T.; Tomohara, K.; Kawabata, T., Asymmetric Induction via Short-Lived Chiral Enolates with Chiral C-O Axis, *J. Am. Chem. Soc.*, **135,** 7102-7105 (2013).

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).

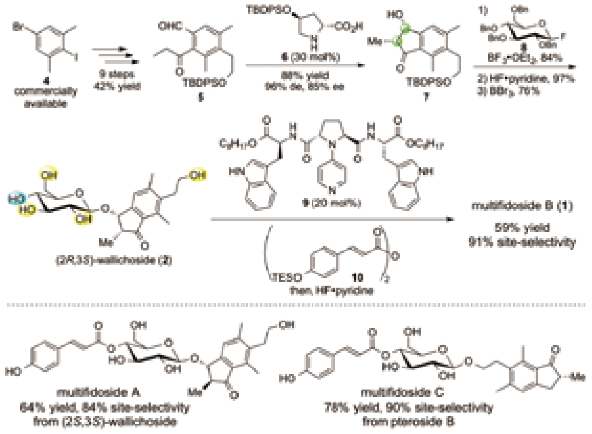
Ueda, Y.; Furuta, T.; Kawabata, T., Final-Stage Site-Selective Acylation for the Total Syntheses of Multifidosides A-C, *Angew. Chem. Int. Ed.*, **54,** 11966-11970 (2015).

An Unconventional Retrosynthesis of Acylated Natural Glycosides: Final-stage Site-selective Acylation of Unprotected Glycosides

Several hundreds of acylated glycosides such as phenylethanoid glycosides and ellagitannins exist in nature. Some of them show potent biological activities including antivirus, antitumor, and antiallergic activities, and have attracted interest for synthesis. Multifidosides A-C, isolated from whole plants used in traditional Chinese medicine, possess a *p*-coumaroyl group at C(4)–OH of the glucopyranose moiety. Properly protected precursor **3** with free C(4)–OH is a rational precursor for the synthesis of multifidoside B (**1**) based on the conventional protection/deprotection strategy. In contrast, we propose an unconventional strategy based on final-stage site-selective acylation: the *p*-coumaroyl group can be introduced directly onto the C(4)–OH of the unprotected precursor **2** at the final step of total synthesis. The expected advantages of the proposed strategy would be: 1) streamlining for fewer steps for the total synthesis and 2) avoidance of the risks of the undesired side reactions during the removal of the protecting groups (PGs) at a later stage of the conventional synthetic scheme.

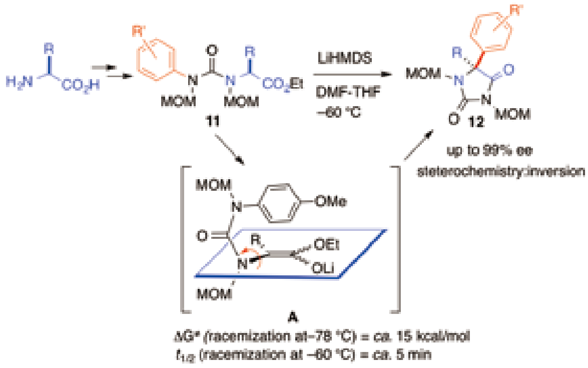


Unprotected precursor **2** was readily prepared by a thirteen-step transformation from commercially available **4**, in which an intramolecular asymmetric aldol reaction of **5** catalyzed by organocatalyst **6** was performed as a key step. As we expected, acylation of **2** promoted by our originally developed organocatalyst **9** took place at the intrinsically less reactive C(4)–OH of the glucopyranose substructure even in the presence of two primary hydroxy groups. Thus, multifidoside C was obtained in one step from the unprotected precursor **2** by the removal of the TES group during the work-up process. Notably, the synthetic route has a one-step conversion from a natural glycoside into another natural glycoside, since **2** is also a naturally occurring glycoside named (2*R*,3*S*)-wallichoside. Similarly, the first total syntheses of multifidosides A and C have been achieved by final-stage site-selective acylation of the precursor natural glycosides, (2*S*,3*S*)-wallichoside and pteroside B, respectively. Considering the predictability and reliability of the site-selective acylation promoted by catalyst **9**, the proposed strategy could provide a general synthetic route to 4-O-acylglycosides.



Asymmetric α−Arylation of Amino Acid Derivatives by Intramolecular Aryl Migration of Ester Enolates via Memory of Chirality

Asymmetric α−arylation of amino acids has been a challenge in current organic synthesis. We have developed a method for asymmetric α−arylation of amino acid derivatives via intramolecular aryl migration (Clayden rearrangement) of chiral enolates generated from amino acid esters, based on the protocol of memory of chirality. The reaction took place through inversion of configuration via chiral enolate intermediate **A**, whose racemization barrier was ~15 kcal/mol at −78 °C. The half-life of racemization of the axially chiral enolate was estimated to be ~5 min at −60 °C (reaction temperature). This method provides chiral hydantoins with aryl-substituted tetrasubstituted carbon, potentially useful chiral building blocks in the field of medicinal chemistry, and are structural equivalents to amino acids with aryl-substituted tetrasubsituted carbon.



Division of Synthetic Chemistry
– Advanced Inorganic Synthesis –

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

Prof
TERANISHI, Toshiharu
(D Eng)

Assoc Prof
SAKAMOTO, Masanori
(D Eng)

Assist Prof
SATO, Ryota
(D Sc)

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

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

PD
WU, Hsin-Lun
(D Sc)

PD
NGUYEN, Viet Long
(D Eng)

Students

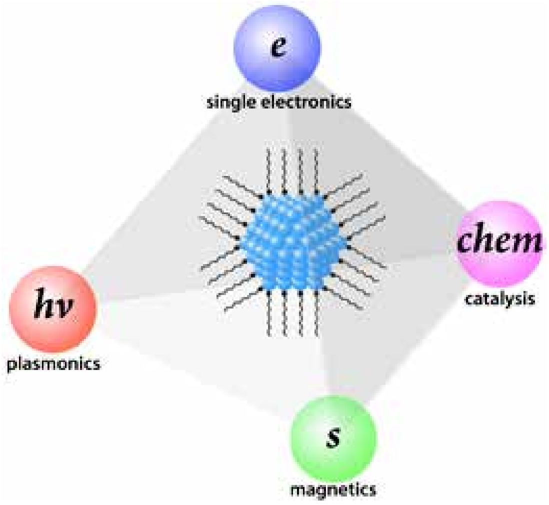
CHEN, Lihui (D3)
KIM, Sungwon (D3)
EGUCHI, Daichi (D2)
LIAN, Zichao (D1)
KIMURA, Masato (M2)
MATSUMOTO, Kenshi (M2)
TABUCHI, Michimasa (M2)

Guest Scholars

LIN, Zhiqun	Georgia Institute of Technology, U.S.A., 12 June-13 June
PRASAD, B. L. V.	National Chemical Laboratory, India, 17 November-20 November

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
Plasmonics
Photocatalysts
Single Electronics
Nanocomposite Magnet

Selected Publications

Sakamoto, M.; Chen, L.; Okano, M.; Tex, D. M.; Kanemitsu, Y.; Teranishi, T., Photoinduced Carrier Dynamics of Nearly Stoichiometric Oleylamine-protected Copper Indium Sulfide Nanoparticles and Nanodisks, *J. Phys. Chem. C*, **119,** 11100-11105 (2015).

Chen, L.; Sakamoto, M.; Sato, R.; Teranishi, T., Determination of a Localized Surface Plasmon Resonance Mode of Cu_7S_4 Nanodisks by Plasmon Coupling, *Faraday Discuss*., **181,** 355-364 (2015).

Frake, J. C.; Kano, S.; Ciccarelli, C.; Griffiths, J.; Sakamoto, M.; Teranishi, T.; Majima, Y.; Smith, C. G.; Buitelaar, M. R., Radio-frequency Capacitance Spectroscopy of Metallic Nanoparticles, *Sci. Rep.*, **5,** 10858 (2015).

Trinh, T. T.; Sato, R.; Sakamoto, M.; Fujiyoshi, Y.; Haruta, M.; Kurata, H.; Teranishi, T., Visible to Near-Infrared Plasmon-Enhanced Catalytic Activity of Pd Hexagonal Nanoplates for the Suzuki Coupling Reaction, *Nanoscale*, **7,** 12435-12444 (2015).

Photo-induced Carrier Dynamics of Nearly Stoichiometric Oleylamine-protected Copper Indium Sulfide Nanoparticles and Nanodisks

Copper indium sulfide ($CuInS_2$) nanocrystals (NCs) are nontoxic and inexpensive, making them attractive for use in high-efficiency solar cells. However, direct observations of the photo-induced carrier dynamics of $CuInS_2$ NCs to examine the relationship between carrier dynamics and structural parameters, with the aim of optimizing NC properties for specific applications, are limited. Here, we synthesized nearly stoichiometric oleylamine-protected $CuInS_2$ NCs using two convenient one-pot methods to produce $CuInS_2$ nanoparticles and nanodisks. Transient absorption measurements using femtosecond laser flash photolysis revealed that the use of oleylamine as a protecting ligand leads to the formation of vacancy-doped NCs. The rapid decay of the photogenerated excitons in the oleylamine-protected NCs was not sensitive to the crystal structure or shape of NCs, and could be explained by defect trapping and energy transfer to the hole-based localized surface plasmon resonance in the oleylamine-protected NCs. Our results confirm that careful selection of a protecting ligand is important to obtain $CuInS_2$ NCs with optimized properties for specific applications.

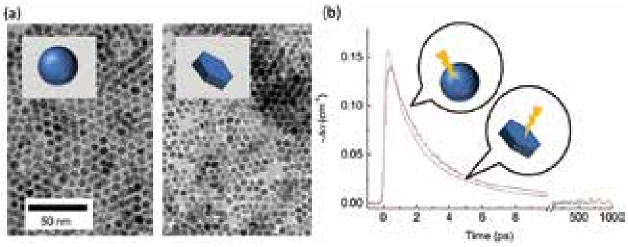


Figure 1. TEM images (a) and decay profile of photogenerated excitons in the $CuInS_2$ nanoparticles and nanodisks (b).

Simple Surfactant Concentration–Dependent Shape Control of Polyhedral Fe_3O_4 Nanoparticles and Their Magnetic Properties

Magnetite (Fe_3O_4) is one of the most studied magnetic nanoparticle (NP) materials, with uses in magnetic resonance imaging (MRI), drug delivery, biosensors, magnetic separation, and medical diagnostics. Characteristic magnetic features of Fe_3O_4 NPs depend strongly on their shape and size because of shape- and size-determined differences in surface states such as exposed crystal planes and specific surface area of NPs. In this study, we developed a facile solution approach to synthesize a series of polyhedral Fe_3O_4 NPs with sizes between 20 and 200 nm using cetylpyridinium chloride (CPC) and oleic acid (OAc) as surfactants. The concentrations of CPC and OAc in the reaction solution play an essential role in the shape and size evolution. The shape of Fe_3O_4 NPs is tuned simply by the amount of CPC. Cubic Fe_3O_4 NPs surrounded by six {100} planes are obtained in the absence of CPC. Increasing the CPC content during synthesis causes the shape of the resulting Fe_3O_4 NPs to change from cubic to truncated cubic, cuboctahedral, truncated octahedral, and finally octahedral. During this evolution, the predominantly exposed planes of the Fe_3O_4 NPs vary from {100} to {111}. The shape control results from the synergistic effect of the chloride anions, pyridinium cations, and long-chain alkyl groups of CPC. The size of the cubic Fe_3O_4 NPs can also be tuned from 50 to 200 nm by changing the concentration of OAc. These polyhedral Fe_3O_4 NPs clearly exhibit shape- and size-dependent magnetic properties, including saturation magnetization, remanent magnetization, and coercivity.

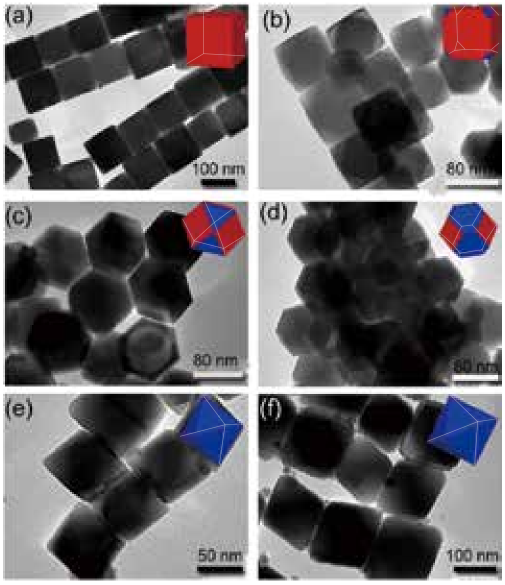


Figure 2. TEM images of (a) cubic, (b) truncated cubic, (c) cuboctahedral, (d) truncated octahedral, and (e,f) octahedral Fe_3O_4 NPs synthesized by varying only the amount of CPC. Insets show the {100} and {111} planes in red and blue, respectively.

Division of Materials Chemistry
– Chemistry of Polymer Materials –

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

Prof
TSUJII, Yoshinobu
(D Eng)

Assoc Prof
OHNO, Kohji
(D Eng)

Assist Prof
SAKAKIBARA, Keita
(D Agr)

PD
BAEK, Sung Chul
(Ph D)

Assist Techn Staffs

NAKANISHI, Yohei
TANISHIMA, Miho

Researchers(pt)

HSU, Shu-Yao
NAKAMICHI, Kimiyo
MORIKI, Yoshito
SAKAUE, Motokazu
NAKAJIMA, Yuuki
SEO, Haruna

Students

YAHATA, Yoshikazu (D3)
KINOSE, Yuji (D1)
SHIMIZU, Yoshihiko (D1)
NOGAMI, Naotsugu (M2)
MASUDA, Shota (M2)
WADA, Ryota (M2)
EGI, Kohki (M1)
YAMASHITA, Kohei (M1)
YASUDA, Shuma (M1)
ZHAO, Chenzhou (M1)
FUJIMORI, Tomoya (UG)
HISATOMI, Tatsuya (UG)
NISHIUMI, Kosuke (UG)

Scope of Research

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

KEYWORDS
Precision Polymerization
Living Radical Polymerization
Polymer Brush
Hybrid Materials
Biointerface

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).

Synthesis of Iron Oxide Rods Coated with Polymer Brushes and Control of Their Assembly in Thin Films

We investigated surface-initiated atom transfer radical polymerization (SI-ATRP) of methyl methacrylate (MMA) using monodisperse rod-type particles of iron oxide, β-FeOOH. The slow hydrolysis of iron(III) chloride yielded monodisperse β-FeOOH rods with an average length-to-width ratio, L/W, of 6 ($L = 210$ nm and $W = 35$ nm on average). The surface of the β-FeOOH rods was modified with a triethoxysilane derivative as an ATRP-initiating site, namely, (2-bromo-2-methyl)propionyloxypropyl triethoxysilane. The SI-ATRP of MMA, mediated by a copper complex, was performed using the initiator-coated β-FeOOH rods in the presence of a sacrificial free initiator. Well-defined poly(methyl methacrylate) (PMMA) brushes with molecular weights of up to 700,000 could be grafted on the β-FeOOH rods with a surface density as high as 0.3 chains/nm^2. The resultant polymer-brush afforded hybrid rods exhibited high dispersibility in various solvents for PMMA without forming aggregates. Thin films were prepared by dip-coating from a suspension of the hybrid rods and the rods were oriented in a specific direction in the films. The arrangement of the rods could be controlled by varying the chain length of the polymer brush and the withdrawal speed during the dip-coating process.

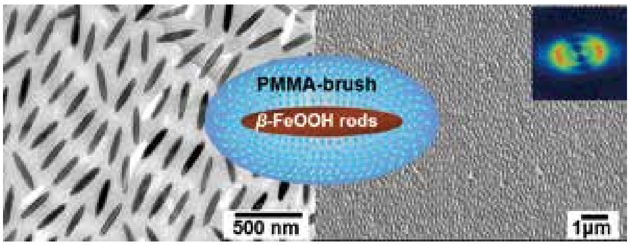


Figure 1. Transmission and scanning electron microscopy images of films of β-FeOOH rods end-grafted with PMMA.

Preparation of Polymer Monolith Materials by Using Block Copolymer Surfactants

The use of block copolymer-based surfactants has been proposed as a methodology for creation of various polymeric monolith materials, where monolith means bi-continuous skeletal and pore space with meso-/macroporous sizes. For example, freestanding epoxy-based monolith membranes have been developed through polymerization induced phase separation based on the spinodal decomposition with an assist of a PVA sacrifice film. The membranes are 10–20 μm thick and a few centimeters on each side (Figure 2a), which could be applied for heat resistant separators of lithium ion secondary batteries. To improve their mechanical properties, cellulose nanofibers (CNFs) were introduced as a reinforcement filler, leading Young's modulus to be about 1.3 times higher than that of a neat monolith membrane. In addition, by using suitable block copolymers as a surfactant, the modulus increase was about twice higher than for a neat monolith, because the interfacial strength between monolith and CNFs was strong. Another example showed that block copolymer–stabilized emulsion could be used for the preparation of polymer monolith particles without a surface skin layer (Figure 2b). The composition of the block copolymer was crucial for the formation of skin on the surface, as well as the size of particles, interpreted by the interfacial tension parameter. These particles are promising for separation materials with application in chromatography, water purification, and adsorption of toxic substances.

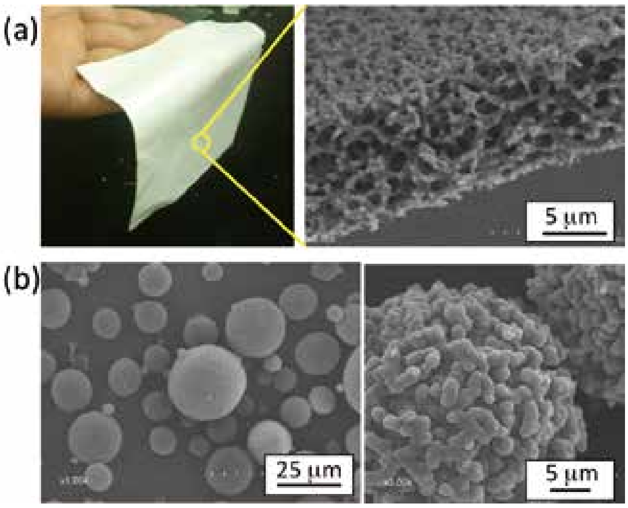


Figure 2. SEM images of polymer monolith materials in the form of (a) a sheet and (b) particles without a surface skin layer.

Division of Materials Chemistry
– Polymer Controlled Synthesis –

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


Prof
YAMAGO, Shigeru
(D Sc)


Assoc Prof
TOSAKA, Masatoshi
(D Eng)


Program-Specific Assoc Prof
NAKAMURA, Yasuyuki
(D Sc)


Assist Prof
KAYAHARA, Eiichi
(D Eng)


Program-Specific Assist Prof
HASHIMOTO, Sigma
(D Eng)


Program-Specific Res
SUGIHARA, Yusuke
(D Eng)


PD
PATEL, Vijay Kumar
(D Sc)


PD
YU, Mengmeng
(D Sc)


PD
LI, Wenjuan
(D Sc)

Researcher(pt)

NISHINO, Hideo (D Eng)

Students

FUJITA, Takehiro (D3)
LU, Yangtian (D1)
SUN, Liansheng (D1)
NOGUCHI, Naoki (M2)
OHNISHI, Hiroaki (M2)
OGIHARA, Tasuku (M2)
KONO, Taro (M2)
FAN, Weijia (M2)
QU, Rui (M2)
HUA SHEN, Zhiren (M1)
SEKI, Toyomitsu (M1)
TSUKIMI, Ryosuke (M1)
Li, Xiaopei (RS)
UEMURA, Seigo (UG)
KAISE, Misaki (UG)
KATOH, Masakazu (UG)
MIYOSHI, Shunichiro (UG)

Scope of Research

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

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

Selected Publications

Nakamura, Y.; Yamago, S., Termination Mechanism in the Radical Polymerization of Methyl Methacrylate and Styrene Determined by the Reaction of Structurally Well-defined Polymer End Radicals, *Macromolecules*, **48,** 6450-6456 (2015).
Patel, V. K.; Kayahara, E.; Yamago, S., Practical Synthesis for [*n*]Cycloparaphenylenes (n = 5, 7-12) by H_2SnCl_4-Mediated Aromatization of 1,4-Dihydroxylcyclo-2,5-diene Precursors, *Chem. Eur. J.*, **21,** 5742-5749 (2015).
Toriumi, N.; Muranaka, A.; Kayahara, E.; Yamago, S.; Uchiyama, M., In-Plane Aromaticity in Cycloparaphenylene Dications: A Magnetic Circular Dichroism and Theoretical Study, *J. Am. Chem. Soc.*, **137,** 82-85 (2015).
Sugihara, Y.; Yamago, S.; Zetterlund, P., An Innovative Approach to Implementation of Organotellurium-Mediated Radical Polymerization (TERP) in Emulsion Polymerization, *Macromolecules*, **48,** 4312-4318 (2015).
Gros, A.; Tosaka, M.; Huneau, B.; Verron, E.; Poompradub, S.; Senoo, K., Dominating Factor of Strain-induced Crystallization in Natural Rubber, *Polymer*, **76,** 230-236 (2015).

Topics

Modular Synthesis of Mid-Chain-Functionalized Polymers by Photoinduced Diene- and Styrene-Assisted Radical Coupling Reaction of Polymer-End Radicals

An array of precisely located functional groups in natural macromolecules, such as nucleotides and proteins, plays a pivotal role in their well-defined three-dimensional structure and numerous functions. Therefore, controlling the position and number of reactive functional groups in a structurally well-defined synthetic polymer has been an important challenge in order to create novel functional polymer materials with enhanced or new properties. Photo-irradiation of structurally well-defined "living" polymers prepared by organotellurium-mediated living radical polymerization in the presence of dienes or styrenes induced selective polymerend coupling reaction with the concomitant insertion of the dienes or styrenes with >90% coupling efficiency. The number of inserted dienes or styrenes could be highly controlled to two molecules when acrylic polymers were used. Therefore, various mid-chain-functionalized polymers with well-controlled molecular and macromolecular structure in terms of their molecular weight, molecular weight distribution, functionality, and position were successfully synthesized by employing functionalized dienes or styrenes. The method was applied to the facile synthesis of mid-chain-functionalized telechelic polymers and a 4-miktoarm star polymer with a well-controlled structure.

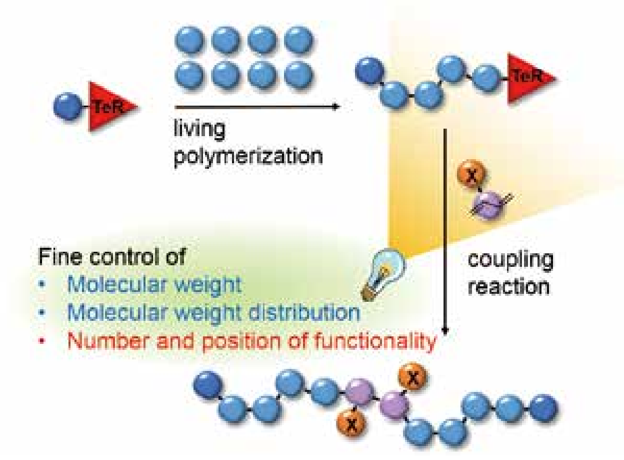


Figure 1. Novel synthetic strategy for mid-chain-functionalized polymers.

Practical Synthesis of [*n*]Cycloparaphenylenes (*n* = 5, 7–12) by H_2SnCl_4-mediated Aromatization of 1,4-Dihydroxycyclo-2,5-diene Precursors

Cyclic precursors of cycloparaphenylenes (CPPs) containing 1,4-dihydroxy-2,5-cyclohexadien-1,4-diyl units were prepared by modifying the synthesis method of corresponding 1,4-dimethoxy derivatives, which was developed by Jasti and co-workers. Reductive aromatization of the diyl moieties by $SnCl_2/2\,HCl$ took place under mild conditions and afforded CPPs incorporating 5 or 7–12 phenylene units with good yield. Highly strained [5]CPP was synthesized at more than 0.3 g. ^{119}Sn NMR spectroscopy clarified the *in situ* formation of an ate complex, H_2SnCl_4, upon mixing a 2:1 ratio of HCl and $SnCl_2$, which serves as a highly active reducing agent under nearly neutral conditions. When more than two equivalents of HCl, in relation to $SnCl_2$, were used, acid-catalyzed decomposition of the CPP precursors took place. The stoichiometry of HCl and $SnCl_2$ was found to be critical in achieving the desired aromatization reaction of highly strained CPP precursors.

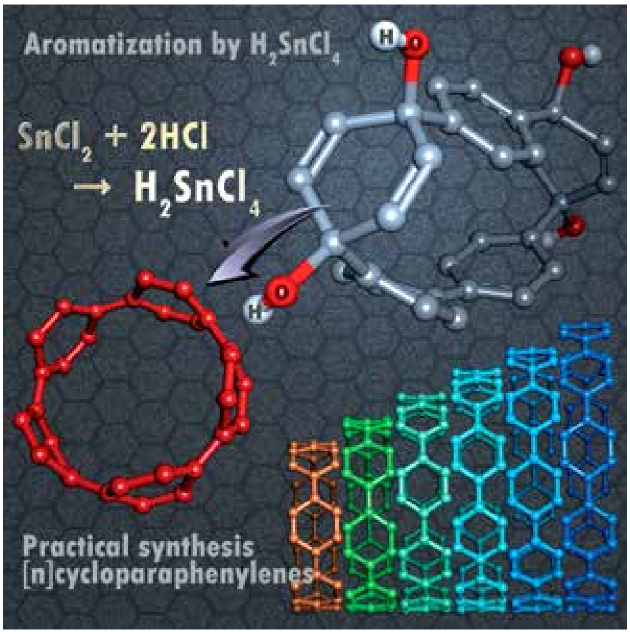


Figure 2. Synthesis of [*n*]Cycloparaphenylenes (*n* = 5, 7–12)

Division of Materials Chemistry
– Inorganic Photonics Materials –

http://mizuochilab.kuicr.kyoto-u.ac.jp/websites/

Assoc Prof
TOKUDA, Yomei
(D Eng)

Assist Prof
MASAI, Hirokazu
(D Eng)

Students

UEDA, Yuki (M2)
USUI, Takaaki (M2)
TAKAHASHI, Yuya (M1)
KANEKO, Shunichi (M1)
TORIMOTO, Aya (M1)
DANJO, Takuya (UG)

Scope of Research

In this laboratory, the main subject is to create novel functional amorphous materials, such as organic–inorganic hybrids, polycrystalline, and amorphous inorganic oxides. The amorphous structure and its properties are investigated by XRD, MAS NMR, thermal and optical analysis, and quantum chemical calculations. Currently, we are trying to prepare novel amorphous-based optical functional materials such as a proton conducting membrane, optical biosensor, and amorphous phosphor.

KEYWORDS

Organic-inorganic Hybrid
Oxide Glass
Solid State NMR
Photoluminescence

Selected Publications

Tokuda, Y.; Takahashi, Y.; Masai, M.; Kaneko, S.; Ueda, Y.; Fujimura, S.; Yoko, T., Local Structure of Alkalis in Mixed Alkali Borate Glass to Elucidate the Origin of Mixed-alkali Effect, *J. Asian Ceram. Soc.*, 10.1016/j.jascer.2015.09.002 (2015).

Tokuda, Y.; Norikawa, Y.; Masai, H.; Ueda, Y.; Nihei, N.; Fujimura, S.; Ono, Y., Nuclear Magnetic Resonance Study of Cs Adsorption onto Clay Minerals, *Radiological Issues for Fukushima's Revitalized Future*, *Springer*, 79-88 (2015).

Masai, H.; Yamada, Y.; Okumura, S.; Yanagida, T.; Fujimoto, Y.; Kanemitsu, Y.; Ina, T., Photoluminescence of Monovalent Indium Centres in Phosphate Glass, *Scientific Reports*, **5,** 13646 (2015).

Masai, H.; Yanagida, T.; Mizoguchi, T.; Ina, T.; Miyazaki, T.; Kawaguti, N.; Fukuda, K., Local Coordination State of Rare Earth in Eutectic Scintillators for Neutron Detector Applications, *Scientific Reports*, **5,** 13332 (2015).

Masai, H.; Miyata, H.; Yamada, Y.; Okumura, S.; Yanagida, T.; Kanemitsu, Y., Tin-Doped Inorganic Amorphous Films for Use as Transparent Monolithic Phosphors, *Scientific Reports*, **5,** 11224 (2015).

Structural Analysis of Alkali Cations in Silicate Glasses

Structural analysis of alkali ions in glass is an important topic in glass science because of the mixed alkali effect (MAE) that arises when the composition of a glass is altered by gradual substitution of one alkali for another. More specifically, the MAE is characterized by the deviation from the linear additive properties of alkali silicate glasses, which can be attributed to structural, thermodynamic, and electrodynamic factors, among others.

Recently, we investigated the heterogeneous distribution of Na_+ in mixed alkali silicate glasses (Na_2O–K_2O–SiO_2 glass) by performing $_{23}Na$ multiple-quantum magic-angle spinning (MQMAS) nuclear magnetic resonance (NMR) studies. The results were also supported by Na_+ elution analysis, which showed that Na_+ is extracted faster from more aggregated sites than from less aggregated sites. Nevertheless, in the previous study, the local structure of K_+ in Na_2O–K_2O–SiO_2 glass could not be investigated, as the $_{39}K$ sensitivity of NMR is extremely low. In order to understand the precise mechanisms underlying the MAE, analyses of the local structure of both alkali ions are required.

Here, we report structural analysis of Na_+ and Cs_+ in sodium cesium silicate glass by using $_{23}Na$ and $_{133}Cs$ magic-angle spinning (MAS) NMR spectroscopy. In the NMR spectra of cesium silicate crystals, the peak position shifted to a higher magnetic field for structures with larger Cs_+ coordination numbers and to lower magnetic field for smaller Cs_+ coordination numbers. The MAS NMR spectra of xNa_2O–yCs_2O–$2SiO_2$ ($x = 0, 0.2, 0.33, 0.5, 0.66, 0.8$, and 1.0; $x+y = 1$) glass reveal that the average coordination number of both alkali cations decreases with an increasing $Cs_+/(Na_++Cs_+)$ ratio. In addition, the coordination number of Na+ in xNa_2O–yCs_2O–$2SiO_2$ glass is smaller than that of Cs+. This difference between the average coordination numbers of the alkali cations is considered to be one structural reason for the mixed alkali effect.

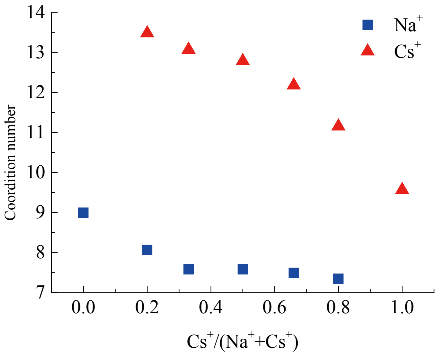


Figure 1. Average coordination numbers of Na^+, Cs^+ in xNa_2O–yCs_2O–$2SiO_2$ glasses ($x = 1.0, 0.8, 0.66, 0.5, 0.33$, and 0.2; $x+y = 1$).

Oxide Glasses: The Structure, Physical Property, and Functionalization

Glass is a solidified liquid that can possess characteristics of both solid and liquid. Although glass is an isotropic material from macroscopic viewpoint, it is indeed anisotropic in terms of microscopic scale. Various compositions of inorganic glasses have random networks that allow diversity in local structure. This diversity is the origin of various functionalities of inorganic glass.

Emitting solid-state matter is one of the main applications of transparent amorphous materials. Since oxide glass consists of a random network structure, metastable species can be introduced easily, compared with ordered crystals. We have recently focused on the ns^2-type emission center as an activator in amorphous materials. The emission centers take the metastable valence state of each element, and their emissions are strongly affected by the coordination field because of the electrons in the outermost shell. However, there is no detailed understanding of the dispersion and energy diagram in oxide glasses, although it is expected that the random networks of the glasses have strong influence on the emission property of the ns^2-type emission centers.

Recently, we have reported the highest quantum efficiency (QE) for amorphous Sn^{2+}-doped ZnO–P_2O_5 glass (Figure 2a). In addition, photoluminescence of the metastable In^+ centers (non-conventional ns^2-type center) is demonstrated (Figure 2b). On the other hand, the photoluminescence of the Sn^{2+} center can be demonstrated in amorphous film prepared by a liquid phase reaction (Figure 2c and 2d). It is notable that an energy transfer from Sn^{2+} (donor) to Mn^{2+} (acceptor) is observed even in the film shape (Figure 2d). Because some glasses show luminescence with a high value of quantum efficiency comparable to crystalline phosphor, RE-free glass phosphor is a fascinating material from the viewpoint of unique emission mechanisms in a random matrix.

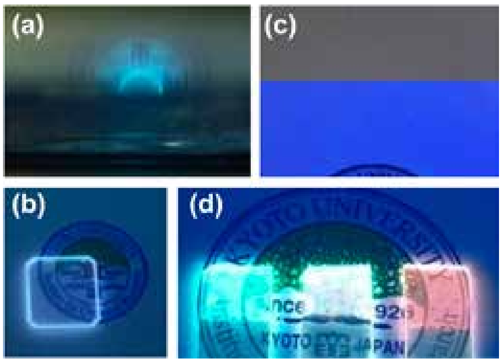


Figure 2. Amorphous materials containing ns^2-type emission centers. (a) Sn^{2+}-doped bulk glass, (b) In^+-doped bulk glass, and (c), (d) Sn^{2+}-doped films. The emission color of the film can be controlled by co-doping of Mn^{2+} cations.

Division of Materials Chemistry
– Nanospintronics –

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


Prof
ONO, Teruo
(D Sc)


Assist Prof
MORIYAMA, Takahiro
(Ph D)


Assist Prof
KIM, Kab-Jin
(D Sc)


Techn Staff *
KUSUDA, Toshiyuki


PD
KIM, Sanghoon
(Ph D)

*Re-employed Staff


PD
FUJIMOTO, Junji
(D Sc)

Lect (pt)

NAKAMURA, Kohji (D Sc) Mie University

Students

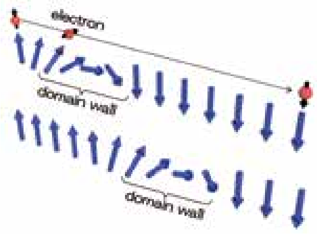
KAWAGUCHI, Masashi (D3)
YOSHIMURA, Yoko (D3)
KAKIZAKAI, Haruka (D2)
YAMADA, Kihiro (D2)
TANAKA, Kensho (D1)
TANIGUCHI, Takuya (D1)
KAMIYA, Michinari (D1)
MATSUZAKI, Noriko (M2)
MIZUNO, Hayato (M2)
TONO, Takayuki (M2)
ANDO, Fuyuki (M1)
OKUNO, Takaya (M1)
ODA, Kento (M1)

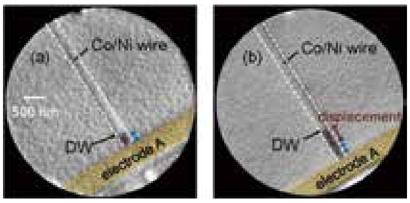
Scope of Research

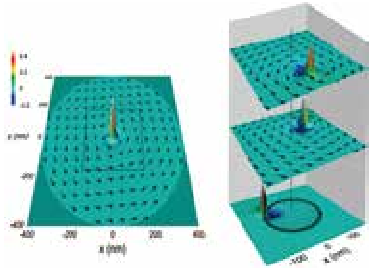
Conventional electronics uses only the charge of electrons, while traditional magnetic devices use only the spin degree of freedom of electrons. Aiming at complete control of both charge and spin in single solid-state devices, an emerging field called spintronics is rapidly developing and having an impact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

KEYWORDS

Spintronics
Quantum Transport
Nano-fabrication
Artificial Materials







Selected Publications

Moriyama, T.; Takei, S.; Nagata, M.; Yoshimura, Y.; Matsuzaki, N.; Terashima, T.; Tserkovnyak, Y.; Ono, T., Anti-damping Spin Transfer Torque through Epitaxial Nickel Oxide, *Appl. Phys. Lett.*, **106,** [162406-1]-[162406-4] (2015).

Yoshimura, Y.; Kim, K.-J.; Taniguchi, T.; Tono, T.; Ueda, K.; Hiramatsu, R.; Moriyama, T.; Yamada, K.; Nakatani, Y.; Ono, T., Soliton-like Magnetic Domain Wall Motion Induced by the Interfacial Dzyaloshinskii–Moriya Interaction, *Nat. Phys.*, doi:10.1038/nphys3535 (2015)(in press).

Matsuo, S.; Takeshita, S.; Tanaka, T.; Nakaharai, S.; Tsukagoshi, K.; Moriyama, T.; Ono, T.; Kobayashi, K., Edge Mixing Dynamics in Graphene p–n Junctions in the Quantum Hall Regime, *Nat. Commun.*, **6,** [8066-1]-[8066-6] (2015).

Tanabe, K.; Matsumoto, R.; Ohe, J.; Murakami, S.; Moriyama, T.; Chiba, D.; Kobayashi, K.; Ono, T., Real-time Observation of Snell's Law for Spin Waves in Thin Ferromagnetic Films, *Applied Physics Express*, **7,** [053001-1]-[053001-4] (2014).

Chiba, D.; Fukami, S.; Shimamura, K.; Ishiwata, N.; Kobayashi, K.; Ono, T., Electrical Control of the Ferromagnetic Phase Transition in Cobalt at Room Temperature, *Nature Materials*, **10,** 853-856 (2011).

Soliton-like Magnetic Domain Wall Motion Induced by the Interfacial Dzyaloshinskii-Moriya Interaction

Topological spin structures such as magnetic domain walls (DWs), vortices, and skyrmions often appear in magnetic materials. Since the stability of spin structure is strongly protected by its topological nature, such topological objects can be exploited in the production of memory devices. Recently, a novel type of antisymmetric exchange interaction, namely Dzyaloshinskii-Moriya interaction (DMI), has been uncovered and found to influence the formation of topological objects. Exploring how DMI affects the dynamics of topological objects is therefore an important task. Here we investigate experimentally the dynamics of the magnetic DW under DMI and found that DMI boosts DW velocity. Furthermore, enhanced DW velocity is maintained at a constant for a wide range of magnetic fields. Such distinct behavior of DW velocity can be explained in terms of a magnetic soliton with its topology protected during its motion. Our results therefore shed light on the physics of dynamic topological objects, paving the way for future work in topology-based memory applications.

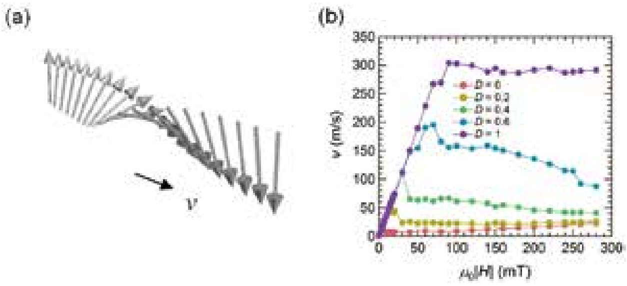


Figure 1. Magnetic soliton and its velocity. (a) Topologically protected magnetic soliton spin structure. (b) Magnetic soliton velocity *v* as a function of magnetic field $\mu_0 H$. Different colors correspond to different strengths of the Dzyaloshinskii-Moriya interaction *D* as denoted in the legend. The units of *D* are mJ/m^2.

Anti-damping Spin Transfer Torque through Antiferromagnetic Material

Spin transfer torque (STT) has been an efficient and promising technique to control magnetization of ferromagnetic materials in modern spintronic devices. This novel technique is based on an interaction between electron spin and local magnetic moments. The same interaction should be conserved in antiferromagnets in which there are microscopic local magnetic moments that compensate each other to exhibit no net magnetization. In this work, we prepared MgO(001) substrate / Pt 5nm / NiO 10nm / FeNi 3nm / SiO2 5nm multilayers, in which the films are epitaxially grown until the NiO layer, and performed a spin torque ferromagnetic resonance (ST-FMR) measurement to quantify the anti-damping spin torque transported between the Pt and the FeNi through the antiferromagnetic NiO layer. A pure spin current is created by the spin Hall effect of the Pt and injected into the NiO. As shown in Figure 2(a), we found that the FMR linewidth monotonously varies with the spin current injection. As the ST-FMR measurement is only sensitive to the linewidth (i.e., magnetic damping) of the FeNi layer, this change in the linewidth in Pt/NiO/FeNi can be interpreted in a way that the spin current is transferred through the NiO and interacts with the FeNi. This intriguing spin current transport can be explained by the angular-momentum transfer mediated by the antiferromagnetic magnons as shown in Figure 2(b). Our results assure that the spin current exerts a spin torque on the NiO magnetic moments and excites their dynamics. The results open up a new field of antiferromagnetic spintronics.

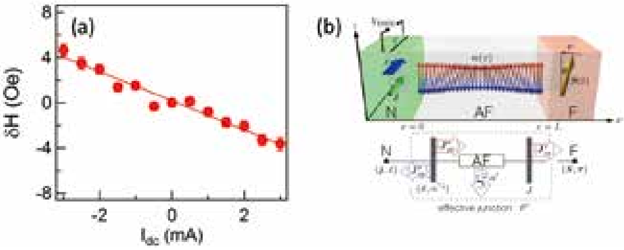


Figure 2. (a) FMR linewidth δH as a function of the dc current. Due to the spin Hall effect of Pt, the spin current injection is proportional to the dc current. (b) Schematic illustration of the N (Pt) / AF (NiO) / F (FeNi) structure in which the anti-damping spin transfer torque takes place. N (Pt) layer injects the spin current J^s_{stt} toward AF (NiO). The antiferromagnetic magnon in AF (NiO) carries the spin current J^s_{ex} toward F (FeNi).

Division of Biochemistry
– Biofunctional Design-Chemistry –

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


Prof
FUTAKI, Shiroh
(D Pharm Sc)


Senior Lect
IMANISHI, Miki
(D Pharm Sc)


Assist Prof
TAKEUCHI, Toshihide
(D Pharm Sc)


Program-Specific Res
NAKANO, Yukiko
(D Sc)

Students

KAWAGUCHI, Yoshimasa (D3)
OKU, Akihiko (D3)
MURAYAMA, Tomo (D2)
TSUJI, Shogo (D2)
AKISHIBA, Misao (M2)
SASAKI, Yuichiro (M2)
SHINODA, Kouki (M2)
ARAFILES, Jan Vincent (M1)
IINO, Masatomo (M1)
ISE, Shoko (M1)
MASUDA, Toshihiro (M1)
TAKAGI, Shun (M1)
WATANABE, Kensuke (M1)
HAYASHI, Syuhei (UG)
NOMURA, Kayo (UG)
SAKAMOTO, Kentaro (UG)

Scope of Research

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

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

Selected Publications

Takeuchi, T.; Suzuki, M.; Fujikake, N.; Popiel, H. A.; Kikuchi, H.; Futaki, S.; Wada, K.; Nagai, Y., Intercellular Chaperone Transmission via Exosomes Contributes to Maintenance of Protein Homeostasis at the Organismal Level. *Proc. Natl. Acad. Sci. U.S.A.*, **112,** E2497-E2509 (2015).
Azuma, Y.; Kükenshöner, T.; Ma, G.; Yasunaga, J.; Imanishi, M.; Tanaka, G.; Nakase, I.; Maruno, T.; Kobayashi, Y.; Arndt, K. M.; Matsuoka, M.; Futaki, S., Controlling Leucine-Zipper Partner Recognition in Cells through Modification of a-g Interactions, *Chem. Commun.*, **50,** 6364-6367 (2014).
Tsuji, S.; Futaki, S.; Imanishi, M., Creating a TALE Protein with Unbiased 5’-T Binding, *Biochem. Biophys. Res. Commun.*, **441,** 262-265 (2013).
Pujals, S.; Miyamae, H.; Afonin, S.; Murayama, T.; Hirose, H.; Nakase, I.; Taniuchi, K.; Umeda, M.; Sakamoto, K.; Ulrich, A. S.; Futaki, S., Curvature Engineering: Positive Membrane Curvature Induced by Epsin N-Terminal Peptide Boosts Internalization of Octaarginine, *ACS Chem. Biol.*, **8,** 1894-1899 (2013).
Futaki, S.; Noshiro, D.; Kiwada, T.; Asami, K., Extramembrane Control of Ion Channel Peptide Assemblies, Using Alamethicin as an Example, *Acc. Chem. Res.,* **46,** 2924-2933 (2013).

Topics

Intercellular Chaperone Transmission via Exosomes Contributes to Maintenance of Organismal Protein Homeostasis

Heat shock response (HSR) is a protective system necessary for cell survival in a stressful environment, to maintain protein homeostasis (proteostasis). Recent studies, however, have indicated that HSR is not ubiquitous at the organismal level, but depends highly on the cell types. Despite such imbalanced HSR upon stress, it is unclear as to how organismal proteostasis is maintained. We addressed this issue by analyzing cell culture and *Drosophila* models that mimic the imbalanced state of HSR by expressing molecular chaperones in limited groups of cells. We found that increased expression of molecular chaperones such as Hsp70 and Hsp40 in a group of cells improves proteostasis in other groups of cells in a cell-nonautonomous manner. We also found that exosome-mediated secretion and intercellular transmission of molecular chaperones are crucial for this cell-nonautonomous improvement of proteostasis. Our study reveals a novel cell-nonautonomous mechanism for organismal proteostasis that relies on cell-to-cell communication of molecular chaperones via exosomes, which could functionally compensate the imbalanced HSR between cells and tissues.

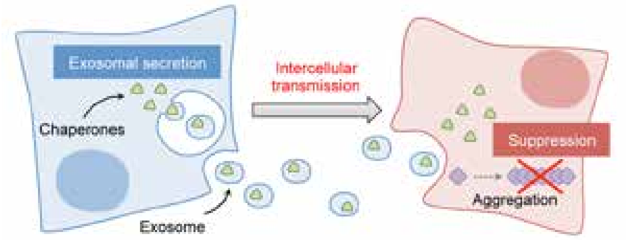


Figure 1. Molecular chaperones are secreted via exosomes and transmitted to the other cells, where they show chaperoning activity.

Effects of Amino Acid Substitution in the Hydrophobic Face of N-terminal Helix of Adenovirus Internal Protein VI on the Membrane Perturbation

Amphiphilic helices in membrane-interacting peptides and proteins often play crucial roles in their bioactivities. Understanding the roles of each amino acid in helical structural formation and membrane interaction is important since the functions of these peptides can be decided by the amino acid composition. We used the N-terminal helical segment of adenovirus internal protein VI positions 33–55 (WT) as a model amphipathic peptide to study the roles of hydrophobic amino acids. The leucine residue at position 40 has been suggested to be critical for viral infectious activity. The phenylalanine-substituted peptide (L40F) yielded less helicity on membrane binding and showed a shallower membrane-bound structure than WT. However, the liposomal leakage assay indicated that WT and L40F had similar degrees of membrane perturbation activity. Both peptides could induce positive membrane curvature and possessed higher affinities to membranes with high curvature, but no apparent curvature-sensitive membrane perturbation was observed.

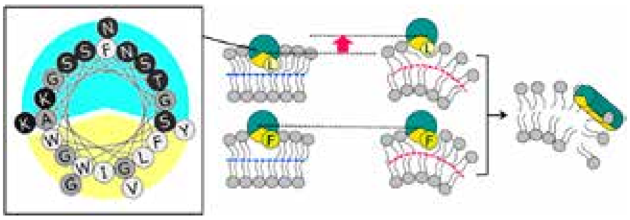


Figure 2. Helical wheel projection of N-terminal segment of adenovirus internal protein VI (left). WT and L40F peptide may have different membrane-bound states but the same extent of membrane perturbation activity (right).

Division of Biochemistry
– Chemistry of Molecular Biocatalysts –

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

Prof
HIRATAKE, Jun
(D Agr)

Assist Prof
WATANABE, Bunta
(D Agr)

Students

AKASHI, Takuya (M2)
KURODA, Kou (M2)
YIN, Ziewi (M2)

ITO, Shota (M1)
SAITO, Shingo (M1)
NAESHIRO, Kazuki (M1)

LI, Xian (M1)

Scope of Research

Our research focuses on the molecular design and synthesis of specific inhibitors of physiologically important enzymes (biocatalysts). Enzyme inhibitors are used for probing reaction mechanisms, three-dimensional structures, and identifying the physiological roles of the enzymes. Finely designed inhibitors are further elaborated to develop useful bioactive substances that could knock out specific enzymes *in vivo* to develop lead compounds for novel pharmaceuticals, agrochemicals, and cosmetic ingredients. Our current research includes the design, synthesis, and application of transition-state analogues and/or mechanism-based inhibitors of such enzymes as γ-glutamyl transpeptidase, a key enzyme in glutathione metabolism; asparagine synthetase, an important enzyme for cancer chemotherapy; and 4-coumaroyl CoA ligase, which plays a pivotal role in the biosynthesis of a vast array of phenylpropanoids in plants. The identification of the genes of hitherto unknown enzymes for biosynthesis of phenylpropanoid volatiles in plants are also pursued to shed light on the detailed reaction mechanisms and physiological functions of the biosynthetic enzymes for plant secondary metabolites.

KEYWORDS

Enzyme Reaction Mechanisms
Transition-State Analogue Inhibitors
Mechanism-Based Enzyme Inhibitors
Glutathione Homeostasis
Bioactive Substance

Selected Publications

Tuzova, M.; Jean, J.-C.; Hughey, R. P.; Brown, L. A. S.; Cruikshank, W. W.; Hiratake, J.; Joyce-Brady, M., Inhibiting Lung Lining Fluid Glutathione Metabolism with GGsTop as a Novel Treatment for Asthma, *Front. Pharmacol*, **5,** 1-8 (2014).

Saino, H.; Shimizu, T.; Hiratake, J.; Nakatsu, T.; Kato, H.; Sakata, K.; Mizutani, M., Crystal Structures of β-Primeverosidase in Complex with Disaccharide Amidine Inhibitors, *J. Biol. Chem.*, **289,** 16826-16834 (2014).

Nakajima, M.; Watanabe, B.; Han, L.; Shimizu, B.; Wada, K.; Fukuyama, K.; Suzuki, H.; Hiratake, J., Glutathione-Analogous Peptidyl Phosphorus Esters as Mechanism-Based Inhibitors of γ-Glutamyl Transpeptidase for Probing Cysteinyl-Glycine Binding Site, *Bioorg. Med. Chem.*, **22,** 1176-1194 (2014).

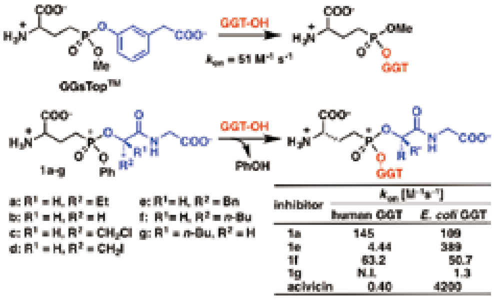
Kodan, A.; Yamaguchi, T.; Nakatsu, T.; Sakiyama, K.; Hipolito, C. J.; Fujioka, A.; Hirokane, R.; Ikeguchi, K.; Watanabe, B.; Hiratake, J.; Kimura, Y.; Suga, H.; Ueda, K.; Kato, H., Structural Basis for Gating Mechanisms of a Eukaryotic P-Glycoprotein Homolog, *Proc. Natl. Acad. Sci. U.S.A.*, **111,** 4049-4054 (2014).

Koeduka, T.; Sugimoto, K.; Watanabe, B.; Someya, N.; Kawanishi, D.; Gotoh, T.; Ozawa, R.; Takabayashi, J.; Matsui, K.; Hiratake, J., Bioactivity of Natural *O*-Prenylated Phenylpropenes from *Illicium anisatum* Leaves and Their Derivatives Against Spider Mites and Fungal Pathogens, *Plant Biol.*, **16,** 451-456 (2013).

Development and Applications of Specific Inhibitors of γ-Glutamyl Transpeptidase, a Key Enzyme in Glutathione Metabolism

Glutathione (GSH, γ-Glu–Cys–Gly) is a ubiquitous redox active tripeptide containing Cys and plays central roles in detoxification of reactive oxygen species (ROS) and toxic xenobiotics, in the front line of the cellular defense system. γ-Glutamyl transpeptidase (GGT) is a key enzyme in GSH metabolism that catalyzes the cleavage of γ-glutamyl peptide bond of extracellular GSH to supply cells with Cys, a rate-limiting substrate for intracellular GSH biosynthesis. Hence, GGT is implicated in many physiological disorders such as drug resistance of cancer cells, cardiovascular diseases and asthma. We have developed a mechanism-based inhibitor, named GGsTop™, that was a highly specific and non-toxic inhibitor of GGT. A series of phosphonate-based GGT inhibitors with a peptidyl side chain have also been synthesized for evaluation as inhibitors of human and *E. coli* GGTs to probe the Cys–Gly binding site (Figure 1).

Interestingly, GGsTop™, a highly efficient inhibitor of human GGT, induces the cellular anti-oxidative stress response. As a result, this compound exhibited interesting biological activities, such as increasing the biosynthesis of type I collagen, elastin, and HSP47 of human dermal fibroblasts (Figure 2). These properties, along with its non-toxic nature, allowed GGsTop™ to serve as a novel active ingredient for anti-ageing cosmetics. This compound is now marketed under the trade name Nahlsgen® and has attracted significant interest from the cosmetic market.



inhibitor	k_{on} [M⁻¹s⁻¹]	
	human GGT	*E. coli* GGT
1a	145	109
1e	4.44	389
1f	63.2	50.7
1g	N.I.	1.3
acivicin	0.40	4200

Figure 1. Mechanism-based inhibition of GGT by GGsTop™ and peptidyl phosphonate inhibitors **1a–g**.

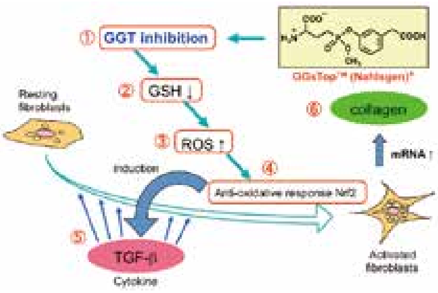
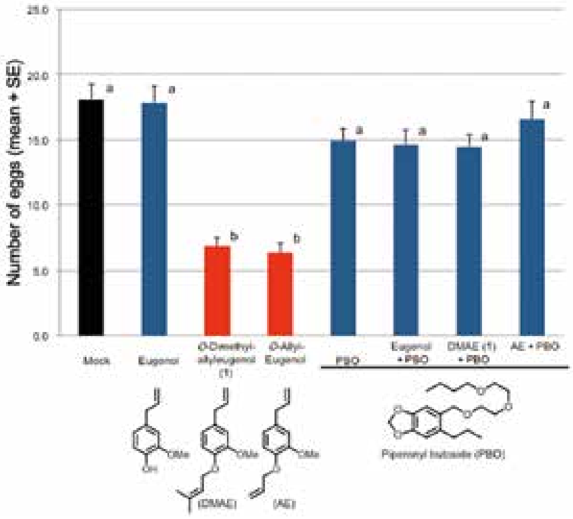


Figure 2. Mechanism for activation of human fibroblasts by GGT inhibitor, GGsTop™.

Biological Activities of Plant Second Metabolite Phenylpropenes and Their Mode of Action

Phenylpropenes having a C6–C3 unit carbon skeleton with a variety of substituents on the benzene ring (C6) and the propene side chain (C3) are one of the most prevalent plant secondary metabolites that exhibit various biological activities such as bacteriocidal, anti-fungal, anti-viral, antioxidative, and anti-tumor activities. Eugenol and its derivatives such as estragole, *O*-methyleugenol, and safrole are typical volatile phenylpropenes found widely across the plant kingdom and are considered to be a part of the chemical self-defense system of plants. Among them, *O*-dimethylallyleugenol (DMAE) is a unique eugenol derivative found in enormous quantities in leaves of Japanese star anise (*Illicium anisatum*) and exhibits the unique activity of suppression of ovipositon of mites, which its parent compound eugenol does not. We therefore are interested in the mode of action of DMAE and performed structure–activity relationship studies.

O-alkylated eugenols like estragole, methyleugenol, and safrole did not show any ovipositon suppression activity at 2 mM; only *O*-allyl-based alkenyl derivatives including DMAE exhibited significant activity. Furthermore, the activity was observed only for the allyl benzene with *O*-allyl substituent at the para position. Interestingly, the activities of DMAE and *O*-allyleugenol (AE) were totally abolished in the presence of piperonyl butoxide (PBO), a competitive inhibitor of cytochrome P450 enzyme, suggesting that the metabolic activation of *O*-allyleugenols involving P450 is responsible for the biological activity. The formation of *p*-quinone methide is inferred as an active entity.



Division of Biochemistry
– Molecular Biology –

http://seitaibunshijyoho-e.weebly.com


Prof
AOYAMA, Takashi
(D Sc)


Assoc Prof
TSUGE, Tomohiko
(D Sc)


Assist Prof
FUJIWARA-KATO, Mariko
(D Agr)


Techn Staff
YASUDA, Keiko

Students

GOTO, Kakeru (D2)
ZHANG, Xiao-Juan (D1)
SHIMAMURA, Ryota (D1)
WATARI, Machiko (M2)
KURODA, Ryo (M1)

Guest Res Assoc

LIN, Qing   Peking University, China, P.R., 25 September 2014-24 September 2015

Scope of Research

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

KEYWORDS
Morphogenesis
Phospholipid
Cytokinin
Signal Transduction
COP9 Signalosome

Selected Publications

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

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

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

Kato, M.; Aoyama, T.; Maeshima, M., The Ca2^{+}-binding Protein PCaP2 Located on the Plasma Membrane is Involved in Root Hair Development as a Possible Signal Transducer, *Plant J.*, **74,** 690-700 (2013).

Aki, S.; Nakai, H.; Aoyama, T.; Oka, A.; Tsuge, T., *AtSAP130/AtSF3b-3* Function is Required for Reproduction in *Arabidopsis thaliana*, *Plant Cell Physiol.*, **52,** 1330-1339 (2011).

GLABRA2 Targets Basic Helix-Loop-Helix Transcription Factor Genes to Suppress Root Hair Development

The morphological differentiation and deposition patterns of cells are crucial determinants of plant structures. Among the plant tissues composed of multiple types of cells, the root epidermis of *Arabidopsis thaliana* has served as an excellent model system for studying morphological differentiation and pattern formation of plant cells. In *Arabidopsis*, the root epidermis is composed of non-hair (N) and hair (H) cell files, and only cells in H cell files develop root hairs. For this cell pattern formation and subsequent cell differentiation, numerous transcription factor genes, including *GLABRA2* (*GL2*), constitute the regulatory networks. *GL2* encodes a homeodomain-leucine-zipper transcription factor and is thought to be a negative regulator of root hair development because it is expressed preferentially in N cell files and mutant defects in *GL2* result in ectopic root hair formation in N cell files. Furthermore, because the expression of a modified GL2 with constitutive transactivating function (VP16-GL2ΔN) resulted in the formation of root hair-like structures from various epidermal cells, including leaf pavement cells, GL2 is thought to recognize a set of genes sufficient for root hair development. This line of evidence clarifies the role of *GL2* as a genetic switch that suppresses root hair development through the suppression of its target genes.

Despite the pivotal role of *GL2* in suppressing root hair development, the molecular basis of the suppression remains obscure because, to date, few GL2 target genes are known and none of them are connected to the gene regulatory network for root hair cell differentiation. The *PHOSPHOLIPASE Dζ1* gene is suppressed directly by GL2 in N cell files and its ectopic expression causes root hair bulges in N cell files, suggesting its involvement in promoting root hair development. *CELLULOSE SYNTHASE5* and *XYLOGLUCAN ENDOTRANSGLYCOSYLASE17*, both of which encode enzymes involved in polysaccharide synthesis, are also GL2 target genes, but their roles in root hair development are unclear. *GL2* and *MYB23* constitute a positive feedback loop in the shoot epidermis where GL2 directly recognizes *MYB23*. Upstream regions of these genes typically contain the L1 box–like sequence 5’-TAAATGT-3’. Although GL2 physically interacted with DNA regions containing this sequence, whether the sequence is necessary and/or sufficient for recognition by GL2 *in planta* remains unclear.

In this study, we identified five *Arabidopsis* bHLH transcription factor genes, *ROOT HAIR DEFECTIVE6 (RHD6), ROOT HAIR DEFECTIVE6-LIKE1 (RSL1), RSL2, Lotus japonicus ROOTHAIRLESS1-LIKE1 (LRL1)*, and *LRL2*, as direct targets of GL2 using transcriptional and post-translational induction systems with chimeric transcription factors VP16-GL2ΔN and GR-VP16-GL2ΔN, respectively. Chromatin immunoprecipitation (ChIP) analysis using a green fluorescence protein (GFP)-fused GL2 protein confirmed the physical interaction of GL2 with these genes *in planta*. Expression analyses showed that the genes are suppressed by *GL2* in N cell files and are expressed in various developmental stages of root hair development. Moreover, the phenotypes caused by the ectopic expression of their GFP-fusion proteins differed among them: *GL2* promoter-driven GFP-LRL1 and GFP-LRL2, but not the other GFP-bHLH proteins, conferred root hair development on non-hair cells. These results indicate that GL2 targets these bHLH genes, which have diverse functions, to robustly suppress root hair development via multimodal pathways.

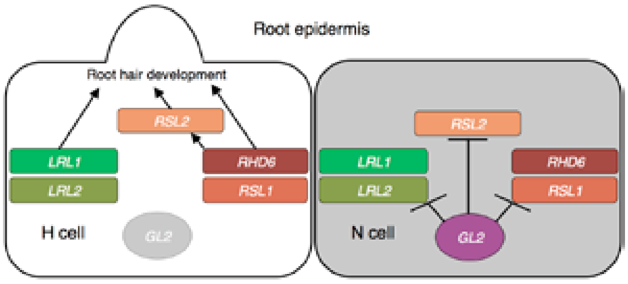


Figure 1. A model of the transcriptional network surrounding *GL2* in root epidermal cells. In N cells (gray color), GL2 directly suppresses the bHLH transcription factor genes *RHD6*, *RSL1*, *RSL2*, *LRL1*, and *LRL2*. In H cells (white), *GL2* is not activated and the bHLH genes remain active to promote root hair development.

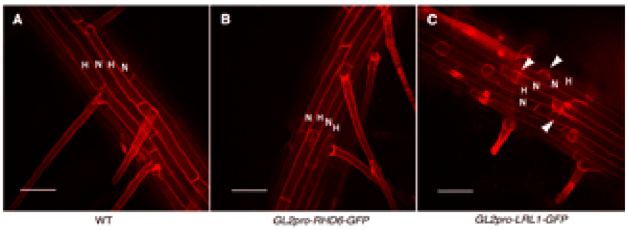


Figure 2. Root hair development patterns of transgenic plants harboring the *GL2* promoter-driven bHLH-GFP genes. PI-stained epidermal cells of wild-type **(A)**, and transgenic roots with *GL2pro-RHD6-GFP* **(B)** and *GL2pro-LRL1-GFP* **(C)** are shown. H and N cell files are marked by “H” and “N”, respectively. Ectopic root hairs developing from N cell files are indicated by arrowheads. Bar = 25 µm.

Division of Biochemistry
– Chemical Biology –

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


Prof
UESUGI, Motonari
(D Pharm Sc)


Assoc Prof
OHKANDA, Junko
(D Eng)


Senior Lect
PERRON, Amelie
(Ph D)


Assist Prof
TAKEMOTO, Yasushi
(D Eng)


Assist Prof
WATANABE, Mizuki
(D Pharm Sc)


Proj Res*
SATO, Shinichi
(D Eng)


Proj Res**
KATSUDA, Yousuke
(D Sc)


Proj Res**
TAKASHIMA, Ippei
(D Pharm Sc)


Proj Res**
TAKENOYA, Mihoko
(D Eng)


Guest Res Assoc
PARVATKAR, Prakash Tukaram
(Ph D)

Researchers
FURUTA, Tomoyuki***
OKUDA, Satoshi***

Researchers(pt)
AKIZUKI, Maika
QIN, Ying***

Assist Techn Staff
MAO, Di***

Assist Res Staff
NAKASHIMA, Mitsue***

*Assoc Prof of iCeMS **PD of iCeMS ***iCeMS

Students
TAKAYA, Junichiro (D4)
ASANO, Risa (D2)
LIAO, Youqi (D2)
PUNZALAN, Louvy Lynn (D1)
YATSUZUKA, Kenji (D1)
MBENZA, Mbambi Naasson (M2)
CHUNG, Watson Xie Khim (M1)
MENDOZA, Aileen de-Leon (RS) ***
LE, Toan Khanh (RS)
PE, Kathleen Beverly Alog (RS) ***
VU, Hue Thi (RS) ***

Scope of Research

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

KEYWORDS
Cell Therapy
Chemical Biology
Small Molecules
Chemical Library
Chemical Genetics

Selected Publications

Takaya, J.; Mio, K.; Shiraishi, T.; Kurokawa, T.; Otsuka, S.; Mori, Y.; Uesugi, M., A Potent and Site-Selective Agonist of TRPA1, *J. Am. Chem. Soc.*, **137,** 15859-15864 (2015).

Parvatkar, P.; Kato, N.; Uesugi, M.; Sato, S.; Ohkanda, J., Intracellular Generation of a Diterpene-Peptide Conjugate that Inhibits 14-3-3-Mediated Interactions, *J Am Chem Soc.*, **137,** 15624-15627 (2015).

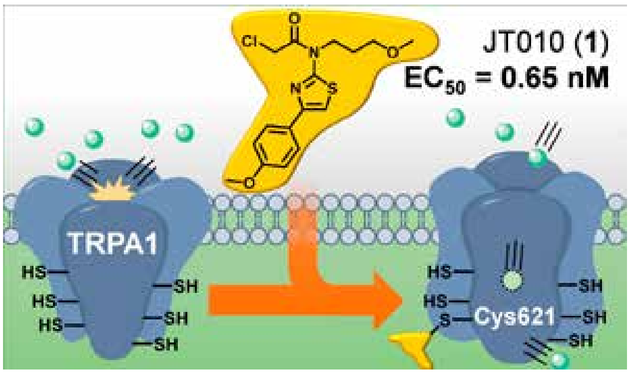
Sato, S.; Watanabe, M.; Katsuda, Y.; Murata, A.; Wang, D. O.; Uesugi, M., Live-cell Imaging of Endogenous mRNAs with a Small Molecule, *Angew. Chem. Int. Ed.*, **54,** 1855-1858 (2015).

Frisco-Cabanos, H. L.; Watanabe, M.; Okumura, N.; Kusamori, K.; Takemoto, N.; Takaya, J.; Sato, S.; Yamazoe, S.; Takakura, Y.; Kinoshita, S.; Nishikawa, M.; Koizumi, N.; Uesugi, M., Synthetic Molecules that Protect Cells from Anoikis and Their Use in Cell Transplantation, *Angew. Chem. Int. Ed.*, **126(42),** 11390-11395 (2014).

Kuo, T. F.; Mao, D.; Hirata, N.; Khambu, B.; Kimura, Y.; Kawase, E.; Shimogawa, H.; Ojika, M.; Nakatsuji, N.; Ueda, K.; Uesugi, M., Selective Elimination of Human Pluripotent Stem Cells by a Marine Natural Product Derivative, *J. Am. Chem. Soc.*, **136(28),** 9798-9801 (2014).

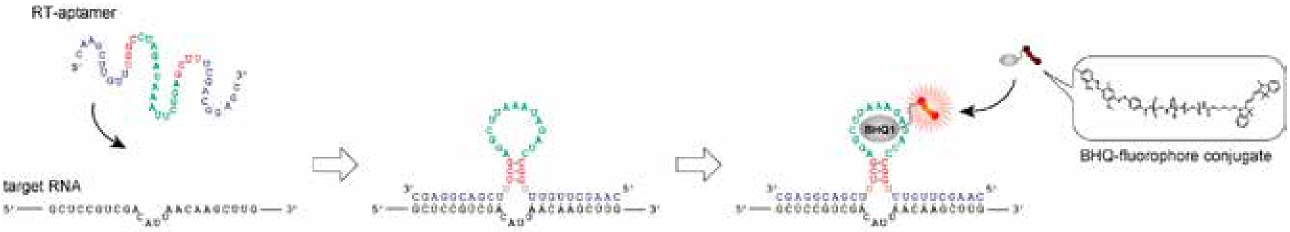
A Potent and Site-Selective Agonist of TRPA1

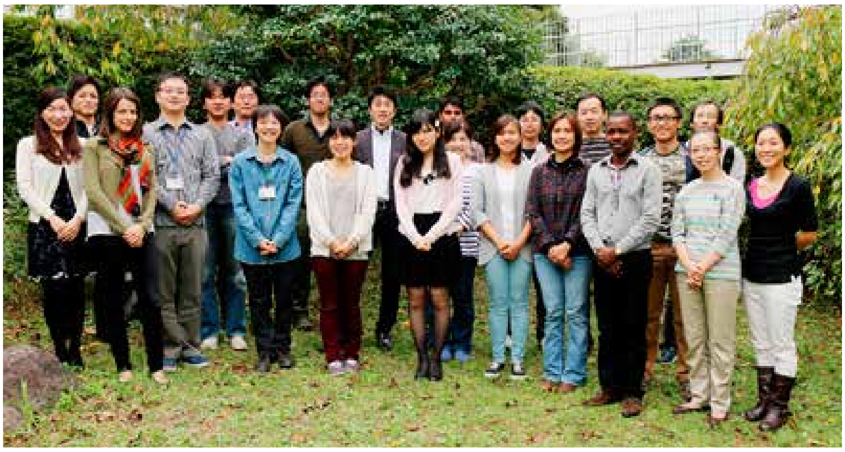
TRPA1 is a member of the transient receptor potential (TRP) cation channel family that is expressed primarily on sensory neurons. This chemo-sensor is activated through covalent modification of multiple cysteine residues with a wide range of reactive compounds including allyl isothiocyanate (AITC), the spicy component of wasabi. The present study reports on potent and selective agonists of TRPA1, discovered through screening 1,657 electrophilic molecules. In an effort to validate the mode of action of hit molecules, we noted a new TRPA1-selective agonist, JT010 (molecule 1), which opens the TRPA1 channel by covalently and site-selectively binding to Cys621 (EC50 = 0.65 nM). The results suggest that a single modification of Cys621 is sufficient to open the TRPA1 channel. The TRPA1-selective probe described herein might be useful for further mechanistic studies of TRPA1 activation.



Live-cell Imaging of Endogenous mRNAs with a Small Molecule

Determination of subcellular localization and dynamics of mRNA is increasingly important for understanding gene expression. A new convenient and versatile method is reported that permits spatiotemporal imaging of specific non-engineered RNAs in living cells. The method uses transfection of a plasmid encoding a gene-specific RNA aptamer, combined with a cell-permeable synthetic small molecule, the fluorescence of which is restored only when the RNA aptamer hybridizes with its cognitive mRNA. The method was validated by live-cell imaging of the endogenous mRNA of β-actin. Application of the technology to mRNAs of a total of 84 human cytoskeletal genes allowed us to observe cellular dynamics of several endogenous mRNAs including arfaptin-2, cortactin, and cytoplasmic FMR1-interacting protein 2. The RNA-imaging technology and its further optimization might permit live-cell imaging of any RNA molecule.





Division of Environmental Chemistry
– Molecular Materials Chemistry –

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


Prof
KAJI, Hironori
(D Eng)


Assist Prof
FUKUSHIMA, Tatsuya
(D Eng)


Assist Prof
SHIZU, Katsuyuki
(D Eng)


Techn Staff
OHMINE, Kyoko


Techn Staff
MAENO, Ayaka


PD
SUZUKI, Katsuaki
(D Hum Env Sc)

Researchers
ISHIYAMA, Norihiro (D Eng)
NAKAGAWA, Hiromichi (D Eng)

Assist Techn Staff
MIYAKE, Harumi

Lect (pt)
NISHIYAMA, Yusuke (D Sc) JEOL Resonance
YOSHIMURA, Ken (D Eng) Sumitomo Chemical Co., Ltd.

Students
ISHIBASHI, Hirotaka (M2)
KUBO, Shosei (M2)
MIWA, Takuya (M2)
OGATA, Isamu (M1)
MIURA, Tsutomu (M1)
WADA, Yoshimasa (M1)
URATANI, Hiroki (UG)
KIDO, Tsuyoshi (UG)

Scope of Research

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

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

Selected Publications

Suzuki, K.; Kubo, S.; Shizu, K.; Fukushima, T.; Wakamiya, A.; Murata, Y.; Adachi, C.; Kaji, H., Triarylboron-based Fluorescent Organic Light-emitting Diodes with External Quantum Efficiencies Exceeding 20%, *Angew. Chem. Int. Ed.*, **54,** 15231-15235 (2015).

Wada, Y.; Shizu, K.; Kubo, S.; Suzuki, K.; Tanaka, H.; Adachi, C.; Kaji, H., Highly Efficient Electroluminescence from a Solution-processable Thermally Activated Delayed Fluorescence Emitter, *Appl. Phys. Lett.*, **107,** [183303-1]-[183303-4] (2015).

Kaji, H.; Suzuki, H.; Fukushima, T.; Shizu, K.; Suzuki, K.; Kubo, S.; Komino, T.; Oiwa, H.; Suzuki, F.; Wakamiya, A.; Murata, Y.; Adachi, C., Purely Organic Electroluminescent Material Realizing 100% Conversion from Electricity to Light, *Nat. Commun.*, **6,** [8476-1]-[8476-8] (2015).

Shizu, K.; Tanaka, H.; Uejima, M.; Sato, T.; Tanaka, K.; Kaji, H.; Adachi, C., Strategy for Designing Electron Donors for Thermally Activated Delayed Fluorescence Emitters, *J. Phys. Chem. C*, **119,** 1291-1297 (2015).

Fukushima, T.; Yamamoto, J.; Fukuchi, M.; Hirata, S.; Jung, H. H.; Hirata, O.; Shibano, Y.; Adachi, C.; Kaji, H., Material Degradation of Liquid Organic Semiconductors Analyzed by Nuclear Magnetic Resonance Spectroscopy, *AIP Advances*, **5,** [087124-1]-[087124-5] (2015).

Suzuki, F.; Shizu, K.; Kawaguchi, H.; Furukawa, S.; Sato, T.; Tanaka, K.; Kaji, H., Multiscale Simulation of Charge Transport in a Host Material, *N,N'*-dicarbazole-3,5-benzene (mCP), for Organic Light-emitting Diodes, *J. Mater. Chem. C*, **3,** 5549-5555 (2015).

Environmentally Friendly Emitter for Organic Light-emitting Diodes Realizing 100% Conversion from Electricity to Light

Organic light-emitting diodes (OLEDs) are solid-state light-emitting devices applied to display and lighting applications. In OLEDs, singlet and triplet excitons are theoretically generated in a 1:3 ratio by electron–hole recombinations. Triplet excitons are typically deactivated through a non-emissive process. Only singlet excitons are converted into photons, meaning that the conversion from carriers to light is limited to 25%. To overcome this issue, thermally activated delayed fluorescent (TADF) materials are proposed, which have a small energy gap between singlet and triplet excited states (ΔE_{ST}) to convert triplet into singlet excitons at room temperature. In this study, we have developed a new TADF material (DACT-II) with approximately 100% up-conversion of the triplet to singlet excitons as well as approximately 100% photoluminescence quantum efficiency, by fine-tuning the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) distributions. OLEDs containing DACT-II show a maximum external electroluminescence quantum efficiency (EQE) of 29.6%, indicating an internal quantum efficiency (conversion of excitons to photons) of ~100%. An external EQE of 41.5% is obtained by the use of an out-coupling sheet. At a high luminance of 3,000 cd/m^2, the external EQE is 30.7%.

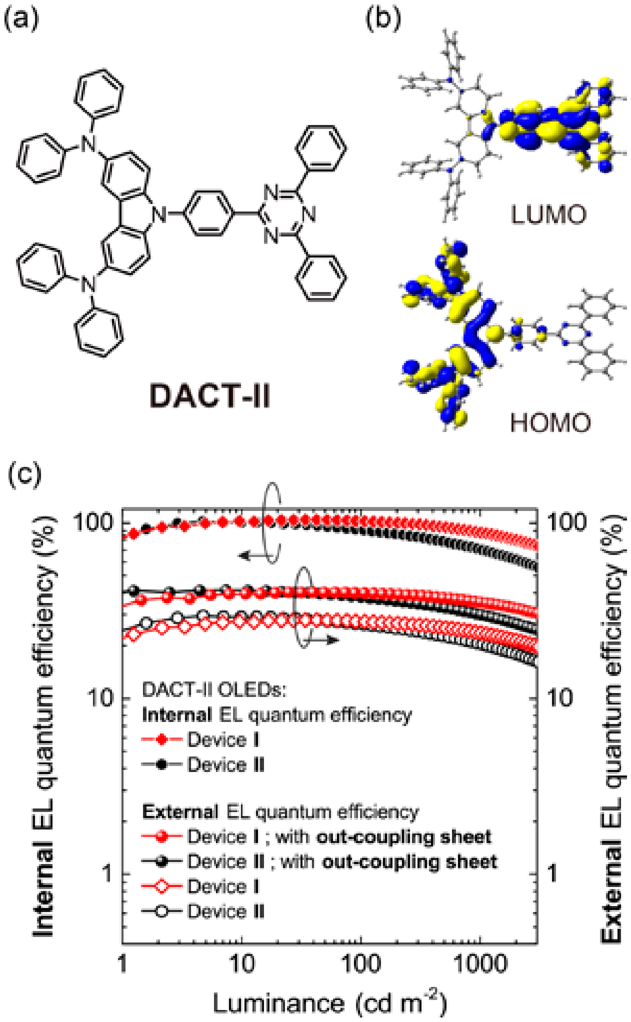


Figure 1. (a) Chemical structure of DACT-II. (b) HOMO and LUMO distributions in DACT-II. (c) Internal EQE–luminance–external EQE characteristics for the DACT-II OLEDs.

Carrier Transport Simulation in an Amorphous mCP Thin Film for Organic Light-emitting Diodes

Carrier injection and carrier blocking at each interface, as well as carrier transport in each layer need to be optimized to improve the performance of OLEDs. Among these processes, the energy levels of the HOMO and the LUMO of organic molecules for injection and blocking of carriers are important and can be well-estimated using quantum chemical calculations for isolated molecules. However, carrier transport in organic films depends strongly on both the intramolecular and intermolecular structures. In this study, multiscale carrier transport simulations were performed for the amorphous structure *N*,*N'*-dicarbazole-3,5-benzene (mCP), which has been used as a host material for OLEDs. We investigated the contribution of respective molecular pairs to carrier transport in an amorphous structure constructed by molecular dynamics. Molecular-level analysis of the carrier transport simulations demonstrates that molecular pairs with large electronic couplings are not the most important factor in carrier transport processes. Carriers are transported effectively in the forward direction via other molecular pairs that do not have substantially large electronic couplings.

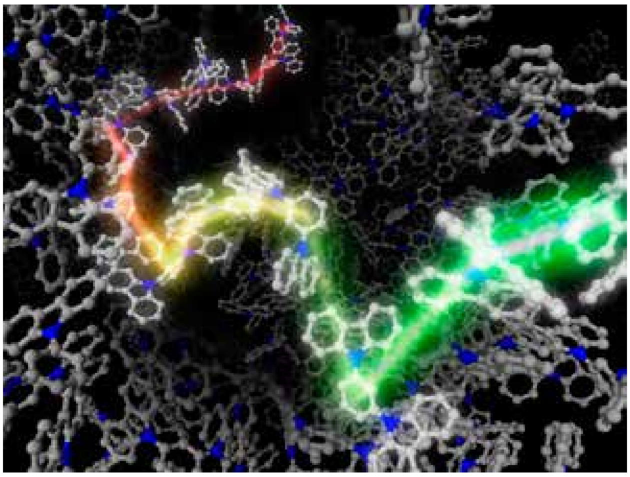


Figure 2. Carrier transport in amorphous mCP films.

Division of Environmental Chemistry
– Hydrospheric Environment Analytical Chemistry –

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

Prof
SOHRIN, Yoshiki
(D Sc)

Assoc Prof
UMETANI, Shigeo
(D Sc)

Assist Prof
TAKANO, Shotaro
(D Sc)

Techn Staff
MINAMI, Tomoharu
(D Eng)

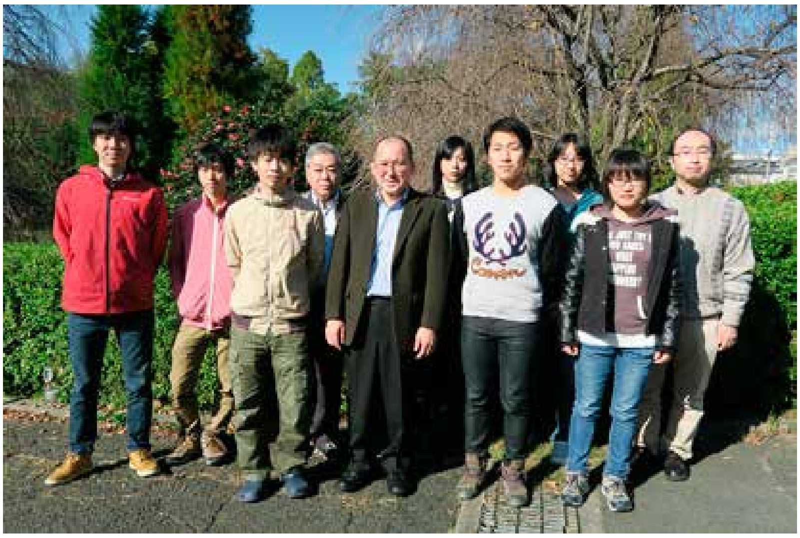
Students

ZHENG, Linjie (D1)
MURATA, Rena (M2)
SASAKI, Masanobu (M2)
TSUJISAKA, Makoto (M1)
UEHARA, Wataru (M1)

Scope of Research

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

(ii) Ion recognition: Novel ligands and ion recognition system are designed, synthesized, and characterized.



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

Selected Publications

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).
Nägler, T. F.; Anbar, A. D.; Archer, C.; Goldberg, T.; Gordon, G. W.; Greber, N. D.; Siebert, C.; Sohrin, Y.; Vance, D., Proposal for an International Molybdenum Isotope Measurement Standard and Data Representation, *Geostand. Geoanal. Res.*, **38,** 149-151 (2014).
Takano, S.; Tanimizu, M.; Hirata, T.; Sohrin, Y., Determination of Isotopic Composition of Dissolved Copper in Seawater by Multi-collector Inductively Coupled Plasma Mass Spectrometry after Pre-concentration Using an Ethylenediaminetriacetic Acid Chelating Resin, *Anal. Chim. Acta*, **784,** 33-41 (2013).
Vu, H. T. D.; Sohrin, Y., Diverse Stoichiometry of Dissolved Trace Metals in the Indian Ocean, *Sci. Rep.*, **3,** [1745-1]-[1745-5] (2013).
Firdaus, M. L.; Minami, T.; Norisuye, K.; Sohrin, Y., Strong Elemental Fractionation of Zr-Hf and Nb-Ta across the Pacific Ocean, *Nature Geosci.*, **4,** 227-230 (2011).

Trace Elements Influenced by Environmental Changes in Lake Biwa: (I) Seasonal Variations under Suboxic Hypolimnion Conditions during 2007 and 2009

Dissolved oxygen (DO) in the Lake Biwa hypolimnion reached its lowest level of < 1 mg kg^{-1} in 2007. Here we report the variations of total dissolvable (TD), dissolved (D), and labile particulate (LP) fractions of Al, Si, P, V, Cr, Mn, Fe, Ni, Cu, Zn, As, Mo, W, and U in Lake Biwa between 2007 and 2009. Al and Fe species were predominantly in the form of LP-Al and LP-Fe, with a strong correlation with one another ($r = 0.99$), suggesting that weathering of aluminous minerals and supply of clay mineral particles mainly control the distribution of Al and Fe. Although D-Al increased in the summer epilimnion, D-Fe was relatively low, probably as a result of uptake by plants. Reductive release of Fe from the bottom was not seen. Mn was also dominated by LP-Mn, but this fraction showed a different distribution than LP-Al and LP-Fe. The D-Mn and LP-Mn concentrations varied by factors of 700–1000, showing marked increases in bottom water during stratification in 2007. We expect Mn^{2+} to have been released from the sediments and oxidized by DO in bottom water. Ni, Cu, Zn, and Cr, which exist as cationic species, had LP/TD ratios of 0.1–0.7 and relatively uniform distributions. Si, P, V, As, Mo, W, and U, which form oxoacid species, had LP/TD ratios of 0–0.8. Si, P, and As were characterized by a nutrient-like profile; V, W, and U showed summer maxima in the epilimnion; and Mo had a uniform distribution. TD-Mo increased in bottom water in company with TD-Mn, while TD-V and TD-W showed significant decreases. The results are likely attributed to differences in adsorption of these elements onto manganese oxides and iron hydroxides.

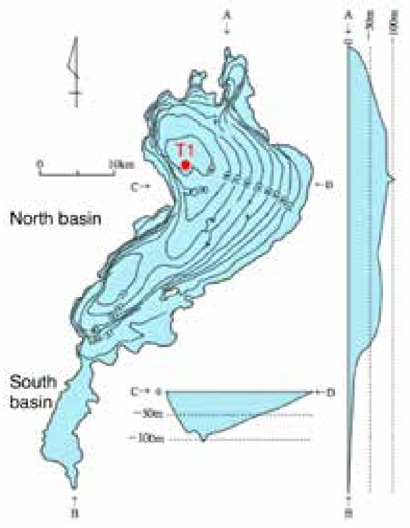


Figure 1. Location of the sampling station T1.

Trace Elements Influenced by Environmental Changes in Lake Biwa: (II) A Regime Shift in the Hypolimnion over the Last Half-century

The history of the deep north basin of Lake Biwa extends over 430,000 years. Although it has probably been oxic and oligotrophic since its formation, human impact has been changing lake conditions. In this paper, we discuss long-term changes in the chemistry of bottom water by compiling literature and through our own data over the last half-century. Long-term records show an increase in temperature, a decrease in DO, and an increase in nutrients in bottom water. The stoichiometry between oxygen and nutrients indicates that changes are basically consistent with aerobic decomposition of organic matter. These changes are most likely the result of global warming and local eutrophication. Of particular note, yearly minimum DO concentrations of less than 50 µmol kg^{-1} have started to occur frequently at ~90 m depth since 1999. Manganese concentrations in bottom water are at their minimum during the turnover period and at a maximum during the late stratification period each year. Yearly minimum Mn concentration has been within a narrow range over the last 30 years (0.25 ± 0.07 µmol kg^{-1}, $n = 12$). However, abnormally high Mn concentrations (up to 9.3 µmol kg^{-1}) were observed in 2007, caused by reductive release of a substantial amount of Mn from suboxic sediments and subsequent oxidation in bottom water. The concentration of arsenic has gradually increased over the last 20 years in a similar manner with a homologous element of phosphorus, resulting in an observed range of 17–29 nmol kg^{-1} in 2010. The accumulation rate was ~0.8 nmol kg^{-1} yr^{-1} for As and ~6 nmol kg^{-1} yr^{-1} for P.

Figure 2. Mr. Nakajima and a water sampling bottle on board the training investigation ship Hassaka, belonging to the University of Shiga Prefecture.

Division of Environmental Chemistry
– Solution and Interface Chemistry –

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

Prof
HASEGAWA, Takeshi
(Ph D)

Assist Prof
WAKAI, Chihiro
(D Sc)

Assist Prof
SHIMOAKA, Takafumi
(D Sc)

Students

SHIOYA, Nobutaka (D1)
TANAKA, Yuki (D1)
IZUMI, Naoki (M1)
UKAI, Hironori (M1)
HADA, Miyako (M1)

Scope of Research

To understand the chemical structure and property in a molecular aggregated system, the keywords of molecular interactions and/or orientation are focused on, and the molecular aggregates are investigated by using originally developed spectroscopic techniques. The current major topics are: (1) Stratified Dipole-Arrays (SDA) theory accounting for bulk and molecular properties of perfluoroalkyl compounds; (2) the molecular orientation and conformation analysis in a thin film of an organic semiconductor; (3) the molecular structure and dynamics analysis of molecular water involved in a Nafion membrane.

KEYWORDS
Infrared and Raman Spectroscopy
Perfluoroalkyl Compounds
Polymer Electrolyte Membrane
Surface and Interface Chemistry
Organic Semiconductor

Selected Publications

Hasegawa, T.; Shimoaka, T.; Tanaka, Y.; Shioya, N.; Morita, K.; Sonoyama, M.; Amii, H.; Takagi, T.; Kanamori, T., An Origin of Complicated Infrared Spectra of Perfluoroalkyl Compounds Involving a Normal Alkyl Group, *Chem. Lett.*, **44,** 834-836 (2015).

Hasegawa, T., Understanding of the Intrinsic Difference between Normal- and Perfluoro-alkyl Compounds toward Total Understanding of Material Properties, *Chem. Phys. Lett.*, **626,** 64-66 (2015).

Shioya, N.; Shimoaka, T.; Eda, K.; Hasegawa, T., A New Schematic of Poly(3-alkylthiophene) in an Amorphous Film Studied Using a Novel Structural Index on Infrared Spectroscopy, *Phys. Chem. Chem. Phys.*, **17,** 13472-13479 (2015).

Shimoaka, T.; Wakai, C.; Sakabe, T.; Yamazaki, S.; Hasegawa, T., Hydration Structure of the Strongly Bound Water on the Sulfonic Acid Group in a Nafion Membrane Studied by Infrared Spectroscopy and Quantum Chemical Calculation, *Phys. Chem. Chem. Phys.*, **17,** 8843-8849 (2015).

Wakai, C.; Shimoaka, T.; Hasegawa, T., ^{1}H NMR Analysis of Water Freezing in Nanospace Involved in a Nafion Membrane, *J. Phys. Chem. B,* **119,** 8048-8053 (2015).

Ishizuka, R.; Matubayasi, N.; Tu, K.-M.; Umebayashi, Y., Energetic Contributions from Cation and Anion to the Stability of Carbon Dioxide Dissolved in Imidazolium-Based Ionic Liquids, *J. Phys. Chem.* B, **119,** 1579-1587 (2015).

An Origin of Complicated Infrared Spectra of Perfluoroalkyl Compounds Involving a Normal Alkyl Group

Perfluoroalkyl (Rf) compounds containing a normal alkyl group often yield highly complicated infrared (IR) spectra especially in the CF stretching vibration (νC-F) region. To reveal the reason behind this, the IR p-polarized multiple-angle incidence resolution spectrometry (pMAIRS) is employed to measure a monolayer of $CF_3(CF_2)_9(CH_2)_3COOH$ deposited on a silicon substrate. The compound is known to spontaneously aggregate to form a molecular assembly with the closest packing, in which the molecules are oriented perpendicular to the substrate. The IR pMAIRS spectra apparently prove that the complexity of the νC-F region is due to the normal alkyl part directly connected to the Rf group because the carbons in the Rf group are vibrated as a coupled oscillator, and the oscillation of the alkyl part propagates to the Rf part along the molecular axis.

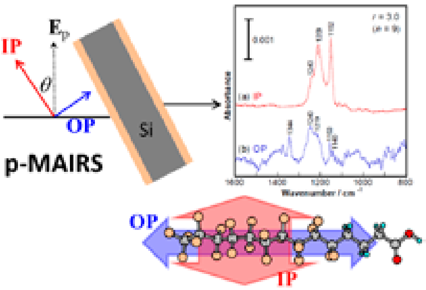


Figure 1. Schematic image of the CF stretching vibration mode. The complicated band is induced by the vibration along the molecular axis.

A New Schematic for Poly(3-alkylthiophene) in an Amorphous Film Studied Using a Novel Structural Index in Infrared Spectroscopy

The molecular structure of poly(3-alkylthiophene-2,5-diyl) in an amorphous film reveals that the short axis of the thiophene ring is kept highly oriented parallel to the substrate, whereas the long axis along the polymer chain is largely disordered. This is unveiled by infrared p-polarized multiple-angle incidence resolution spectroscopy (pMAIRS), achieved by analyzing the orientation angles of three mutually orthogonal vibrational modes localized on the thiophene ring with the aid of a newly developed structural index. This new analytical technique is useful irrespective of the crystallinity of the thin film. As a result, the intrinsic chemical parameters controlling the molecular orientation are understood in a unified manner, and the reason that the hexyl group gives the best results for a photovoltaic cell is also revealed.

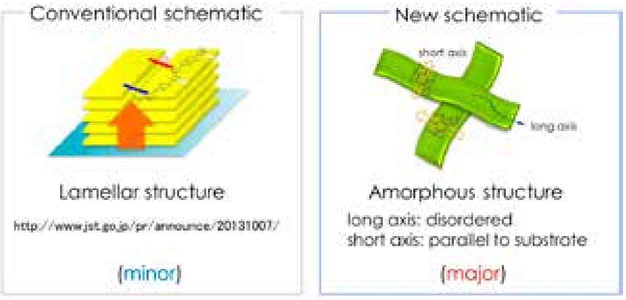


Figure 2. A new schematic of the face-on orientation in a thin film of poly(3-alkylthiophene).

Hydration Structure of Strongly Bound Water on the Sulfonic Acid Group in a Nafion Membrane Studied by Infrared Spectroscopy and Quantum Chemical Calculation

The hydration structure of the 'strongly bound water' around the sulfonic acid (SA) groups in Nafion, which has recently been revealed by 1H NMR spectroscopy (*Anal. Chem.*, **85,** 7581 (2013)), is studied using infrared spectroscopy with the aid of quantum chemical (QC) calculations. During a heated drying process, bulky water is firstly dehydrated, which is followed by the disappearance of the hydronium ion and the appearance of bands that have been assigned to the fully dehydrated species at 140 °C. However, a spectral simulation based on QC reveals that the spectrum at 140 °C comes from the SA group associated with a single-water molecule via two H-bonds. This implies that a thoroughly dried membrane is unavailable even at 140 °C, and the involved water corresponds to the 'strongly bound water.' The QC-analytical results are experimentally confirmed by evolved gas analysis mass spectrometry (EGA-MS). At ca. 300 °C, which is the temperature where the SA group is selectively decomposed, the molecular fragment of SO_2 is observed accompanying water molecules as expected. This confirms that the last single-water molecule can remain on the SA group until the thermal decomposition.

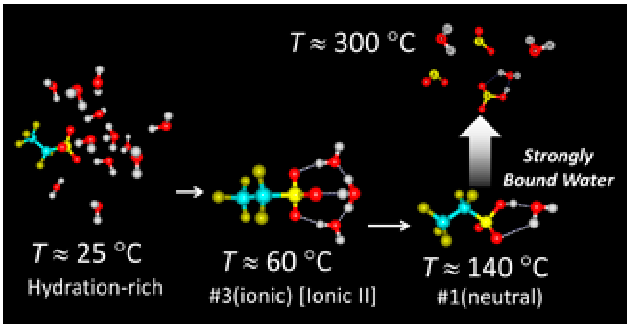


Figure 3. Dehydration and deionization process about sulfonic acid group in a Nafion membrane on heating.

Division of Environmental Chemistry
– Molecular Microbial Science –

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

Prof
KURIHARA, Tatsuo
(D Eng)

Assist Prof
KAWAMOTO, Jun
(D Agr)

Assist Prof
OGAWA, Takuya
(D Agr)

PD
CHO, Hyun-Num
(D Agr)

Assist Res Staff

KITAYAMA, Kaori

Students

SUGIURA, Miwa (D3)
KAWAI, Soichiro (D2)
OHKE, Yoshie (D2)
CHEN, Chen (D1)
TOKUNAGA, Tomohisa (D1)
TOYOTAKE, Yosuke (M2)
NINOMIYA, Takemasa (M2)
OTA, Masaki (M1)
KUMAGAI, Fumihito (M1)
SUGIMOTO, Saki (M1)
CHEN, Tsai-min (M1)
FURUKAWA, Takahiro (M1)
YOKOYAMA, Fumiaki (M1)

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-adaptation Mechanism
Polyunsaturated Fatty Acid
Membrane Proteins
Acyltransferase

Selected Publications

Goto, S.; Kawamoto, J.; Sato, S. B.; Iki, T.; Watanabe, I.; Kudo, K.; Esaki, N.; Kurihara, T., Alkyl Hydroperoxide Reductase Enhances the Growth of *Leuconostoc mesenteroides* Lactic Acid Bacteria at Low Temperatures, *AMB Express*, **5,** 11 (2015).
Kawamoto, J.; Kurihara, T., Cold-adaptation Mechanism of Psychrophiles, *Seibutsu-Kogaku Kaishi*, **93,** 477-480 (2015).
Park, J.; Yamaura, T.; Kawamoto, J.; Kurihara, T.; Sato, S. B., Reciprocal Modulation of Surface Expression of Annexin A2 in a Human Umbilical Vein Endothelial Cell-derived Cell Line by Eicosapentaenoic Acid and Docosahexaenoic Acid, *PLoS One*, **9,** (1):e85045 (2014).
Kawamoto, J.; Kurihara, T., Proteins and Lipids of Cold-Adapted Microorganisms, *CSJ Current Review*, **17,** 55-61 (2014).
Kurihara, T.; Kawamoto, J., Chemical Approach to Analyze the Physiological Function of Phospholipids with Polyunsaturated Fatty Acyl Chain, *Yakugaku Zasshi*, **134,** 507-513 (2014).

Synthesis of Omega-ethynyl Eicosapentaenoic Acid and Its Application

Eicosapentaenoic acid (EPA) is an ω-3 polyunsaturated fatty acid (ω-3 PUFA) with a 20-carbon chain and five *cis* double bonds; the first double bond is located at the third carbon from the omega end. EPA acts as a precursor for a group of physiologically active lipid compounds and has many physiological functions, such as anti-inflammatory and anti-tumor. Although EPA commonly exists in membrane phospholipids as an acyl chain, how EPA behaves *in vivo* has not been elucidated in detail. Here, we developed an efficient synthesis method for ω-ethynyl EPA with an ethynyl group at omega position of EPA. This synthetic EPA analog is available for direct visualization by Raman microscopy and allows *in situ* chemical modification of EPA via click chemistry. To evaluate the usability of synthesized ω-ethynyl EPA, we used an Antarctic bacterium, *Shewanella livingstonensis* Ac10, as a model organism. This strain inducibly produces EPA at low temperatures, and the EPA-less mutant (ΔEPA) shows growth retardation and abnormal morphology at low temperatures. When EPA or ω-ethynyl EPA was exogenously supplemented to ΔEPA, both growth retardation and abnormal morphology were suppressed at 4 °C. Under the same conditions, membrane phospholipids of ΔEPA contained ω-ethynyl EPA as an acyl chain, and the amount of ω-ethynyl EPA was about 7% of total fatty acids in the membrane. These results reveal that ω-ethynyl EPA, similar to the natural form, is incorporated into *S. livingstonensis* Ac10 and performs the required physiological functions, suggesting that ω-ethynyl EPA can be used for *in situ* functional studies of EPA.

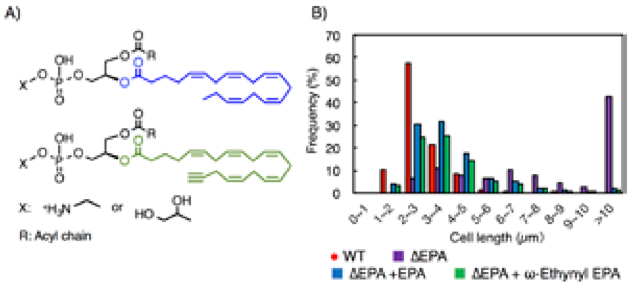


Figure 1. Structure of EPA-/ω-ethynyl EPA–containing phospholipids (A) and cell-size distribution of *S. livingstonensis* Ac10 and the EPA-less mutant grown with EPA/ω-ethynyl EPA (B). The EPA-less mutant forms filamentous cells with an average cell length of ΔEPA > 10 µm. In the presence of EPA/ω-ethynyl EPA, the average cell length of ΔEPA was 2-4 µm, similar to that of the parent strain (wild type).

Physiological Function of a Novel Acyltransferase of an Antarctic Bacterium, *Shewanella livingstonensis* Ac10

In bacterial cell membrane biogenesis, phospholipid synthesis is catalyzed by two acyltransferases, PlsB and PlsC. The second acyltransferase PlsC catalyzes the acylation of the *sn*-2 position of the glycerol backbone of 1-acylglycerol phosphate. These two enzymes contribute to an asymmetric distribution of fatty acids between the *sn*-1 and 2 positions of the glycerol phosphate backbone. In *Shewanella livingstonensis* Ac10, a cold-adapted microorganism isolated from Antarctic seawater, eicosapentaenoic acid (EPA)-containing phospholipids play important roles in cell division at low temperatures. *S. livingstonensis* Ac10 has five putative PlsC proteins, PlsC1–5, in which PlsC1 is a key enzyme for EPA-containing phospholipids at low temperatures. On the other hand, the physiological functions of other PlsCs are still unclear. We generated gene-deletion mutants of each *plsC* gene and analyzed their phospholipid compositions. In the *plsC4*-deletion mutant (Δ*plsC4*), the amount of phospholipids containing the saturated fatty acid, 11-methyllauric acid (isoC13:0), was significantly decreased. The *plsC4*-expression vector restored the production of isoC13:0-containing phospholipids. An *in vitro* acyltransferase assay using 18:1-containing lysophosphatidic acid and various acyl donors indicated that PlsC4 has PlsC activity for relatively short-chain saturated acyl groups, 12:0, 13:0, and 14:0, but not for relatively long-chain saturated and unsaturated acyl groups, demonstrating that PlsC4 has a different substrate specificity from that of PlsC1 and is essential for the synthesis of isoC13:0-containing phospholipids.

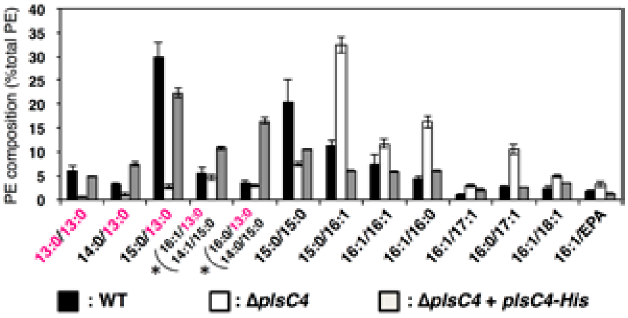


Figure 2. Composition of phosphatidylethanolamine of *S. livingstonensis* Ac10 (wild type), the *plsC4*-deleted mutant (Δ*plsC4*), and the *plsC4*-exoression strain (Δ*plsC4* + *plsC4-His* expression vector). The cells were harvested at 4 °C, and the membrane phospholipids were extracted. Phospholipid extracts were analyzed by ESI-MS. Red characters indicate the phospholipids containing 11-methyllauric acid (13:0). Asterisks indicate the isomers.

Division of Multidisciplinary Chemistry
– Polymer Materials Science –

http://www.scl.kyoto-u.ac.jp/~kanaya2/e_index.html

Prof
KANAYA, Toshiji
(D Eng)

Assoc Prof
NISHIDA, Koji
(D Eng)

Assist Prof
OGAWA, Hiroki
(D Eng)

Students

MASHITA, Ryo (D3)
KISHIMOTO, Mizuki (M2)
FUJISHIMA, Yudai (M2)
MURAKAMI, Momoko (M2)
MIYATAKE, Yuki (M1)
OKIHARA, Tetsuya (UG)
OKAMOTO, Masanori (UG)
SAIGA, Mari (UG)

Scope of Research

The structure and molecular motion of polymer substances are studied, mainly using scattering methods such as neutron, X-ray, and light with intent to solve fundamentally important problems in polymer science. The main projects are studies on 1) the mechanism of structural development in crystalline polymers from glassy or molten state to spherulites, 2) the dynamics in disordered polymer materials including low-energy excitation, 3) glass transition and local segmental motions, 4) formation processes and structure of polymer gels, and 5) the structure and molecular motion of polyelectrolyte solutions.

KEYWORDS
Polymer Physics
Polymer Properties
Scattering
Neutron Scattering
Synchrotron X-ray Scattering

Selected Publications

Kanaya, T.; Ogawa, H.; Kishimoto, M.; Inoue, R.; Suter, A.; Prokscha, T., Distribution of Glass Transition Temperatures T_g in Polystyrene Thin Films as Revealed by Low-energy Muon Spin Relaxation: A Comparison with Neutron Reflectivity Results, *Phys. Rev. E*, **92,** 022604-1-022604-7 (2015).
Nishida, K.; Zhuravlev, E.; Yang, B.; Schick, C.; Shiraishi, Y.; Kanaya, T., Vitrification and Crystallization of Poly(butylene-2,6-naphthalate), *Thermochim. Acta*, **603,** 110-115 (2015).
Ogawa, H.; Nishikawa, Y.; Fujiwara, A.; Takenaka, M.; Wang, Y.-C.; Kanaya, T.; Takata, M., Visualizing Patterned Thin Films by Grazing-incidence Small Angle X-ray Scattering (GISAXS) Coupled with Computed Tomography (CT)., *J. Appl. Cryst.*, **48,** 1645-1650 (2015).
Matsuura, T.; Murakami, M.; Inoue, R.; Nishida, K.; Ogawa, H.; Ohta, N.; Kanaya, T., Microbeam Wide-Angle X-ray Scattering Study on Precursor of Shish Kebab. Effects of Shear Rate and Annealing on Inner Structure, *Macromolecules*, **48,** 3337−3343 (2015).
Osaka, O.; Benten, H.; Ohkita,H.; Ito, S.; Ogawa, H.; Kanaya, T., Nanostructures for Efficient Hole Transport in Poly(3- hexylthiophene) Film: A Study by Conductive Atomic Force Microscopy, *J. Phys. Chem. C*, **43,** 24307−24314 (2015).

Distribution of Glass Transition Temperature T_g in Polystyrene Thin Films as Revealed by Low-energy Muon Spin Relaxation (μSR)

Information on T_g distribution is very useful for understanding the interesting but unusual properties of polymer thin films. However, one problem that we have to clarify is whether there are effects of deuterium labeling on T_g or not. To tackle the problem, we performed low-energy muon spin relaxation (μSR) measurements on the aforementioned deuterium-labeled 5-layer PS thin film as well as dPS and hPS single layer thin films ~100 nm thick as a function of muon implantation energy. It was found that deuterium labeling had no significant effect on T_g distribution, guaranteeing that we can safely discuss the unusual thin-film properties based on the T_g distribution revealed by neutron reflectivity on the deuterium-labeled thin films. In addition, the μSR result suggested that the higher T_g near the Si substrate is due to the strong orientation of phenyl rings.

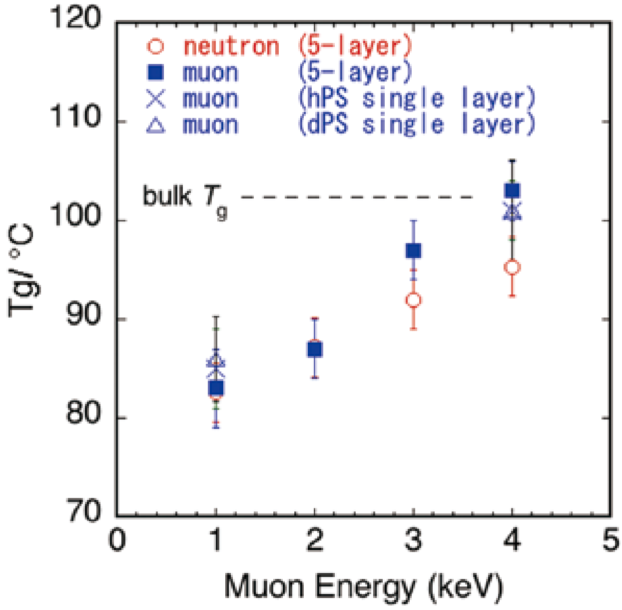


Figure 1. Distributions of the average neutron $\langle T_g \rangle_{ME}$ (o), the muon T_g evaluated (■) for the 5-layer dPS/hPS/dPS/hPS/dPS thin film, and the muon T_g for the single layer hPS (×) and dPS (△) thin films, as a function of muon implantation energy.

Perfect Vitrification, Mesophase Formation, and Crystallization of Poly (buthlene-2,6-naphthalate)

It was very difficult to obtain the glassy state of poly(butylene-2,6-naphthalate) (PBN), because PBN crystallizes very quickly on cooling from the molten state. The differential fast scanning calorimetry (DFSC) technique has been successfully applied to study the vitrification of PBN and crystallization from the glassy state. A cooling rate of more than 6000 K/s could prevent PBN from crystallizing and more than 30000 K/s effectively reduced the development of active nuclei. A heating rate faster than 7000 K/s could prevent cold crystallization from the proper glassy state. In cooling and heating rates less severe than 30000 K/s and 7000 K/s, respectively, a variety of structure formations, such as nucleation, mesophase formation, crystallization, and their multiple melting behaviors, have been observed (Figure 2). The present work has been performed through the collaborative research with Professor Schick's laboratory at Rostock University in Germany and supported by Researcher Exchange Program between Japan Society for the Promotion of Science (JSPS) and Deutscher Akademischer Austausch Dienst (DAAD) awarded to K.N.

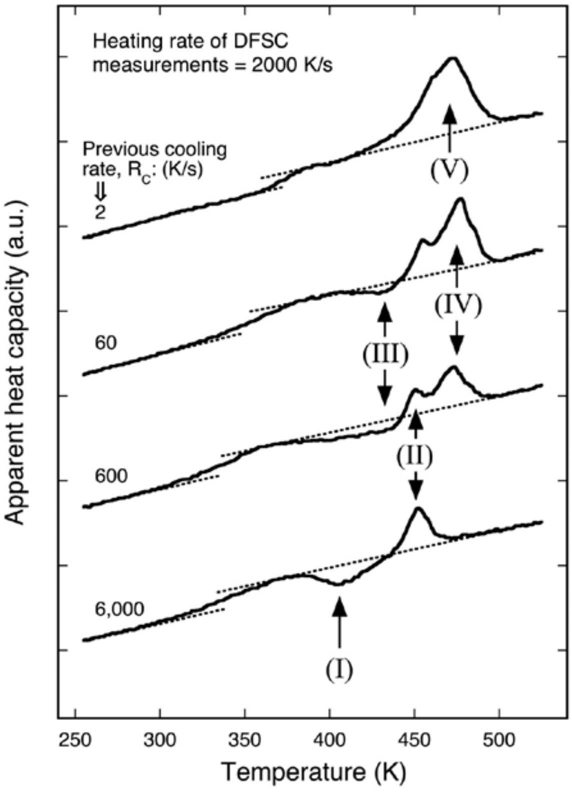


Figure 2. Representative DFSC curves illustrating five categories of exo- and endothermic peaks. (I) Mesophase formation from (devitrified) amorphous, (II) melting of mesophase, (III) cold crystallization on heating, (IV) melting of crystal formed on heating, and (V) melting of the original crystal that formed on previous cooling.

Division of Multidisciplinary Chemistry
– Molecular Rheology –

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

Prof
WATANABE, Hiroshi
(D Sc)

Assist Prof
MATSUMIYA, Yumi
(D Eng)

Techn Staff*
OKADA, Shinichi

*Re-employed Staff

Students

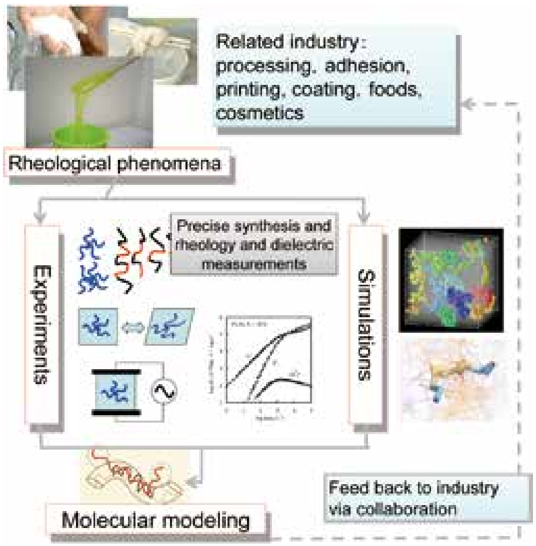
HIROTSU, Soichiro (M2)
TANAKA, Takeya (M2)
ISHIBASHI, Takuma (M1)
KUBO, Kosei (M1)
OHKITA, Yuya (M1)
ISHIMOTO, Ryushin (UG)

Guest Scholars

KWON, Youngdon (Ph D)	Sungkyunkwan University, Korea, R., 8 April-25 July
RAKKAPAO, Natthida (Ph D)	Prince of Songkla University, Thailand, 1 May-31 October

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

Matsumiya, Y.; Rakkapao, N.; Watanabe, H., Entanglement Length in Miscible Blends of cis-Polyisoprene and Poly(p-tert-butylstyrene), *Macromolecules*, **48(21),** 7889–7908 (2015).

Timachova, K.; Watanabe, H.; Balsara, N. P., Effect of Molecular Weight and Salt Concentration on Ion Transport and the Transference Number in Polymer Electrolytes, *Macromolecules*, **48(21),** 7882–7888 (2015).

Watanabe, H.; Matsumiya, Y.; Inoue, T., Revisit the Stress-Optical Rule for Entangled Flexible Chains: Overshoot of Stress, Segmental Orientation, and Chain Stretch on Start-up of Flow, *J. Soc. Rheol. Jpn*, **43(3-4),** 105-112 (2015).

Schauser, N. S.; Harry, K. J.; Parkinson, D. Y.; Watanabe, H.; Balsara, N. P., Lithium Dendrite Growth in Glassy and Rubbery Nanostructured Block Copolymer Electrolytes, *J. Electochem. Soc.*, **162(3),** A398-A405 (2015).

Watanabe, H.; Matsumiya, Y.; Masubuchi, Y.; Urakawa, O.; Inoue, T., Viscoelastic Relaxation of Rouse Chains undergoing Head-to-Head Association and Dissociation: Motional Coupling through Chemical Equilibrium, *Macromolecules*, **48(9),** 3014–3030 (2015).

Entanglement Length in Miscible Blends of cis-Polyisoprene and Poly (p-tert-butylstyrene)

The entanglement length *a*, being equivalent to the plateau modulus G_N ($\propto M_e^{-1} \propto a^{-2}$), is one of the most basic parameters that determine the slow dynamics of high molecular weight (*M*) polymers. In miscible blends of chemically different chains, the components should have the common *a* value. However, changes of *a* with the blend composition have not been fully elucidated. For this problem, this study conducted linear viscoelastic tests for miscible blends of high-*M* *cis*-polyisoprene (PI) and poly(*p*-*tert*-butylstyrene) (PtBS) and analyzed the storage and loss moduli (G' and G") data in a purely empirical way, considering the very basic feature that unentangled and entangled blends having the same composition exhibit the same local relaxation. (From a molecular point of view, this local relaxation reflects the chain motion *within* the length scale of *a*.) On the basis of this feature, a series of barely entangled low-*M* PI/PtBS blends having various component molecular weights and a given composition were utilized as references for well-entangled high-*M* PI/PtBS blends with the same composition, and the modulus data of the reference were subtracted from the data of the high-*M* blends. For an optimally chosen reference, the storage modulus of the high-*M* blends obtained after the subtraction ($G_{\mathrm{ent}}' = G_{\mathrm{high}\text{-}M\,\mathrm{blend}}' - G_{\mathrm{ref}}'$) exhibited a clear plateau at high angular frequencies ω. The corresponding loss modulus G_{ent}" decreased in proportion to ω^{-1} at high ω, which characterized the short-time onset of the global entanglement relaxation: A mischoice of the reference gave no plateau of $G_{\mathrm{high}\text{-}M\,\mathrm{blend}}' - G_{\mathrm{ref}}'$ and no ω^{-1} dependence of $G_{\mathrm{high}\text{-}M\,\mathrm{blend}}" - G_{\mathrm{ref}}"$ at high ω, but a survey for various low-*M* PI/PtBS blends allowed us to find the optimum reference (Figure 1). With the aid of such an optimum reference, the entanglement plateau modulus G_N of the high-*M* PI/PtBS blends was accurately obtained as the high-ω plateau value of G_{ent}'. G_N thus obtained was well described by a linear mixing rule of the entanglement length *a* with the weighing factor being equated to the number fraction of Kuhn segments of the components, not by the reciprocal mixing rule utilizing the component volume fraction as the weighing factor (Figure 2). This result, not explained by a mean-field picture of entanglement (constant number of entanglement strands in a volume a^3), is discussed in relation to local packing efficiency of bulky PtBS chains and skinny PI chains.

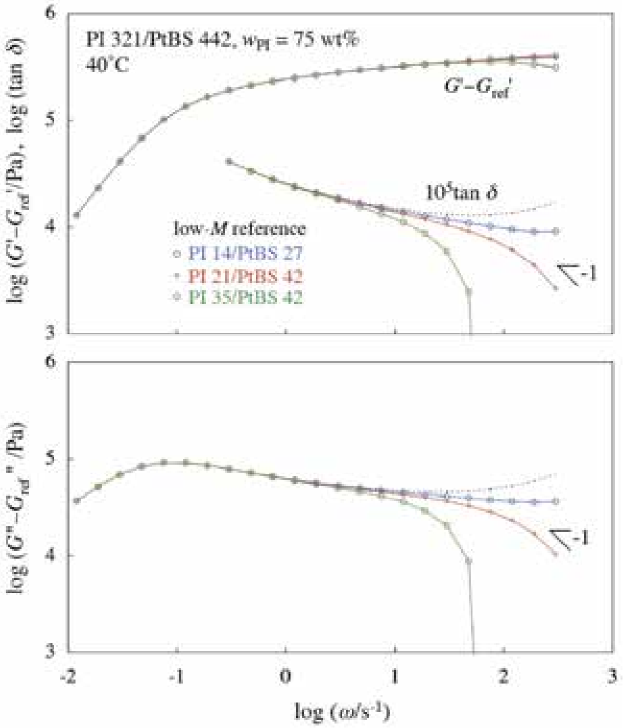


Figure 1. Test of the modulus difference $G^* - G_{\mathrm{ref}}^*$ for high-*M* PI 321/PtBS 442 blend with w_{PI} = 75 wt%.

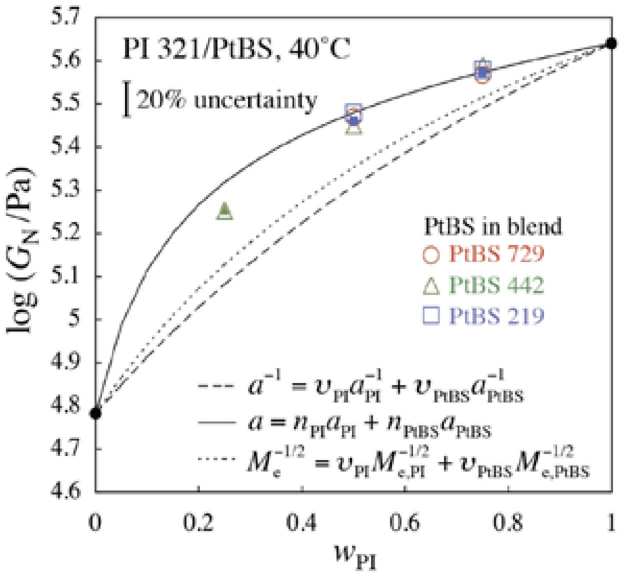


Figure 2. Entanglement plateau modulus G_N of high-*M* PI/PtBS blends evaluated by subtraction of G^* data of low-*M* reference blends (large unfilled symbols) and by phenomenological fitting with the aid of G^* data of two PI samples and/or two PtBS samples (small filled squares and small filled triangle).

Division of Multidisciplinary Chemistry
– Molecular Aggregation Analysis –

http://www.kuicr.kyoto-u.ac.jp/labos/is2/scope.html

Prof
SATO, Naoki
(D Sc)

Assist Prof
MURDEY, Richard James
(Ph D)

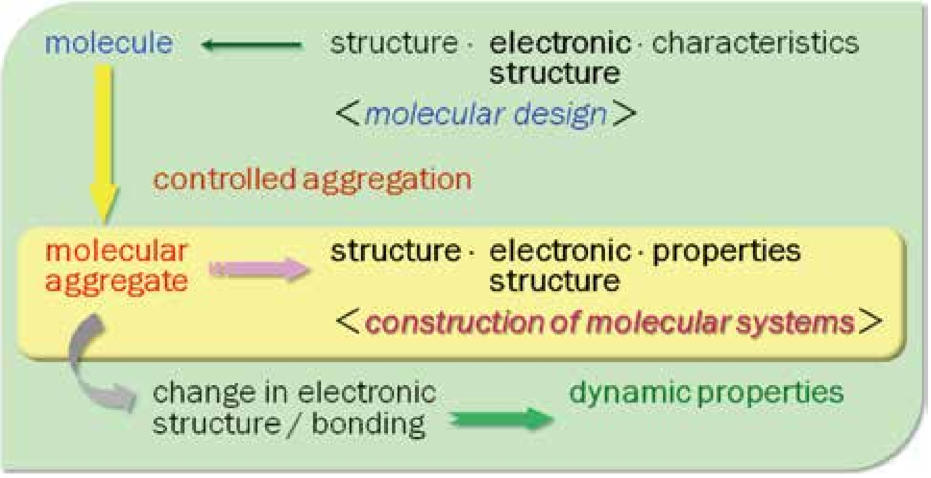
Student

NAKAO, Kazuto (M2)

Scope of Research

The research of this subdivision is devoted to correlation studies on structures and properties of molecular aggregates, in particular, organic semiconductor solids and thin films, from two main standpoints: photoelectric and electric properties. The electronic structure of organic thin films is studied using photoemission and inverse photoemission spectroscopies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with fabrication of organic electronic devices; elucidation of charge carrier generation and transport, examination of trapping states, understanding of interface electronic behaviors, and so on.

KEYWORDS
Charge Carrier Transport
Electronic Structure
Frontier Electronic State
Organic Semiconductor
Thin Film



Selected Publications

Murdey, R.; Sato, N., Photocurrent Action Spectra of Organic Semiconductors, *In "Advances in Organic Crystal Chemistry, Comprehensive Reviews 2015", Tamura. R.; Miyata, M. Eds., Springer, Tokyo*, 627-652 (2015).

Yoshida, H.; Yamada, K.; Tsutsumi, J.; Sato, N., Complete Description of Ionization Energy and Electron Affinity in Organic Solids: Determining Contributions from Electronic Polarization, Energy Band Dispersion and Molecular Orientation, *Phys. Rev. B*, **92,** 075145 (2015).

Photocurrent Action Spectra of Organic Semiconductor Thin Films

Photocurrent action spectra were measured for vacuum-deposited pentacene thin films 20 nm to 100 nm in thickness, as functions of incident photon energy, applied bias, photon flux, film thickness, and measurement temperature, in order to better understand the mechanisms underpinning photo-induced charge carrier generation, injection, and transport in molecular semiconductors. A strong dependence on the electrode material was found, and, for aluminum electrodes, the measured photocurrent was determined to originate from an intrinsic mechanism, where photogenerated electron-hole geminate pairs are created in the bulk film. For gold or titanium electrodes, a substantial contribution to the photocurrent from extrinsic, or injected, photocurrents was observed. The intrinsic photocurrent spectrum of pentacene thin film resembled the previous measurements obtained for thick films and single crystals (Figure 1). The onset of the intrinsic photocurrent, taken to indicate the transport energy gap, E_G, was determined to be 2.25 eV, the same value as in previous studies. Aluminum electrodes form blocking contacts that substantially reduce extrinsic photocurrents attributed to exciton-enhanced charge injection and transport, enhancing the visibility of the intrinsic processes. The dependence of the intrinsic photocurrent on temperature, photon flux, and applied field is consistent with a mechanism in which optical generation of a charge transfer state is followed by the thermally assisted dissociation of the geminate electron–hole pair into independent charge carriers.

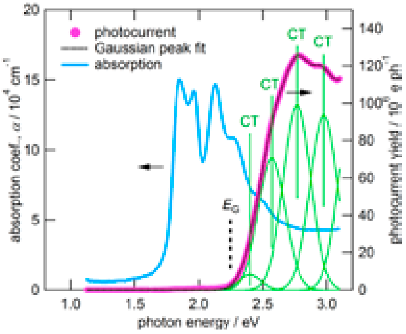


Figure 1. Photocurrent action spectra and absorption coefficient obtained for the 100 nm pentacene film / aluminum electrode device. Photocurrents are normalized to the incident photon flux. The transport energy gap is E_G = 2.25 eV, estimated from the threshold onset of the photocurrent yield.

Complete Description of Ionization Energy and Electron Affinity in Organic Solids: Determining Contributions from Electronic Polarization, Energy Band Dispersion, and Molecular Orientation

Ionization energy and electron affinity in organic solids are understood in terms of electronic energy levels of a single molecule perturbed by solid-state effects such as polarization energy, band dispersion, and molecular orientation as primary factors. We have precisely determined the electron affinities of pentacene (PEN) and perfluoropentacene (PFP) thin films with different molecular orientations (lying on HOPG and standing on SiO_2) to a precision of 0.1 eV using low-energy inverse photoemission spectroscopy (LEIPS) to confirm their molecular orientation dependence (Figure 2). On the basis of the determined electron affinities and the corresponding data of ionization energies in the solid state, and other relevant energy parameters, we evaluate the individual contribution of these effects quantitatively, with the aid of theoretical calculations. It turns out that the bandwidth ($2w_+$ and $2w_-$ for HOMO- and LUMO-derived bands, respectively) as well as the polarization energy (P_+ and P_- for a hole and an electron, respectively), in particular, the polarization energy of the thin film (P_+^{film} and P_-^{film}), which depends on the molecular orientation, contributes to the ionization energy (I_s) and electron affinity (A_s) in the solid state, while the effect of the surface dipole d is a few tenths of an eV at most and does not vary with the molecular orientation (Figure 3). As a result, we conclude that the I_s and A_s values of an organic thin film—key energy parameters characterizing the electronic structure of its frontier electronic states—are determined by corresponding values of component molecules under polarization energy and the energy dispersion, and that the molecular orientation dependence of the ionization energy and electron affinity of organic solids originates from the orientation-dependent polarization energy in the film.

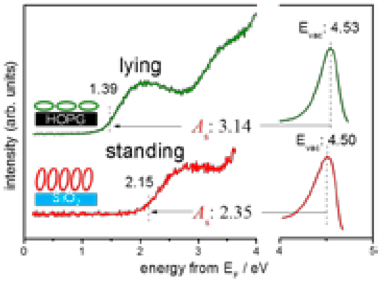


Figure 2. LEIPS spectra of pentacene thin films on HOPG and SiO_2 substrates together with the first derivatives of the sample current spectra to determine the vacuum level E_{vac}.

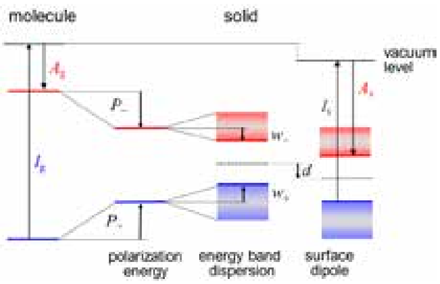


Figure 3. Schematic energy-level correlation diagram showing ionization energy and electron affinity in gaseous and solid states.

Advanced Research Center for Beam Science
– Particle Beam Science –

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

Assoc Prof
IWASHITA, Yoshihisa
(D Sc)

Techn Staff
TONGU, Hiromu

Researchers(pt)

HOKONOHARA, Hisao
KAZAMA, Ichiro

Lect (pt)

SHIMIZU, Hirohiko M. (D Sc) Laboratory for Particle Properties, Department of Physics, Nagoya University

Students

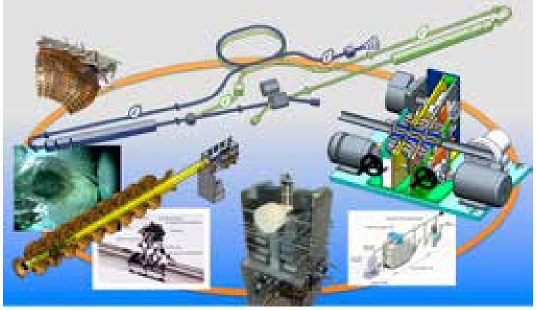
IMAJO, Sohei (D3)
FUWA, Yasuhiro (D3)
KITAHARA, Ryunosuke (D2)
IKEDA, Hideki (M2)

Guest Scholar

JAMESON, Robert A. (Ph D) Goethe University, Frankfurt Germany, 8 April-11 April. 10 November-30 November.

Scope of Research

Particle accelerators have contributed to the progress of science in a variety of fields. Our current research is in neutron science and participation in the International Linear Collider (ILC) project. The following subjects are our focus: 1) neutron beam focusing by modulating sextupole magnets, 2) neutron acceleration/deceleration, 3) compact neutron source including ion source, 4) permanent quadrupole magnets for final focusing of ILC, 5) nondestructive inspections for superconducting accelerating tube towards higher yield and performance and multi layered film structure for RF, and 6) their subsidiary subjects.



KEYWORDS
Beam Physics
Phase Rotation
Accelerator Physics
International Linear Collider
Neutron Optics

Selected Publications

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.*, **043G01,** (2015).

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

Fuwa, Y.; Iwashita, Y.; Tongu, H.; Kitahara, R.; Matsumoto, T.; Michizono, S.; Fukuda, S., Focusing System with Permanent Magnets for Klystrons, *IEEE Trans. on Applied Supercond.*, **24,** 0502005 (2014).

White, G. R.; Ainsworth, R.; Akagi, T.; Alabau-Gonzalvo, J.; Angal-Kalinin, D.; Araki, S.; Aryshev, A.; Bai, S.; Bambade, P.; Bett, D. R.; Blair, G.; Blanch, C.; Blanco, O.; Blaskovic-Kraljevic, N.; Bolzon, B.; Boogert, S.; Burrows, P. N.; Christian, G.; Corner, L.; Davis, M. R.; Faus-Golfe, A.; Fukuda, M.; Gao, J.; Garc´ıa-Morales, H.; Geffroy, N.; Hayano, H.; Heo, A. Y.; Hildreth, M.; Honda, Y.; Huang, J. Y.; Hwang, W.H.; Iwashita, Y.; Jang, S.; Jeremie, A.; Kamiya, Y.; Karataev, P.; Kim, E. S.; Kim, H. S.; Kim, S. H.; Kim, Y. I.; Komamiya, S.; Kubo, K.; Kume, T.; Kuroda, S.; Lam, B.; Lekomtsev, K.; Liu, S.; Lyapin, A.; Marin, E.; Masuzawa, M.; McCormick, D.; Naito, T.; Nelson, J.; Nevay, L. J.; Okugi, T.; Omori, T.; Oroku, M.; Park, H.; Park, Y. J.; Perry, C.; Pfingstner, J.; Phinney, N.; Rawankar, A.; Renier, Y.; Resta-L´opez, J.; Ross, M.; Sanuki, T.; Schulte, D.; Seryi, A.; Shevelev, M.; Shimizu, H.; Snuverink, J.; Spencer, C.; Suehara, T.; Sugahara, R.; Takahashi, T.; Tanaka, R.; Tauchi, T.; Terunuma, N.; Tom´as, R.; Urakawa, J.; Wang, D.; Warden, M.; Wendt, M.; Wolski, A.; Woodley, M.; Yamaguchi, Y.; Yamanaka, T.; Yan, J.; Yokoya, K.; Zimmermann, F., Experimental Validation of a Novel Compact Focusing Scheme for Future Energy Frontier Linear Lepton Colliders, *PHYSICAL REVIEW LETTERS*, **112,** 034802 (2014).

RF Synchronized Short Pulse Laser Ion Source

In order to enhance the accelerating efficiency of a front-end ion accelerator and develop a compact ion beam injector, we were studying an RF synchronized short pulse laser ion source.

The interaction between lasers and matter is promising for producing high current ion beams. In conventional laser ion sources, laser plasma is produced in a field-free region with a laser pulse whose pulse duration is more than a few nanoseconds. In this case, laser plasma expands before ions are extracted and the pulse length of obtained ion beams is over a few microseconds. Since the operating frequencies of RF ion accelerators are usually between a few tenths of MHz and a few hundred MHz, the ion beam must be bunched before acceleration. To keep beam emittance low, bunching should be performed adiabatically and the length of bunching section must be long. If an ion source can produce a short pulse ion beam, ions can be accelerated without the bunching process and the bunching section is no longer needed. An interaction between matter and ultra-short (femto-second) pulse laser would allow production of plasma with a short pulse structure (<5 ns). If the production of the plasma occurs in RF electric field, ions can be extracted without expanding, and pulse length of obtained ion beam would be shorter than 5 ns. Ion beams can be accelerated as micro bunches (Figure 1) by connecting an RFQ (radio frequency quadrupole) linear accelerator to this ion source directly.

A proof-of-principle experiment was performed to produce a short pulse laser ion beam. In this experiment, hydrogen gas was ionized with 40 fs laser in RF electric field. To generate the longitudinal RF electric field, a 53.3 MHz RF resonator was designed and fabricated (Figure 2 and 3). The Q factor of the resonator was 190 and the gap voltage was 2.5 kV with 250 W input power. A pulse gas valve unit with a piezoelectric element was set in the resonator and a H_2 gas jet was supplied into the laser interaction region just before laser irradiation.

Tuning the laser power density to 10^{14}–10^{15} W/cm^2, charge particles extracted by RF electric field were detected by the ion probe at the exit of RF resonator. The detected current was changed depending on initial RF phase (Figure 4). Positive current was detected in a phase range between 180 degrees and 270 degrees. The pulse length of the ion beam was 3.1 ns (FWHM) and the peak current was up to 1.2 mA with an initial RF phase of 240 degrees. This pulse length is short enough to inject into the accelerating section of RFQ to enhance its accelerating efficiency of RFQ.

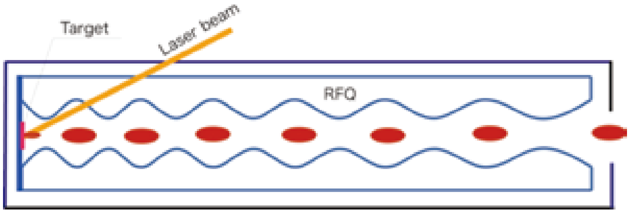


Figure 1. A schematic image of direct injection of bunched ion beam into RFQ.

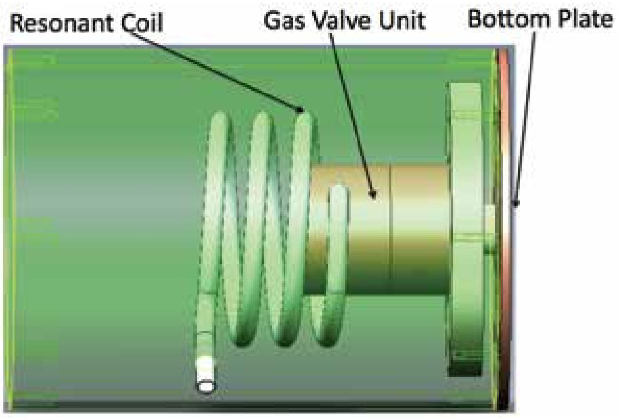


Figure 2. Design of RF resonator.

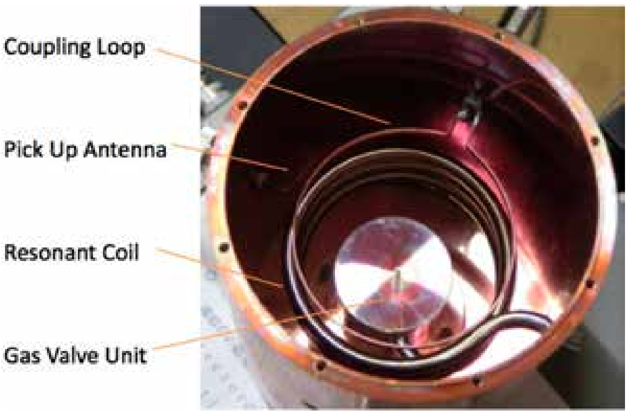


Figure 3. Fabricated RF resonator.

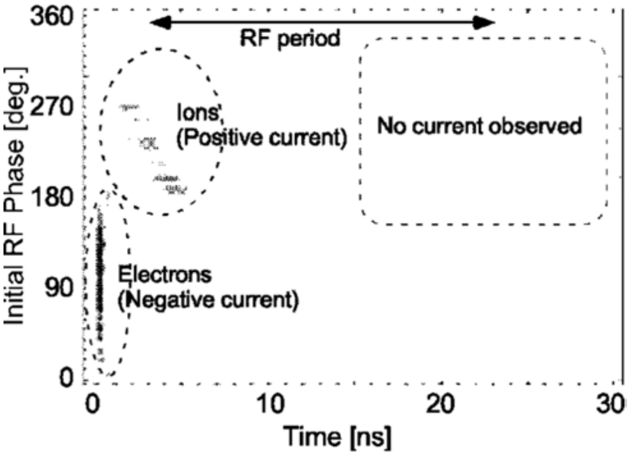


Figure 4. Measured current at the exit of the RF resonator with various RF phases.

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

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

Prof
SAKABE, Shuji
(D Eng)

Assoc Prof
HASHIDA, Masaki
(D Eng)

Assist Prof
INOUE, Shunsuke
(D Sc)

PD
NAKAMIYA, Yoshihide
(D Sc)

Lect (pt)

TOKITA, Shigeki (D Eng)   Osaka University

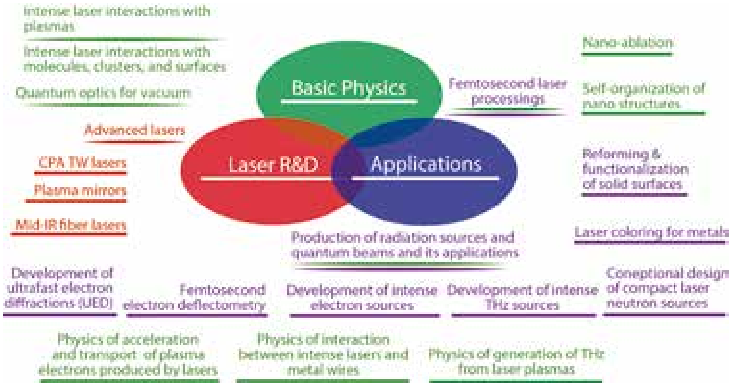
Students

MORI, Kazuaki (D2)	WATANABE, Kota (M2)
TERAMOTO, Kensuke (D1)	NAKAJI, Ryosuke (M1)

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

Miyasaka, Y.; Hashida, M.; Nishii, T.; Inoue, S.; Sakabe, S., *Appl. Phys. Lett.*, **106,** 013101 (2015).
Inoue, S.; Tokita, S.; Hashida, M.; Sakabe, S., *Phys. Rev. E*, **91,** 043101 (2015).
Tokita, S.; Sakabe, S.; Nagashima, T.; Hashida, M.; Inoue, S., *Scientific Reports*, **5,** 8268 (2015).
Hashida, M.; Miyasaka, Y.; Inoue, S.; Nishii, T.; Shimizu, M.; Inoue, S.; Sakabe, S., *IEEJ Trans. FM*, **135,** 575-580 (2015).
Hasebe, T.; Homma, K.; Nakamiya, Y.; Matsuura, K.; Otani, K.; Hashida, M.; Inoue, S.; Sakabe, S., *Prog. Theor. Exp. Phys.*, **2015,** 073C01 (2015).

Intense Laser Interaction with a Thin Foil and Its Induced Surface Wave along a Neighbor Metal Wire

In recent years, generation of intense terahertz pulses has been achieved by intense femtosecond laser pulses, opening up prospects for studying non-linear optics of material at frequencies in the terahertz range. To generate intense terahertz pulses, an essential subject is to understand the optical damage of the wavelength conversion element that converts femtosecond laser pulses into terahertz pulses, such as nonlinear crystal. Laser plasmas, with no optical damage limitation, are an attractive terahertz radiation source. Recently, we demonstrated the generation of strong sub-terahertz surface waves by irradiating a metal wire directly with intense laser pulses. The amplitude and pulse width of the surface wave were evaluated to be 200 MV/m and 7 ps, respectively. It is considered that the sub-terahertz surface waves are driven by mass movement of laser-accelerated electrons and the waves are transmitted along the laser-irradiated wire. To separate the generation and transmission parts of the sub-terahertz surface waves is significant from an application standpoint, because it would improve the repetition rate and ease-of-use of the transmission part. We provide a new technique to separate the generation and transmission parts of strong terahertz waves. By placing the metal wire (i.e., the transmission part) near the intense laser plasma (i.e., the generation part), we succeeded in measuring the sub-terahertz surface waves propagated along the metal wire.

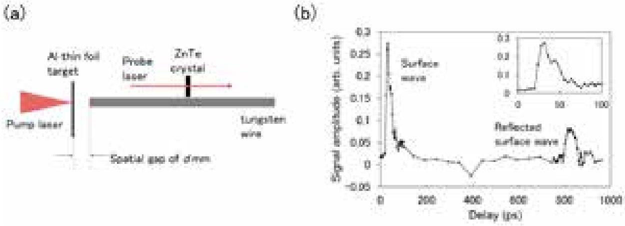


Figure 1. (a) Schematic of the experimental setup; (b) Surface wave measured by electro-optical sampling.

Orientation of Periodic Grating Structures Controlled by Double-pulse Irradiations

The experiment for the formation of laser induced periodic surface structures (LIPSS) has been demonstrated on a titanium surface irradiated by a double-pulse beam cross-polarized in a time delay of Δτ = 0 to 40ps. The first pulse fluence F_1 and the delayed pulse fluence F_2 were always kept below the formation threshold F_{TH} = 65mJ/cm^2 of the periodic grating structure on Ti. We found that the periodic grating structures with a LIPSS orientation of 45° relative to both polarizations were produced with a time delay of 0–120 fs. To control the LIPSS orientation, the experiment of double pulse beam with a time delay of 0 fs has been demonstrated, in which a beam composed of a first pulse with constant fluence of F_1 = 70 mJ/cm^2 and a delayed pulse varying from F_2 = 0 to 70 mJ/cm^2. The LIPSS orientations were in the range of 0–45° and decreasing as the normalized fluence F_2/F_1 decreases. We found that the orientation of LIPSS produced by double pulse irradiations was in relatively good agreement with the direction obtained by the vector sum of laser fields, $E_1{}^4$ and $E_2{}^4$. The tendency suggests that the orientation of LIPSS might be characterized by multi-photon process at the metal surface.

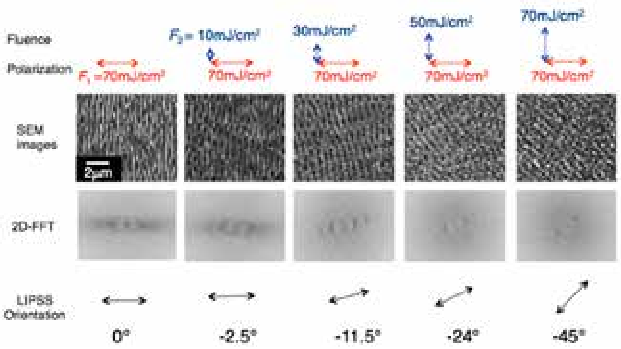


Figure 2. The dependence of periodic structure interspaces on the laser fluence of first pulse F_1 for the delayed pulse fluence of F_2 = 70 mJ/cm^2.

Intense THz Emission from Cluster Plasma Produced by Two-color Laser Pulse

Terahertz (THz) waves are expected to have use in great variety of applications, such as information and communication technology, safety and security, bio-sensing, and medicine. To make these applications practicable, more intense THz pulses are desired. Some concepts and techniques to generate intense THz pulses have been proposed. However, incidental laser energy is limited by the damage threshold of the materials used for the THz source. Laser plasmas have the benefit of being damage-free as a THz-wave source. Therefore, THz radiation from plasmas produced by intense femtosecond laser pulses has been studied to explore the potential of future intense THz sources. We have studied THz radiation from argon cluster plasmas produced by an intense two-color laser pulse. The angular distribution of THz radiation has been measured for laser energy of 10 mJ and laser pulse durations of 200 fs. The THz emission generated from argon cluster plasma is enhanced by irradiation with fundamental and second harmonic pulses.

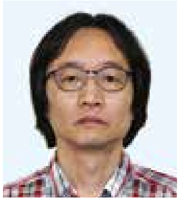
Advanced Research Center for Beam Science
– Electron Microscopy and Crystal Chemistry –

http://eels.kuicr.kyoto-u.ac.jp:8080/Root/English


Prof
KURATA, Hiroki
(D Sc)


Assist Prof
NEMOTO, Takashi
(D Sc)


Assist Prof
HARUTA, Mitsutaka
(D Sc)


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


Program-specific Res*
KIYOMURA, Tsutomu

*Nanotechnology Platform

Assist Techn Staff

HIRAIZUMI, Yuri

Students

FUJIYOSHI, Yoshifumi (D3)
YAMAGUCHI, Atsushi (D2)
LAI, Ming Wei (D1)
TOMISAKI, Yuriko (M2)
INOUE, Shota (M1)

Scope of Research

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

KEYWORDS
AREELS
Surface Plasmon
Dispersion Relation
Waveguide
Transverse Magnetic Mode

Selected Publications

Minari, T.; Nemoto, T.; Isoda, S., Temperature and Electric-field Dependence of the Mobility of a Single-grain Pentacene Field-effect Transistor, *J. Appl. Phys.*, **99,** [034506-1]-[034506-5] (2006).

Haruta, M.; Kurata, H.; Komatsu, H.; Shimakawa, Y.; Isoda, S., Site-resolved Oxygen K-edge ELNES of Layered Double Perovskite La_2CuSnO_6: *Physical Review B*, **80,** [165123-1]-[165123-6] (2009).

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).

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

Saito, H.; Namura, K.; Suzuki, M.; Kurata, H., Dispersion Relations for Coupled Surface Plasmon-polariton Modes Excited in Multilayer Structures, *Microscopy*, **63,** 85-93 (2014)

Formation of a Hybrid Plasmonic Waveguide Mode Probed by Dispersion Measurement

Guiding light with subwavelength confinement is a critical challenge for nanoscale optical applications. Hybrid waveguides, i.e., dielectric waveguides combined with plasmonic waveguides, have great potential for concomitantly exhibiting subwavelength confinement and long range propagation, enabling a highly integrated photonic circuit. This waveguide mode has been regarded as a coupling of the dielectric waveguide and the surface plasmon-polaritons (SPPs). We report the characterization of hybrid waveguide modes excited in Si/SiO_2/Al films by dispersion measurement using angle-resolved electron energy-loss spectroscopy (AREELS).

Figure 1(a) shows a schematic diagram of AREELS. A narrow slit is placed to be perpendicular to the direction of energy dispersion for the spectrometer at the entrance plane where the angular dispersive (electron diffraction) pattern is formed. The observed two-dimensional AREELS pattern allows us to directly visualize the energy-loss probability as a function of the energy loss E and the component of the scattering vector perpendicular to the direction of incident electrons $q_\perp$ (E–q map). When the incident electrons are normal to the multilayered films, $q_\perp$ can be assumed to be the wave vector k (propagation constant) of the propagating waves in waveguide structures. Therefore, the E–q map directly yields the dispersion relations of the waveguide modes.

The waveguide structures consisting of the multilayered semiconductor–insulator (SI) and semiconductor–insulator–metal (SIM) films were prepared as shown in Figure 1(b). Silicon (Si), silicon dioxide (SiO_2), and aluminum (Al) were chosen as the semiconductor layer, the insulator gap, and the metal layer, respectively. Since the SPP mode supported by the plane surface is the transverse magnetic (TM) mode, we consider the dispersion relations for TM modes only in the present study.

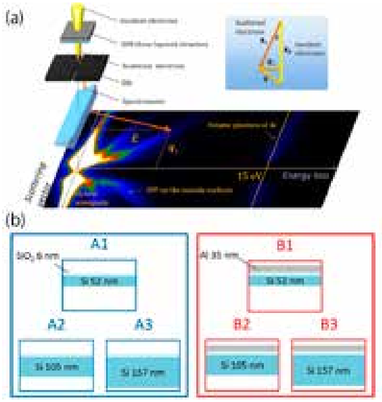


Figure 1. (a) Schematic diagram of AREELS method. k_0 and k_1 represent the wave vectors of incident and scattered electrons, respectively. An angular selection slit is placed at the entrance plane of the spectrometer to limit electron collection to those scattered perpendicular to the direction of energy dispersion. The gap in the center of the slit is closed to prevent the intense direct beam from saturating the CCD detector. The inserted E–q map is taken from B2. (b) Schematics of the specimens.

Figure 2 shows the E–q maps of the SI films (A1, A2, and A3) and SIM films (B1, B2, and B3), in which they are compared with the calculated dispersion relations of light in vacuum, bulk amorphous SiO_2, and Si crystal (white solid lines and curves). On the E–q map in Figure 2(b), the dispersion curve of the lowest TM mode (TM_0) appears in the region between the light lines in vacuum and Si bulk. This is a feature of Si waveguide modes. When the thickness of the Si film is increased, dispersion curves of two TM modes are observed, as shown in Figure 2(c). The dispersion curve of the TM_0 mode shifts to the lower energies with increasing Si thickness. This behavior is characteristic of dielectric waveguide modes. Figures 2(d)–2(f) show the E–q maps measured from SIM films (B1, B2, and B3). A new dispersion curve clearly appears in the E–q map of Figure 2(d), whereas no dispersion curve was detected for the corresponding SI film (A1), as seen in Figure 2(a). This dispersion curve might be related to the SPP excited on the Al/SiO_2 interface. Moreover, when the thickness of the Si film in SIM structures is increased, the dispersion curves shift to lower energies (see Figure 2(e) and 2(f)), similar to SI films. The new peaks observed in the SIM film (B2) are lower than those of the Si waveguide (TM_0) mode in the SI film (A2), which suggests that the new excitation mode arises from the coupling between the SPPs on the Al/SiO_2 interface and the TM_0 modes in the Si film, representing a hybrid waveguide mode.

A hybrid mode can be characterized in terms of the effective index, defined as the propagation constant of waveguide mode divided by the wave vector in vacuum. With increasing Si waveguide layer thickness, the critical energy, where effective indexes of the TM_0 and SPP modes intersect, giving maximum coupling seems to decrease, which suggests that the energy of effective hybrid coupling can be controlled by adjusting the thickness of the dielectric waveguide layer.

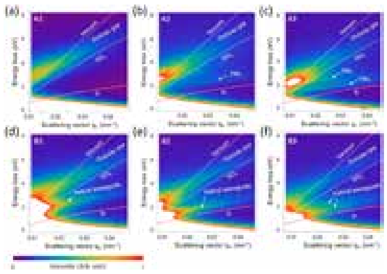


Figure 2. E–q maps of (a) A1, (b) A2, (c) A3, (d) B1, (e) B2, and (f) B3. White solid curves and lines are calculated dispersion relations of light in bulk Si, bulk SiO_2, and vacuum. The red curve represents the relationship between the energy and $q_\perp$ of Čerenkov radiation excited by 200 keV electrons in bulk Si.

Advanced Research Center for Beam Science
– Structural Molecular Biology –

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

Prof
HATA, Yasuo
(D Sc)

Assoc Prof
ITO, Yoshiaki
(D Sc)

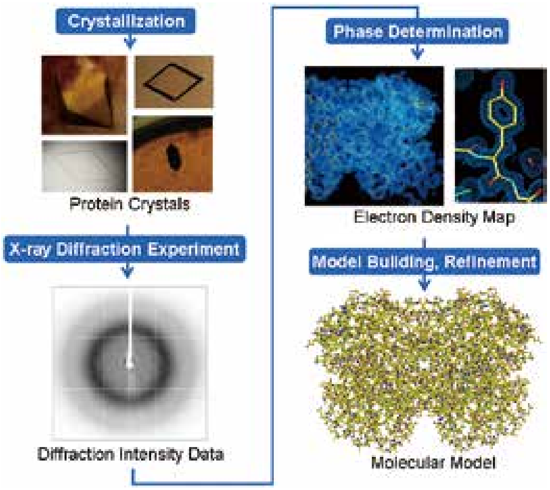
Assist Prof
FUJII, Tomomi
(D Sc)

PD
YAMAUCHI, Takae
(D Agr)

Scope of Research

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

The research activities in this laboratory are on X-ray structural analyses of biological macromolecules and the investigation of the electronic state in materials as follows: 1) the main subjects of the biomacromolecular crystallography are crystallographic studies on the reaction mechanism of enzymes, 2) the relationship between the multiform conformation and the functional variety of proteins, and 3) the mechanisms underlying the thermostabilization of proteins. In the investigation of the chemical state in materials, the characteristics of the chemical bonding in the atom and molecules are investigated in detail using a newly developed X-ray spectrometer with high-resolution in order to elucidate the property of materials. The theoretical analysis of the electronic states with DV-Xα and WIEN2k, and the development of a new type of X-ray spectrometer with ultra high resolution have also been carried out.



Selected Publications

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

Hayashida, M.; Fujii, T.; Hamasu, M.; Ishiguro, M.; Hata, Y., Similarity between Protein-Protein and Protein-Carbohydrate Interactions, Revealed by Two Crystal Structures of Lectins from the Roots of Pokeweed, *J. Mol. Biol.*, **334,** 551-565 (2003).

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

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

Fujii, T.; 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).

Crystallographic Structure Analysis of Aspartate Racemase from *Thermococcus litoralis* DSM 5473

Amino-acid racemases are responsible for the racemization of amino acids and can be mainly grouped into two families, pyridoxal 5'-phosphate (PLP) dependent and PLP independent. Aspartate racemase catalyzes the interconversion between L- and D-aspartate and belongs to the PLP-independent racemase group. The enzyme is thought to employ a two-base mechanism to catalyze both the directions of racemization and utilize two cysteine residues as the conjugated catalytic acid and base in the catalytic reaction. To elucidate the structure-function relationship and the thermostability of aspartate racemase, we have determined the crystal structure of aspartate racemase from *Thermococcus litoralis* DSM 5473 (TlAspR). TlAspR has maximum activity at 95 °C.

Initial crystallization experiments were performed by the sitting-drop vapour-diffusion method using Crystal Screen, Crystal Screen 2, PEGRx 1, PEGRx 2 (Hampton Research), Wizard I, and Wizard II (Emerald BioSystems). Crystals were obtained after several days with the solution PEGRx 2 #17. The crystallization conditions were optimized based on those of the solution. The final conditions produced plate-shaped crystals with approximate dimensions of 0.15 × 0.06 × 0.03 mm at 20 °C in 1 week using the sitting-drop vapour-diffusion method with seeding technique (Figure 1). Drops of 1 µl protein solution at 12 mg/ml (in 20 mM Tris-HCl buffer pH 8.0, 0.01%(v/v) β-mercaptoethanol) and 1 µl reservoir solution were equilibrated against 500 µl reservoir solution consisting of 24% (w/v) PEG1500, 0.2 M L-proline, and 0.1 M HEPES pH 7.5.

Figure 1. Crystal of aspartate racemase from *Thermococcus litoralis* DSM 5473.

Diffraction experiments were performed at beamline BL-5A, Photon Factory (Tsukuba, Japan). The crystal was flash-cooled in a nitrogen stream at 100 K. Diffraction data were collected at a wavelength of 1.000 Å using a Quantum 315r CCD detector set to 142.3 mm in a crystal-to-detector distance. The crystals belonged to space group $P2_12_11$ with unit cell parameters of $a = 90.26$, $b = 125.78$, and $c = 40.64$ Å. The data set was collected at 1.6 Å resolution and has 65,774 independent reflections with 98.3% completeness. The asymmetric unit contained one dimeric molecule of TlAspR with a corresponding crystal volume per protein mass (V_M) of 2.32 Å^3/Da and a solvent content of 47%. The crystal structure has been determined by molecular replacement. The current model was refined at 1.6 Å resolution to an R-factor of 19.3% (R_{free} = 24.0%).

In crystals, TlAspR adopts a homodimeric form. The subunit consists of two domains: the N-terminal domain (residues 1–101 and 213–228) and the C-terminal domain (residues 102–212). In each domain, a central four-stranded parallel β-sheet is flanked by six α-helices. The spatial arrangement of the strictly conserved residues Cys83 and Cys194 strongly indicates that the active site of TlAspR must be located in the cleft between the two domains.

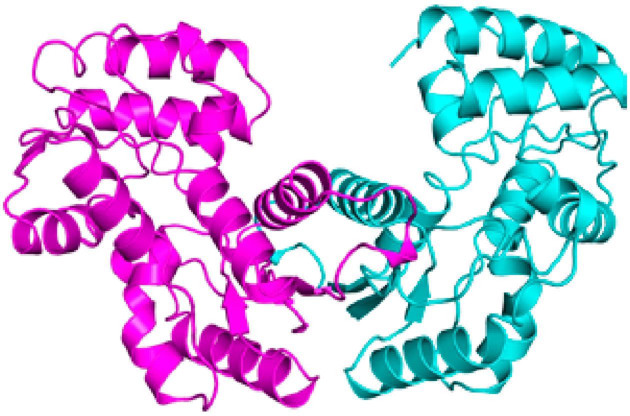


Figure 2. Dimeric molecular structure of aspartate racemase from *Thermococcus litoralis* DSM 5473.

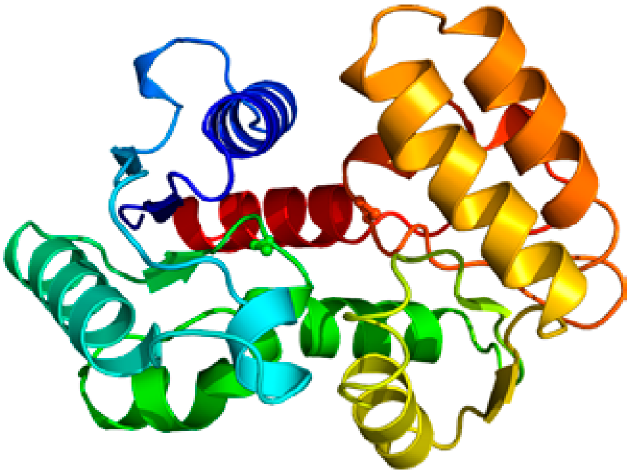


Figure 3. Subunit structure of aspartate racemase from *Thermococcus litoralis* DSM 5473. The strictly conserved residues Cys83 and Cys194 are shown as ball-and-stick models.

International Research Center for Elements Science
– Organic Main Group Chemistry –

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


Prof
NAKAMURA, Masaharu
(D Sc)


Assoc Prof
TAKAYA, Hikaru
(D Eng)


Assist Prof
ISOZAKI, Katsuhiro
(D Eng)


Program-Specific Assist Prof
IWAMOTO, Takahiro
(D Eng)


Program-Specific Res
SUZUKI, Tsuyoshi
(Ph D)


PD
ADAK, Laksmikanta
(Ph D)

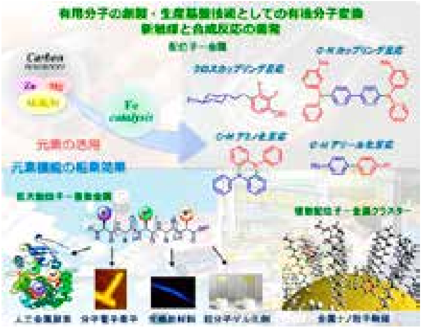

PD
MISHRA, Vijay Lakshmi
(Ph D)

Students

NAKAJIMA, Sho (D2)
YOSHIDA, Ryota (D2)
AGATA, Ryosuke (D1)
AOKI, Yuma (D1)
ISHIBASHI, Kosuke (M2)
SAITO, Shota (M2)
OKUZONO, Chiemi (UG)

Scope of Research

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



KEYWORDS
Selective Organic Reaction Iron Catalyst Metalated Peptide Catalyst Metallic Nanoparticle Catalyst Organic Synthesis

Selected Publications

Kawamura, S.; Agata, R.; Nakamura, M., Regio- and Stereoselective Multisubstituted Olefin Synthesis via Hydro/carboalumination of Alkynes and Subsequent Iron-catalysed Cross-coupling Reaction with Alkyl Halides, *Org. Chem. Front.*, **2,** 1053-1058 (2015).

Jin, M.; Adak, L.; Nakamura, M., Iron-Catalyzed Enantioselective Cross-Coupling Reactions of α-Chloroesters with Aryl Grignard Reagents, *J. Am. Chem. Soc.*, **137,** 7128-7134 (2015).

Agata, R.; Iwamoto, T.; Nakagawa, N.; Isozaki, K.; Hatakeyama, T.; Takaya, H.; Nakamura, M., Iron Fluoride/N-Heterocyclic Carbene Catalyzed Cross Coupling between Deactivated Aryl Chlorides and Alkyl Grignard Reagents with or without β-Hydrogens, *Synthesis*, **47,** 1733-1740 (2015).

Nakagawa, N.; Hatakeyama,T.; Nakamura, M., Iron-Catalyzed Suzuki-Miyaura Coupling Reaction of Unactivated Alkyl Halides with Lithium Alkynylborates, *Chem. lett.*, **44,** 486-488 (2015).

Nakagawa, N.; Hatakeyama, T.; Nakamura, M., Iron-Catalyzed Diboration and Carboboration of Alkynes, *Chem. Eur. J.*, **21,** 4257-4261 (2015).

Takaya, H.; Nakajima, S.; Nakagawa, N.; Isozaki, K.; Iwamoto, T.; Imayoshi, R.; Gower, N.; Adak, L.; Hatakeyama, T.; Honma, T.; Takagi, M.; Sunada, Y.; Nagashima, H.; Hashizume, D.; Takahashi, O.; Nakamura, M., Investigation of Organoiron Catalysis in Kumada-Tamao-Corriu-Type Cross-Coupling Reaction Assisted by Solution-Phase X-ray Absorption Spectroscopy, *Bull. Chem. Soc. Jpn.*, **88,** 410-418 (2015).

Topics

Iron-catalyzed Enantioselective Cross-Coupling Reactions of Alkyl Halides with Aryl Grignard Reagents

Transition-metal-catalyzed enantioselective cross-coupling reactions are powerful tools in the asymmetric synthesis of functional chiral molecules. Recently, we developed the first iron-catalyzed enantioselective cross-coupling reaction. The present reaction provides easy access to a variety of chiral α-aryl esters, which are easily converted to important pharmaceutical compounds such as ibuprofen and naproxen.

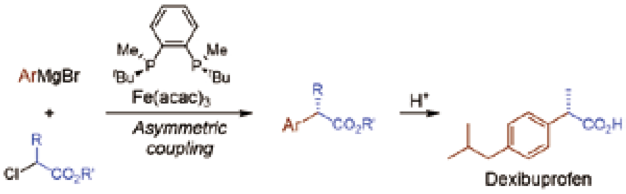


Figure 1. Iron-catalyzed enantioselective cross-coupling reaction of α-chloroesters with aryl Grignard reagents.

Characterization of Solution-phase Organoiron Catalyst by Synchrotron X-ray Absorption Spectroscopy

In the past few decades, iron catalysts have regained much attention in cross-coupling chemistry due to their unprecedented reactivity and practical advantages. However, understanding of their mechanisms remains limited because characterization of organoiron intermediates has been hampered by their paramagnetic character and instability toward air and moisture. Recently, we discovered *in situ* XAFS analysis to be a feasible method to characterize iron intermediates in solution. The methods would also provide valuable mechanistic insight for a variety of transition-metal catalyses as well as iron catalysis. Now, we are trying to clarify the mechanism of several metal-catalyzed reactions by XAFS analysis to investigate effective catalysts and novel reactions.

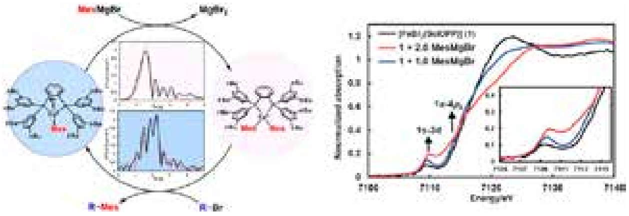


Figure 2. Reaction mechanism of iron-catalyzed KTC-coupling of an arylmagnesium halide with an alkylhalide and the Fe K-edge XAFS spectra of organoiron intermediates.

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-point intermolecular interaction, 3) size-selective synthesis of metallic nanoparticles and clusters, and 4) utilization of plasmonic resonance with light.

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

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

Prof
SHIMAKAWA, Yuichi
(D Sc)

Assoc Prof
KAN, Daisuke
(D Sc)

Assist Prof
SAITO, Takashi
(D Sc)

Program-Specific Assist Prof
ICHIKAWA, Noriya
(D Eng)

PD (JPSJ)
FABIO, Denis Romero
(Ph D)

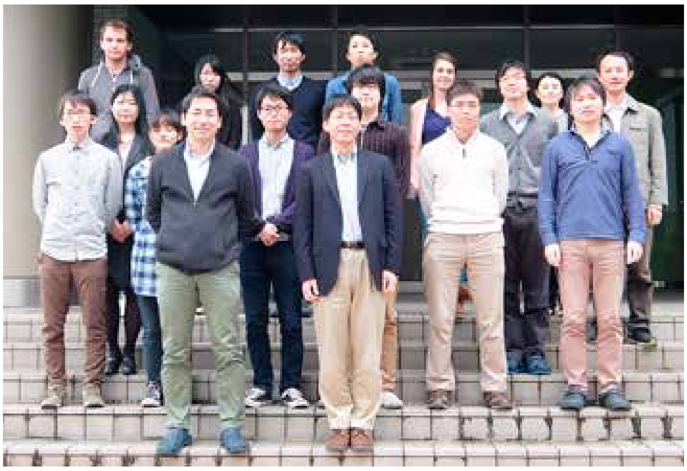
Students

SEKI, Hayato (D3)
HOSAKA, Yoshiteru (D2)
GUO, Haichuan (D2)
XIONG, Peng (D1)
SASAKI, Takahiro (M2)
BABA, Erina (M2)
OZAKI, Yusuke (M1)
NISHIMURA, Tomoe (M1)
WADA, Tamaki (M1)

Scope of Research

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

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



Selected Publications

Hosaka, Y.; Ichikawa, N.; Saito, T.; Manuel, P.; Khalyavin, D.; Attfield, J. P.; Shimakawa, Y., Two-dimensional Charge Disproportionation of the Unusual High-valence State Fe^{4+} in a Layered Double Perovskite, *J. Am. Chem. Soc.*, **137**, 7468-7473 (2015).

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

Matsumoto, K.; Haruta, M.; Kawai, M.; Sakaiguchi, A.; Ichikawa, N.; Kurata, H.; Shimakawa, Y., Selective Reduction of Layers at Low Temperature in Artificial Superlattice Thin Films, *Sci. Rep.*, **1,** [27-1]-[27-14] (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).

Two-dimensional Charge Disproportionation of the Unusual High Valence State Fe^{4+} in a Layered Double Perovskite

Many iron oxides contain Fe^{2+} or Fe^{3+} because these oxidation states are very stable in octahedral and tetrahedral oxygen coordination. In the simple perovskite $AFe^{4+}O_3$ (A = Ca^{2+}, Sr^{2+}, Ba^{2+}) synthesized under strongly oxidizing conditions, however, unusual high oxidation states of Fe like Fe^{4+} can be stabilized. The low-lying Fe-3d orbitals strongly hybridize with O-2p orbitals, and as a result, oxygen p holes (ligand holes, L) are produced in the electronic structure of the perovskites. These ligand holes are the reason that Fe^{4+}, which is expected to have $t_{2g}{}^3e_g{}^1$ electron configuration, does not induce Jahn–Teller distortion like the isoelectronic Mn^{3+} does. The ligand holes are mobile at high temperatures, leading to metallic conduction, but often become unstable at low temperatures. The instability of the high oxidation state of Fe^{4+} is relieved by charge disproportionation (CD) from Fe^{4+} to Fe^{3+} and Fe^{5+}. In the ground state, the ligand holes are localized alternately at the Fe sites, and the CD transition ($2Fe^{4+} \rightarrow Fe^{3+} + Fe^{5+}$) can be described as $2d^5\underline{L} \rightarrow d^5 + d^5\underline{L}^2$.

In this paper, we investigated the CD and magnetic transition behaviors in the newly discovered layered double-perovskite Ca_2FeMnO_6 with a two-dimensional arrangement containing high valence Fe^{4+} at room temperature. The new compound, Ca_2FeMnO_6, is a fully oxygenated double perovskite Ca_2FeMnO_6 with a layered arrangement of $Fe^{4+}O_6$ and $Mn^{4+}O_6$ octahedra (Figure 1) and is the first compound that has an isolated two-dimensional layered arrangement of high valent Fe^{4+}. This oxide was obtained by low-temperature topochemical oxidation of the brownmillerite Ca_2FeMnO_5. Our analysis of the low-temperature neutron diffraction patterns revealed that below 95 K, the charge-disproportionated Fe^{3+} and Fe^{5+} are ordered in a checkerboard pattern in the two-dimensional FeO_6 octahedral layers and the checkerboard-type layers stack in an in-phase manner. Two-dimensional localization of the ligand holes with effective spins plays an important role in the noncollinear magnetic structure of Ca_2FeMnO_6.

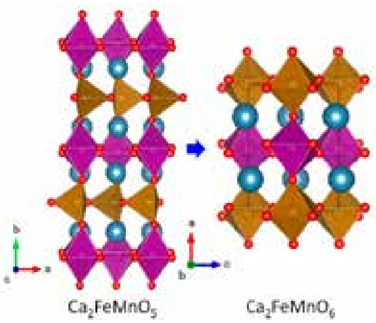


Figure 1. Crystal structure of layered double perovskite Ca_2FeMnO_6 (right) obtained by topochemical oxidation of brownmillerite $CaFe_2MnO_5$ (left) at a low temperature. Blue, brown, purple, and red spheres represent Ca, Fe, Mn, and O ions, respectively.

Significant Strain-induced Increase in Metal–Insulator Transition Temperature in Oxygen-deficient Fe Oxide Epitaxial Thin Films

Transition-metal oxide epitaxial thin films, which often exhibit behaviors different from those of the bulk oxide, have attracted a great deal of attention as a platform for exploring novel functionalities. This is in part because strong correlations between charges, spins, and lattices determine the functional properties of the films, and these correlations are affected by structural distortions from substrate-induced strain effects. While these strain effects have been studied in many fully oxygenated oxides, such as ABO_3 perovskites, those in oxygen-deficient oxides consisting of various oxygen coordination environments like tetrahedra and pyramids as well as octahedra remain unexplored. Substrate-induced modifications of such various oxygen coordination units would provide additional routes to controlling the strong correlations and consequently to modifying or even enhancing the functional properties.

We focused here on oxygen-deficient Fe-based perovskite oxides, $SrFeO_x$ (SFOx), which exhibit a variety of structural and physical properties, depending on their oxygen vacancy concentration, and discovered that an oxygen-deficient $SrFeO_x$ (x~2.8) epitaxial thin film shows a transport behavior markedly different from the corresponding behavior in the bulk material. The present thin film under substrate-induced tensile strain shows a metal-insulator transition associated with charge disproportionation of $Fe^{3.66+}$ into Fe^{4+} and Fe^{3+} at 620 K. This transition temperature is much higher than the 70 K reported for the transition in the bulk material and is also much higher than room temperature. We also found the transition to be accompanied by oxygen-vacancy ordering. This significant increase in the metal-insulator transition temperature demonstrates that epitaxial growth of oxygen-deficient oxides under substrate-induced strain is a promising route for exploring novel functionality.

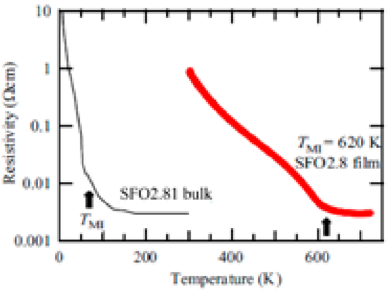


Figure 2. Temperature dependence of the electrical resistivity of SFO2.8 film from 720 to 300 K in air (red line) and $SrFeO_x$ (x ~ 2.81) bulk from 300 to 5 K (black line). The arrows denote the metal-insulator transition temperatures (T_{MI}). The resistivity data of the SFO2.81 bulk were taken from a report by P. Adler et al. (*Phys. Rev. B*, **73**, 094451 (2006)).

International Research Center for Elements Science
– Organotransition Metal Chemistry –

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

Prof
OZAWA, Fumiyuki
(D Eng)

Assist Prof
WAKIOKA, Masayuki
(D Eng)

Assist Prof
TAKEUCHI, Katsuhiko
(D Sc)

Researcher(pt)

ICHIHARA, Nobuko

Students

TAGUCHI, Hiro-omi (D1)
IIZUKA, Eisuke (M2)
TANIGAWA, Ippei (M2)
SASAKI, Daichi (M1)
TAKAHASHI, Rina (M1)
XU, Kai (RS)
TANAKA, Yuto (UG)
YAMASHITA, Natsumi (UG)

Scope of Research

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

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

Selected Publications

Chang, Y.-H.; Tanigawa, I.; Taguchi, H.; Takeuchi, K.; Ozawa, F., Iridium(I) Complexes Bearing a Noninnocent PNP-Pincer Type Phosphaalkene Ligand: Catalytic Application to Base-Free N-Alkylation of Amines with Alcohols, *Eur. J. Inorg. Chem.* (in press).

Chang, Y.-H.; Takeuchi, K.; Wakioka, M.; Ozawa, F., C-H Bond Cleavage of Acetonitrile by Iridium Complexes Bearing PNP-Pincer Type Phosphaalkene Ligands, *Organometallics*, **34,** 1957-1962 (2015).

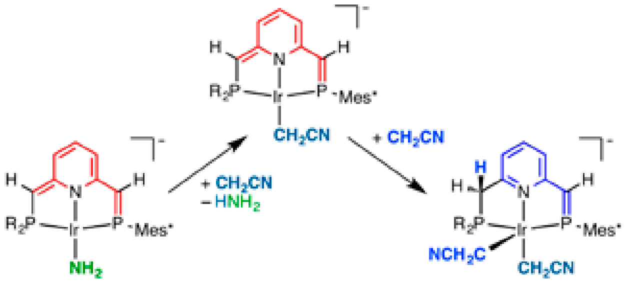
Iizuka, E.; Wakioka, M.; Ozawa, F., Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Synthesis of Donor-Acceptor Polymers with Dithienosilole (DTS) and Thienopyrroledione (TPD) Units, *Macromolecules*, **48,** 2989-2993 (2015).

Taguchi, H.; Chang, Y.-H.; Takeuchi, K.; Ozawa, F., Catalytic Synthesis of an Unsymmetrical PNP-Pincer Type Phosphaalkene Ligand, *Organometallics*, **34,** 1589-1596 (2015).

Wakioka, M.; Nakamura, Y.; Montgomery, M.; Ozawa, F., Remarkable Ligand Effect of $P(2\text{-}MeOC_6H_4)_3$ on Palladium-Catalyzed Direct Arylation, *Organometallics*, **34,** 198-205 (2015).

C–H Bond Cleavage of Acetonitrile by Iridium Complexes Bearing PNP-pincer Type Phosphaalkene Ligands

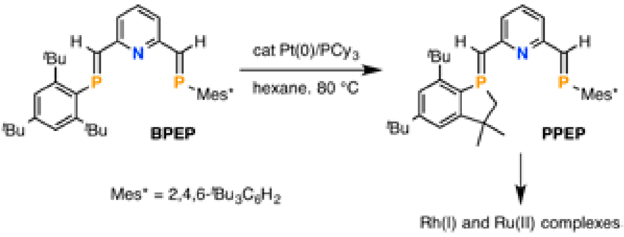
A novel parent amido complex of iridium(I), K[Ir(NH_2)(PPEP*)], coordinated with a dearomatized PNP-pincer-type phosphaalkene ligand (PPEP*) has been prepared by deprotonation with KHMDS from [Ir(NH_2)(PPEP)], with benzophospholanylmethyl and phosphaethenyl groups at the 2,6-positions of pyridine. K[Ir(NH_2)(PPEP*)] has two base points at PPEP* and NH_2 ligands and, thus, successively reacts with two molecules of CH_3CN via heterolytic cleavage of the C–H bond. X-ray structural analysis of the product complex K[Ir(CH_2CN)$_2$(PPEP)] reveals remarkable elongation of the P=C bond, indicative of the occurrence of strong π-back-donation from iridium to PPEP.



Scheme 1. Reaction of [Ir(NH_2)(PPEP)] with acetonitrile.

Catalytic Synthesis of an Unsymmetrical PNP-pincer Type Phosphaalkene Ligand

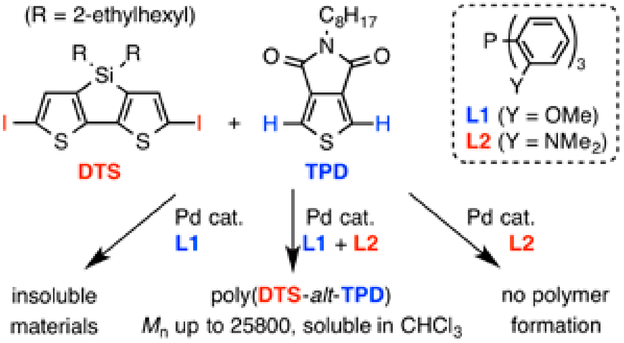
An unsymmetrical PNP-pincer-type phosphaalkene ligand, 2-(phospholanylmethyl)-6-(2-phosphaethenyl)-pyridine (PPEP), has been prepared from 2,6-bis(2-phosphaethenyl)pyridine (BPEP) by intramolecular C–H addition/cyclization of the 2-phosphaethenyl group with a 2,4,6-tri-tert-butylphenyl substituent (CH=PMes*). The reaction proceeds in hexane in the presence of a catalytic amount of [Pt(PCy_3)$_2$] (20 mol %) at 80 °C in a sealed tube, giving PPEP in 32% isolated yield, along with a byproduct of 2,6-bis(phospholanylmethyl)pyridine (BPMP) and a Pt(II) phosphanido complex. The PPEP ligand reacts with [Rh(μ-Cl)(C_2H_4)$_2$]$_2$ and [$RuCl_2$(PPh_3)$_3$] to afford [RhCl(PPEP)] (**1**) and [$RuCl_2$(PPh_3)(PPEP)] (**2**), respectively. Complex **1** easily undergoes C–H addition/cyclization at the other CH=PMes* group to afford the 2,6-bis(phospholanylmethyl)pyridine complex [RhCl(BPMP)] (**3**), whereas **2** is stable against C–H addition/cyclization. Treatment of **2** with ^{t}BuOK forms [RuCl(PPh_3)(PPEP*)] (**4**), coordinated with an unsymmetrical PNP-pincer-type phosphaalkene ligand containing a dearomatized pyridine unit (PPEP*).



Scheme 2. Pt(0)/PCy_3 catalyzed C–H addition/cyclization of BPEP to give PPEP.

A Mixed-ligand Approach to Palladium-catalyzed Direct Arylation Polymerization: Synthesis of Donor–Acceptor Polymers with Dithienosilole (DTS) and Thienopyrroledione (TPD) Units

We examined the synthesis of an alternating copolymer with dithienosilole (DTS) and thienopyrroledione (TPD) units via palladium-catalyzed direct arylation polymerization (DArP). Although DArP is attractive as an easy preparation method of π-conjugated polymers without the need for pre-preparation of organometallic monomers, a major problem is that the resulting polymers are occasionally insolubilized in catalytic systems. We have found that the combined use of P(2-$MeOC_6H_4$)$_3$ (**L1**) and P(2-$Me_2NC_6H_4$)$_3$ (**L2**) ligands enables the synthesis of poly(DTS-*alt*-TPD) with good solubility and high molecular weight (M_n up to 25800), and high yield. NMR investigation into the early stage of polymerization revealed two types of side reactions affording structural defects, oxidative coupling (homocoupling) of TPD-H groups and reduction of DTS-I to DTS-H. The combined use of **L1** and **L2** was also effective in preventing these side reactions.



Scheme 3. Synthesis of donor–acceptor polymers with DTS and TPD units via DArP.

International Research Center for Elements Science
– Photonic Elements Science –

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

Prof
KANEMITSU, Yoshihiko
(D Eng)

Assist Prof
IHARA, Toshiyuki
(D Sc)

Assist Prof
TAHARA, Hirokazu
(D Sc)

PD
TEX, David Michael
(D Eng)

PD
LE, Phuong Quang
(D Sc)

Students

OHNO, Kai (M2)
IBUKI, Hiroto (M2)
YAMADA, Takumi (M2)
HANDA, Taketo (M1)
HIROSHIGE, Nao (M1)

Scope of Research

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

KEYWORDS
Femtosecond Laser Spectroscopy
Carbon Nanotubes
Semiconductor Nanoparticles
Transition Metal Oxides
Semiconductor Nanostructures

Selected Publications

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).

Yamada,Y.; Sato, H. K.; Hikita, Y.; Hwang, H. Y.; Kanemitsu, Y., Measurement of the Femtosecond Optical Absorption of $LaAlO_3/SrTiO_3$ Heterostructures: Evidence for an Extremely Slow Electron Relaxation at the Interface, *Phys. Rev. Lett.*, **111,** [047403-1]-[047403-5] (2013).

Matsunaga, R.; Matsuda, K.; Kanemitsu, Y., Observation of Charged Excitons in Hole-doped Carbon Nanotubes Using Photoluminescence and Absorption Spectroscopy, *Phys. Rev. Lett.*, **106,** [037404-1]-[037404-4] (2011).

Excitation Spectroscopy of Photoluminescence Properties of Single CdSe/ZnS Nanocrystals

The absorption spectrum represents an important aspect of single semiconductor nanocrystals (NCs), revealing their morphology and orientation. By conducting quantitative photoluminescence excitation spectroscopy based on a single-photon counting method, we succeed in clarifying the absorption cross-section spectrum of neutral excitons in single CdSe/ZnS NCs. With the absorption cross section, we reveal that the intensity saturation of the neutral-exciton emission can be explained by the Poisson statistics for incident photons and by the small quantum yield of the biexciton emission. We also quantitatively evaluated the biexciton emission contribution and the ionization rate of NCs that appear at increased incident photon fluxes.

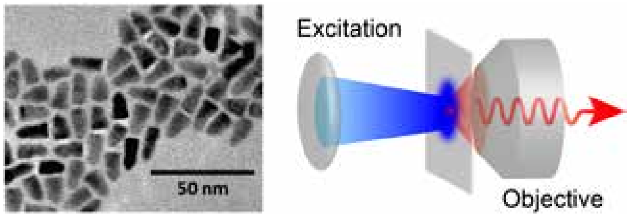


Figure 1. A TEM image of the sample and a schematic diagram of the excitation geometry.

Contactless Characterization of Electrical Subcell Performance for Tandem Solar Cells

Tandem solar cells absorb different spectral parts in several subcells, which are grown in a multilayer structure. World-record conversion efficiencies have been realized, yet there is a significant gap between ideal and realized efficiencies. For optimization, the current generation process must be analyzed. Due to the layered subcell design, it is impossible to physically contact only one subcell and measure its electrical properties, such as current–voltage curves. We proposed a new method to determine the subcell's electrical performance from the power dependence of time-resolved photoluminescence decays.

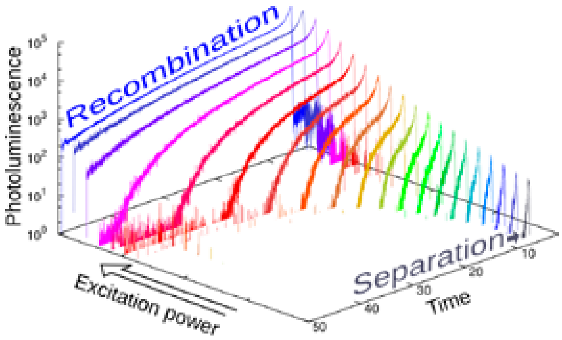


Figure 2. Power dependence of time-resolved photoluminescence decays from the middle subcell of a triple-junction solar cell.

Since this method does not require any contact, all subcells can be probed individually. The charge separation and carrier recombination rates are determined from the photoluminescence decays, allowing us to understand the physics of the current generation in each subcell.

Coherent Control of Photocurrent Dynamics in Bulk GaAs Using Phase-locked Pulses

Photocarrier generation in semiconductors is an essential process that determines the photon-to-current conversion efficiency. To analyze the carrier generation sites in semiconductors, we developed an ultrafast photocurrent spectroscopy using a phase-lock of excitation pulses. In this technique, the relative phase between two excitation pulses is locked to yield constructive or destructive interference. The ultrafast photocurrent dynamics are analyzed by measuring the photocurrent intensity as a function of the delay time between the excitation pulses. By analyzing the time-resolved photocurrent of bulk GaAs, we found that the shallow acceptors are dominant carrier generation sites at room temperature. Furthermore, the photocurrent intensity and direction were successfully controlled by changing the phase-lock conditions.

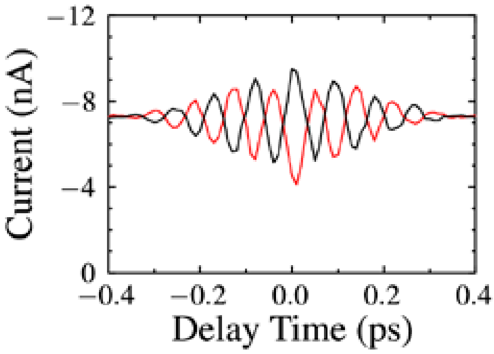


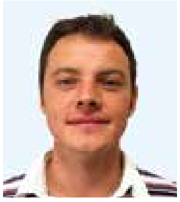
Figure 3. Photocurrent intensity under the constructive (black line) and destructive (red line) phase-lock conditions.

Bioinformatics Center
– Chemical Life Science –

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


Prof
OGATA, Hiroyuki
(D Sc)


Assoc Prof
GOTO, Susumu
(D Eng)


Assist Prof
BLANC-MATHIEU, Romain
(D Sc)


Program-Specific Res
YOSHIZAWA, Akiyasu
(D Sc)

Researchers(pt)

SHIMIZU, Yugo
YAMAMOTO, Rumiko

Lect (pt)

MOGUSHI, Kaoru (D Sc)	Juntendo University

Students

NISHIMURA, Yosuke (D3)
MIHARA, Tomoko (D3)
YOSHIKAWA, Genki (M1)
NISHIYAMA, Hiroki (M1)
KUMABE, Akihiko (UG)
ABDUL HALIM, Arhaime Hamezze (UG)
KHAIRIL ANUAR, Mohammad Fahmi Arieef (UG)
MOHD HASRI, Nurul Nadzirah (UG)
MUHAMAD, Rafidah (UG)

Scope of Research

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

KEYWORDS

GenomeNet
(Meta)genomics
Pharmacoinformatics
Bioinformatics
Evolutionary Biology

Selected Publications

Ogata, H.; Takemura, M., A Decade of Giant Virus Genomics: Surprising Discoveries Opening New Questions, *In "Global Virology I - Identifying and Investigating Viral Diseases", Shapshak, P. et al., Eds., Springer, New York Heidelberg Dordrecht London*, 147-160 (2015).

Takemura, M.; Yokobori, S.; Ogata, H., Evolution of Eukaryotic DNA Polymerases via Interaction between Cells and Large DNA Viruses, *J. Mol. Evol.*, **81,** 24-33 (2015).

Sunagawa, S., *et al.*, Structure and Function of the Global Ocean Microbiome, *Science*, **348,** 1261359 (2015).

Brum, J. R., *et al.*, Patterns and Ecological Drivers of Ocean Viral Communities, *Science*, **348,** 1261498 (2015).

Mihara, T.; Goto, S.; Ogata, H., Diversity and Ecology of Marine Giant Viruses Uncovered from Their Genomes, *Seibutsu no Kagaku, Iden*, **69,** 318-325 (2015) (in Japanese).

Phylogenetic Diversity of Multi-domain Type III Polyketide Synthases in Protists

Polyketides (PKs) are natural products that have diverse chemical structures and biological functions as well as a wide variety of pharmacologically valuable properties. PKs are biosynthesized by polyketide synthases (PKSs) which are classified into three types (I, II, and III) according to their domain structures and subunit organizations. Type III PKSs consist of only a single ketosynthase (KS) domain whereas type I and II PKSs are either multi-domain proteins or protein complexes. Exceptional multi-domain type III PKSs, which contain type I PKS domains and catalyze both type I and III PKS reactions consecutively, have been isolated from a social amoeba (*Dictyostelium discoideum*).

We extracted 1,044 type III PKSs by homology-based genome mining against KEGG GENES to investigate the diversity of the type III PKS. While 1,034 type III PKSs from bacteria, plants, and fungi are single domain proteins, only seven out of ten type III PKSs from the other mostly unicellular eukaryotes (called "protists") are multi-domain proteins. Since the sequenced protist genomes are still taxonomically biased and limited, we further surveyed sequences of the Marine Microbial Eukaryote Transcriptome Sequencing Project, which represents a large number of protist transcriptome sequences. A phylogenetic tree of the resulting 307 protist sequences showed five distantly related clades, suggesting that the protist type III PKSs are more diverse than previously recognized (Figure 1). Among the five clades, four clades contain multi-domain proteins with novel domain organization. Therefore, multi-domain type III PKSs are frequent in and unique to protists. The function of these novel PKSs should be elucidated.

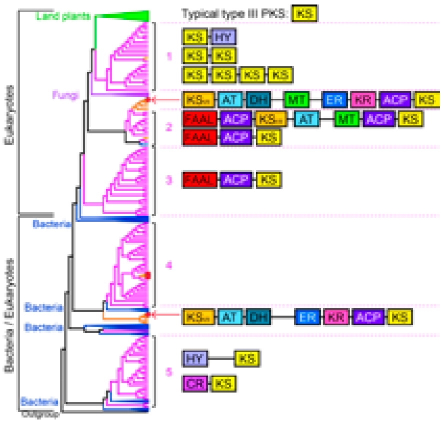


Figure 1. Phylogenetic tree and domain organization diversity of protist type III PKSs. The maximum likelihood tree based on KS domain sequences in type III PKSs and typical multi-domain structures for each clade are indicated. Sequences from genomic data and transcriptomic data are colored orange and magenta, respectively. Experimentally characterized sequences are indicated by red circles.

Investigation of Binding Sites of Arabidopsis Response Regulator Through Chromatin Immunoprecipitation Sequencing

Arabidopsis response regulator 1 (ARR1) is a response regulator in His-Asp phosphorelay. The motif 5'-GAT(C/T)-3' (referred to as the "core motif") is essential for ARR1 to bind to DNA strands. Furthermore, the extended version of the motif, 5'-AAGAT(C/T)TT-3' ("extended core motif"), appears more frequently in promoters directly regulated by ARR1 than in randomly chosen promoters. However, the genomic context of ARR1-binding sites is yet to be fully elucidated.

In this perspective, we used chromatin immunoprecipitation sequencing (ChIP-Seq) data of non-treated (control), water-treated (negative control), and benzyl adenine (activator of ARR1) –treated *Arabidopsis thaliana* (*At*) plants to investigate the binding sites of ARR1. These datasets and *At* reference genome data were used for normalization, and to determine a set of DNA sequences that are preferentially bound by ARR1.

Our initial analysis by MEME performed on the raw dataset did not yield any strongly conserved motifs due to complexity of the data. Therefore, we attempted to reduce data complexity by analyzing the relationship between different variables. As a result, a correlation between sequence length and quality score was found (Figure 2A). We also observed that sequences with scores above 40 contain the reference core motif at a relatively high density (Figure 2B). This result encourages us to continue to refine our dataset to achieve reliable detection of ARR1 binding site features. Alternatively, we are thinking about applying the Motif Centrality Analysis of ChIP-Seq (MOCCS) tool to clarify DNA-binding motif ambiguity. This method comprehensively analyzes and describes the frequency of every k-mer around the binding sites (bound by ARR1 in our case) determined as "peaks" by mapping the ChIP-Seq reads onto the *At* reference genome sequence.

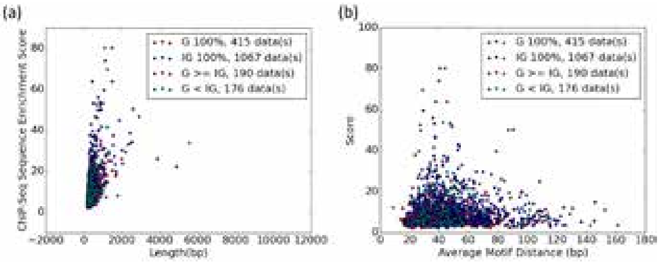


Figure 2. Relationships among different parameters characterizing the binding regions. (A) Relationship between sequence length and ChIP-Seq sequence enrichment score. (B) Relationship between ChIP-Seq sequence enrichment score and average motif distance. G and IG represent genic region and intergenic region, respectively. "G 100%" means that the DNA strand corresponds entirely to genic regions. "IG 100%" means that the DNA strand corresponds entirely to intergenic areas. "G ≥ IG" and "G < IG" mean that the genic regions overlapping with the DNA strands are, respectively, longer or shorter than the intergenic regions.

Bioinformatics Center
– Mathematical Bioinformatics –

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

Prof
AKUTSU, Tatsuya
(D Eng)

Assist Prof
HAYASHIDA, Morihiro
(D Inf)

Assist Prof
TAMURA, Takeyuki
(D Inf)

Students

- NAKAJIMA, Natsu (RF)
- RUAN, Peiying (RF)
- JIRA, Jindalertudomdee (D3)
- BAO, Yu (D2)
- CAO, Yue (M2)
- NGOUV, Hayliang (M2)
- KAWAKAMI, Yuko (M1)
- FUKUSAKO, Yuta (M1)
- LI, Ruiming (RS)

Guest Scholars

HOU, Wenpin (Ph D)	The University of Hong Kong, China, P.R., 25 March–22 August
MÜNZNER, Ulrike (Ph D)	Humboldt University, Germany, 15 April–15 June
CHENG, Xiaoqing (Ph D)	The University of Hong Kong, China, P.R., 22 June–13 July

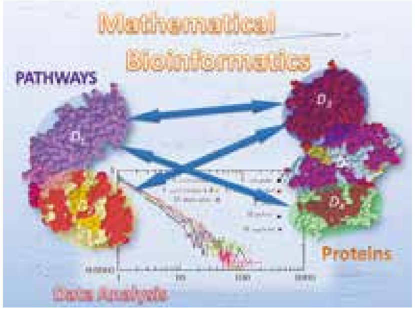
Guest Res Assoc

MELKMAN, Avraham (Ph D)	Ben Gurion University of the Negev, Israel, 18 February-18 April

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
Scale-free Networks
Boolean Networks
Chemical Graphs
Grammar-based Compression
Protein Complexes



Selected Publications

Akutsu, T.; Tamura, T.; Melkman, A. A.; Takasu, A., On the Complexity of Finding a Largest Common Subtree of Bounded Degree, *Theoretical Computer Science*, **590,** 2-16 (2015).
Nacher, J. C.; Akutsu, T., Structurally Robust Control of Complex Networks, *Physical Review E*, **91,** 012826 (2015).
Mori, T.; Takasu, A.; Jansson, J.; Hwang, J.; Tamura, T.; Akutsu, T., Similar Subtree Search Using Extended Tree Inclusion, *IEEE Transactions on Knowledge and Data Engineering*, **27,** 3360-3373 (2015).
Hayashida, M.; Jindalertudomdee, J.; Zhao, Y.; Akutsu, T., Parallelization of Enumerating Tree-like Chemical Compounds by Breadth-first Search Order, *BMC Medical Genomics*, **8(Suppl 2),** S15 (2015).
Kagami, H.; Akutsu, T.; Maegawa, S.; Hosokawa, S.; Nacher, J. C., Determining Associations between Human Diseases and non-coding RNAs with Critical Roles in Network Control, *Scienfitic Reports*, **5,** 14577 (2015).

Similar Subtree Search Using Extended Tree Inclusion

In this research, we consider the problem of identifying all locations of subtrees in a large tree or in a large collection of trees that are similar to a specified pattern tree, where all trees are assumed to be rooted and node-labeled. To calculate the similarity of two trees, tree edit distance is widely used, but it is NP-hard (Non-deterministic Polynomial-time hard) to compute for unordered trees. Therefore, we propose a new similarity measure that extends the concept of unordered tree inclusion by taking the costs of insertion and substitution operations on the pattern tree into account, and present an algorithm for computing it. The proposed algorithm has the same time complexity as the original one for unordered tree inclusion: i.e., it runs in $O(|T1||T2|)$ time, where $T1$ and $T2$ denote the pattern tree and the text tree, respectively, when the maximum outdegree of $T1$ is bounded by a constant. The experimental evaluation conducted using synthetic and real datasets confirms that the proposed algorithm is fast and scalable and very useful for bibliographic matching, which is a typical entity resolution problem for tree-structured data. Moreover, we extend our algorithm to also allow a constant number of deletion operations on $T1$ while still running in $O(|T1||T2|)$ time.

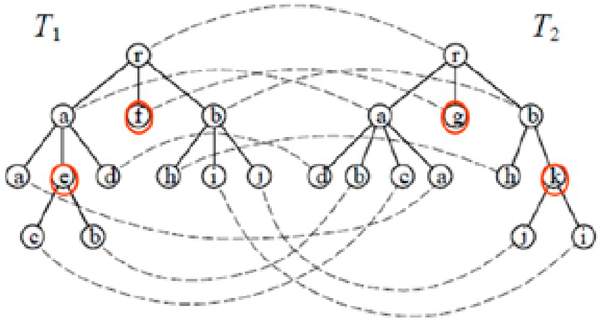


Figure 1. In unordered trees, T_2 is obtained by deletion of the node 'e', insertion of a node 'k', and substitutions of nodes 'f' to 'g' from T_1.

Parallelization of Enumerating Tree-like Chemical Compounds by Breadth-first Search Order

Enumeration of chemical structures is useful for designing and finding new drugs, and determining chemical structures from mass spectrometry. We previously developed efficient algorithms, BfsMulEnum and BfsSimEnum, for enumerating tree-like chemical compounds with and without multiple bonds, respectively. In many instances, the algorithms were able to enumerate chemical structures faster than other existing methods.

Modern computers have multiple processing cores, and are able to execute many tasks simultaneously. In this work, we developed three parallelized algorithms, BfsEnumP1–3, by modifying BfsSimEnum to further reduce execution time. BfsSimEnum constructs a family tree in which each vertex denotes a molecular tree. BfsEnumP1–3 divide a set of vertices with some given depth of the family tree into several subsets, each of which is assigned to a core.

For evaluation, we performed several experiments with varying division depth and number of cores, and showed that BfsEnumP1–3 are useful to reduce the execution time for enumeration of tree-like chemical compounds. In addition, we showed that BfsEnumP3 achieved more than 80% parallelization efficiency using up to 11 cores, and reduced the execution time using 12 cores to about 1/10 of that by BfsSimEnum.

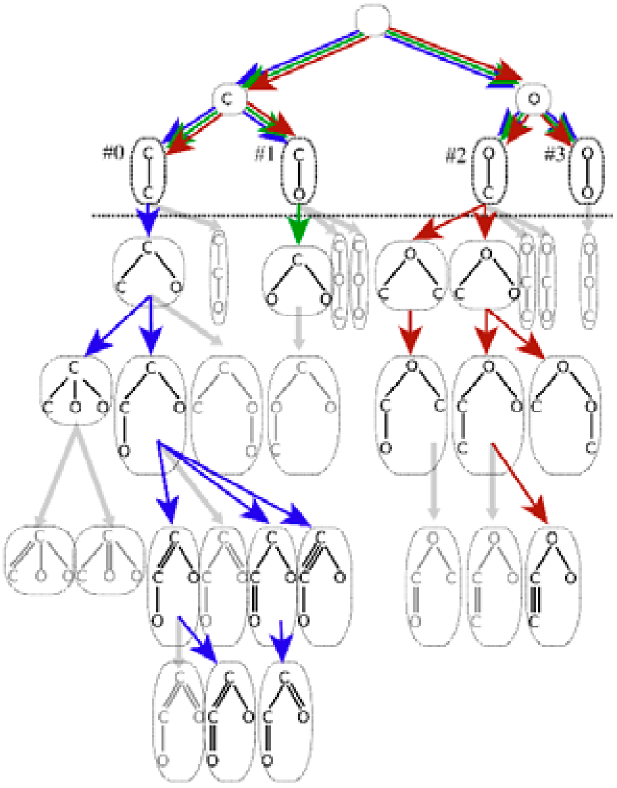


Figure 2. Example of a family tree created by BfsSimEnum and BfsMulEnum for $C_2O_2H_2$ and its separation by BfsEnumP1 with three cores and division depth 2.

Bioinformatics Center
– Bio-knowledge Engineering –

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

Prof
MAMITSUKA, Hiroshi
(D Sc)

Assist Prof
NGUYEN, Canh Hao
(D Knowledge Science)

Assist Prof
YAMADA, Makoto
(D Statistical Science)

Students

MOHAMED, Ahmed (D3)   YOTSUKURA, Sohiya (D3)   TOHZAKI, Yudai (UG)

Guest Scholar

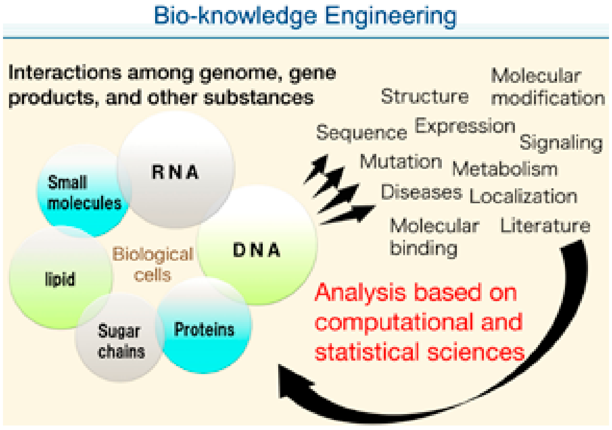
KASKI, Samuel	Aalto University, Finland, 13 October-22 December

Guest Res Assoc

GAO, Junning	Fudan University, China, P.R., 14 October 2015-8 January 2016
KANGASRÄÄSIÖ, Antti	Aalto University, Finland, 26 October-23 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

Zheng, X.; Zhu, S.; Gao, J.; Mamitsuka, H., Instance-wise Weighted Nonnegative Matrix Factorization for Aggregating Partitions with Locally Reliable Clusters, *Proceedings of the 24th International Joint Conference on Artificial Intelligence (IJCAI 2015)*, 4091-4097 (2015).

Liu, K.; Peng, S.; Wu, J.; Zhai, C.; Mamitsuka, H.; Zhu S., MeSHLabeler: Improving the Accuracy of Large-scale MeSH indexing by Integrating Diverse Evidence, *Bioinformatics 31 (12) (Proceedings of the 23rd International Conference on Intelligent Systems for Molecular Biology (ISMB/ECCB 2015))*, i339-i347 (2015).

Yotsukura, S.; Mamitsuka, H., Evaluation of Serum-based Cancer Biomarkers: A Brief Review from a Clinical and Computational Viewpoint, *Critical Reviews in Oncology/Hematology*, **93 (2),** 103-115 (2015).

Shiga, M.; Mamitsuka, H., Non-negative Matrix Factorization with Auxiliary Information on Overlapping Groups, *IEEE Transactions on Knowledge and Data Engineering*, **27 (6),** 1615-1628 (2015).

Mohamed, A.; Nguyen, C. H.; Mamitsuka, H., Current Status and Prospects of Computational Resources for Natural Product Dereplication, (in press).

Selecting Graph Cut Solutions Using Global Graph Similarity

A graph is a general way to represent complex data for analysis. It is a natural way to represent networks, especially in biology, such as metabolic, protein–protein interactions or regulatory networks. Graphs are particularly useful for analyzing high-dimensional data with complicated distributions encountered in various situations in high-throughput biological experiments. Graphs are an integrated framework to analyze expression data of many genes at various time points under many different conditions.

A common data analysis task is *clustering*, which groups similar data points into the same cluster. In the context of graph, similar data points are well-connected clusters with many short paths within the clusters. By grouping these nodes, it is equivalent to *cutting* the edges between the clusters to retain well-connected clusters. Hence, clustering is usually considered a graph cut method.

Clustering on graphs is usually formulated as an optimization problem, of which the objective functions are usually the cut's quality on graphs involving small cut's value (the number of edges being cut) and the balance of a clustering solution in terms of sizes of clusters. However, easily computable objective functions are usually not expressive enough to capture many different scenarios of data. A serious problem is that optimizing the objective functions does not always lead to well-connected clusters. In fact, optimal clustering solutions may even contain disconnected clusters, which defeats the purpose of clustering (Figure 1). Furthermore, detecting disconnected clusters is computationally too expensive to be used in objective functions of clustering algorithms.

Our idea to solve this problem is to use a *global graph similarity* measure named *ged*. It is a measure that, even though computationally too demanding to be used as a clustering objective function, is more expressive for distinguishing undesired clustering solutions that usual objective functions cannot recognize. The motivation is that undesired solutions with disconnected clusters are topologically more different from ones with well-connected clusters. Therefore, global graph similarity of the original graph with clustering solutions could show undesired clustering solutions, even though they could be as optimal as the desired ones.

The measure is formulated with eigenvectors and eigenvalues of the graph Laplacians. It was proved that the measure is equivalent to embedding graphs into a space, then comparing the embedded node sets on the space. In fact, it is equivalent to the standard method for independence measure of HSIC. The global graph similarity measure was used in simulated and real networks and shows that it could detect undesired clustering solutions.

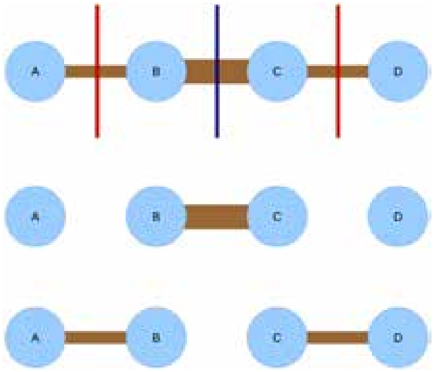


Figure 1. Equally optimal solutions of graph cut clustering on the original graph (top), resulting in an undesired clustering solution (middle), as well as a desired solution (bottom).

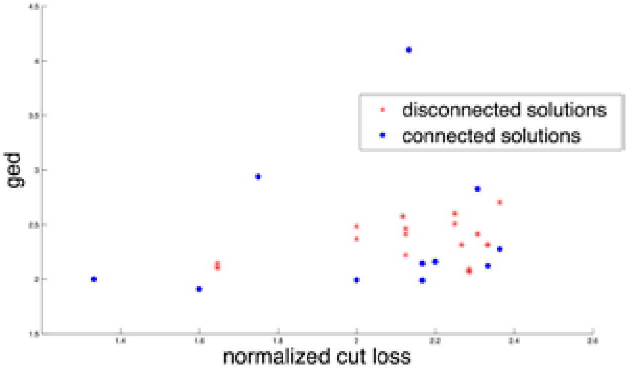


Figure 2. In karate data, *ged* can show that desired solutions with connected clusters tend to have small *ged* compared with the original graph, and can be a candidate for selecting clustering solutions.

HAKUBI RESEARCHERS' ACTIVITIES IN ICR

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

Research Topic

Algorithmic Graph Theory with Applications to Bioinformatics

Host Laboratory Laboratory of Mathematical Bioinformatics

Host Professor AKUTSU, Tatsuya

Program-Specific Assoc Prof
JANSSON, Jesper
(Ph D)

Outline of Research

During 2015, I have worked on several research topics involving graph algorithms, data compression, and bioinformatics together with researchers in Japan, Singapore, and Sweden. One project introduced four graph orientation problems that we call “Max W-Light”, “Min W-Light”, “Max W-Heavy”, and “Min W-Heavy”, where W can be any fixed non-negative integer. In each of these four problems, the input is an undirected, unweighted graph and the objective is to assign a direction to every edge so that the number of vertices with outdegree at most W or at least W in the resulting directed graph is maximized or minimized. A number of results on the computational complexity and polynomial-time approximability of these problems for different values of W and various classes of graphs were derived. In particular, we observed that the special cases Max 0-Light and Min 1-Heavy are identical to the well-known Maximum Independent Set and Minimum Vertex Cover problems, respectively, so by allowing the value of W to vary, we obtained a new, natural generalization of the two latter problems.

ACTIVITIES OF JOINT USAGE/RESEARCH CENTER

JURC Cooperative Research Subjects 2015

(1 April 2015 ~ 31 March 2016)

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

A Study of Magneto-optic and Electro-optic Effects by Laser Induced Pico-second Electromagnetic Pulses
YASUHARA, Ryo, National Institutes of Natural Sciences, National Institute for Fusion Science
Host in JURC SAKABE, Shuji

Fundamental Study on “Stochastic Vacuum Heating” Mechanism in Laser-driven Ion Acceleration
YOGO, Akihumi, Institute of Laser Engineering, Osaka University
Host in JURC SAKABE, Shuji

Development of the Methodology for the Removal of Carbon Contaminant on the Metal Target for the Laser-driven High Energy Heavy Ion Acceleration
NISHIUCHI, Mamiko, Japan Atomic Energy Agency, Quantum Beam Science Directorate
Host in JURC HASHIDA, Masaki

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

Development of Middle Beta Accelerator for the Precise Measurement of Muon g-2/EDM
MIBE, Tsutomu, Institute of Particle and Nuclear Studies, High Energy Accelerator Research Organization
Host in JURC IWASHITA, Yoshihisa

Development of Gas Load Reduction Method for Pulse Ion Sources
ICHIKAWA, Masahiro, Japan Atomic Energy Agency
Host in JURC IWASHITA, Yoshihisa

Development of Neutron Resonance Spin Flipper at BL06(VIN ROSE) at J-PARC/MLF
HINO, Masahiro, Research Reactor Institute, Kyoto University
Host in JURC IWASHITA, Yoshihisa

Study of 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, Faculty of Engineering, Hokkaido University
Host in JURC IWASHITA, Yoshihisa

Synthesis of π-extension Building Block by Iron-catalyzed Diboration of Strained Cyclic Acelylenes
ORITA, Akihiro, Department of Applied Chemistry, Okayama University
Host in JURC NAKAMURA, Masaharu

Development of Silane Alcoholysis Reaction with 2D-arrayed Gold Nanoparticle Catalyst
MIKI, Kazushi, Polymer Materials Unit, National Institute for Materials Science
Host in JURC ISOZAKI, Katsuhiro

Mechanistic Studies of C–H Bond Functionalization Reactions Using Iron and Related Base Metal Catalysts
YOSHIKAI, Naohiko, Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University
Host in JURC NAKAMURA, Masaharu

Development of Novel Pincer-Type Phosphaalkene Ligands and Their Application to Catalytic Reactions
MATSUO, Tsukasa, Faculty of Science and Engineering / Graduate School of Science and Engineering Research, Kinki University
Host in JURC TAKEUCHI, Katsuhiko

Synthesis of Metal Complexes with a High Spin State and Their Applications to Catalysis
NAKAJIMA, Yumiko, Interdisciplinary Research Center for Catalytic Chemistry, National Institute of Advanced Industrial Science and Technology
Host in JURC OZAWA, Fumiyuki

Synthesis of Novel Low-Coordinated Phosphine-Metal Catalysts Based on the Chemistry of Diphosphene
ITO, Shigekazu, Graduate School of Science and Engineering, Tokyo Institute of Technology
Host in JURC OZAWA, Fumiyuki

Investigation of Photoconversion Mechanism in Halide-perovskite Solar Cells
YAMADA, Yasuhiro, Department of Physics, Graduate School of Science Chiba University
Host in JURC KANEMITSU, Yoshihiko

Study for Dielectric Function and Exciton Binding Energy in Semiconductors
SUZUURA, Hidekatsu, Graduate School of Engineering, Hokkaido University
Host in JURC KANEMITSU, Yoshihiko

Characterization of Self-assembled Peptides on Two-dimensional Semiconductor Nanomaterials by Microscopic Photoluminescence Lifetime Measurements
HAYAMIZU, Yuhei, Graduate School of Engineering, Tokyo Institute of Techonology
Host in JURC KANEMITSU, Yoshihiko

Development of PCR-primers Specific to Megaviridae
YOSHIDA, Takashi, Graduate School of Agriculture, Kyoto University
Host in JURC OGATA, Hiroyuki

Pathway Database for Human Gut Microbiome
YAMADA, Takuji, Graduate School of Bioscience and Biotechnology, Tokyo Institute of Technology
Host in JURC GOTO, Susumu

Comparative Genomic Analysis of Parmales and Diatom
KUWATA, Akira, Tohokku National Fisheries Research Institute
Host in JURC OGATA, Hiroyuki

Flexible and Efficient Search Algorithms for Structured Data in Bioinformatics
TAKASU, Atsuhiro, National Institute of Informatics Digital Content and Media Sciences Research Division
Host in JURC AKUTSU, Tatsuya

Analysis and Control of Complex Bipartite Networks
JOSE, C. Nacher, Department of Science, Toho University
Host in JURC AKUTSU, Tatsuya

Biological Data Analysis Based on Statistical Machine Learning Approach
SHIGA, Motoki, Informatics Course, Department of Electrical, Electronic and Computer Engineering, Faculty of Engineering, Gifu University
Host in JURC MAMITSUKA, Hiroshi

Knowledge Discovery from Life-Science Data with Discrete Structures
TAKIGAWA, Ichigaku, Graduate School of Information Science and Technology, Hokkaido University
Host in JURC MAMITSUKA, Hiroshi

Development of Novel Nonalternant Heterocycles toward Electronic Materials
KUROTOBI, Kei, National Institute of Technology, Kurume College
Host in JURC MURATA, Yasujiro

Transition Metal-Catalyzed Dehydrogenative Cyclization Leading to Dithienosiloles and Their Properties
SUGA, Seiji, Graduate School of Natural Science and Technology, Okayama University
Host in JURC MURATA, Yasujiro

Synthesis and Properties of the Supramolecular Spiral Staircase
KURAMOCHI, Koji, Graduate School of Life and Environmental Sciences, Kyoto Prefectural University
Host in JURC KAWABATA, Takeo

Fabrication of Novel Photoacoustic Imaging Probes Using Functional Metal Nanoparticles
ISHIHARA, Miya, National Defense Medical College
Host in JURC TERANISHI, Toshiharu

Dynamical Correlations between Molecules in Polymeric Liquids
SUKUMARAN, Sathish Kumar, Graduate School of Science and Engineering, Yamagata University
Host in JURC MASUBUCHI, Yuichi

Precise Analysis during Processing of Bi-axial Drawing Films
MATSUBA, Go, Faculty of Engineering, Yamagata University
Host in JURC KANAYA, Toshiji

Study on Transportation and Separation of Metal Ions through a Liquid Membrane by Complex Formation with Multidentate
MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education
Host in JURC SOHRIN, Yoshiki

Molecular Studies on Highly Efficient and Colorful Dye-sensitized Solar Cell Device Oriented by Natural Anthocyanins
YOSHIDA, Kumi, Department of Complex Systems Science, Guraduate School of Information Science, Nagoya University
Host in JURC MURATA, Yasujiro

Study on Size- and Shape-dependent Hydrogen Storage in Pd Nanoparticles by Time-resolved Synchrotron XRD Technique
YAMAUCHI, Miho, Kyushu University
Host in JURC TERANISHI, Toshiharu

Analysis of Molecular Structure in a Monolayer of Fluorinated Amphiphilic Molecules
SONOYAMA, Masashi, Graduate School of Engineering, Gunma University
Host in JURC HASEGAWA, Takeshi

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

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

Development of Devices for Ultra-cold Neutrons
KITAGUCHI, Masaaki, Center for Experimental Studies, Kobayashi-Maskawa Institute for the Origin of Particles and the Universe (KMI), Graduate School of Science, Nagoya University
Host in JURC IWASHITA, Yoshihisa

X-ray Analysis of Structure-Function Relationship of Resorcinol Monooxygenase
OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University
Host in JURC FUJII, Tomomi

X-ray Structural Studies on Environmental Adaptation of Psychrophilic Aspartate Racemase
MATSUI, Daisuke, Faculty of Engineering, Toyama Prefectural University
Host in JURC HATA, Yasuo

X-ray Crystallographic Studies on Structure-Function of L-Asparaginase from *T. litoralis*
KATO, Shiro, Organization for Research and Development of Innovative Science and Technology, Kansai University
Host in JURC FUJII, Tomomi

Design and Synthesis of Thermally Activated Delayed Fluorescence Materials and the Organic Light-Emitting Diodes
ADACHI, Chihaya, Center for Organic Photonics and Electronics Research, Kyushu University
Host in JURC KAJI, Hironori

Development of Lignin-binding Metalated Peptide Catalysts for Oxidative Degradation of Wooden Biomasses
WATANABE, Takashi, Research Institute for Sustainable Humanosphere, Kyoto University
Host in JURC NAKAMURA, Masaharu

Synthesis of Cyclic π-conjugated Molecules and Their Properties
SUZUKI, Toshiyasu, Institute for Molecular Science, National Institute of Natural Sciences
Host in JURC YAMAGO, Shigeru

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

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

Colloidal Microparticles with Polymer Brushes for Laser Applications
FURUMI, Seiichi, Faculty of Science Division 1, Tokyo University of Science
Host in JURC OHNO, Kohji

Development of Novel Hole Transport Polymers Based on Carbazole Chromophore
TANI, Keita, Division of Natural Science, Osaka Kyoiku University
Host in JURC TSUJII, Yoshinobu

Molecular Simulation of Cellulosic Janus-type Bottlebrushes toward Chiral Microphase Separation
YAMANE, Chihiro, Faculty of Home Economics, Kobe Women's University
Host in JURC TSUJII, Yoshinobu

Fabrication of Oxide Glass Containing Li for Radiation Applications
YANAGIDA, Takayuki, Kyushu Institute of Technology
Host in JURC MASAI, Hirokazu

Development of Cystine/glutamate Antiporter xCT Inhibitors and Regulation of Cellular Oxidative Stress
SATO, Hideyo, Faculty of Medicine, Niigata University
Host in JURC HIRATAKE, Jun

Elucidation of Oxidation Properties for [N]Cycloparaphenylenes
NISHINAGA, Tohru, Graduate School of Science and Engineering, Tokyo Metropolitan University
Host in JURC YAMAGO, Shigeru

Simulation of Dielectric Relaxation of Polymer Melt under Fast Shear
UNEYAMA, Takashi, Division of Natural Sciences, Graduate School of Natural Science and Technology, Kanazawa University
Host in JURC MASUBUCHI, Yuichi

Fundamental Study on the Characteristics of Molecular Rotor in Clathrate Crystal of Syndiotactic Polystyrene
URAKAWA, Osamu, Graduate School of Science, Osaka University
Host in JURC MATSUMIYA, Yumi

Colloidal Crystallization Dynamics of Aqueous Dispersion of Polymer Microgels
TAKESHITA, Hiroki, Department of Materials Science and Technology, Nagaoka University of Technology
Host in JURC KANAYA, Toshiji

Co-crystallization of Syndiotactic Polystyrene Delta-phase Crystal and Carboxylic Acid
KAWAGUCHI, Tatsuya, Graduate School of Science, Osaka University
Host in JURC KANAYA, Toshiji

Elucidation of Transport Process of Bioactive Trace Metals in the South Pacific Ocean and the Antarctic Ocean(2)
NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kinki University
Host in JURC SOHRIN, Yoshiki

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

Development of Functional Materials Highly Selective for the Separation of Rare Metals
YAMAZAKI, Shoko, Department of Chemistry, Nara University of Education
Host in JURC UMETANI, Shigeo

Synergistic Effect of Surfactants for Solvent Extraction of Rare Metal Elements
KURAHASHI, Kensuke, Environmental and Materials Chemistry Course, Osaka Prefecture University College of Technology
Host in JURC SOHRIN, Yoshiki

Development of Organic Functional Materials Based on Nitrogen-containing π-Conjugated Compounds
IWANAGA, Tetsuo, Department of Chemistry, Faculty of Science, Okayama University of Science
Host in JURC MURATA, Yasujiro

Development of Biofunctional Peptide-modified Exosomes for Drug Delivery
NAKASE, Ikuhiko, Nanoscience and Nanotechnology Research Center, Osaka prefecture University
Host in JURC FUTAKI, Shiroh

Development of a Method Using Cell Penetrating Peptides for Detection of Poly(ADP-ribose) in Breast Cancer Cells
OKUDA, Akiko, Graduate School of Health Sciences, Niigata University
Host in JURC FUTAKI, Shiroh

Material Delivery into Gastrointestinal Epithelium Using Cell-penetrating Peptide (CPP)
OHASHI, Wakana, Graduate School of Medicine and Pharmaceutical Sciences for Research, University of Toyama
Host in JURC FUTAKI, Shiroh

Characterization of Fine Bubbles and Ion Uptake Efficiency of Agricultural Plants
NIHEI, Naoto, Graduate School of Agricultural and Life Sciences, The University of Tokyo
Host in JURC TOKUDA, Yomei

Examination of Randomness of Oxide Glasses using Light-scattering Spectroscopy
KOREEDA, Akitoshi, Ritsumeikan University
Host in JURC MASAI, Hirokazu

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

Introduction of Nanoparticles into Nanogap Electrodes Using Localized Surface Plasmon Resonance Radiation Force
MAJIMA, Yutaka, Tokyo Institute of Technology
Host in JURC TERANISHI, Toshiharu

Study for Local Magnetism of Ferromagnetic Films and Tunnel Magnetoresistance Effect for Development of High Spin Polarized Current Source
TANAKA, Masaaki, Department of Engineering Physics, Electronics and Mechanics, Nagoya Institute of Technology
Host in JURC ONO, Teruo

Effect of Dzyaloshinskii-Moriya-Interaction on Domain Wall Motion
NAKATANI, Yoshinobu, Department of Communication Engineering and Informatics, The University of Electro-Comuunications
Host in JURC ONO, Teruo

Development of the Anticancer Drug Targeting Gamma-glutamylcyclotransferase (GGCT)
KAGEYAMA, Susumu, The Department of Urology, Shiga University of Medical Science
Host in JURC HIRATAKE, Jun

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

Functional Analysis of Miraculin Using *Arabidopsis thaliana*
INOUE, Hiroyasu, Department of Food Science and Nutrition, Nara Women's University
Host in JURC AOYAMA, Takashi

Role of PIP5K and ROP-GTPase in Plant Cell Morphogenesis
KUSANO, Hiroaki, Department of Technology and Science, Tokyo University of Science
Host in JURC AOYAMA, Takashi

Discovery of New Cellular Functions of Acyldopamine
ITO, Akihiro, RIKEN Center for Sustainable Resource Science
Host in JURC UESUGI, Motonari

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

Control of Chromophore Orientation by Means of Dipole-Arrays of Perfluoroalkyl Amphiphile
YAMADA, Norihiro, Graduate School of Education, Chiba University
Host in JURC HASEGAWA, Takeshi

Elucidating Mechanism of the Structural Phase Transition Transforming Optical Properties of Photo-functional Organic Crystals
AMIMOTO, Kiichi, Graduate School of Education, Hiroshima University
Host in JURC SATO, Naoki

Photoconduction Behavior of Radical Dissociative Photochromic Compounds in the Thin-Film State
KATOH, Keiichi, Graduate School of Science, Tohoku University
Host in JURC MURDEY, Richard

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Intense THz Emission for Nonlinear Interaction Physics
NAGASHIMA, Takeshi, Faculty of Science and Engineering, Setsunan University
Host in JURC HASHIDA, Masaki

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

Synthesis and Entanglement Relaxation of Jellyfish-shaped Polymers
TAKANO, Atsushi, Graduate School of Engineering, Nagoya University
Host in JURC WATANABE, Hiroshi

Elucidation of Anisotropic Charge Transport Mechanism in Organic/Inorganic Hybrid Perovskite Single Crystal
SAEKI, Akinori, Graduate School of Engineering, Osaka University
Host in JURC WAKAMIYA, Atsushi

Exploration of Exotic Phenomena Emerged at Oxide Heterointerface by Transmission Electron Microscopy
Aso, Ryotaro, The Institute of Scientific and Industrial Research, Osaka University
Host in JURC KAN, Daisuke

Magnetic and Electric Properties of Complex Iron Oxide Thin Films
FUJII, Tatsuo, Graduate School of Natural Science and Technology, Okayama University
Host in JURC SAITO, Takashi

Mechanisms of Cs Adsorption in Soil and Uptake Behavior of Cs in Agricultural Plants
FUJIMURA, Shigeto, NARO Tohoku Agricultural Research Center
Host in JURC TOKUDA, Yomei

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

The Control of the Antiphase Boundary and the Magnetotransport Property in Ferrimagnetic Spinel Ultrathin Films
NAGAHAMA, Taro, Laboratory of Advanced Materials Chemistry, Graduate School of Engineering, Hokkaido University
Host in JURC ONO, Teruo

Discovery and Modulation of New Cellular Functions of Vitamin D
NAGASAWA, Kazuo, Faculty of Engineering, Tokyo University of Agriculture and Technology
Host in JURC UESUGI, Motonari

Mechanistic Studies of Microbial Degradation of Unsaturated Aliphatic Organohalogen Compounds
KURATA, Atsushi, Faculty of Agriculture, Kinki University
Host in JURC KURIHARA,Tatsuo

Functional Studies on Proteins Involved in the Microbial Metal Respiration
MIHARA, Hisaaki, Department of Biotechnology, College of Life Sciences, Ritsumeikan University
Host in JURC KURIHARA,Tatsuo

SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

Melting Kinetics of Polymer Crystals by Ultra-fast-scan Calorimetry
TODA, Akihiko, Graduate School of Integrated Arts and Sciences, Hiroshima University
Host in JURC KAJI, Hironori

Structure and Function of Polymer for Solar Cell
SATO, Toshifumi, Graduate School of Engineering, Hokkaido University
Host in JURC KAJI, Hironori

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

Elucidation of Properties of Unsymmetrically-Substituted Disilynes
IWAMOTO, Takeaki, Graduate School of Science, Tohoku University
Host in JURC TOKITOH, Norihiro

Synthesis and Structure of Aromatic Compounds Containing a Heavier Group 16 Element
NAGAHORA, Noriyoshi, Department of Chemistry, Fuculty of Science, Fukuoka University
Host in JURC SASAMORI, Takahiro

Study on the Chemical Bonding of Hypervalent Group 15 and 16 Element Compounds Using Precise X-Ray Analysis
MINOURA, Mao, Fuculty of Science, Rikkyo University
Host in JURC TOKITOH, Norihiro

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

Fabrication of Metal Nanowires and Nanomeshes and Their Catalytic Activity
KAWAI, Takeshi, Faculty of Engineering, Tokyo University of Science
Host in JURC KURATA, Hiroki

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

Band Structures of Near-field Coupled Metal Particle Arrays
SANNOMIYA, Takumi, Interdisciplinary School of Science and Engineering, Tokyo Institute of Technology
Host in JURC KURATA, Hiroki

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

Study on Novel Bimetal Nanoclusters by Using High-resolution Mass Spectrometry
NEGISHI, Yuichi, Department of Applied Chemistry, Tokyo University of Science
Host in JURC NAKAMURA, Masaharu

SUBJECTS ENCOURAGING JOINT PROGRAM

The Eleventh International Workshop for East Asian Young Rheologists
TAKAHASHI, Yoshiaki, Institute for Materials Chemistry and Engineering, Kyushu University
Host in JURC WATANABE, Hiroshi

Analysis of Organic Device Materials Using Ultrasensitive Solid-state DNP-NMR
GAËL, De Paëpe, Laboratoire de Resonances Magnetiques, Service de Chimie Inorganique et Biologique, CEA Grenoble
Host in JURC KAJI, Hironori

Investigations of Oxygen Ion Transport by Synchrotron X-ray
MIZUMAKI, Masaichiro, Japan Synchrotron Radiation Research Institute, SPring-8
Host in JURC ICHIKAWA, Noriya; SHIMAKAWA, Yuichi

Korea-Japan Interdisciplinary Collaboration in Chemical Biology and Pharmaceutical Sciences
YOUNGJOO, Kwon, Ewha Womans University, College of Pharmacy
Host in JURC FUTAKI, Shiroh

JURC Publications (Selected Examples)

(until 31 May 2015)

Molecular Interplays Involved in the Cellular Uptake of Octaarginine on Cell Surfaces and the Importance of Syndecan-4 Cytoplasmic V Domain for the Activation of Protein Kinase Cα
Nakase, I.; Osaki, K.; Tanaka, G.; Utani, A.; Futaki, S., *Biochem. Biophys. Res. Commun.*, **446(4),** 857-862 (2014).
Abstract
Arginine-rich cell-penetrating peptides (CPPs) are promising carriers for the intracellular delivery of various bioactive molecules. However, many ambiguities remain about the molecular interplays on cell surfaces that ultimately lead to endocytic uptake of CPPs. By treatment of cells with octaarginine (R8), enhanced clustering of syndecan-4 on plasma membranes and binding of protein kinase Cα (PKCα) to the cytoplasmic domain of syndecan-4 were observed; these events potentially lead to the macropinocytic uptake of R8. The cytoplasmic V domain of syndecan-4 made a significant contribution to the cellular uptake of R8, whereas the cytoplasmic C1 and C2 domains were not involved in the process.

Relaxation Transition in Glass-forming Polybutadiene as Revealed by Nuclear Resonance X-ray Scattering
Kanaya, T.; Inoue, R.; Saito, M.; Seto, M.; Yoda, Y., *J. Chem. Phys.*, **140,** [144906-1]-[044906-5] (2014).
Abstract
We investigated the arrest mechanism of molecular motions in a glass forming polybutadiene near the glass transition using a new nuclear resonance synchrotron X-ray scattering technique to cover a wide time range (10^{-9} to 10^{-5} s) and a scattering vector Q range (9.6–40 nm^{-1}), which have never been accessed by other methods. Owing to the wide time and Q ranges it was found for the first time that a transition of the α -process to the slow β -process (or the Johari-Goldstein process) was observed in a Q range higher than the first peak in the structure factor S (Q) at the critical temperature T_c in the mode coupling theory. The results suggest the important roles of hopping motions below T_c, which was predicted by the recent extended mode coupling theory and the cooperative motions due to the strong correlation at the first peak in S (Q) in the arrest mechanism.

Dielectric and Viscoelastic Behavior of Star-Branched Polyisoprene: Two Coarse-Grained Length Scales in Dynamic Tube Dilation
Matsumiya, Y.; Masubuchi, Y.; Inoue, T.; Urakawa, O.; Liu, C.-Y.; van Ruymbeke, E.; Watanabe, H., *Macromolecules*, **47,** 7637-7652 (2014).
Abstract
cis-Polyisoprene (PI) chain has the type A dipole parallel along the backbone so that its large-scale (global) motion results in not only viscoelastic but also dielectric relaxation. Utilizing this feature of PI, this paper examined dielectric and viscoelastic behavior of star PI probe chains (arm molecular weight $10^{-3}M_a = 9.5–23.5$, volume fraction $\upsilon_1 = 0.1$) blended in a matrix of long linear PI ($M = 1.12 \times 10^6$). The constraint release (CR)/dynamic tube dilation (DTD) mechanism was quenched for those dilute probes entangled with the much longer matrix, as evidenced from coincidence of the frequency dependence of the dielectric and viscoelastic losses of the probe in the blend. Comparison of the probe data in the blend and in monodisperse bulk revealed that the star probe relaxation is retarded and broadened on blending and the retardation/broadening is enhanced exponentially with M_a. This result in turn demonstrates significant CR/DTD contribution to the dynamics of star PI in bulk. The magnitude of retardation was quantitatively analyzed within the context of the tube model, with the aid of the dielectrically evaluated survival fraction of the dilated tube, $\varphi'(t)$, and the literature data of CR time, τ_{CR}. In the conventional molecular picture of partial-DTD, the tube is assumed to dilate laterally, but not *coherently* along the chain backbone. The corresponding *lateral* partial-DTD relationship between $\varphi'(t)$ and the normalized viscoelastic relaxation function μ(t), $\mu(t) = \varphi'(t)/\beta(t)$ with $\beta(t)$ being the number of entanglement segments per laterally dilated segment (that was evaluated from the $\varphi'(t)$ and τ_{CR} data), held for the $\mu(t)$ and $\varphi'(t)$ data of star PI in bulk. Nevertheless, the observed retardation of the star probe relaxation on blending was *less significant* compared to the retardation expected for the arm motion (retraction) along the laterally dilated tube in bulk PI. This result suggests that the relaxation time of the probe in bulk is governed by the longitudinal partial-DTD that occurs *coherently* along the chain backbone. In fact, the magnitude of retardation evaluated from the $\varphi'(t)$ and τ_{CR} data on the basis of this *longitudinal* partial-DTD picture was close to the observation. These results strongly suggest that the star PI chains in monodisperse bulk have two different coarse-grained length scales: the diameter of laterally dilated tube that determines the modulus level and the diameter of longitudinally dilated tube that reflects the path length for the arm retraction and determines the relaxation time. Thus, the star PI chains in bulk appear to move along the longitudinally dilated tube that wriggles in the laterally dilated tube. This molecular scenario is consistent with the previous finding for bulk linear PI [Matsumiya et al. Macromolecules 2013, 46, 6067].

Synthesis and Properties of Butterfly-Shaped Expanded Naphthofuran Derivatives
Nakanishi, K.; Sasamori, T.; Kuramochi, K.; Tokitoh, N.; Kawabata, T.; Tsubaki, K., *J. Org. Chem.*, **79,** 2625-2631 (2014).
Abstract
The construction of dinaphtho[2,1-*b*;2',3'-*d*]furan-6-ol was developed via a dehydration reaction involving two molecules of 2,3-dihydroxynaphthalene in the presence of a strong acid. Starting from the dinaphthofuran, a variety of butterfly shaped derivatives were synthesized. The optical properties of these compounds were investigated with special attention to the dihedral angle formed by adjacent dinaphthofuran rings and/or the sizes of the fused aromatic rings.

Interface Magnetism of Co_2FeGe Heusler Alloy Layers and Magnetoresistance of $Co_2FeGe/MgO/Fe$ Magnetic Tunnel Junctions
Tanaka, A. M.; Maezaki, D.; Ishii, T.; Okubo, A.; Hiramatsu, R.; Ono, T.; Mibu, K., *J. of Appl. Phys.*, **116,** [163902-1]-[163902-5] (2014).
Abstract
The interface magnetism between Co_2 FeGe Heusler alloy layers and MgO layers was investigated using ^{57}Fe Mö ossbauer spectroscopy. Interface-sensitive samples, where the ^{57}Fe isotope was used only for the interfacial atomic layer of the Co_2 FeGe layer on the MgO layer, were prepared using atomically controlled alternate deposition. The ^{57}Fe Mö ossbauer spectra of the interface-sensitive samples at room temperature were found similar to those of the bulk-sensitive Co_2FeGe films in which the ^{57}Fe isotope was distributed throughout the films. On the other hand, the tunnel magnetoresistance effect of magnetic tunnel junctions with Co_2FeGe layers as the ferromagnetic

electrodes showed strong reduction at room temperature. These results indicate that the strong temperature dependence of the tunneling magnetoresistance of magnetic tunnel junctions using Heusler alloy electrodes cannot be attributed simply to the reduction of the magnetization at the interfaces between the Heusler alloy and insulator layers.

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
MATANO, Yoshihiro
(D Sc)

Division of Synthetic Chemistry

Professor, Department of Chemistry, Faculty of Science, Niigata University
(8050, Ikarashi 2-no-cho, Nishi-ku, Niigata 950-218)

Lecture at *ICR*
Synthesis and Optical Properties Highly Fluorescent π-Conjugated Phosphole Derivatives

Vis Prof
HAYASHI, Ken-ichiro
(D Agr)

Division of Biochemistry

Professor, Department of Biochemistry, Faculty of Science, Okayama University of Science
(1-1 Ridai-Cho, Kita-ku, Okayama, Okayama 700-0005)

Lecture at *ICR*
The Crosstalk between Auxin Signaling and Transport

Vis Prof
TAKAHARA, Atsushi
(D Eng)

Division of Multidisciplinary Chemistry

Professor, Institute for Materials Chemistry and Engineering, Kyushu University
(744 Motooka, Nishi-ku, Fukuoka, 819-0395)

Lecture at *ICR*
Analysis of Soft Material Structure by using Synchrotron X-ray Scattering and Spectroscopy

Vis Prof
UOZUMI, Yasuhiro
(D Pharm Sc)

International Research Center for Elements Science
Professor, Department of Life and Coordination-Complex Molecular Science, Institute for Molecular Science
(Higashiyama 5-1, Myodaiji, Okazaki, Aichi 444-8787)
Lecture at *ICR*
Development of Functional Polymer-Fixed Metal Catalysts
Synthesis and Function of Novel Pincer Type Pd Complex

Vis Assoc Prof
NAKAMURA, Kohji
(D Eng)

Division of Materials Chemistry

Associate Professor, Graduate School of Engineering, Mie University
(1577 Kurimamachiya-cho, Tsu, Mie 514-8507)

Lecture at *ICR*
Decision of Material Chemistry Nanospintoronics

Vis Assoc Prof
Yoshimura, Ken
(D Eng)

Division of Environmental Chemistry

Senior Research Scientist, Tsukuba Research Laboratory, Sumitomo Chemical Co., Ltd.,
(6 Kitahara Tsukuba Ibaraki 300-3294)

Lecture at *ICR*
Development of Organic Photovoltaics and its Application

Vis Assoc Prof
AGO, Hideo
(D Sc)

Advanced Research Center for Beam Science

Senior Research Scientist, RIKEN SPring-8 Center, RIKEN
(1-1-1 Kouto, Sayo, Hyogo 679-5148)

Lecture at *ICR*
Advanced Beamline Technology Enabling Breakthrough in Protein Crystallography

Vis Assoc Prof
IWASAKI, Wataru
(D Sc)

Bioinformatics Center

Assoc Prof, Graduate School of Science, The University of Tokyo
(2-11-16 Yayoi, Bunkyo-ku, Tokyo 113-0032)

Lecture at *ICR*
Bioinformatic Approaches for Comprehensive Description of Biological Systems

Vis Assoc Prof
HINGAMP, Pascal Michel
(D Sc)

Bioinformatics Center

Assoc Prof, Aix-Marseille University
(163 Avenue de Luminy, Case 934, 13288 Marseille cedex 9, France)

Lecture at *ICR*
First insights from the *Tara Oceans* global plankton sampling expedition

Prof Em KANEHISA, Minoru (D Sc)

Appointed as Res (pt) at ICR,
1 April 2012–31 March 2016

PERSONAL

Retirement

Professor SATO, Naoki

Division of Multidisciplinary Chemistry

– Molecular Aggregation Analysis –

On 31 March 2016, Dr. SATO, Naoki will retire from the Institute for Chemical Research (ICR), Kyoto University after about 24 years of service to be honored with the title of Professor Emeritus of Kyoto University.

Dr. Sato was born in Tokyo in February 1951. He graduated from Faculty of Science, The University of Tokyo in 1974 and went on graduate school to study organic solid-state chemistry under the supervision of the late Professor Hiroo Inokuchi at The Institute for Solid State Physics. In 1976, he received a master's and was employed as a technical associate in the Institute for Molecular Science. He earned his Doctor of Science degree for the thesis entitled "Photoemission spectroscopic studies of aromatic solids - Polarization energy and electronic states" from The University of Tokyo in 1983 and was re-assigned to an assistant professor at the Faculty of Science, Kumamoto University next year. He transferred to the College of Arts and Sciences, The University of Tokyo to serve as an associate professor for about five years between 1987 and 1992. Meanwhile, he was sent to the Department of Physics, Chemistry and Biology, Linköping University in Sweden to collaborate with Professor William R. Salaneck under the International Scientific Research Program in 1989. In May 1992, he was appointed professor of the Division of Interface Science II, ICR and came to serve concurrently as a professor at the Division of Chemistry, Graduate School of Science, Kyoto University. Since the reorganization of ICR in 2004 he has held the chair of the Laboratory of Molecular Aggregation Analysis, Division of Multidisciplinary Chemistry. He served as a Vice-Director of ICR between June 2005 and March 2010 and also as the Director of Kyoto University Uji Library between April 2006 and March 2010. After he served as the Director of ICR between April 2012 and September 2014, he was appointed as the Executive Vice-President for finance, facilities, and environmental health and safety in October 2014.

Throughout his academic career, Dr. Sato devoted himself to the investigation in the field of organic solid-state chemistry and/or physical chemistry. His research interests have focused on three topics: Analyzing electronic structures of frontier electronic states in organic solids and thin films with their surfaces and interfaces, fabricating molecular systems with novel electronic properties, and searching organic solid-state reactions to be followed by dynamic electronic functions. Among them he has been active especially in the first topic, that is, elucidation of the structure - electronic structure correlation in organic semiconductors in the solid and thin-film states, in particular, using photoemission and inverse photoemission spectroscopies with developing their experimental apparatus on his own. He has disclosed main factors contributing to the evolution of the electronic structure in organic semiconductor thin films, with paying close attention to the difference of electronic structures between a film and its component molecule whose electrostatic characteristics should also be recognized. While developing such studies, he has been an active member of domestic and international academic societies, such as the Division of the Organic Crystals, The Chemical Society of Japan.

Dr. Sato's educational contribution in Kyoto University is also noteworthy. He has supervised 43 graduate students to send them out into society, especially industry and academia. He has contributed to education of undergraduate students as well through giving lectures in the liberal arts and general education courses from time to time. In addition, he has given intensive lectures in response to requests from other national universities in Japan.

Finally, his various contribution to the administration of Kyoto University as well as ICR so far goes without saying and will still devote himself to the university as an Executive Vice-President after April 2016 for a while.

Thus, Dr. Sato's contribution to Kyoto University and the ICR through his scientific research, education of students and graduate students, and institute and university operations is highly appreciated. His sincere attitude toward everything including nature will remain in the memory of all the people knowing him for a long time in the future.

Retirement

Professor HATA, Yasuo

Advanced Research Center for Beam Science

– Structural Molecular Biology –

On March 31, 2016, Dr. Yasuo Hata retired from Kyoto University after 25 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Hata was born in Nara Prefecture on January 6th, 1951. He graduated from Faculty of Science, Osaka University in 1974 and went on to the Department of Macromolecular Science, Graduate School of Science to study protein crystallography under the supervision of the late Professor Masao Kakudo in the Institute for Protein Research. In 1979, he graduated from the doctoral course and was granted the doctoral degree of science for the thesis "X-ray Crystal Structure Analysis of Lipase at 2.8 Å Resolution". Concurrently, he was appointed Assistant Professor and continued his research activity at the Institute for Protein Research. In 1991, he moved to the Institute for Chemical Research, Kyoto University, as Associate Professor and started up a research of X-ray structural biology. In 2002, he was promoted Professor directing the Laboratory of Atomic and Molecular Physics in Division of States and Structures. The laboratory was re-organized as the Laboratory of Structural Molecular Biology in Advanced Research Center for Beam Science in 2004. He served as the head of this center in 2007-2009 and 2013-15.

Throughout his academic career, Dr. Hata devoted himself to X-ray structure determination of novel proteins and clarification of vital phenomena wrapped in mystery, such as mechanisms of enzymatic reaction and protein-protein interaction, based on the structure-function relationship of protein. He succeeded in broadening the research field in structural biology by introducing advanced techniques of SR science and protein engineering into protein science. Moreover, he succeeded in developing research techniques which enabled detailed structural studies on reaction mechanism of enzymes and physical properties of proteins. Notably, he demonstrated that two kinds of one-electron different metals, such as Cu^{2+} and Zn^{2+}, in a protein can be physically distinguished from each other by using wavelength-tunable SR X-ray beams. This distinguishment is quite difficult to be done by chemical methods. In previous studies of Cu^{2+}, Zn^{2+}-SOD, the locations of these metal ions in the protein were speculated by the difference in distribution of the amino-acid residues coordinated to the ion. His method is strictly based on physical principles and evaluated highly all over the world. In addition, he succeeded in revealing the existence and biological role of an unexpected metal ion in a protein by the same technique.

He subsequently undertook the elucidation of reaction mechanism of enzymes by using the methods of X-ray structural biology and genetic mutation. He fulfilled the world-first success in X-ray structure determination of L-2-haloacid dehalogenase. This result led to the structural determination of the P-type Ca-ATPase found in Japan. In addition, he succeeded in preparation of reaction-intermediate by using a mutant of the dehalogenase, X-ray structure determination of the intermmediate and elucidation of enzymatic-reaction mechanism of the enzyme.

He also performed the study of protein adaptation to temperature environment. He determined X-ray structures of several kinds of proteins from thermophile and psychrophile and succeeded in explanation of adaptation strategies of these proteins to temperature environment from their structural differences. He established the validity of explanation by using mutant proteins. He also succeeded in structure determination of enzymes involved in resorcinol catabolism and elucidation of their reaction mechanism based on their structural changes during the reaction processes in catabolism. His research achievements were reported in a lot of scientific papers of high quality and have been highly evaluated all over the world.

Dr. Hata has supervised many graduate students including doctoral students who took a doctoral degree. He enthusiastically guided his students in the field of X-ray structural biology and let them have valuable experience in that field. His students assume important roles and are active in various fields of industry and academia.

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

Awards

MORINAKA, Yuta; WAKAMIYA, Atsushi; TANABE, Fumiyuki; MURATA, Michihisa; KOMATSU, Koichi; KATO, Tatsuhisa[1]; NAGASE, Shigeru[2]; MURATA, Yasujiro; SATO, Satoru[3]; NIKAWA, Hidefumi[3]; MIZOROGI, Naomi[3]; FURUKAWA, Ko[4]; AKASAKA, Takeshi[3]

Six Major Results of 2013 from Nanotechnology Platform Japan

"ESR and X-ray Observation of a Helium Atom and Placing a Nitrogen Atom inside He@C_{60} and He@C_{70}"

Nanotechnology Platform Japan, MEXT, Japan

30 January 2015

[1] Institute for the Promotion of Excellence in Higher Education, Kyoto University
[2] Fukui Institute for Fundamental Chemistry, Kyoto University
[3] Life Science Center of Tsukuba Advanced Research Alliance, University of Tsukuba
[4] Institute for Molecular Science

WAKAMIYA, Atsushi

2015 Step-up Award of Japan Association for Chemical Innovation

"Development of Innovative Oranic Semi Conductors and Organic-Inorganic Hybrid Materials that Enable Highly Efficient Photoelectronic Conversion"

Japan Association for Chemical Innovation (JACI)

27 May 2015

The Nozoe Memorial Award for Young Organic Chemists

26th Symposium on Physical Organic Chemistry

"Development of Functional Materials Based on Fine-tuning of pi-Orbitals"

The Society of Physical Organic Chemistry

25 September 2015

MURATA, Michihisa

ICR Award for Young Scientists

"Electron-deficient Tetrabenzo-fused Pyracylene and Conversions into Curved and Planar π-systems Having Distinct Emission Behaviors"

Institute for Chemical Research, Kyoto University

11 December 2015

UEDA, Yoshihiro

ICR Award for Young Scientists

"Final-stage Site-selective Acylation for the Total Syntheses of Multifidosides A-C"

Institute for Chemical Research, Kyoto University

11 December 2015

KASAMATSU, Koji

Best Presentation Award

The 135th Annual Meeting of the Pharmaceutical Society of Japan

"Asymmetric α-Fluorination of Amino Acid Derivatives via Memory of Chirality"

The Pharmaceutical Society of Japan

31 March 2015

TAKEUCHI, Hironori

ICR Award for Graduate Students

"Total Synthesis of Ellagitannins via Regioselective Sequential Functionalization of Unprotected Glucose"

Institute for Chemical Research, Kyoto University

11 December 2015

SAKAMOTO, Masanori

Japanese Photochemistry Association Prize for Young Scientist for 2015

Japanese Photochemistry Association

10 September 2015

SATO, Ryota

Presentation Award for Young Scientists

The 66th Divisional Meeting on Colloid & Interface Chemistry

"Novel and Versatile Alloying Route of Nanoparticle via Phosphorus Compound"

Division of Colloid and Surface Chemistry, The Chemical Society of Japan

3 October 2015

YOSHIZUMI, Toshihiro

CSJ Presentation Award 2015

The 95th Annual Meeting of the Chemical Society of Japan

"Photocatalytic Activities of Transition Metal Oxide Nanoparticles for Water Oxidation"

The Chemical Society of Japan

13 April 2015

EGUCHI, Daichi

CSJ Presentation Award 2015

The 95th Annual Meeting of the Chemical Society of Japan

"Structural Control of Gold Clusters Using Porphyrin Derivatives"

The Chemical Society of Japan

13 April 2015

YAMAGO, Shigeru

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

"Research of Excellent Novel Living Radical Polymerization Reaction to Practicality"

The Minister of Education, Culture, Sports, Science and Technology

15 April 2015

TOSAKA, Masatoshi

Prize of the Society of Fiber Science and Technology, Japan

2015 Annual Meeting of the Society of Fiber Science and Technology, Japan

"Strain-induced Crystallization of Polymer Network"

The Society of Fiber Science and Technology, Japan

10 June 2015

Progress Award

The 53rd Annual Meeting of the Adhesion Society of Japan

"Kinetics of Strain-induced Crystallization in Cross-linked Natural Rubber"

The Adhesion Society of Japan

19 June 2015

NAKAMURA, Yasuyuki

Excellence Lecture Award

The 95th Chemical Society of Japan Annual Meeting

"Elucidation of the Termination Reaction Mechanism in the Radical Polymerization of (Meth) Acrylic Acid Ester"

The Chemical Society of Japan

13 April 2015

Young Scientist Lecture Award

The 61st Annual Kobe Polymer Research Symposium

"Control of Radical Reaction by Light - Living Radical Polymerization, Polymer Reactions and Reaction Mechanism Analysis"

The Society of Polymer Science, Japan, Kansai Regional Chapter

17 July 2015

PATEL, Vijay Kumar

ICR Award for Young Scientists

"Practical Synthesis of [*n*]cycloparaphenylenes (n=5, 7-12) by H_2SnCl_4-mediated Aromatization of 1,4-dihydroxycyclo-2,5-diene Precursors"

Institute for Chemical Research, Kyoto University

11 December 2015

ONO, Teruo

The IEEE Magnetics Society 2016 Distinguished Lecturer

"Spin Dynamics in Inhomogeneously Magnetized Systems"

The IEEE Magnetics Society

28 September 2015

YOSHIMURA, Yoko

NIHON LOREAL Scientific Award

"Development of Magnetic Domain-wall Based Memory for Next Generation Memory Device"

8 July 2015

TAKEUCHI, Toshihide

The Young Investigator Award

The 7th Annual Meeting of the Japanese Association for RNAi and the 2nd Annual Meeting of the Japanese Society of Extracellular Vesicles

"Intercellular Chaperone Transmission via Exosomes Contributes to Non-cell autonomous Maintenance of Organismal Proteostasis"

The Japanese Association for RNAi, The Japanese Society of Extracellular Vesicles

28 August 2015

The Young Investigator Award

The 10th Annual Meeting of the Biomedical Society for Stress Response

"Maintenance of Organismal Protein Homeostasis by Intercellular Transmission of Molecular Chaperones via Exosomes"

The Biomedical Society for Stress Response

6 November 2015

MURAYAMA, Tomo

Good Stone Award, Annual Meeting of JPS

The 52nd Japanese Peptide Symposium

"Membrane-Remodeling Amphipathic Helical Peptides Accelerate Direct Penetration of Octaarginine"

The Japanese Peptide Society

17 November 2015

Best Presentation Award

37th Symposium on Interactions between Biomembranes and Drugs

"Curvature-Inducing Amphipathic Helical Peptides Accelerate Membrane Translocation of Octaarginine"

The Division of Physical Sciences of the Pharmaceutical Society of Japan

20 November 2015

WATANABE, Bunta

Society Awards 2015 (on high prospectiveness)

"Structure-activity relationship studies of insect and plant steroid hormones"

Pesticide Science Society of Japan

18 March 2015

TAKAYA, Junichiro

Outstanding Presentation Award

The 7th Young Researchers Workshop, Chemical Biology of Natural Products: Target ID and Regulation of Bioactivity

"A Selective Agonist of TRPA1 and Direct Observation of its Binding"

Chemical Biology of Natural Products: Target ID and Regulation of Bioactivity

9 June 2015

TAKANO, Shotaro

Sasakawa Scientific Research Encouragement Prize

"Biogeochemical Cycling of Nickel, Copper, and Zinc Isotopes in the Ocean"

The Japan Science Society

13 April 2015

HASEGAWA, Takeshi

The 32nd Academic Award from the Chemical Society of Japan

The 95th Annual Meeting of the Chemical Society Japan

"Development of Multiple-Angle Incidence Resolution Spectrometry and Its Application to Structural Analysis of Two-Dimensional Molecular Assemblies"

The Chemical Society of Japan

28 March 2015

SAS Fellow

SciX2015

"Outstanding service to the field of spectroscopy and the Society for Applied Spectroscopy"

The Society for Applied Spectroscopy

29 September 2015

SHIOYA, Nobutaka

Award for Encouragement of Research in Materials Science

25th Annual Meeting of MRS-J

"Preparation of a Highly Oriented Thin Film of a Functionalized Compound Using a Simple Spin-coating Technique"

The Materials Research Society of Japan

10 December 2015

ICR Award for Graduate Students

"A New Schematic for Poly(3-alkylthiophene) in an Amorphous Film Studied Using a Novel Structural Index in Infrared Spectroscopy"

Institute for Chemical Research, Kyoto University

11 December 2015

WATANABE, Hiroshi

The Bingham Medal

The Society of Rheology 87th Annual Meeting

The Society of Rheology (USA)

13 October 2015

IWASHITA, Yoshihisa

The JSNS Technology Prize

The 15th Annual Meeting of the Japanese Society for Neutron Science

“Efficient Utilization of Neutrons by Active Focusing of Pulse White Neutron”

The Japanese Society for Neutron Science

10 December 2015

SAKABE, Shuji

Fellow Award of The Laser Society of Japan

The Laser Society of Japan

29 May 2015

MIYASAKA, Yasuhiro

The distinguished Paper Award

The Papers of Technical Meeting on “Fundamentals and Materials”, IEE Japan.

“Femtosecond Laser Ablation Rate for Materials”

The Institute of Electrical Engineering of Japan.

17 September 2015

WATANABE, Kota

Award for the Presentation of an Excellent Paper

The 35th Annual Meeting of the Laser Society of Japan

“Ultrafast electron Diffraction with Laser-assisted Electrons Produced by an Intense Short Pulse Laser”

The Laser Society of Japan

29 May 2015

HARUTA, Mitsutaka

Research Encouragement Award

The 71st Annual Meeting of the Japanese Society of Microscopy

“Local State Analysis and Mapping by STEM-EELS”

The Japanese Society of Microscopy

14 May 2015

SEKI, Hayato

CSJ Student Presentation Award 2015

The Chemical Society of Japan

“Crystal Structures and Physical Properties of New Perovskites $SrFe_{1-x}Ni_xO_3$”

The Chemical Society of Japan

13 April 2015

IHARA, Toshiyuki

Young researcher award

“Photoluminescence Properties of Excitons in Nanocrystals Revealed by Single Molecule Spectroscopy”

174th Committee on Molecular Nanotechnology JSPS University-Industry Cooperative Research Committees

3 March 2015

SHIMIZU, Yugo, et al.

Research Awards

Informatics in Biology, Medicine and Pharmacology 2015

“Relating the Reaction Types and Phylogeny of Type III Polyketide Synthases”

Program Committee of Information in Biology, Medicine and Pharmacology 2015

31 October 2015

NISHIMURA, Yosuke, et al.

Research Awards

Informatics in Biology, Medicine and Pharmacology 2015

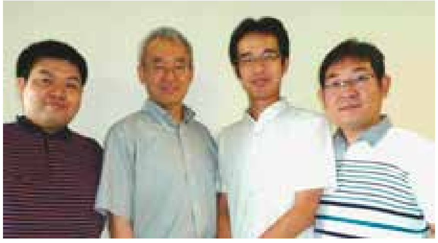
The 2015 Annual Conference of the Japanese Society for Bioinformatics (JSBi2015)

“Revealing Complete Genomes from Metagenomes: a Case Study for Viruses in the Ocean”

Program Committee of Information in Biology, Medicine and Pharmacology 2015

31 October 2015

Paper Awards



YAMADA, Yasuhiro;
NAKAMURA, Toru;
ENDO, Masaru;
WAKAMIYA, Atsushi;
KANEMITSU, Yoshihiko;

37th (2015) Best Paper Award of the Japan Society of Applied Physics

"Near-band-edge Optical Responses of Solution-processed Organic–inorganic Hybrid Perovskite $CH_3NH_3PbI_3$ on Mesoporous TiO_2 Electrodes"

The Japan Society of Applied Physics

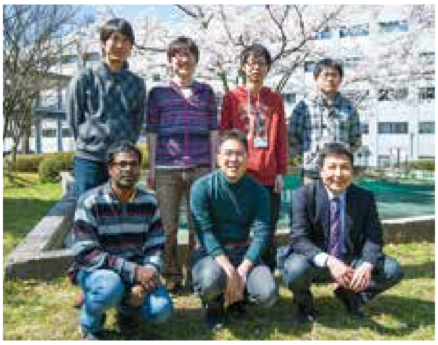
13 September 2015

TANIGUCHI, Takuya

JPS paper award

"Dimensional Crossover Characterized by Distribution of Magnetic Domain Wall Creep Velocity"

1 November 2015



TAKAYA, Hikaru et. al.

BCSJ Award

"Investigation of Organoiron Catalysis in Kumada-Tamao-Corriu-Type Cross-Coupling Reaction Assisted by Solution-Phase X-ray Absorption Spectroscopy"

Takaya, H.; Nakajima, S.; Nakagawa, N.; Isozaki, K.; Iwamoto, T.; Imayoshi, R.; Gower, N.; Adak, L.; Hatakeyama, T.; Honma, T.; Takagi, M.; Sunada, Y.; Nagashima, H.; Hashizume, D.; Takahashi, O.; Nakamura, M.

Bull. Chem. Soc. Jpn. **2015,** 88, 410-418

15 March 2015

ISOZAKI, Katsuhiro;
PINCELLA, Francesca[1];
MIKI, Kazushi[2]

LSA top 10 paper award in 2014

"A visible light-driven plasmonic photocatalyst"

Light: Science & Applications

7 July 2015

[1] Polymer Materials Unit, National Institute for Materials Science
[2] Department of Pure and Applied Sciences, University of Tsukuba

KANEMITSU, Yoshihiko

Award for Best Review Paper

37th JSAP AWARDS

"Multiple Carrier Interactions in Semiconductor Nanostructures for High-efficiency Solar Cell Applications"

The Japan Society of Applied Physics

13 September 2015

TAHARA, Hirokazu

Seiichi Tejima Doctoral Dissertation Award

"Coherent Transients of Excitons Generated in Semiconductors"

Tokyo Institute of Technology

17 February 2015

Poster Awards

NAGATA, Koichi

Award for Best Poster

The 14th International Symposium on Inorganic Ring Systems

"Reactions of a Barrelene-type Dialumane Bearing Bulky Aryl Substituents with Lewis Bases"

European Journal of Inorganic Chemistry

31 July 2015

FUJIMORI, Shiori

Best Poster Award

Meeting for Young Scientists on Organic Reactions

"Synthesis and Properties of Germabenzenylpotassium"

Organizing Committee of Meeting for Young Scientists on Organic Reactions

31 July 2015

Poster Award

57th Symposium on Organometallic Chemistry, Japan

"Synthesis and Structures of Germabenzenylpotassium"

The Kinki Chemical Society, Japan

28 September 2015

Best Poster Award

The 5th Asian Silicon Symposium

"Synthesis and Structure of a Stable Germabenzenylpotassium Derivative"

ASiS International Committee

20 October 2015

Poster Award

The 19th Symposium of the Society of Silicon Chemistry Japan

"Structure and Reactivity of Germabenzenylpotassium"

The Society of Silicon Chemistry Japan

23 October 2015

SUGAHARA, Tomohiro

Poster Award

The 19th Symposium of the Society of Silicon Chemistry Japan

"Reactivity of Stable Diaryldigermynes with Alkenes and Alkynes"

The Society of Silicon Chemistry Japan

23 October 2015

ZHANG, Rui

Best Poster Award

16th International Symposium on Novel Aromatic Compounds (ISNA-16)

"X-ray Structure and Properties of Endohedral C_{70} Encapsulating Water Molecule(s)"

10 July 2015

FUTAGOISHI, Tsukasa

Poster Award

26th Symposium on Physical Organic Chemistry

"Insertion of a Molecule of MeOH into an Open-Cage C_{60} Derivative and Its X-ray Structure"

The Society of Physical Organic Chemistry

26 September 2015

HASHIKAWA, Yoshifumi

Best Young Scientists Poster Awards, JEOL RESONANCE Award

The 54th Annual Meeting of the NMR Society of Japan

"^{1}H NMR Relaxation Times of H_2O and H_2 Entrapped inside Carbon-Cluster Cages of C_{60} and $C_{59}N$"

The Nuclear Magnetic Resonance Society of Japan, JEOL RESONANCE INC.

7 November 2015

KASAMATSU, Koji

Best Poster Award

Symposium on Molecular Chirality 2015

"Asymmetric α-Fluorination of Amino Acid Derivatives via long-lived Chiral Enolate Intermediates based on Memory of Chirality"

Molecular Chirality Research Organization (MCRO)

13 June 2015

CHEN, Lihui

Poster award

The 13th Annual Meeting of Society of Nano Science and Technology

"Investigation on Carrier Dynamics of Oleylamine-Capped Copper Indium Sulfide Nanocrystals Using Femtosecond Laser Flash Photolysis"

Society of Nano Science and Technology

12 May 2015

MATSUMOTO, Kenshi

Poster Award

The 66th Divisional Meeting on Colloid and Interface Chemistry

“High-Performance $L1_0$-FePd/<-Fe Nanocomposite Magnets with Controlled Crystal Grain Size”

Division of Colloid and Surface Chemistry, The Chemical Society of Japan

11 September 2015

YAHATA, Yoshikazu

CSJ Poster Presentation Award 2015 for Excellent Research

5th CSJ Chemistry Festa

“Polymer-brush-grafted Particles for Control of Phase Separation in Polymer/ionic-liquid Blend Films”

The Chemical Society of Japan

12 November 2015

KAKIZAKAI, Haruka

Poster Award

5th CSJ Chemistry Festa

The 76th JSPS Autumn Meeting, 2015

“Approach to Electric Field Induced Domain Wall Motion in MgO/Co/Pt System”

1 October 2015

KAWAGUCHI, Yoshimasa

Award for Excellence at Poster Presentation

The 52nd Japanese Peptide Symposium

“Syndecan-4 as a Possible Octaarginine Receptor for Its Clathrin-Mediated Endocytic Uptake”

The Japanese Peptide Society

17 November 2015

AKISHIBA, Misao

Best Poster Award

7th International Peptide Symposium

“Novel Endsome-destabilizing Peptide for Intracellular Delivery of Exogenous Antibodies”

11 December 2015

WATANABE, Mizuki

Molecular BioSystem Poster Prize

10th Annual Meeting of Japanese Society for Chemical Biology

“The Action Mechanism of Endogenous Small Molecules That Suppress the Lipid Biosynthesis”

Royal Society of Chemistry

12 June 2015

TAKAYA, Junichiro

Student Poster Competition Award

“Discovery of a potent and selective agonist of TRPA1 and direct observation of its binding to TRPA1 by electron microscopy”

International Chemical Congress of Pacific Basin Societies (Pacifichem 2015)

18 December 2015

HADA, Miyako

Poster prize

The 66th Divisional Meeting on Colloid & Interface Chemistry

“Structural Analysis of a Thin Film of a porphyrin Derivative Using Visible MAIRS”

Division of Colloid and Surface Chemistry, Chemical Society of Japan

11 September 2015

KISHIMOTO, Mizuki

The Poster Presentation Award

70th Autumun Meeting

“Effect of Substrate Surface Modification on the Glass Transition Temperature of Polymer Thin Films”

The Society of Fiber Science and Technology

22 October 2015

SAITO, Shota

Poster Award

The 62nd Symposium on Organometallic Chemistry

“Iron-Catalyzed Enantioselective Carbometalation of Azabicyclic Alkenes with Arylzinc Reagents”

Division of Organometallic Chemistry, The Kinki Chemical Society

28 September 2015

IBUKI, Hiroto

Region5 Poster Awards

The Physical Society of Japan 2015 Autumn Meeting

"Photoluminescence Blinking and Spectral Diffusion of Single CdSe/ZnS Nanocrystals: Charge Fluctuation Effects"

The Physical Society of Japan

18 September 2015

YAMADA, Takumi

Region5 Poster Awards

The Physical Society of Japan 2015 Autumn Meeting

"Photocarrier Diffusion and Recombination Dynamics in Lead-halide Perovskite $CH_3NH_3PbX_3$(X=I,Br) Single Crystals"

The Physical Society of Japan

18 September 2015

AKUTSU, Tatsuya; ISHITSUKA Masayuki[1]; NACHER, Jose[1]

Best Poster Award

Informatics in Biology, Medicine and Pharmacology 2015

"On the Efficient Identification of Proteins with Control Roles in Large Networks"

Japanese Society for Bioinformatics

31 October 2015

[1] Toho University

Obituary

Professor Emeritus

Dr. OKANO, Masaya (1920-2015)

Dr. Masaya Okano, Professor Emeritus of Kyoto University, passed away on June 8, 2015, in Ohtsu, at the age of 94.

Dr. Masaya Okano was born in Shiga on November 7, 1920. He graduated from the Department of Industrial Chemistry, Faculty of Engineering, Kyoto Imperial University in 1947 and continued his research on organic chemistry as a special graduate student under the supervision of Professor Yoshiro Ogata. In 1953, he was appointed a full-time lecturer of the Department of Industrial Chemistry, Faculty of Engineering, Kyoto University and started his academic career majoring in theoretical organic chemistry. He was conferred a doctoral degree (Doctor of Engineering) form Kyoto University in 1954 for his studies on the mechanism of organic reactions clarified by kinetics. After the promotion to an Associate Professor of the same Department in 1955, Dr. Okano joined the member of the Institute for Chemical Research, Kyoto University in 1956. In 1966, on leave from Kyoto University, he stayed at Yale University, USA to work on synthetic organic chemistry in co-operation with Professor K. B. Wiberg. In 1967, Dr. Okano was promoted to a Full Professor of Kyoto University to hold a chair of Laboratory of Petroleum Chemistry in the Institute for Chemical Research.

Dr. Okano retired from Kyoto University on April 1, 1984 and was honored with the title of Professor Emeritus, Kyoto University on the same day. After retirement, Dr. Okano served as the President of Kyoto Polytechnic College (established by Ministry of Labor for the training to get employment) until 1988.

Dr. Okano has shown that kinetic analysis is very effective method to clarify the mechanism of the reactions valuable to synthesize industrially important compounds such as melamine resin and azo dye. He further developed these findings to control the reaction course of reactive carbon species bearing heteroatom such as nitrogen, phosphine, sulfur, or halogens on the carbon atom.

Dr. Okano has opened a new methodology of organic syntheses by the use of inorganic salts. He discovered novel selectivity which was not realized by the traditional methods during halogenation reactions using antimony(V) or molybdenum(V) chlorides. Thus, *cis*-dihalogenated products were produced selectively from olefins and acetylenes and unsymmetrically substituted *para*-dihalogenobenzenes were produced selectively from halogenobenzenes. He also discovered the unique catalytic activity of thallium(III) salts in the conversion of isonitriles to isothiocyanates and carboxylation of aromatic compounds.

Dr. Okano also contributed to establish another new methodology in organic synthesis by the use of organo-metallic and -semimetallic compounds as intermediates. Thus, he succeeded in the isolation of so far unknown organothallium(III) compounds from olefins, acetylenes, and aromatic compounds and clearly showed that carbon-thallium bonds in these compounds were easily cleaved by the reaction with copper salts to introduce halogen atoms or pseudohalogeno groups into the carbon atoms. He also discovered that anchimeric assistance of selenium atom is useful to introduce various functional groups into olefins. This finding was utilized in the selective construction of unique bicyclic ethers and in the convenient procedure to synthesize allylic amides and alcohols.

Due to these excellent achievements, Dr. Okano was prized with Synthetic Organic Chemistry Award, Japan in 1983.

He delivered lectures on stereochemistry and chemistry of reactive intermediates at the Department of Hydrocarbon and Synthetic Chemistry, Graduate School of Kyoto University and was charged with supervising dissertation works of graduate students, during which he trained many doctor candidates.

Dr. Okano's superiority in research and education, deep insight into science and warm hospitality not only have attracted and stimulated many young and talented students but also have won him the respect of many friends and colleagues. He also served as a director or an executive board of scientific societies such as the Society of Synthetic Organic Chemistry, Japan.

For his outstanding professional activities in research, education and academic society, Dr. Okano received the Third Order of Merit with the Order of Rising Sun, Gold Rays with Neck Ribbon from Japanese Government in April, 1995.

PUBLICATIONS
INTERNATIONAL RESEARCH COLLABORATIONS
SELECTED GRANTS
THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Tokitoh, N.; Mizuhata, Y.; Egawa, Y.; Sasamori, T., Synthesis of 1,2-Dialkynyldisilanes Incorporated in 10-Membered-Ring System, *Heterocycles*, **90,** 1111-1123 (2015).

Sasamori, T.; Sugahara, T.; Agou, T.; Sugamata, K.; Guo, J.-D.; Nagase, S.; Tokitoh, N., Reaction of a Diaryldigermyne with Ethylene, *Chem. Sci.*, **6,** 5526-5530 (2015).

Agou, T.; Wasano, T.; Sasamori, T.; Tokitoh, N., Syntheses and Structures of a Stable Gallole Free of Lewis Base Coordination and Its Dianion, *J. Phys. Org. Chem.*, **28,** 104-107 (2015).

Fuku-en, S.; Furukawa, K.; Sasamori, T.; Tokitoh, N.; Abe, M.; Yamamoto, Y., Oxidation of an Allene Compound Bearing 1,8-Dichloroacridene Moieties and Photolysis of the Halogenated Allene Compound for the Generation of Triplet Carbenes, *J. Phys. Org. Chem.*, **28,** 79-87 (2015).

Egawa, Y.; Mizuhata, Y.; Sasamori, T.; Tokitoh, N., Unexpected Photochemical Reactions of 2-Aryl-2-ethynyltrisilane Derivative, *Main Gr. Met. Chem.*, **38,** 51-55 (2015).

Ota, M.; Sasamori, T.; Tokitoh, N.; Onodera, T.; Mizushina, Y.; Kuramochi, K.; Tsubaki, K., Synthesis, Photochemical Properties, and Cytotoxicities of 2 *H* -Naphtho[1,2- *b*]pyran and Its Photodimers, *J. Org. Chem.*, **80,** 5687-5695 (2015).

Sasamori, T.; Sugahara, T.; Agou, T.; Guo, J.-D.; Nagase, S.; Streubel, R.; Tokitoh, N., Synthesis and Characterization of a 1,2-Digermabenzene, *Organometallics*, **34,** 2106-2109 (2015).

Miyake, H.; Sasamori, T.; Tokitoh, N., Sulfurization of 4,5,6-Triphospha[3]radialene, *Phosphorus Sulfur Silicon Relat. Elem.*, **190,** 1247-1250 (2015).

Agou, T.; Wasano, T.; Sasamori, T.; Guo, J.-D.; Nagase, S.; Tokitoh, N., Ring Expansion to 1-Bromo-1-alumacyclonona-2,4,6,8-tetraene by Insertion of Two Alkyne Molecules into the Al–C Bonds, *Angew. Chem. Int. Ed.*, **54,** 9568-9571 (2015).

Swarnakar, A. K.; Hering-Junghans, C.; Nagata, K.; Ferguson, M. J.; McDonald, R.; Tokitoh, N.; Rivard, E., Encapsulating Inorganic Acetylene, HBNH, Using Flanking Coordinative Interactions, *Angew. Chem. Int. Ed.*, **54,** 10666-10669 (2015).

Sasamori, T.; Hirano, K.; Miyake, H.; Tokitoh, N., Photochemical (*E*)–(*Z*) Isomerization of the P=C Double Bond in Triphospha[3]radialene–[M(CO)$_5$] (M = W, Cr) Complexes, *Chem. Lett.*, **44,** 1240-1242 (2015).

Nagata, K.; Agou, T.; Sasamori, T.; Tokitoh, N., Formation of a Diaminoalkyne Derivative by Dialumane-mediated Homocoupling of *t*-Butyl Isocyanide, *Chem. Lett.*, **44,** 1610-1612 (2015).

Yamaguchi, K.; Murai, T.; Hasegawa, S.; Miwa, Y.; Kutsumizu, S.; Maruyama, T.; Sasamori, T.; Tokitoh, N., 5-*N*-Arylaminothiazoles as Highly Twisted Fluorescent Monocyclic Heterocycles: Synthesis and Characterization, *J. Org. Chem.*, **80,** 10742-10756 (2015).

— Structural Organic Chemistry —

Futagoishi, T.; Murata, M.; Wakamiya, A.; Murata, Y., Trapping N$_2$ and CO$_2$ on the Sub-Nano Scale in the Confined Internal Spaces of Open-Cage C$_{60}$ Derivatives: Isolation and Structural Characterization of the Host–Guest Complexes, *Angew. Chem. Int. Ed.*, **54,** 14791-14794 (2015).

Nishimura, H.; Ishida, N.; Shimazaki, A.; Wakamiya, A.; Saeki, A.; Scott, L. T.; Murata, Y., Hole-Transporting Materials with a Two-Dimensionally Expanded π-System around an Azulene Core for Efficient Perovskite Solar Cells, *J. Am. Chem. Soc.*, **137,** 15656-15659 (2015).

Wakamiya, A.; Yamaguchi, S., Designs of Functional π-Electron Materials based on the Characteristic Features of Boron, *Bull. Chem. Soc. Jpn.*, **88,** 1357-1377 (2015).

Chaolumen, Murata, M.; Sugano, Y.; Wakamiya, A.; Murata, Y., Electron Deficient Tetrabenzo-fused Pyracylene and Conversions into Curved and Planar π-Systems with Distinct Emission Behaviors, *Angew. Chem. Int. Ed.*, **54,** 9308-9312 (2015).

Nishimura, H.; Eliseeva, M. N.; Wakamiya, A.; Scott, L. T., 1,3,5,7-Tetra(Bpin)azulene by Exhaustive Direct Borylation of Azulene and 5,7-Di(Bpin)azulene by Selective Subsequent Deborylation, *Synlett*, **26,** 1578-1580 (2015).

Yamada, Y.; Endo, M.; Wakamiya, A.; Kanemitsu, Y., Spontaneous Defect Annihilation in CH$_3$NH$_3$PbI$_3$ Thin Films at Room Temperature Revealed by Time-resolved Photoluminescence Spectroscopy, *J. Phys. Chem. Lett.*, **6,** 482-486 (2015).

Uemura, T.; Nakanishi, R.; Mochizuki, S.; Murata, Y.; Kitagawa, S., Radical Polymerization of 2,3-Dimethyl-1,3-butadiene in Coordination Nanochannels, *Chem. Commun.*, **51,** 9892-9895 (2015).

Yamada, Y.; Yamada, T.; Le, P. Q.; Maruyama, N.; Nishimura, H.; Wakamiya, A.; Murata, Y.; Kanemitsu, Y., Dynamic Optical Properties of CH$_3$NH$_3$PbI$_3$ Single Crystals as Revealed by One- and Two-Photon Excited Photoluminescence Measurements, *J. Am. Chem. Soc.*, **137,** 10456-10459 (2015).

Kaji, H.; Suzuki, H.; Fukushima, T.; Shizu, K.; Suzuki, K.; Kubo, S.; Komino, T.; Oiwa, H.; Suzuki, F.; Wakamiya, A.; Murata, Y.; Adachi, C., Purely Organic Electroluminescent Material Realizing 100% Conversion from Electricity to Light, *Nat. Commun.*, **6,** [8476-1]-[8476-8] (2015).

Yamada, Y.; Nakamura, T.; Endo, M.; Wakamiya, A.; Kanemitsu, Y., Photoelectronic Responses in Solution-Processed Perovskite CH$_3$NH$_3$PbI$_3$ Solar Cells Studied by Photoluminescence and Photoabsorption Spectroscopy, *J. Photovoltaics*, **5,** 401-405 (2015).

Wang, S.; Yang, D.-T.; Lu, J.; Shimogawa, H.; Gong, S.; Wang, X.; Mellerup, S. K.; Wakamiya, A.; Chang, Y.-L.; Yang, C.; Lu, Z.-H., In Situ Solid-State Generation of (BN)$_2$-Pyrenes and Electroluminescent Devices, *Angew. Chem. Int. Ed.*, **54,** 15074-15078 (2015).

Maroto, E. E.; Mateos, J.; Garcia-Borras, M.; Osuna, S.; Filippone, S.; Herranz, M. A.; Murata, Y.; Sola, M.; Martin, N., Enantiospecific cis-trans Isomerization in Chiral Fulleropyrrolidines: H-Bonding Assistance in the Carbanion Stabilization in $H_2O@C_{60}$, *J. Am. Chem. Soc.*, **137,** 1190-1197 (2015).

[Others]

Murata, Y.; Wakamiya, A.; Murata, M., Laboratory Introduction, *Organometallic News*, 64-65 (2015) (in Japanese).

Murata, Y., Endohedral Fullerene Encapsulating Molecule(s), *Kotai Butsuri*, **50,** 141-147 (2015) (in Japanese).

— Synthetic Organic Chemistry —

Fujita, D.; Yokoyama, H.; Ueda, Y.; Sato, S.; Fujita, M., Geometrically Restricted Intermediates in the Self-Assembly of an M12L24 Cuboctahedral Complex, *Angew. Chem. Int. Ed.*, **54,** 155-158 (2015).

Lehr, K.; Schulthoff, S.; Ueda, Y.; Mariz, R.; Leseurre, L.; Gabor, B.; Fürstner, A., A New Method for the Preparation of Non-Termial Alkynes: Application to the Total Syntheses of Tulearin A and C, *Chem. Eur. J.*, **21,** 219-227 (2015).

Yamanaka, M.; Yoshida, U.; Sato, M.; Shigeta, T.; Yoshida, K.; Furuta, T.; Kawabata, T., Origin of High E-Selectivity in 4-Pyrrolidinopyridine-Catalyzed Tetrasubstituted α, α'-Alkenediol: A Computational and Experimental Study, *J. Org. Chem.*, **80,** 3075-3082 (2015).

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).

Yokoyama, H.; Ueda, Y.; Fujita, D.; Sato, S.; Fujita, M., Finely Resolved Threshold for the Sharp M12L24/M24L48 Structural Switch in Multi-Component MnL2n Polyhedral Assemblies: X-ray, MS, NMR, and Ultracentrifugation Analyses, *Chem. Asian. J.*, **10,** 2292-2295 (2015).

— Advanced Inorganic Synthesis —

Veamatahau, A.; Jiang, B.; Seifert, T.; Makuta, S.; Latham, K.; Kanehara, M.; Teranishi, T.; Tachibana, Y., Origin of Surface Trap States in CdS Quantum Dots: Relationship between Size Dependent Photoluminescence and Sulfur Vacancy Trap States, *Phys. Chem. Chem. Phys.*, **17,** 2850-2858 (2015).

Okano, S.; Tanaka, D.; Sakamoto, M.; Teranishi, T.; Majima, Y., Control of Charging Energy in Chemically Assembled Nanoparticle Single-Electron Transistors, *Nanotechnology*, **26,** 45702(1-9) (2015).

Sakamoto, M.; Chen, L.; Okano, M.; Tex, D. M.; Kanemitsu, Y.; Teranishi, T., Photoinduced Carrier Dynamics of Nearly Stoichiometric Oleylamine-protected Copper Indium Sulfide Nanoparticles and Nanodisks, *J. Phys. Chem. C*, **119,** 11100-11105 (2015).

Chen, L.; Sakamoto, M.; Sato, R.; Teranishi, T., Determination of a Localized Surface Plasmon Resonance Mode of Cu_7S_4 Nanodisks by Plasmon Coupling, *Faraday Discuss.*, **181,** 355-364 (2015).

Serdio, V. M. V.; Muraki, T.; Takeshita, S.; Salinas, D. E. H.; Kano, S.; Teranishi, T.; Majima, Y., Gap Separation-Controlled Nanogap Electrodes by Molecular Ruler Electroless Gold Plating, *RSC Advances*, **5,** 22160-22167 (2015).

Frake, J. C.; Kano, S.; Ciccarelli, C.; Griffiths, J.; Sakamoto, M.; Teranishi, T.; Majima, Y.; Smith, C. G.; Buitelaar, M. R., Radio-frequency Capacitance Spectroscopy of Metallic Nanoparticles, *Sci. Rep.*, **5,** 10858 (2015).

NGUYEN, V. L.; Yang, Y.; Teranishi, T.; Cao, T. M.; Nogami, M., Synthesis and Related Magnetic Properties of $CoFe_2O_4$ Cobalt Ferrite Particles by Polyol Method with $NaBH_4$ and Heat Treatment: New Micro and Nanoscale Structures, *RSC Advances*, **5,** 56560-56569 (2015).

NGUYEN, V. L.; Yang, Y.; Teranishi, T.; Cao, T. M.; Cao, Y.; Nogami, M., Biomedical Applications of Advanced Multifunctional Magnetic Nanoparticles, *J. Nanosci. Nanotech.*, **15,** (2015).

NGUYEN, V. L.; Yang, Y.; Teranishi, T.; Cao, T. M.; Cao, Y.; Nogami, M., Synthesis and Magnetism of Hierarchical Particles, *Mater. Design*, **86,** 797-808 (2015).

Ge, W.; Sato, R.; Teranishi, T., Simple Surfactant Concentration-dependent Shape Control of Polyhedral Fe_3O_4 Nanoparticles and Their Magnetic Properties, *ChemPhysChem*, **16,** 3200-3205 (2015).

Trinh, T. T.; Sato, R.; Sakamoto, M.; Fujiyoshi, Y.; Haruta, M.; Kurata, H.; Teranishi, T., Visible to Near-Infrared Plasmon-Enhanced Catalytic Activity of Pd Hexagonal Nanoplates for the Suzuki Coupling Reaction, *Nanoscale*, **7,** 12435-12444 (2015).

Kano, S.; Maeda, K.; Tanaka, D.; Sakamoto, M.; Teranishi, T.; Majima, Y., Chemically Assembled Double-Dot Single-Electron Transistors Analyzed by the Orthodox Model Considering Offset Charges, *J. Appl. Phys.*, **118,** 134304(1-6) (2015).

[Others]

Reguera, J.; Malachosky, E.; Martin, M.; Tebbe, M.; Law, B.; Isa, L.; Moehwald, H.; Liu, Y.; Bresme, F.; Ganeshan, D.; Sorensen, C.; Ghosh, S.; Fery, A.; Kr´al, P.; Widmer-Cooper, A.; Graf, C.; Gallego, A.; Schiffrin, D.; Korgel, B.; Okram, G.; Sankaranarayanan, S.; Wang, Y.; Teranishi, T.; Salerno, K. M.; McBride, S.; Lin, X.-M., Properties of Self-assembled Nanostructures: General Discussion, *Faraday Discuss.*, **181,** 365-381 (2015).

Reguera, J.; Scarabelli, L.; Petit, C.; Siramdas, R.; Wolf, H.; Chanana, M.; Liu, X.; Martin, M.; Tebbe, M.; Lin, X.-M.; Isa, L.; Moehwald, H.; Sshurtenberger, P.; Velev, O.; Liu, Y.; Fattah, A. R. A.; Bumajdad, A.; Ganeshan, D.; Faivre, D.; Bresme, F.; Sorensen, C.; Coll, P. G.; Ghosh, S.; Fery, A.; Haddassi, F. E.; Salerno, K. M.; Graf, C.; Cardinal, M. F.; Schiffrin, D.; Li, Z.; Shevchenko, E.; Teranishi, T.; Shubiao, Z.; Talapin, D.; Alivisatos, A. P.; Duguet, E.; Philipse, A.; Bianchi, E.; Latsuzbaia, R., New Routes to Control Nanoparticle Synthesis: General Discussion, *Faraday Discuss.*, **181,** 147-179 (2015).

DIVISION OF MATERIALS CHEMISTRY
— Chemistry of Polymer Materials —

Arafune, H.; Kamijo, T.; Morinaga, T.; Honma, S.; Sato, T.;Tsujii, Y., A Robust Lubrication System Using an Ionic Liquid Polymer Brush, *Adv. Mater. Interfaces*, **2,** 1500187 (2015).

Huang, Y.; Ishige, R.; Tsujii, Y.; Ohno, K., Synthesis of Iron Oxide Rods Coated with Polymer Brushes and Control of Their Assembly in Thin Films, *Langmuiri*, **31,** 1172-1179 (2015).

Nomura, K.; Makino, H.; Nakaji-Hirabayashi, T.; Kitano, H.; Ohno, K., Temperature-responsive Copolymer Brush Constructed on a Silica Microparticle by Atom Transfer Radical Polymerization, *Colloid Poly. Sci.*, **293,** 851-859 (2015).

Sato, T.; Marukane, S.; Morinaga, T.; Kamijo, T.; Arafune, H.; Tsujii, Y., High Voltage Electric Double Layer Capacitor Using a Novel Solid-state Polymer Electrolyte, *J. Power Sources*, **295,** 108-116 (2015).

Ogura, K.; Morioka, K.; Tsujii, Y.; Hsu, S. Y.; Wagner, M. H., Uniaxial Extensional Flow Behavior of Comb-shaped Poly(methyl methacrylate), *Rheologica Acta*, **54,** 637-645 (2015).

Kawata, Y.; Yamamoto, T.; Kihara, H.; Ohno, K., Dual Self-Healing Abilities of Composite Gels Consisting of Polymer-Brush-Afforded Particles and an Azobenzene-Doped Liquid Crystal, *ACS Appl. Mater. Interfaces*, **7,** 4185-4191 (2015).

Sato, O.; Iwata, N.; Kasai, T.; Tsujii, Y.; Kang, S. M.; Watanabe, J.; Tokita, M., Nematic Liquid Crystal Anchoring Strengths of High Density Polymer Brush Surfaces, *Liquid Crystals*, **42,** 181-188 (2015).

Moraes, J.; Ohno, K.; Maschmeyer, T.; Perrier, S., Selective Patterning of Gold Surfaces by Core/Shell, Semisoft Hybrid Nanoparticles, *Small*, **11,** 482-488 (2015).

Mori, Y.; Chen, T.; Fujisawa, T.; Kobashi, S.; Ohno, K.; Yoshida, S.; Tago, Y.; Komai, Y.; Hata, Y.; Yoshioka, Y., From Cartoon to Real Time MRI: in vivo Monitoring of Phagocyte Migration in Mouse Brain, *Sci. Rep.*, **4,** 6697 (2015).

Lin, C.-C.; Ohno, K.; Clarke, N.; Winey, K. I.; Composto, R. J., Macromolecular Diffusion through a Polymer Matrix with Polymer-Grafted Chained Nanoparticles, *Macromolecules*, **47,** 5357-5364 (2015).

[Others]

Sakakibara, K.; Tsujii, Y.; Harada, T., Interface Control of Wood-Derived Nanocelluloses by Using Novel Polymer Dispersant toward High Performance Resin Nanocomposite Materials, *Nippon Gomu Kyokaishi*, **88,** 443-446(2015) (in Japanese).

— Polymer Controlled Synthesis —

PeñaAlvarez, M.; Burrezob, P. M.; Iwamoto, T.; Taravilloa, M.; Baonzaa, V. G.; Navarreteb, J. T. L.; Yamago, S.; Casado, J., Chameleon-like Behaviour of Cyclo[n]paraphenylenes in Complexes with C_{70}. On Their Impressive Electronic and Structural Adaptability as Probed by Raman spectroscopy, *Faraday Discuss.*, **173,** 157-171 (2014).

Nakamura, Y.; Yamago, S., Termination Mechanism in the Radical Polymerization of Methyl Methacrylate and Styrene Determined by the Reaction of Structurally Well-defined Polymer End Radicals, *Macromolecules*, **48,** 6450-6456 (2015).

Nakamura, Y.; Yu, M.; Ukai, Y.; Yamago, S., Organotellurium-mediated Radical Polymerization under Photo Irradiation, *ACS Symp. Ser.*, **1187,** 295-309 (2015).

Kayahara, E.; Patel, V. K.; Xia, J.; Jasti, R.; Yamago, S., Selective and Gram-scale Synthesis of [6]Cycloparaphenylene, *Synlett*, **26,** 1615-1619 (2015).

Fujistuka, M.; Tojo, S.; Iwamoto, T.; Kayahara, E.; Yamago, S.; Majima, T., Radical Ions of Cyclopyrenylene: Comparison of Spectral Properties with Cycloparaphenylene, *J. Phys. Chem. Part A*, **119,** 4136-4141 (2015).

Patel, V. K.; Kayahara, E.; Yamago, S., Practical Synthesis for [n] Cycloparaphenylenes (n = 5, 7-12) by H_2SnCl_4-Mediated Aromatization of 1,4-Dihydroxylcyclo-2,5-diene Precursors, *Chem. Eur. J.*, **21,** 5742-5749 (2015).

Toriumi, N.; Muranaka, A.; Kayahara, E.; Yamago, S.; Uchiyama, M., In-Plane Aromaticity in Cycloparaphenylene Dications: A Magnetic Circular Dichroism and Theoretical Study, *J. Am. Chem. Soc.*, **137,** 82-85 (2015).

Tien, N.-D.; Nishikawa, Y.; Hashimoto, M.; Tosaka, M.; Sasaki, S.; Sakurai, S., Three-dimensional Analyses of Spherulite Morphology in Poly(oxyethylene) and Its Blends with Amorphous Poly(d,l-lactic acid) Using X-ray Computerized Tomography, *Polymer J.*, **47,** 37-44 (2015).

Gros, A.; Tosaka, M.; Huneau, B.; Verron, E.; Poompradub, S.; Senoo, K., Dominating Factor of Strain-induced Crystallization in Natural Rubber, *Polymer*, **76,** 230-236 (2015).

Sugihara, Y.; Yamago, S.; Zetterlund, P., An Innovative Approach to Implementation of Organotellurium-Mediated Radical Polymerization (TERP) in Emulsion Polymerization, *Macromolecules*, **48,** 4312-4318 (2015).

Nakagawa, H.; Yamago, S.; Ishihara, K.; Yusa, S., Preparation of Biocompatible Poly(2-methacryloyloxyethyl phosphorylcholine) (PMPC) via Organotellulium-Medicated Radical Polymerization (TERP), *Kobunshi Ronbunshu*, **72,** 335-340 (2015).

Kayahara, E.; Qu, R.; Kojima, M.; Iwamoto, T.; Suzuki, T.; Yamago, S., Ligand-controlled Synthesis of [3]- and [4]Cyclo-9,9-dimethyl-2,7-fluorenes through Triangle- and Square-shaped Platinum Intermediates, *Chem. Eur. J.*, **21,** 18939-18943 (2015).

Fujita, T.; Yamago, S., Lewis-acid-mediated Stereospecific Radical Polymerization of Acrylimides Bearing Chiral Oxazolidinones, *Chem. Eur. J.*, **21,** 18547-18550 (2015).

Yamago, S.; Nakamura, Y., Photo-Induced Living/Controlled Radical Polymerization Reaction, *Kobunshi (High Polymers, Japan)*, **64,** 103-106 (2015) (in Japanese).

Tosaka, M., Kinetics of Strain-induced Crystallization in Cross-linked Natural Rubber, *J. Adhesion Soc. Jpn.*, **51,** 450-455 (2015) (in Japanese).

Nakamura, Y.; Yamago, S., Organotellurium-mediated Living Radical Polymerization, *Finechemical*, **44,** 25-31 (2015) (in Japanese).

Iwamoto, T.; Takaya, H.; Yamago, S., Structural Investigation of Cycloparaphenylene – Fullerene Supramolecular Complexes Using Synchrotron Radiation and Theoretical Calculation, *J. Cryst. Soc. Jpn.*, **57,** 239-244 (2015) (in Japanese).

— Inorganic Photonics Materials —

Masai, H.; Yamada, Y.; Okumura, S.; Yanagida, T.; Fujimoto, Y.; Kanemitsu, Y.; Ina, T., Photoluminescence of Monovalent Indium Centres in Phosphate Glass, *Scientific Reports*, **5,** 13646 (2015).

Ueda, Y.; Tokuda, Y.; Nihei, N.; Sugiyama, A.; Ogawa, Y., Fine Bubble Technology as an Adhesive Agent with Gas-liquid Interface, *Journal of the Adhesion Society of Japan*, **50,** 58-65 (2015).

Ueda, Y.; Tokuda, Y.; Nihei, N.; Sugiyama, A.; Ogawa, Y.; Shiraga, K., Electric and Electrochemical Properties of Fine Bubble Water and Analysis of the Correlation with Applied Research, *THE JAPANESE SOCIETY FOR MULTIPHASE FLOW*, **28,** 555-562 (2015).

Masai, H.; Hino, Y.; Yanagida, T.; Fujimoto, Y.; Tokuda, Y., High Energy-transfer Rate from Sn^{2+} to Mn^{2+} in Phosphate Glasses, *Optical Materials Express*, **5,** 617-622 (2015).

Ueda, Y.; Tokuda, Y.; Goto, H., Remediation Technology of Cesium Using a Micro-bubble Water Containing Sodium Silicate, *Radiological Issues for Fukushima's Revitalized Future, Springer*, 79-88 (2015).

Tokuda, Y.; Norikawa, Y.; Masai, H.; Ueda, Y.; Nihei, N.; Fujimura, S.; Ono, Y., Nuclear Magnetic Resonance Study of Cs Adsorption onto Clay Minerals, *Radiological Issues for Fukushima's Revitalized Future, Springer*, 3-12 (2015).

Tokuda, Y.; Takahashi, Y.; Masai, M.; Kaneko, S.; Ueda, Y.; Fujimura, S.; Yoko, T., Local Structure of Alkalis in Mixed Alkali Borate Glass to Elucidate the Origin of Mxed-alkali Effect, *J. Asian Ceram. Soc*, (2015).

Masai, H.; Yanagida, T.; Mizoguchi, T.; Ina, T.; Miyazaki, T.; Kawaguti, N.; Fukuda, K., Local Coordination State of Rare Earth in Eutectic Scintillators for Neutron Detector Applications, *Scientific Reports*, **5,** 13332 (2015).

Masai, H.; Suzuki, Y.; Yanagida, T.; Mibu, K., Luminescence of Sn^{2+} Center in $ZnO-B_2O_3$ Glasses Melted in Air and Ar Condition, *Bulletin of the Chemical Society of Japan*, **88,** 1047–1053 (2015).

Masai, H.; Yanagida, T., Emission Property of Ce^{3+}-doped $Li_2O-B_2O_3-SiO_2$ Glasses, *Optical Materials Express*, **5,** 1851-1858 (2015).

Kinoshita, M.; Takahashi, Y.; Terakado, N.; Masai, H.; Fujiwara, T., Controllable Photoluminescence by Melting-process Temperature in SnO-containing Glass, *Journal of the Ceramic Society of Japan*, **123,** 614-617 (2015).

Masai, H.; Miyata, H.; Yamada, Y.; Okumura, S.; Yanagida, T.; Kanemitsu, Y., Tin-Doped Inorganic Amorphous Films for Use as Transparent Monolithic Phosphors, *Scientific Reports*, **5,** 11224 (2015).

Nanto, H.; Nakagawa, R.; Takei, Y.; Hirasawa, K.; Miyamoto, Y.; Masai, H.; Kurobori, T.; Yanagida, T.; Fujimoto, Y., Optically Stimulated Luminescence in X-ray Irradiated $xSnO–(25−x)SrO–75B_2O_3$ Glass, *Nuclear Instruments and Methods in Physics Research Section A*, **784,** 14-16 (2015).

Masai, H.; Yanagida, T.; Fujiwara, T., Photo- and Radioluminescence of ZnO-precipitated Glass-Ceramics, *Sensors and Materials*, **37,** 237-245 (2015).

Masai, H.; Hino, Y.; Yanagida, T.; Fujimoto, Y., Photoluminescence and Radioluminescence Properties of MnO-doped $SnO-ZnO-P_2O_5$ Glasses, *Optical Materials*, **42,** 381-384 (2015).

Masai, H.; Miyazaki, T.; Mibu, K.; Takahashi, Y.; Fujiwara, T., Nano-phase Separation and the Effect of SnO Addition in TiO_2-precipitated Glass-ceramics, *Journal of European Ceramics Society*, **35,** 2139-2144 (2015).

Masai, H.; Hino, Y.; Yanagida, T.; Fujimoto, Y.; Tokuda, Y., High Energy-transfer Rate from Sn^{2+} to Mn^{2+} in Phosphate Glasses, *Optical Materials Express*, **5,** 617-622 (2015).

— Nanospintronics —

Hiramatsu, R.; Kim, K.; Taniguchi, T.; Tono, T.; Moriyama, T.; Fukami, S.; Yamanouchi, M.; Ohno, H.; Nakatani, Y.; Ono, T., Localized Precessional Mode of Domain Wall Controlled by Magnetic Field and dc Current, *Appl. Phys. Exp*, **8,** [023003-1] -[023003-4] (2015).

Arakawa, T.; Shiogai, J.; Ciorga, M.; Utz, M.; Schuh, D.; Kohda, M.; Nitta, J.; Bougeard, D.; Weiss, D.; Ono, T.; Kobayashi, K., Shot Noise Induced by Nonequilibrium Spin Accumulation, Phys. *Rev. Lett.*, **114,** [016601-1] -[016601-4] (2015).

Ueda, K.; Hiramatsu, R.; Kim, K.; Taniguchi, T.; Tono, T.; Moriyama, T.; Ono, T., Temperature Dependence of Current-induced Magnetic Domain Wall Motion in an Asymmetric Co/Ni Nanowire, *J.J. of Appl. Phys.*, **54,** [038004-1]-[038004-3] (2015).

Madami, M.; Gubbiotti, G.; Moriyama, T.; Tanaka, K.; Siracusano, G.; Carpentieri, M.; Finocchio, G.; Tacchi, S.; Ono, T.; Carlotti, G., Micro-focused Brillouin Light Scattering Study of the Magnetization Dynamics Driven by Spin Hall Effect in a Transversely Magnetized Rectangular NiFe Nanowire, *J. of Appl. Phys.*, **447,** [17D504-1]-[17D504-4] (2015).

Gubbiotti, G.; Nguyen, H.; Hiramatsu, R.; Tacchi, S.; Cottam, M.; Ono, T., Resonant Spin-wave Modes in Trilayered Magnetic Nanowires Studied in the Parallel and Antiparallel Ground State, *J. Magn. Magn. Mater.*, **384,** 45-48 (2015).

Ueda, K.; Kim, K.; Taniguchi, T.; Tono, T.; Moriyama, T.; Ono, T., In-plane Field-driven Crossover in the Spin-torque Mechanism Acting on Magnetic Domain Walls in Co/Ni, *Phys. Rev. B*, **91,** [060405-1]-[060405-5] (2015).

Tono, T.; Taniguchi, T.; Kim, K.; Moriyama, T.; Tsukamoto, A.; Ono, T., Chiral Magnetic Domain Wall in Ferrimagnetic GdFeCo Wires, *Appl. Phys. Exp.*, **8,** [073001-1]-[073001-4] (2015).

Mizuno, H.; Moriyama, T.; Kawaguchi, M.; Nagata, M.; Tanaka, K.; Koyama, T.; Chiba, D.; Ono, T., Ferromagnetic Resonance Measurements in Sub-nanometer Fe Films, *Appl. Phys. Exp.*, **8,** [073003-1]-[073003-4] (2015).

Taniguchi, T.; Kim, K.; Tono, T.; Kim, S.; Moriyama, T.; Ono, T., Dimensional Crossover Characterized by Distribution of Magnetic Domain Wall Creep Velocity, *Appl. Phys. Exp.*, **8,** [073004-1]-[073004-4] (2015).

Taniguchi, T.; Kim, K.; Tono, T.; Moriyama, T.; Nakatani, Y.; Ono, T., Precise Control of Magnetic Domain Wall Displacement by a Nanosecond Current Pulse in Co/Ni Nanowires, *Appl. Phys. Exp.*, **8,** [073008-1]-[073008-4] (2015).

Hata, H.; Moriyama, T.; Tanabe, K.; Kobayashi, K.; Matsumoto, R.; Murakami, S.; Ohe, J.; Chiba, D.; Ono, T., Micromagnetic Simulation of Spin Wave Propagation in a Ferromagnetic Film with Different Thicknesses, *J. of Magn. Soc. Japan*, **39,** 151-154 (2015).

Moriyama, T.; Yoon, S.; McMichael, R. D., Ferromagnetic Resonance Measurement Using Stroboscopic Magneto-optical Kerr, *J. of Appl. Phys.*, **117,** [213908-1]-[213908-4] (2015).

Matsuzaki, N.; Moriyama, T.; Nagata, M.; Kim, K.; Suzuki, I.; Taniyama, T.; Ono, T., Current Induced Antiferro-ferromagnetic Transition in FeRh Nanowires, *J.J. of Appl. Phys.*, **54,** 54- (2015).

Moriyama, T.; Takei, S.; Nagata, M.; Yoshimura, Y.; Matsuzaki, N.; Terashima, T.; Tserkovnyak, Y.; Ono, T., Anti-damping Spin Transfer Torque through Epitaxial Nickel Oxide, *Appl. Phys. Lett.*, **106,** [162406-1]-[162406-4] (2015).

Kawaguchi, M.; Moriyama, T.; Koyama, T.; Chiba, D.; Ono, T., Layer Thickness Dependence of Current Induced Effective Fields in Ferromagnetic Multilayers, *J. of Appl. Phys.*, **117,** [17C730-1]-[17C730-4] (2015).

Mishra, P.; Hill, P., J.; Vijayaraghavan, S.; Rossom, V. W.; Yoshizawa, S.; Grisolia, M.; Echeverria, J.; Ono, T.; Ariga, K.; Nakayama, T.; Joachim, C.; Uchihashi, T., Current-Driven Supramolecular Motor with In Situ Surface Chiral Directionality Switching, *Nano Lett.*, **15,** 4793-4798 (2015).

Matsuo, S.; Nakaharai, S.; Komatsu, K.; Tsukagoshi, K.; Moriyama, T.; Ono, T.; Kobayashi, K., Parity Effect of Bipolar Quantum Hall Edge Transport around Graphene Antidots, *Sci. Rep.*, **5,** [11723-1]-[11723-5] (2015).

Matsuo, S.; Takeshita, S.; Tanaka, T.; Nakaharai, S.; Tsukagoshi, K.; Moriyama, T.; Ono, T.; Kobayashi, K., Edge Mixing Dynamics in Graphene p–n Junctions in the Quantum Hall Regime, *Nat. Commun.*, **6,** [8066-1]-[8066-6] (2015).

Moriyama, T.; Matsuzaki, N.; Kim, K.; Suzuki, I.; Taniyama, T.; Ono, T., Sequential Write-read Operations in FeRh Antiferromagnetic Memory, *Appl. Phys. Lett.*, **107,** [122403-1]-[122403-4] (2015).

Takei, S.; Moriyama, T.; Ono, T.; Tserkovnyak, Y., Antiferromagnet-mediated Spin Transfer between Metal and Ferromagnet, *Phys. Rev. B*, **92,** [020409-1]-[020409-4] (2015).

DIVISION OF BIOCHEMISTRY
— Biofunctional Design-Chemistry —

Kuroda, Y.; Kato-Kogoe, N.; Tasaki, E.; Yuasa-Sunagawa, M.; Yamanegi, K.; Nakasyo, K.; Nakase, I.; Futaki, S.; Tohyama, Y.; Hirose, M., Suppressive Effect of Membrane-permeable Peptides Derived from Autophosphorylation Sites of the IGF-1 Receptor on Breast Cancer Cells, *Eur. J. Pharm.*, **765,** 24-33 (2015).

Takeuchi, T.; Suzuki, M.; Fujikake, N.; Popiel, H. A.; Kikuchi, H.; Futaki, S.; Wada, K.; Nagai, Y., Intercellular Chaperone Transmission via Exosomes Contributes to Maintenance of Protein Homeostasis at the Organismal Level, *Proc. Natl. Acad. Sci. U.S.A.*, **112,** E2497-E2506 (2015).

Nakase, I.; Futaki, S., Combined Treatment with a pH-sensitive Fusogenic Peptide and Cationic Lipids Achieves Enhanced Cytosolic Delivery of Exosomes, *Sci. Rep.*, **5,** 10112 (2015).

Nakase, I.; Takeuchi, T.; Futaki, S., Cell Penetrating Peptides for Chemical Biological Studies, *Methods Mol. Biol.*, **1324,** 387-396 (2015).

Nakase, I.; Kawaguchi, Y.; Nomizu, M.; Futaki, S., Cellular Uptake of Arginine-Rich Cell-Penetrating Peptides and the Contribution of Membrane-Associated Proteoglycans, *Trends Glycosci. Glycotech.*, **27,** 81-88 (2015).

— Chemistry of Molecular Biocatalysts —

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).

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).

[Others]

Watanabe, B., Structure-Activity Relationship Studies of Insect and Plant Steroid Hormones, *J. Pestic. Sci.*, **40,** 146-151 (2015).

— Molecular Biology —

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

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

Li, N.; Teranishi, M.; Yamaguchi, H.; Matsushita, T.; Watahiki, M. K.; Tsuge, T.; Li, S. S.; Hidema, J., UV-B-Induced CPD Photolyase Gene Expression is Regulated by UVR8-Dependent and -Independent Pathways in Arabidopsis, *Plant Cell Physiol.*, **56,** 2014-2023 (2015).

— Chemical Biology —

Sato, S.; Watanabe, M.; Katsuda, Y.; Murata, A.; Wang, D. O.; Uesugi, M., Live-cell Imaging of Endogenous mRNAs with a Small Molecule, *Angew. Chem. Int. Ed.*, **54,** 1855-1858 (2015).

Sato, S.; Katsuda, Y.; Uesugi, M., Biochemical Purification of Target Proteins with Biotin Conjugates, *CSJ Current Review - Chemical Biology of Bioactive Small Molecules: Target Identification and Mechanism-of-Action Studies*, **19,** 42-47 (2015) (in Japanese).

Parvatkar, P.; Kato, N.; Uesugi, M.; Sato, S.; Ohkanda, J., Intracellular Generation of a Diterpene-Peptide Conjugate that Inhibits 14-3-3-Mediated Interactions, *J. Am. Chem. Soc.*, **137,** 15624-15627 (2015).

Takaya, J.; Mio, K.; Shiraishi, T.; Kurokawa, T.; Otsuka, S.; Mori, Y.; Uesugi, M., A Potent and Site-selective Agonist of TRPA1, *J. Am. Chem. Soc.*, **137,** 15859-15864 (2015).

DIVISION OF ENVIRONMENTAL CHEMISTRY

— Molecular Materials Chemistry —

Shizu, K.; Tanaka, H.; Uejima, M.; Sato, T.; Tanaka, K.; Kaji, H.; Adachi, C., Strategy for Designing Electron Donors for Thermally Activated Delayed Fluorescence Emitters, *J. Phys. Chem. C*, **119,** 1291-1297 (2015).

Kotani, M.; Dohi, H.; Kimura, H.; Muraoka, K.; Kaji, H., Distribution Ratio of Carbon Black in Polyisobutyrene/Polyisoprene Rubber Blends Using High-Resolution Solid-state ^{13}C NMR, *Polym. J.*, **47,** 422-427 (2015).

Kaji, H.; Suzuki, H.; Fukushima, T.; Shizu, K.; Suzuki, K.; Kubo, S.; Komino, T.; Oiwa, H.; Suzuki, F.; Wakamiya, A.; Murata, Y.; Adachi, C., Purely Organic Electroluminescent Material Realizing 100% Conversion from Electricity to Light, *Nat. Commun.*, **6,** [8476-1]-[8476-8] (2015).

Fukushima, T.; Yamamoto, J.; Fukuchi, M.; Hirata, S.; Jung, H. H.; Hirata, O.; Shibano, Y.; Adachi, C.; Kaji, H., Material Degradation of Liquid Organic Semiconductors Analyzed by Nuclear Magnetic Resonance Spectroscopy, *AIP Adv.*, **5,** [087124-1]-[087124-5] (2015).

Asakura, T.; Ohata, T.; Kametani, S.; Okushita, K.; Yazawa, K.; Nishiyama, Y.; Nishimura, K.; Aoki, A.; Suzuki, F.; Kaji, H.; Ulrich, A. S.; Williamson, M. P., Intermolecular Packing in *B. mori* Silk Fibroin: Multinuclear NMR Study of the Model Peptide (Ala-Gly)$_{15}$ Defines a Heterogeneous Antiparallel Antipolar Mode of Assembly in the Silk II Form, *Macromolecules*, **48,** 28-36 (2015).

Suzuki, F.; Shizu, K.; Kawaguchi, H.; Furukawa, S.; Sato, T.; Tanaka, K.; Kaji, H., Multiscale Simulation of Charge Transport in a Host Material, *N,N'*-Dicarbazole-3,5-benzene (mCP), for Organic Light-emitting Diodes, *J. Mater. Chem. C*, **3,** 5549-5555 (2015).

Shizu, K.; Uejima, M.; Nomura, H.; Sato, T.; Tanaka, K.; Kaji, H.; Adachi, C., Enhanced Electroluminescence from a Thermally Activated Delayed-Fluorescence Emitter by Suppressing Nonradiative Decay, *Phys. Rev. Appl.*, **3,** [014001-1]-[014001-7] (2015).

Shizu, K.; Lee, J.; Tanaka, H.; Nomura, H.; Yasuda, T.; Kaji, H.; Adachi, C., Highly Efficient Electroluminescence from Purely Organic Donor-acceptor Systems, *Pure. Appl. Chem.*, **87,** 627-638 (2015).

Sato, T.; Uejima, M.; Tanaka, K.; Kaji, H.; Adachi, C., A Light-emitting Mechanism for Organic Light-emitting Diodes: Molecular Design for Inverted Singlet-triplet Structure and Symmetry-controlled Thermally Activated Delayed Fluorescence, *J. Mater. Chem. C*, **3,** 870-878 (2015).

Ohtsuki, A.; Lei, L.; Tanishima, M.; Goto, A.; Kaji, H., Photocontrolled Organocatalyzed Living Radical Polymerization Feasible over a Wide Range of Wavelengths, *J. Am. Chem. Soc.*, **137,** 5610-5617 (2015).

Lee, J.; Shizu, K.; Tanaka, H.; Nakanotani, H.; Yasuda, T.; Kaji, H.; Adachi, C., Controlled Emission Colors and Singlet-triplet Energy Gaps of Dihydrophenazine-Based Thermally Activated Delayed Fluorescence Emitters, *J. Mater. Chem. C*, **3,** 2175-2181 (2015).

Sagara, Y.; Shizu, K.; Tanaka, H.; Miyazaki, H.; Goushi, K.; Kaji, H.; Adachi, C., Highly Efficient Thermally Activated Delayed Fluorescence Emitters with a Small Singlet-Triplet Energy Gap and Large Oscillator Strength, *Chem. Lett.*, **44,** 360-362 (2015).

Shizu, K.; Sakai, Y.; Tanaka, H.; Hirata, S.; Adachi, C.; Kaji, H., Meta-linking Strategy for Thermally Activated Delayed Fluorescence Emitters with a Small Singlet-Triplet Energy Gap, *ITE Trans. on MTA*, **3,** 108-113 (2015).

Suzuki, K.; Kubo, S.; Shizu, K.; Fukushima, T.; Wakamiya, A.; Murata, Y.; Adachi, C.; Kaji, H., Triarylboron-based Fluorescent Organic Light-emitting Diodes with External Quantum Efficiencies Exceeding 20%, *Angew. Chem. Int. Ed.*, **54,** 15231–15235 (2015).

Shizu, K.; Noda, H.; Tanaka, H.; Taneda, M.; Uejima, M.; Sato, T.; Tanaka, K.; Kaji, H.; Adachi, C., Highly Efficient Blue Electroluminescence Using Delayed-Fluorescence Emitters with Large Overlap Density between Luminescent and Ground States, *J. Phys. Chem. C*, (2015)(in press).

Wada, Y.; Shizu, K.; Kubo, S.; Suzuki, K.; Tanaka, H.; Adachi, C.; Kaji, H., Highly Efficient Electroluminescence from a Solution-Processable Thermally Activated Delayed Fluorescence Emitter, *Appl. Phys. Lett.*, **107,** [183303-1]-[183303-4] (2015).

Taneda, M.; Shizu, K.; Tanaka, H.; Adachi, C., High Efficiency Thermally Activated Delayed Fluorescence Based On 1,3,5-Tris(4-(Diphenylamino)Phenyl)-2,4,6-Tricyanobenzene, *Chem. Commun.*, **51,** 5028-5031 (2015).

Tanaka, H.; Shizu, K.; Lee, J.; Adachi, C., Effect of Atom Substitution in Chalcogenodiazole-Containing Thermally Activated Delayed Fluorescence Emitters on Radiationless Transition, *J. Phys. Chem. C*, **119,** 2948-2955 (2015).

Hirata, S.; Sakai, Y.; Masui, K.; Tanaka, H.; Lee, S. Y.; Nomura, H.; Nakamura, N.; Yasumatsu, M.; Nakanotani, H.; Zhang, Q.; Shizu, K.; Miyazaki, H.; Adachi, C., Highly Efficient Blue Electroluminescence Based on Thermally Activated Delayed Fluorescence, *Nat. Mater.*, **14,** 330-336 (2015).

— Hydrospheric Environment Analytical Chemistry —

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).

[Others]

Takano, S., Isotopic Study for Biogeochemical Cycling of Cu in the Ocean, *Transactions of the Research Institute of Oceanochemistry*, **28,** 10-16 (2015) (in Japanese).

Minami, T., Sectional Distributions of Bioactive Trace Metals in the Southern Ocean and the Western Pacific, *Transactions of the Research Institute of Oceanochemistry*, **28,** 70-76 (2015) (in Japanese).

— Solution and Interface Chemistry —

Shioya, N; Shimoaka, T.; Eda, K.; Hasegawa, T., A New Schematic of Poly(3-alkylthiophene) in an Amorphous Film Studied by Using a Novel Structural Index on Infrared Spectroscopy, *Phys. Chem. Chem. Phys.*, **17,** 13472-13479 (2015).

Shimoaka, T.; Wakai, C.; Sakabe, T.; Yamazaki, S.; Hasegawa, T, Hydration Structure of the Strongly Bound Water on the Sulfonic Acid Group in a Nafion Membrane Studied by Infrared Spectroscopy and Quantum Chemical Calculation, *Phys. Chem. Chem. Phys.*, **17,** 8843-8849 (2015).

Wakai, C.; Shimoaka, T.; Hasegawa, T., ^{1}H NMR Analysis of Water Freezing in Nanospace Involved in a Nafion Membrane, *J. Phys. Chem. B*, **119,** 8048-8053 (2015).

Hasegawa, T., Understanding of the Intrinsic Difference between Normal- and Perfluoro-alkyl Compounds toward Total Understanding of Material Properties, *Chem. Phys. Lett.*, **627,** 64-66 (2015).

Hasegawa, T.; Shimoaka, T.; Tanaka, Y.; Shioya, N.; Morita, K.; Sonoyama, M.; Amii, H.; Takagi, T.; Kanamori, T., An Origin of Complicated Infrared Spectra of Perfluoroalkyl Compounds Involving a Normal Alkyl Group, *Chem. Lett.*, **44,** 834-836 (2015).

Ishizuka, R.; Matubayasi, N.; Tu, K.-M.; Umebayashi, Y., Energetic Contributions from Cation and Anion to the Stability of Carbon Dioxide Dissolved in Imidazolium-Based Ionic Liquids, *J. Phys. Chem. B*, **119,** 1579-1587 (2015).

— Molecular Microbial Science —

Goto, S.; Kawamoto, J.; Sato, S. B.; Iki, T.; Watanabe, I.; Kudo, K.; Esaki, N.; Kurihara, T., Alkyl Hydroperoxide Reductase Enhances the Growth of *Leuconostoc mesenteroides* Lactic Acid Bacteria at Low Temperatures, *AMB Express*, **5,** 11 (2015).

Kawamoto, J.; Kurihara, T.; Cold-adaptation mechanism of Psychrotrophic Bacteria, *Seibutsu Kogaku Kaishi*, **93,** 477-480 (2015) (in Japanese).

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

— Polymer Materials Science —

Kanaya, T.; Ogawa, H.; Kishimoto, M.; Inoue, R.; Suter, A.; Prokscha, T., Distribution of Glass Transition Temperatures T-g in Polystyrene Thin Films as Revealed by Low-energy Muon Spin Relaxation: A Comparison with Neutron Reflectivity Results, *Phys. Rev. E*, **92,** [022604-1]-[022604-7] (2015).

Miyazaki, T.; Shimokita, K.; Ogawa, H.; Yamamoto, K., System for in Situ Observation of Three-dimensional Structural Changes in Polymer Films during Uniaxial Deformation, *J. Appl. Cryst.*, **48,** 1016-1022 (2015).

Shinohara, T.; Higaki, Y.; Nojima, S.; Masunaga, H.; Ogawa, H.; Okamoto, Y.; Aoki, T.; Takahara, A., Molecular Aggregation States and Wetting Behavior of a Poly{2-(perfluorooctyl)ethyl acrylate} Brush-immobilized Nano-imprinted Surface, *Polymer*, **69,** 42293 (2015).

Matsuura, T.; Murakami, M.; Inoue, R.; Nishida, K.; Ogawa, H.; Ohta, N.; Kanaya, T., Microbeam Wide-Angle X-ray Scattering Study on Precursor of Shish Kebab. Effects of Shear Rate and Annealing on Inner Structure, *Macromolecules*, **48,** 3337-3343 (2015).

Ishige, R.; Higuchi, T.; Jiang, X.; Mita, K.; Ogawa, H.; Yokoyama, H.; Takahara, A.; Jinnai, H., Structural Analysis of Microphase Separated Interface in an ABC-Type Triblock Terpolymer by Combining Methods of Synchrotron-Radiation Grazing Incidence Small-Angle X-ray Scattering and Electron Microtomography, *Macromolecules*, **48,** 2697-2705 (2015).

Nishida, K.; Zhuravlev, E.; Yang, B.; Schick, C.; Shiraishi, Y.; Kanaya T., Vitrification and Crystallization of Poly(butylene-2,6-naphthalate), *Thermochim. Acta*, **603,** 110-115 (2015).

Osaka, O.; Benten, H.; Ohkita, H.; Ito, S.; Ogawa, H.; Kanaya, T., Nanostructures for Efficient Hole Transport in Poly(3- hexylthiophene) Film: A Study by Conductive Atomic Force Microscopy, *J. Phys. Chem. C*, **43,** 24307-24314 (2015).

Ogawa, H.; Nishikawa, Y.; Fujiwara, A.; Takenaka, M.; Wang, Y.-C.; Kanaya, T.; Takata, M., Visualizing Patterned Thin Films by Grazing-incidence Small Angle X-ray Scattering (GISAXS) Coupled with Computed Tomography (CT), *J. Appl. Cryst.*, **48,** 1645-1650 (2015).

Chatani, E.; Inoue, R.; Imamura, H.; Sugiyama, M.; Kato, M.; Yamamoto, M.; Nishida, K.; Kanaya, T., Early Aggregation Preceding the Nucleation of Insulin Amyloid Fibrils as Monitored by Small Angle X-ray Scattering, *Sci. Rep.*, **5,** [15485-1]-[15485-14] (2015).

Nishida, K.; Hirabayashi, T.; Tanaka, K.; Morita, H.; Matsuba, G.; Kanaya, T., Salting-In and Salting-Out Effects on Cloud Point of Aqueous Methylcellulose by Addition of Monomeric and Polymeric Sodium Styrene Sulfonate, *Sen'i Gakkaishi (J. Soc. Fiber Sci. Technol., Jpn)*, **71,** 297-301 (2015) (in Japanese).

[Others]

Kanaya, T.; Takahashi, N.; Inoue, R.; Nishida, K.; Matsuba, G., Flow and Deformation-induced Polymer Crystallization by SANS and SAXS, *Nihon Kessho Gakkaishi*, **57,** 27-33 (2015) (in Japanese).

— Molecular Rheology —

Matsumiya, Y.; Rakkapao, N.; Watanabe, H., Entanglement Length in Miscible Blends of cis-Polyisoprene and Poly(p-tert-butylstyrene), *Macromolecules*, **48,** 7889-7908 (2015).

Timachova, K.; Watanabe, H.; Balsara, N. P., Effect of Molecular Weight and Salt Concentration on Ion Transport and the Transference Number in Polymer Electrolytes, *Macromolecules*, **48,** 7882-7888 (2015).

Umeki, Y.; Mohri, K.; Kawasaki, Y.; Watanabe, H.; Takahashi, R.;Takahashi, Y.; Takakura, Y.; Nishikawa, M., Induction of Potent Antitumor Immunity by Sustained Release of Cationic Antigen from a DNA-based Hydrogel with Adjuvant Activity, *Advanced Functional Materials*, **25,** 5758-5767 (2015).

Watanabe, H.; Matsumiya, Y.; Inoue, T., Revisit the Stress-Optical Rule for Entangled Flexible Chains: Overshoot of Stress, Segmental Orientation, and Chain Stretch on Start-up of Flow, *J. Soc. Rheol. Jpn*, **43,** 105-112 (2015).

Schauser, N. S.; Harry, K. J.; Parkinson, D. Y.; Watanabe, H.; Balsara, N. P., Lithium Dendrite Growth in Glassy and Rubbery Nanostructured Block Copolymer Electrolytes, *J. Electochem. Soc.*, **162,** A398-A405 (2015).

Watanabe, H.; Matsumiya, Y.; Masubuchi, Y.; Urakawa, O.; Inoue, T., Viscoelastic Relaxation of Rouse Chains undergoing Head-to-Head Association and Dissociation: Motional Coupling through Chemical Equilibrium, *Macromolecules*, **48,** 3014-3030 (2015).

— Molecular Aggregation Analysis —

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

Yoshida, H.; Yamada, K.; Tsutsumi, J.; Sato, N., Complete Description of Ionization Energy and Electron Affinity in Organic Solids: Determining Contributions from Electronic Polarization, Energy Band Dispersion and Molecular Orientation, *Phys. Rev. B*, **92,** [075145-]-[075145-13] (2015).

Yoshida, H.; Yoshizaki, K., Electron Affinities of Organic Materials Used for Organic Light-Emitting Diodes: A Low-Energy Inverse Photoemission Study, *Org. Electron.*, **20,** 24-30 (2015).

Zhong, Y.; Izawa, S.; Hashimoto, K.; Tajima, K.; Koganezawa, T.; Yoshida, H., Crystallization-Induced Energy Level Change of [6,6]-Phenyl-C_{61}-Butyric Acid Methyl Ester (PCBM) Film: Impact of Electronic Polarization Energy, *J. Phys. Chem. C*, **119,** 23-28 (2015).

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

— Particle Beam Science —

Arimoto, Y.; Higashi, N.; Igarashi, Y.; Iwashita, Y.; Ino, T.; Katayama, R.; Kitaguchi, M.; Kitahara, R.; Matsumura, H.; Mishima, K.; Nagakura, N.; Oide, H.; Otono, H.; Sakakibara, R.; Shima, T.; Shimizu, H. M.; Sugino, T.; Sumi, N.; Sumino, H.; Taketani, K.; Tanaka, G.; Tanaka, M.;Tauchi, K.; Toyoda, A.; Tomita, T.; Yamada, T.; Yamashita, S.; Yokoyama, H.; Yoshioka, T., Development of Time Projection Chamber for Precise Neutron Lifetime Measurement Using Pulsed Cold Neutron Beams, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, **799,** 187-196 (2015).

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.; Garbe, U.; 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, *Progress of Theoretical and Experimental Physics*, [043G01-1]-[043G01-22] (2015).

[Others]

Iwashita, Y.; Fuwa, Y., New Series of RFQ Vane Shapes, *Proceedings of the 6th International Particle Accelerator Conference, IPAC'15*, 3808-3810 (2015).

Hajima, R.; Sawamura, M.; Kubo, T.; Saeki, T.; Cenni, E.; Iwashita, Y.; Tongu, H., Development of Superconducting Spoke Cavities for Laser Compton Scattered X-ray Sources, *Proceedings of the 6th International Particle Accelerator Conference, IPAC'15*, 2902-2904 (2015).

Kubo, T.; Saeki, T.; Cenni, E.; Iwashita, Y.; Tongu, H.; Hajima, R.; Sawamura, M., Multipactor Simulations in 325 MHz Superconducting Spoke Cavity for an Electron Accelerator, *Proceedings of the 6th International Particle Accelerator Conference, IPAC'15*, 2892-2894 (2015).

Fuwa, Y.; Iwashita, Y.; Tongu, H.; Inoue, S.; Hashida, M.; Sakabe, S.; Okamura, M.; Yamazaki A., RF Acceleration of Ions Produced by Short Pulse Laser, *Proceedings of the 6th International Particle Accelerator Conference, IPAC'15*, 2548-2550 (2015).

Otani, M.; Mibe, T.; Fukao, Y.; Saito, N.; Yoshida, M.; Kitamura, R.; Kondo Y.; Iwashita, Y., Development of Muon LINAC for the Muon g-2/EDM Experiment at J-PARC, *Proceedings of the 6th International Particle Accelerator Conference, IPAC'15*, 2541-2544 (2015).

Yoshida, M.; Naito, F.; Artikova, S.; Kondo, Y.; Hayashizaki, N.; Iwashita, Y.; Torikai, K., Re-acceleration of Ultra Cold Muon in J-PARC MLF, *Proceedings of the 6th International Particle Accelerator Conference, IPAC'15*, 2532-2534 (2015).

Arimoto, Y.; Higashi, N.; Igarashi, Y.; Iwashita, Y.; Ino, T.; Katayama, R.; Kitaguchi, M.; Kitahara, R.; Matsumura, H.; Mishima, K.; Nagakura, N.; Oide, H.; Otono, H.; Sakakibara, R.; Shima, T.; Shimizu, H. M.; Sugino, T. S.; Sumi, N.; Sumino, H.; Taketani, K.; Tanaka, G.; Tanaka, M.; Tauchi, K.; Toyoda, A.; Tomita, T.; Yamada, T.; Yamashita, S.; Yokoyama, H.; Yoshioka, T., Development of Time Projection Chamber for Precise Neutron Lifetime Measurement Using Pulsed Cold Neutron Beams, *Nuclear Instruments and Methods in Physics Research A 799*, 187-196 (2015).

Iwashita, Y.; Fuwa, Y., High Efficiency RFQ Vane Shape, *Proceedings of the 12th Annual Meeting of Particle Accelerator Society of Japan*, 412-415 (2015) (in Japanese).

Fuwa, Y.; Iwashita, Y.; Tongu, H.; Inoue, S.; Hashida, M.; Sakabe, S.; Okamura, M.; Yamazaki. A., RF Synchronized Acceleration of Ions Produced by Short Pulse Laser, *Proceedings of the 12th Annual Meeting of Particle Accelerator Society of Japan*, 501-503 (2015) (in Japanese).

Otani, M.; Kitamura, R.; Iwashita, Y.; Mibe, T.; Kondo, Y.; Yoshida, M.; Saito, N., Demonstration of Muon Acceleration and Cavity Design of the Muon LINAC for J-PARC E34, *Proceedings of the 12th Annual Meeting of Particle Accelerator Society of Japan*, 56-61 (2015) (in Japanese).

Imajo, S.; Iwashita, Y.; Kitaguchi, M.; Shimizu, H. M.; Mishima, K.; Ino, T., Improvement of the Ultracold Neutrons Rebuncher III, *Proceedings of the 12th Annual Meeting of Particle Accelerator Society of Japan*, 416-419 (2015) (in Japanese).

Sawamura, M.; Hajima, R.; Nishimori, N.; Nagai, R.; Iwashita, Y.; Tongu, H.; Kubo, T.; Saeki, T., Status of ERL Superconducting Spoke Cavity Fabrication, *Proceedings of the 12th Annual Meeting of Particle Accelerator Society of Japan*, 583-586 (2015) (in Japanese).

Tongu, H.; Iwashita, Y.; Hayano, H.; Yamamoto, Y.; Hokonohara, H., Development of Defect Scanning System of SC Cavity, *Proceedings of the 12th Annual Meeting of Particle Accelerator Society of Japan*, 604-606 (2015) (in Japanese).

Fuwa, Y.; Iwashita, Y.; Matsumoto, T.; Michizono, S.; Fukuda, S., Permanent Magnet Focusing System for L-band 800kW klystron, *Proceedings of the 12th Annual Meeting of Particle Accelerator Society of Japan*, 1133-1135 (2015) (in Japanese).

— Laser Matter Interaction Science —

Inoue, S.; Tokita, S.; Hashida, M.; Sakabe, S., Transient Changes in Electric Fields Induced by Interaction of Ultraintense Laser Pulses with Insulator and Metal Foils: Sustainable Fields Spanning Several Millimeters, *Phys. Rev. E*, **91,** [043101-1]-[043101-5] (2015).

Tokita, S.; Sakabe, S.; Nagashima, T.; Hashida, M.; Inoue, S., Strong Sub-terahertz Surface Waves Generated on a Metal Wire by High-intensity Laser Pulses, *Sci. Rep.*, **5,** [8268-1]-[8268-6] (2015).

Miyasaka, Y.; Hashida, M.; Nishii, T.; Inoue, S.; Sakabe, S., Derivation of Effective Penetration Depth of Femtosecond Laser Pulses in Metal from Ablation Rate Dependence on Laser Fluence, Incidence Angle, and Polarization, *Appl. Phys. Lett.*, **106,** [013101-1]-[013101-5] (2015).

Gemini, L.; Hashida, M.; Shimizu, M.; Miyasaka, Y.; Inoue, S.; Tokita, S.; Limpouch, J.; Mocek, T.; Sakabe, S., Periodic Surface Structures on Titanium Self-organized upon Double Femtosecond Pulse Exposures, *Appl. Surf. Sci.*, **336,** 349-353 (2015).

— Electron Microscopy and Crystal Chemistry —

Hosaka, Y.; Ichikawa, N.; Saito, T.; Haruta, M.; Kimoto, K.; Kurata, H.; Shimakawa, Y., Ca_2FeMnO_6: a Layered Double Perovskite with Unusually High Valence Fe^{4+} in a Layered Arrangement, *Bull. Chem. Soc. Jpn.*, **88,** 657-661 (2015).

Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Phase Control of a Perovskite Transition-metal Oxide through Oxygen Displacement at the Heterointerface, *Dalton Trans.*, **44,** 10594-10607 (2015).

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

Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Research Update: Interface-engineered Oxygen Octahedral Tilts in Perovskite Oxide Heterostructures, *APL Materials*, **3,** [062302-1]-[062302-9] (2015).

Thuy, T.; Sato, R.; Sakamoto, M.; Fujiyoshi, Y.; Haruta, M.; Kurata, H.; Teranishi, T., Visible to Near-infrared Plasmon-enhanced Catalytic Activity of Pd Hexagonal Nanoplates for the Suzuki Coupling Reaction, *Nanoscale*, **7,** 12435-12444 (2015).

Yoshida, K.; Biskupek, J.; Kurata, H.; Kaiser, U., Critical Conditions for Atomic Resolution Imaging of Molecular Crystals by Aberration-corrected HRTEM, *Ultramicroscopy*, **159,** 73-80 (2015).

Baba, E.; Kan, D.; Yamada, Y.; Haruta, M.; Kurata, H.; Kanemitsu, Y.; Shimakawa, Y., Optical and Transport Properties of Transparent Conducting La-doped $SrSnO_3$ Thin Films, *J. Phys. D: Appl. Phys.*, **48,** [455106-1]-[455106-5] (2015).

Sakabe, S.; Kurata, H.; Hashida, M.; Tokita, S.; Inoue, S.; Nemoto, T.; Haruta, M.; Watanabe, K., Evolution of Electron-Microscopes and the Ultrafast Electron Diffraction with Laser Accelerated Electrons, *The Review of Laser Engineering*, **43,** 138-143 (2015) (in Japanese).

Otani, R.; Inukai, M.; Hijikata, Y.; Ogawa, T.; Takenaka, M.; Ohba, M.; Kitagawa, S., Sequential Synthesis of Coordination Polymersomes, *Angew. Chem.*, **127,** 1155-1159 (2015).

— Structural Molecular Biology —

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).

Yamauchi, T.; Fujii, T.; Oikawa, T.; Hata, Y., Crystal Structure Analysis of GraE Protein from the Gene Cluster of γ-Resorcylate Catabolic System, *SPring-8 / SACLA Res. Rep.*, **3,** 329-332 (2015) (in Japanese).

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Organic Main Group Chemistry —

Kawamura, S.; Agata, R.; Nakamura, M., Regio- and Stereoselective Multisubstituted Olefin Synthesis via Hydro/Carboalumination of Alkynes and Subsequent Iron-catalysed Cross-Coupling Reaction with Alkyl Halides, *Org. Chem. Front*., **2,** 1053-1058 (2015).

Jin, M.; Adak, L.; Nakamura, M., Iron-Catalyzed Enantioselective Cross-Coupling Reactions of α-Chloroesters with Aryl Grignard Reagents, *J. Am. Chem. Soc.*, **137,** 7128-7134 (2015).

Agata, R.; Iwamoto, T.; Nakagawa, N.; Isozaki, K.; Hatakeyama, T.; Takaya, H.; Nakamura, M., Iron Fluoride/N-Heterocyclic Carbene Catalyzed Cross Coupling between Deactivated Aryl Chlorides and Alkyl Grignard Reagents with or without β-Hydrogens, *Synthesis*, **47,** 1733-1740 (2015).

Nakagawa, N.; Hatakeyama, T.; Nakamura, M., Iron-Catalyzed Suzuki-Miyaura Coupling Reaction of Unactivated Alkyl Halides with Lithium Alkynylborates, *Chem. Lett.*, **44,** 486-488 (2015).

Nakagawa, N.; Hatakeyama, T.; Nakamura, M., Iron-Catalyzed Diboration and Carboboration of Alkynes, *Chem. Eur. J.*, **21,** 4257-4261 (2015).

Takaya, H.; Nakajima, S.; Nakagawa, N.; Isozaki, K.; Iwamoto, T.; Imayoshi, R.; Gower, N.; Adak, L.; Hatakeyama, T.; Honma, T.; Takagaki, M.; Sunada, Y.; Nagashima, H.; Hashizume, D.; Takahashi, O.; Nakamura, M., Investigation of Organoiron Catalysis in Kumada-Tamao-Corriu-Type Cross-Coupling Reaction Assisted by Solution-Phase X-ray Absorption Spectroscopy, *Bull. Chem. Soc. Jpn.*, **88,** 410-418 (2015).

Mohri, S.; Ohisa, S.; Isozaki, K.; Yonezawa, N.; Okamoto, A., Hydrogen Bonding between Fluoro Group and Aromatic Hydrogen Leading Stripe Structure of R-Isomeric Column and S-Isomeric One: Crystal Structure of 2,7-Dimethoxynaphthalen-1-yl(3-fluorophenyl) methanone and a Comparison with Its 1-Aroylnaphthalene Analogues, *Acta Cryst.*, **C71,** 344-350 (2015).

Pincella, F.; Isozaki, K.; Taguchi, T.; Song, Y.; Miki, K., Selective Two-Photon-Absorption-Induced Reactions of Anthracene-2-Carboxylic Acid on Tunable Plasmonic Substrate with Incoherent Light Source, *J. Nanosci. Nanotech.*, **15,** 1171-1179 (2015).

— Advanced Solid State Chemistry —

Baba, E.; Kan, D.; Yamada, Y.; Haruta, M.; Kurata, H.; Kanemitsu, Y.; Shimakawa, Y., Optical and Transport Properties of Transparent Conducting La-Doped $SrSnO_3$ Thin Films, *J. Phys. D: Applied Physics*, **48,** [455106-1]-[455106-5] (2015).

Shimakawa, Y., Crystal and Magnetic Structures of $CaCu_3Fe_4O_{12}$ and $LaCu_3Fe_4O_{12}$: Distinct Charge Transitions of Unusual High Valence Fe, *J. Phys. D, special issue on "100 Years of Crystallography"*, **48,** [504006-1]-[504006-13](2015).

Wang, X.; Chai, Y. S.; Zhou, L.; Cao, H.; Cruz, C. D.; Yang, J. Y.; Dai, J. H.; Yin, Y.-Y.; Yuan, Z.; Yu, R. Z.; Azuma, M.; Shimakawa, Y.; Zhang, H. M.; Dong, S.; Sun, Y.; Jin, C. Q.; Long, Y. W., Observation of Magnetoelectric Multiferroicity in a Cubic Perovskite System: $LaMn_3Cr_4O_{12}$, *Phys. Rev. Lett.*, **115,** [087601-1]-[087601-5] (2015).

Hosaka, Y.; Ichikawa, N.; Saito, T.; Manuel, P.; Khalyavin, D.; Attfield, J. P.; Shimakawa, Y., Two-Dimensional Charge Disproportionation of the Unusual High-Valence State Fe^{4+} in a Layered Double Perovskite, *J. Am. Chem. Soc.*, **137,** 7468-7473 (2015).

Toyoda, M.; Saito, T.; Yamauchi, K.; Shimakawa, Y.; Oguchi, T., Superexchange Interaction in the *A*-site Ordered Perovskite $YMn_3Al_4O_{12}$, *Phys. Rev. B*, **92,** [014420-1]-[014420-7] (2015).

Kan, D.; Shimizu, T.; Shimakawa, Y., Influence of Cation Off-Stoichiometry on Transport Properties of Metal/Nb-$SrTiO_3$ Junctions, *J. Appl. Phys.*, **117,** [205305-1]-[205305-5] (2015).

Corallini, S.; Ceretti, M; Silly, G.; Piovano, A.; Singh, S.; Stern, J.; Ritter, C.; Ren, J.; Eckert, H.; Conder, K.; Chen, W. T.; Chou, F. C.; Ichikawa, N.; Shimakawa, Y.; Paulus, W., 1D Oxygen Diffusion Mechanism in Sr_2ScGaO_5 Electrolyte Explored by Neutron and Synchrotron Diffraction, ^{17}O-NMR and DFT Calculations, *J. Phys. Chem. C*, **119,** 11447-11458 (2015).

Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Interface-Engineered Oxygen Octahedral Tilts in Perovskite Oxide Heterostructures, *APL Mater.*, **3,** [062302-1]-[062302-9] (2015).

Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Phase Control of a Perovskite Transition-Metal Oxide through Oxygen Displacement at Heterointerface, *Dalton Trans.*, **44,** 10594-10607 (2015).

Hosaka, Y.; Ichikawa, N.; Saito, T.; Haruta, M.; Kimoto, K.; Kurata, H.; Shimakawa, Y., Ca_2FeMnO_6: a Layered Double Perovskite with Unusually High Valence Fe^{4+} in a Layered Arrangement, *Bull. Chem. Soc. Jpn.*, **88,** 657-661 (2015).

Hirai, K.; Kan, D.; Ichikawa, N.; Mibu, K.; Yoda, Y.; Andreeva, M; Shimakawa, Y., Strain-Induced Significant Increase in Metal-Insulator Transition Temperature in Oxygen-Deficient Fe Oxide Epitaxial Thin Films, *Sci. Rep.*, **5,** [7894-1]-[7894-6] (2015).

Saito, T.; Toyoda, M.; Ritter, C.; Oguchi, T.; Attfield, J. P.; Shimakawa, Y., Symmetry-breaking 60°-Spin order in the *A*-Site-ordered Perovskite $LaMn_3V_4O_{12}$, *Phys. Rev. B*, **90,** [214405-1]-[214405-6] (2014).

Aso, R.; Kan, D.; Shimakawa, Y.; Kurata, H., Strong Dependence of Oxygen Octahedral Distortions in $SrRuO_3$ Films on Types of Substrate-Induced Epitaxial Strain, *Cryst. Growth & Des. (Communication)*, **14,** 5177-5184 (2014).

— Organotransition Metal Chemistry —

Wakioka, M.; Ishiki, S.; Ozawa, F., Synthesis of Donor-Acceptor Polymers Containing Thiazolo[5,4-d]thiazole Units via Palladium-Catalyzed Direct Arylation Polymerization, *Macromolecules*, **48,** 8382-8388 (2015).

Chang, Y.-H.; Takeuchi, K.; Wakioka, M.; Ozawa, F., C-H Bond Cleavage of Acetonitrile by Iridium Complexes Bearing PNP-Pincer Type Phosphaalkene Ligands, *Organometallics*, **34,** 1957-1962 (2015).

Iizuka, E.; Wakioka, M.; Ozawa, F., Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Synthesis of Donor-Acceptor Polymers with Dithienosilole (DTS) and Thienopyrroledione (TPD) Units, *Macromolecules*, **48,** 2989-2993 (2015).

Taguchi, H.; Chang, Y.-H.; Takeuchi, K.; Ozawa, F., Catalytic Synthesis of an Unsymmetrical PNP-Pincer Type Phosphaalkene Ligand, *Organometallics*, **34,** 1589-1596 (2015).

Sugawara, S.; Abe, M.; Fujiwara, Y.; Wakioka, M.; Ozawa, F.; Yamamoto, Y., 1,8-Disubstituted Xanthylidene-Based Remote Carbenes: Photolytic Generation and Isolation of Low-Coordinate Palladium(II) Complex, *Eur. J. Inorg. Chem.*, **3,** 534-541 (2015).

Wakioka, M.; Nakamura, Y.; Montgomery, M.; Ozawa, F., Remarkable Ligand Effect of $P(2\text{-}MeOC_6H_4)_3$ on Palladium-Catalyzed Direct Arylation, *Organometallics*, **34,** 198-205 (2015).

— Photonic Elements Science —

Tex, D. M.; Imaizumi, M.; Kanemitsu, Y., Charge Separation in Subcells of Triple-junction Solar Cells Revealed by Time-resolved Photoluminescence Spectroscopy, *Opt. Express*, **23,** A1687 (2015).

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).

Baba, E.; Kan, D.; Yamada, Y.; Haruta, M.; Kurata, H.; Kanemitsu, Y.; Shimakawa, Y., Optical and Transport Properties of Transparent Conducting La-Doped $SrSnO_3$ Thin Films, *J. Phys. D: Appl. Phys.*, **48,** [455106-1]-[455106-5] (2015).

Okano, M.; Endo, M.; Wakamiya, A.; Yoshita, M.; Akiyama, H.; Kanemitsu, Y., Degradation Mechanism of Perovskite $CH_3NH_3PbI_3$ Diode Devices Studied by Electroluminescence and Photoluminescence Imaging Spectroscopy, *Appl. Phys. Express*, **8,** [102302-1]-[102302-4] (2015).

Le, P. Q.; Okano, M.; Yamashita, G.; Nagai, M.; Ashida, M.; Nagaoka, A.; Yoshino, K.; Kanemitsu, Y., Free-carrier Dynamics and Band Tails in $Cu_2ZnSn(S_xSe_{1-x})_4$: Evaluation of Factors Determining Solar Cell Efficiency, *Phys. Rev. B*, **92,** [115204-1]-[115204-7] (2015).

Masai, H.; Yamada, Y.; Okumura, S.; Yanagida, T.; Fujimoto, Y.; Kanemitsu, Y.; Ina, T., Photoluminescence of Monovalent Indium Centres in Phosphate Glass, *Sci. Rep.*, **5,** [13646-1]-[13646-10] (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.; Tex, D. M.; Kamiya, I.; Kanemitsu, Y., Femtosecond Upconverted Photocurrent Spectroscopy of InAs Quantum Nanostructures, *Appl. Phys. Lett.*, **107,** [013905-1]-[013905-5] (2015).

Masai, H.; Miyata, H.; Yamada, Y.; Okumura, S.; Yanagida, T.; Kanemitsu, Y., Tin-Doped Inorganic Amorphous Films for Use as Transparent Monolithic Phosphors, *Sci. Rep.*, **5,** [11224-1]-[11224-12] (2015).

Le, P. Q.; Okano, M.; Yamashita, G.; Nagai, M.; Ashida, M.; Nagaoka, A.; Yoshino, K.; Kanemitsu, Y., Photocarrier Dynamics in Undoped and Na-Doped Cu_2ZnSnS_4 Single Crystals Revealed by Ultrafast Time-resolved Terahertz Spectroscopy, *Appl. Phys. Express*, **8,** [062303-1]-[062303-4] (2015).

Sakamoto, M.; Chen, L.; Okano, M.; Tex, D. M.; Kanemitsu, Y.; Teranishi, T., Photoinduced Carrier Dynamics of Nearly Stoichiometric Oleylamine-Protected Copper Indium Sulfide Nanoparticles and Nanodisks, *J. Phys. Chem. C*, **119,** 11100-11105 (2015).

Okano, M.; Hagiya, H.; Sakurai, T.; Akimoto, K.; Shibata, H.; Niki, S.; Kanemitsu, Y., Individual Identification of Free Hole and Electron Dynamics in $CuIn_{1-x}Ga_xSe_2$ Thin Films by Simultaneous Monitoring of Two Optical Transitions, *Appl. Phys. Lett.*, **106,** [181903-1]-[181903-4] (2015).

Okano, M.; Le, P. Q.; Kanemitsu, Y., Photocarrier Dynamics in CIGS, CZTS, and Related Materials Revealed by Ultrafast Optical Spectroscopy, *Phys. Status Solidi B*, **252,** 1219-1224 (2015).

Nishihara, T.; Tahara, H.; Okano, M.; Ono, M.; Kanemitsu, Y., Fast Dissociation and Reduced Auger Recombination of Multiple Excitons in Closely Packed PbS Nanocrystal Thin Films, *J. Phys. Chem. Lett.*, **6,** 1327-1332 (2015).

Akiyama, H.; Zhu, L.; Yoshita, M.; Kim, C.; Chen, S.; Mochizuki, T.; Kanemitsu, Y., Multi-junction-solar-cell Designs and Characterizations Based on Detailed-Balance Principle and Luminescence Yields, *Proc. SPIE*, **9358,** 93580B (2015).

Yamada, Y.; Endo, M.; Wakamiya, A.; Kanemitsu, Y., Spontaneous Defect Annihilation in $CH_3NH_3PbI_3$ Thin Films at Room Temperature Revealed by Time-Resolved Photoluminescence Spectroscopy, *J. Phys. Chem. Lett.*, **6,** 482-486 (2015).

Chen, S.; Zhu, L.; Yoshita, M.; Mochizuki, T.; Kim, C.; Akiyama, H.; Imaizumi, M.; Kanemitsu, Y., Thorough Subcells Diagnosis in a Multi-junction Solar Cell via Absolute Electroluminescence-efficiency Measurements, *Sci. Rep.*, **5,** [7836-1]-[7836-6] (2015).

Tex, D. M.; Ihara, T.; Akiyama, H.; Imaizumi, M.; Kanemitsu, Y., Time-resolved Photoluminescence Measurements for Determining Voltage-dependent Charge-separation Efficiencies of Subcells in Triple-junction Solar Cells, *Appl. Phys. Lett.*, **106,** [013905-1]-[013905-4] (2015).

Yamada, Y.; Nakamura, T.; Endo, M.; Wakamiya, A.; Kanemitsu, Y., Photoelectronic Responses in Solution-Processed Perovskite $CH_3NH_3PbI_3$ Solar Cells, *IEEE J. Photovolt.*, **5,** 401-405 (2015).

BIOINFORMATICS CENTER
— Chemical Life Science —

Morimoto, K.; Nishikaze, T.; Yoshizawa, A. C.; Kajihara, S.; Aoshima, K.; Oda, Y.; Tanaka, K., GlycanAnalysis Plug-in: a Database Search Tool for N-Glycan Structures Using Mass Spectrometry, *Bioinformatics*, **31,** 2217-9 (2015).

Kuyama, H.; Yoshizawa, A. C.; Nakajima, C.; Hosako, M.; Tanaka, K., Identification of Human Basic Fetoprotein as Glucose-6-phosphate Isomerase by Using N- and C-Terminal Sequence Tags and Terminal Tag Database, *J. Pharm. Biomed. Anal.*, **112,** 116-25 (2015).

Yoshizawa, A. C.; Fukuyama, Y.; Kajihara, S.; Kuyama, H.; Tanaka, K., Computational Survey of Sequence Specificity for Protein Terminal Tags Covering Nine Organisms and Its Application to Protein Identification, *J. Proteome. Res.*, **14,** 756-67 (2015).

Suzuki, M.; Nakabayashi, R.; Ogata, Y.; Sakurai, N.; Tokimatsu, T.; Goto, S.; Suzuki, M.; Jasinski, M.; Martinoia, E.; Otagaki, S.; Matsumoto, S.; Saito, K.; Shiratake, K., Multi Omics in Grape Berry Skin Revealed Specific Induction of Stilbene Synthetic Pathway by UV-C Irradiation, *Plant. Physiol.*, **168,** 47-59 (2015).

Massana, R.; Gobet, A.; Audic, S.; Bass, D.; Bittner, L.; Boutte, C.; Chambouvet, A.; Christen, R.; Claverie, J.-M.; Decelle, J.; Dolan, J. R.; Dunthorn, M.; Edvardsen, B.; Forn, I.; Forster, D.; Guillou, L.; Jaillon, O.; Kooistra, W. H.; Logares, R.; Mahe, F.; Not, F.; Ogata, H.; Pawlowski, J.; Pernice, M. C.; Prober, I.; Romac, S.; Richards, T.; Santini, S.; Shalchian-Tabrizi, K.; Siano, R.; Simon, N.; Stoeck, T.; Vaulot, D.; Zingone, A.; de Vargas, C., Marine Protist Diversity in European Coastal Waters and Sediments as Revealed by High-throughput Sequencing, *Eniron. Microbiol.*, **17,** 4035-4049 (2015).

Clerissi, C.; Desdevises, Y.; Romac, S.; Audic, S.; de Vargas, C.; Acinas, S. G.; Casotti, R.; Poulain, J.; Wincker, P.; Hingamp, P.; Ogata, H.; Grimsley, N., Deep Sequencing of Amplified Prasinovirus and Host Green Algal Genes from an Indian Ocean Transect Reveals Interacting Trophic Dependencies and New Genotypes, *Eniron. Microbiol. Rep.*, **7,** 979-989 (2015).

Halima, N. B.; Khemakhem, B.; Fendri, I.; Ogata, H.; Baril, P.; Pichon, C.; Abdelkafi, S., Identification of a New Oat Beta-amylase by Functional Proteomics, *Biochim. Biophys. Acta.*, **1864,** 52-61 (2015).

Kopf, A.; Bicak, M.; Kottmann, R.; Schnetzer, J.; Kostadinov, I.; Lehmann, K.; Fernandez-Guerra, A.; Jeanthon, C.; Rahav, E.; Ullrich, M.; Wichels, A.; Gerdts, G.; Polymenakou, P.; Kotoulas, G.; Siam, R.; Abdallah, R. Z.; Sonnenschein, E. C.; Cariou, T.; O'Gara, F.; Jackson, S.; Orlic, S.; Steinke, M.; Busch, J.; Duarte, B.; Cacador, I.; Canning-Clode, J.; Bobrova, O.; Marteinsson, V.; Reynisson, E.; Loureiro, C. M.; Luna, G. M.; Quero, G. M.; Loscher, C. R.; Kremp. A.; DeLorenzo. M. E.; Ovreas, L.; Tolman, J.; LaRoche, J.; Penna, A.; Frischer, M.; Davis, T.; Katherine, B.; Meyer, C. P.; Ramos, S.; Magalhaes, C.; Jude-Lemeilleur, F.; Aguirre-Macedo, M. L.; Wang, S.; Poulton, N.; Jones, S.; Collin, R.; Fuhrman, J. A.; Conan, P.; Alonso, C.; Stambler, N.; Goodwin, K.; Yakimov, M. M.; Baltar, F.; Bodrossy, L.; Van De Kamp, J.; Frampton, D. M. F.; Ostrowski, M.; Van Ruth, P.; Malthouse, P.; Claus, S.; Deneudt, K.; Mortelmans, J.; Pitois, S.; Wallom, D.; Salter, I.; Costa, R.; Schroeder, D. C.; Kandil, M. M, Amaral, V.; Biancalana, F.; Santana, R.; Pedrotti, M. L.; Yoshida, T.; Ogata, H.; Ingleton, T.; Munnik, K.; Rodriguez-Ezpeleta, N.; Berteaux-Lecellier, V.; Wecker, P.; Cancio, I.; Vaulot, D.; Bienhold, C.; Ghazal, H.; Chaouni, B.; Essayeh, S.; Ettamimi, S.; Zaid, E. H.; Boukhatem, N.; Bouali, A.; Chahboune, R.; Barrijal, S.; Timinouni, M.; El Otmani, F.; Bennani, M.; Mea, M.; Todorova, N.; Karamfilov, V.; ten Hoopen, P.; Cochrane, G.; L'Haridon, S.; Bizsel, K. C.; Vezzi, A.; Lauro, F. M.; Martin, P.; Jensen, R. M.; Hinks, J.; Gebbels, S.; Rosselli, R.; De Pascale, F.; Schiavon, R.; dos Santos, A.; Villar, E.; Pesant, S.; Cataletto, B.; Malfatti, F.; Edirisinghe, R.; Silveira, J. A. H.; Barbier, M.; Turk, V.; Tinta, T.; Fuller, W. J.; Salihoglu, I.; Serakinci, N.; Ergoren, M. C.; Bresnan, E.; Iriberri, J.; Nyhus, P. A. F.; Edvardsen, B.; Karlsen, H. E.; Golyshin, P. N.; Gasol, J. M.; Moncheva, S.; Dzhembekova, N.; Johnson, Z.; Sinigalliano, C. D.; Gidley, M. L.; Zingone, A.; Danovaro, R.; Tsiamis, G.; Clark, M. S.; Costa, A. C.; El Bour, M.; Martins, A. M.; Collins, E. R.; Ducluzeau, A.-L.; Martinez, J.; Costello, M. J.; Amaral-Zettler, L. A.; Gilbert, J. A.; Davies, N.; Field, D.; Glockner, F. O., The Ocean Sampling Day Consortium, *Giga Science*, **4,** 27 (2015).

Takemura, M.; Yokobori, S.; Ogata, H., Evolution of Eukaryotic DNA Polymerases via Interaction between Cells and Large DNA Viruses, *J. Mol. Evol.*, **81,** 24-33 (2015).

Pesant, S.; Not, F.; Picheral, M.; Kandels-Lewis, S.; Le Bescot, N.; Gorsky, G.; Iudicone, D.; Karsenti, E.; Speich, S.; Trouble, R.; Dimier, C.; Searson, S.; Tara Oceans Consortium Coordinators, Open Science Resources for the Discovery and Analysis of Tara Oceans Data, *Sci. Data.*, **2,** 150023 (2015).

Sunagawa, S.; Coelho, L. P.; Chaffron, S.; Kultima, J. R.; Labadie, K.; Salazar, G.; Djahanschiri, B.; Zeller, G.; Mende, D. R.; Alberti, A.; Cornejo-Castillo, F. M.; Costea, P. I.; Cruaud, C.; d'Ovidio, F.; Engelen, S.; Ferrera, I.; Gasol, J. M.; Guidi, L.; Hildebrand, F.; Kokoszka, F.; Lepoivre, C.; Lima-Mendez, G.; Poulain, J.; Poulos, B. T.; Royo-Llonch, M.; Sarmento, H.; Vieira-Silva, S.; Dimier, C.; Picheral, M.; Searson, S.; Kandels-Lewis, S.; Tara Oceans Coordinators, Bowler, C.; de Vargas, C.; Gorsky, G.; Grimsley, N.; Hingamp, P.; Iudicone, D.; Jaillon, O.; Not, F.; Ogata, H.; Pesant, S.; Speich, S.; Stemmann, L.; Sullivan, M. B.; Weissenbach, J.; Wincker, P.; Karsenti, E.; Raes, J.; Acinas, S. G.; Bork, P., Structure and Function of the Global Ocean Microbiome, *Science*, **348,** 1261359 (2015).

de Vargas, C.; Audic, S.; Henry, N.; Decelle, J.; Mahe, F.; Logares, R.; Lara, E.; Berney, C.; Le Bescot, N.; Probert, I.; Carmichael, M.; Poulain, J.; Romac, S.; Colin, S.; Aury, J. M.; Bittner, L.; Chaffron, S.; Dunthorn, M.; Engelen, S.; Flegontova, O.; Guidi ,L.; Horak, A.; Jaillon, O.; Lima-Mendez, G.; Lukes, J.; Malviya, S.; Morard, R.; Mulot, M.; Scalco, E.; Siano, R.; Vincent, F.; Zingone, A.; Dimier, C.; Picheral, M.; Searson, S.; Kandels-Lewis, S.; Tara Oceans Coordinators, Acinas, S. G.; Bork, P.; Bowler, C.; Gorsky, G.; Grimsley, N.; Hingamp, P.; Iudicone, D.; Not, F.; Ogata, H.; Pesant, S.; Raes, J.; Sieracki, M. E.; Speich, S.; Stemmann, L.; Sunagawa, S.; Weissenbach, J.; Wincker, P.; Karsenti, E., Eukaryotic Plankton Diversity in the Sunlit Ocean, *Science*, **348,** 1261605 (2015).

Lima-Mendez, G.; Faust, K.; Henry, N.; Decelle, J.; Colin, S.; Carcillo, F.; Chaffron, S.; Ignacio-Espinosa, J. C.; Roux, S.; Vincent, F.; Bittner, L.; Darzi, Y.; Wang, J.; Audic, S.; Berline, L.; Bontempi, G.; Cabello, A. M.; Coppola, L.; Cornejo-Castillo, F. M.; d'Ovidio, F.; De Meester, L.; Ferrera, I.; Garet-Delmas, M. J.; Guidi, L.; Lara, E.; Pesant, S.; Royo-Llonch, M.; Salazar, G.; Sanchez, P.; Sebastian, M.; Souffreau, C.; Dimier, C.; Picheral, M.; Searson, S.; Kandels-Lewis, S.; Tara Oceans Coordinators,; Gorsky, G.; Not, F.; Ogata, H.; Speich, S.; Stemmann, L.; Weissenbach, J.; Wincker, P.; Acinas, S. G.; Sunagawa, S.; Bork, P.; Sullivan, M. B.; Karsenti, E.; Bowler, C.; de Vargas, C.; Raes, J., Determinants of Community Structure in the Global Plankton Interactome, *Science*, **348,** 1262073 (2015).

Villar, E.; Farrant, G. K.; Follows, M.; Garczarek, L.; Speich, S.; Audic, S.; Bittner, L.; Blanke, B.; Brum, J. R.; Brunet, C.; Casotti, R.; Chase, A.; Dolan, J. R.; d'Ortenzio, F.; Gattuso, J. P.; Grima, N.; Guidi, L.; Hill, C. N.; Jahn, O.; Jamet, J. L.; Le Goff, H.; Lepoivre, C.; Malviya, S.; Pelletier, E.; Romagnan, J. B.; Roux, S.; Santini, S.; Scalco, E.; Schwenck, S. M.; Tanaka, A.; Testor, P.; Vannier, T.; Vincent, F.; Zingone, A.; Dimier, C.; Picheral, M.; Searson, S.; Kandels-Lewis, S.; Tara Oceans Coordinators,; Acinas, S.G.; Bork, P.; Boss, E.; de Vargas, C.; Gorsky, G.; Ogata, H.; Pesant, S.; Sullivan, M. B.; Sunagawa, S.; Wincker, P.; Karsenti, E.; Bowler, C.; Not, F.; Hingamp, P.; Iudicone, D., Environmental Characteristics of Agulhas Rings Affect Interocean Plankton Transport, *Science*, **348,** 1261447 (2015).

Brum, J. R.; Ignacio-Espinoza, J. C.; Roux, S.; Doulcier, G.; Acinas, S. G.; Alberti, A.; Chaffron, S.; Cruaud, C.; de Vargas, C.; Gasol, J. M.; Gorsky, G.; Gregory, A. C.; Guidi, L.; Hingamp, P.; Iudicone, D.; Not, F.; Ogata, H.; Pesant, S.; Poulos, B. T.; Schwenck, S. M.; Speich, S.; Dimier, C.; Kandels-Lewis, S.; Picheral, M.; Searson, S.; Tara Oceans Coordinators,; Bork, P.; Bowler, C.; Sunagawa, S.; Wincker, P.; Karsenti, E.; Sullivan, M. B., Patterns and Ecological Drivers of Ocean Viral Communities, *Science*, **348,** 1261498 (2015).

Johannessen, T. V.; Bratbak, G.; Larsen, A.; Ogata, H.; Egge, E. S.; Edvardsen, B.; Eikrem, W.; Sandaa, R.-A., Characterisation of Four Novel Viruses Reveal Huge Diversity among Viruses Infecting Prymnesiales (Haptophyta), *Virology*, **476,** 180-188 (2015).

von Dassow, P.; John, U.; Ogata, H.; Probert, I.; Bendif, E. M.; Kegel, J. U.; Audic, S.; Wincker, P.; Da Silva, C.; Claverie, J.-M.; Doney, S.; Glover, D. M.; Flores, D. M.; Herrera, Y.; Lescot, M.; Garet-Delmas, M.-J.; de Vargas, C., Life Cycle Modification in Open Oceans Accounts for Genome Variability in a Cosmopolitan Phytoplankton, *ISME J.*, **9,** 1365-1377 (2015).

[Others]

Ogata, H.; Takemura, M., A Decade of Giant Virus Genomics: Surprising Discoveries Opening New Questions, *In "Global Virology I - Identifying and Investigating Viral Diseases", Shapshak, P., Sinnott, J. T., Somboonwit, C., Kuhn, J. Eds., Springer-Verlag New York*, pp.147-160 (2015).

Takemura, M.; Ogata, H., Preface: Unveiling the Unknowns in the World of Viruses, *Seibutsu no Kagaku, Iden*, **69,** 264-267 (2015) (in Japanese).

Mihara, T.; Goto, S.; Ogata, H., Diversity and Ecology of Marine Giant Viruses Uncovered from Their Genomes, *Seibutsu no Kagaku, Iden*, **69,** 318-325 (2015) (in Japanese).

— Mathematical Bioinformatics —

Chang, C.-J.; Tamura, T.; Chao, K.-M.; Akutsu, T., A Fixed-parameter Algorithm for Detecting a Singleton Attractor in an AND/OR Boolean Network with Bounded Treewidth, *IEICE Transactions on Fundamentals of Electronics, Communications and Computer Sciences*, **E98-A,** 384-390 (2015).

Nacher, J. C.; Akutsu, T., Structurally Robust Control of Complex Networks, *Phys. Rev. E Stat. Nonlin. Soft. Matter Phys.*, **91,** 12826 (2015).

Uech, L.; Akutsu, T.; Stanley, H. E.; Marcus, A. J.; Kenett, D. Y., Sector Dominance Ratio Analysis of Financial Markets, *Physica A*, **421,** 488-509 (2015).

Lu, W.; Tamura, T.; Song, J.; Akutsu, T., Computing Smallest Intervention Strategies for Multiple Metabolic Networks in a Boolean Model, *J. Comput. Biol.*, **22,** 85-110 (2015).

Hasegawa, T.; Mori, T.; Yamaguchi, R.; Shimamura, T.; Miyano, S.; Imoto, S.; Akutsu, T., Genomic Data Assimilation Using a Higher Moment Filtering Technique for Restoration of Gene Regulatory Networks, *BMC Syst. Biol.*, **9,** 14 (2015).

Zhao, Y.; Hayashida, M.; Cao, Y.; Hwang, J.; Akutsu, T., Grammar-based Compression Approach to Extraction of Common Rules among Multiple Trees of Glycans and RNAs, *BMC Bioinformatics*, **16,** 128 (2015).

Hayashida, M.; Jindalertudomdee, J.; Zhao, Y.; Akutsu, T., Parallelization of Enumerating Tree-like Chemical Compounds by Breadth-First Search Order, *BMC Med. Genomics*, **8(Suppl 2),** S15 (2015).

Tamura, T.; Lu, W.; Akutsu, T., Computational Methods for Modification of Metabolic Networks, *Comput. Struct. Biotechnol. J.*, **13,** 376-381 (2015).

Mori, T.; Flottmann, M.; Krantz, M.; Akutsu, T.; Klipp, E., Stochastic Simulation of Boolean Rxncon Models: Towards Quantitative Analysis of Large Signaling Networks, *BMC Syst. Biol.*, **9,** 45 (2015).

Akutsu, T.; Tamura, T.; Melkman, A. A.; Takasu, A., On the Complexity of Finding a Largest Common Subtree of Bounded Degree, *Theoretical Computer Science*, **590,** 2-16 (2015).

Kagami, H.; Akutsu, T.; Maegawa, S.; Hosokawa, H.; Nacher, J. C., Determining Associations between Human Diseases and Non-coding RNAs with Critical Roles in Network Control, *Sci. Rep.*, **5,** 14577 (2015).

Cong, X.; Akutsu, T., Matrix Network: a New Data Structure for Efficient Enumeration of Microstates of a Genetic Regulatory Network, *Journal of Information Processing*, **23,** 804-813 (2015).

Mori, T.; Takasu, A.; Jansson, J.; Hwang, J.; Tamura, T.; Akutsu, T., Similar Subtree Search Using Extended Tree Inclusion, *IEEE Transactions on Knowledge and Data Engineering*, **27,** 3360-3373 (2015).

[Others]

Chang, H. T.; Akutsu, T.; Draghici, S.; Ray, O.; Pai, T. W., Intelligent Informatics in Translational Medicine, *Biomed. Res. Int.*, **2015,** 717210 (2015).

— Bio-knowledge Engineering —

Zheng, X.; Zhu, S.; Gao, J.; Mamitsuka, H., Instance-wise Weighted Nonnegative Matrix Factorization for Aggregating Partitions with Locally Reliable Clusters, *Proceedings of the 24th International Joint Conference on Artificial Intelligence (IJCAI 2015)*, 4091-4097 (2015)

Zhou, J.; Shui, Y.; Peng, S.; Li, X.; Mamitsuka, H.; Zhu, S., MeSHSim: An R/Bioconductor Package for Measuring Semantic Similarity over MeSH Headings and MEDLINE Documents
J. Bioinform. Comput. Biol., **13(6),** 1542002 (2015).

Liu, K.; Peng, S.; Wu, J.; Zhai, C.; Mamitsuka H.; Zhu S., MeSHLabeler: Improving the Accuracy of Large-scale MeSH indexing by Integrating Diverse Evidence, *Bioinformatics (Proceedings of the 23rd International Conference on Intelligent Systems for Molecular Biology (ISMB/ECCB 2015))*, **31(12),** i339-i347 (2015).

Baba, H.; Takahara, J.; Mamitsuka, H., In Silico Predictions of Human Skin Permeability using Nonlinear Quantitative Structure-Property Relationship Models, *Pharmaceut. Res.*, **32(7),** 2360-2371 (2015).

Shiga, M.; Mamitsuka, H., Non-negative Matrix Factorization with Auxiliary Information on Overlapping Groups, *IEEE Trans. Knowl. Data Eng.*, **27(6),** 1615-1628 (2015).

Wang, B.; Chen, X.; Mamitsuka, H.; Zhu, S., BMExpert: Mining MEDLINE for Finding Experts in Biomedical Domains Based on Language Model, *IEEE/ACM Trans. Comput. Biol. Bioinform.*, **12(6),** 1-9 (2015).

Yotsukura, S.; Mamitsuka, H., Evaluation of Serum-based Cancer Biomarkers: A Brief Review from a Clinical and Computational Viewpoint, *Crit. Rev. Oncol. Hematol.*, **93(2),** 103-115 (2015).

[Others]

Mamitsuka, H., Predicting Drug-Target Interactions through Machine Learning, *SAR News*, **29,** 2-8 (2015) (in Japanese).

HAKUBI PROJECT
—Algorithmic Graph Theory with Applications to Bioinformatics —

Jansson, J.; Sadakane, K.; Sung, W.-K., Linked Dynamic Tries with Applications to LZ-Compression in Sublinear Time and Space, *Algorithmica*, **71,** 4, 969-988 (2015).

Asahiro, Y.; Jansson, J.; Miyano, E.; Ono, H., Graph Orientations Optimizing the Number of Light or Heavy Vertices, *Journal of Graph Algorithms and Applications*, **19,** 1, 441-465 (2015).

Mori, T.; Takasu, A.; Jansson, J.; Hwang, J.; Tamura, T.; Akutsu, T., Similar Subtree Search Using Extended Tree Inclusion, *IEEE Transactions on Knowledge and Data Engineering*, **27,** 12, 3360-3373 (2015).

Jansson, J.; Li, Z.; Sung, W.-K., On Finding the Adams Consensus Tree, *Proc. of the 32nd International Symposium on Theoretical Aspects of Computer Science (STACS 2015), LIPIcs*, **30,** 487-499 (2015).

Jansson, J.; Lingas, A.; Lundell, E.-M., The Approximability of Maximum Rooted Triplets Consistency with Fan Triplets and Forbidden Triplets, *Proc. of the 26th Annual Symposium on Combinatorial Pattern Matching (CPM 2015), Lecture Notes in Computer Science*, **9133,** 272-283 (2015).

Jansson, J.; Rajaby, R., A More Practical Algorithm for the Rooted Triplet Distance, *Proc. of the 2nd International Conference on Algorithms for Computational Biology (AlCoB 2015), Lecture Notes in Computer Science*, **9199,** 109-125 (2015).

INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]
Australian National University, ARC Centre of Excellence for Electromaterials Science, Research School of Chemistry

Bragg Institute, Australian National Nuclear Research and Development Organisation

RMIT University, Mechanical and Manufacturing Engineering

The University of New South Wales, Centre for Advanced Macromolecular Design (CAMD), School of Chemical Engineering

[Canada]
Queen’s University, Department of Chemistry

University of Toronto, Department of MaterialsSciences and Engineering

[China, P.R.]
Beijing Institute of Technology, Beijing Key Laboratory of Photoelectronic/Electrophotonic Conver-sion Materials, School of Chemistry

Fudan University, School of Computer Science

Fudan University, Shanghai Key Lab of Intelligent Information Processing

Peking University, School of Life Science

Wuhan University, Hubei Key Lab on Organic and Polymeric Optoelectronic Materials, Department of Chemistry

Wuhan University of Technology, School of Chemistry, Chemical Engineering, and Life Science

[Czech R.]
ASCR, HiLASE Project, Institute of Physics

Czech Technical University in Prague, FNSPE

[France]
Aix-Marseille University, Mediterranean Institute of Microbiology

Ecole Centrale de Nantes, Institut de Recherche en Genie Civil et Mecanique (GeM)

Institut Laue-Langevin

Oceanological Observatory of Banyuls sur Mer, Integrative Biology of Marine Organisms

Universite´ de Rennes, Sciences Chimiques de Rennes

[Germany]
University of Rostock, Institute of Physics

University of Ulm, Electron Microscopy Group of Materials Science

[Switzerland]
Paul Scherrer Institut, Laboratory for Muon-Spin Spectroscopy

University of Geneva, Department of Organic Chemistry

[Thailand]
Chulalongkorn University, Department of Chemical Technology, Faculty of Science

Prince of Songkla University, Faculty of Science and Industrial Technology

[Tunisia]
University of Sfax, Biological Engineering Department

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

University of Cambridge, Cavendish Laboratory

[U.S.A.]
Boston College, Merkert Chemistry Center, Department of Chemistry

Lawrence Berkeley National Laboratory, Advanced Light Source Division

Lawrence Berkeley National Laboratory, Environmental Energy Technology Division

Lawrence Berkeley National Laboratory, Materials Science Division

The Ohaio State University, Department of Microbiology

University of California, Berkeley, Department of Chemical and Biomolecular Engineering

University of California, Berkeley, Department of Materials Science and Engineering

University of Oregon, Department of Chemistry and Biochemistry and Materials Science Institute

*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 Area "Stimuli-responsive Chemical Species for the Creation of Functional Molecules"
28 June 2012−31 March 2017

Tokitoh, N.
Electron-state Control of Aromatic Compounds Containing Heavier Group 14 Elements by Substituent introduction and Element Substitution
Grant-in-Aid for Scientific Research (B)
1 April 2013−31 March 2016

Tokitoh, N.
Synthesis and Properties of Alumoles Having an Aluminum−Halogen Bond
Grant-in-Aid for Challenging Exploratory Research
1 April 2014−31 March 2016

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 Area "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

Agou, T.
Bottom-up Syntheses of Electron-Deficient Aluminum Clusters and Elucidation of Their Properties
Grant-in-Aid for Scientific Research (C)
1 April 2012−31 March 2015

Agou, T.
Development of Transformation Reactions Beginning with the Bond Activation by Reactive Aluminum Compounds
Grant-in-Aid for Young Scientist (A)
1 April 2015−31 March 2018

— Structural Organic Chemistry —

Murata, Y.
Synthesis of Tailor-made Nanocarbons and Their Application to Electronic Devices
Grants-in-Aid for Scientific Research (A)
1 April 2011−31 March 2016

Murata, Y.
Molecular Interface Science of π-Conjugated Carbon Complexes on Non-Equilibrated States
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2012−31 March 2016

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 2015−31 March 2017

Murata, Y.
Functional Molecular Systems Based on Dynamic Behavior of Active Species
Grant-in-Aid for Scientific Research on Innovative Areas "Stimuli-responsive Chemical Species for the Creation of Functional Molecules"
1 April 2015−31 March 2017

Murata, Y.
Creation of New Reactive Chemical Species by the Ultimate Steric Protection
Grant-in-Aid for Challenging Exploratory Research
1 April 2015−31 March 2017

Abbreviations and acronyms

JST : Japan Science and Technology Agency
MEXT : Ministry of Education, Culture, Sports, Science and Technology
METI : Minister of Economy, Trade and Industry
NEDO : New Energy and Industrial Technology Development Organization

Wakamiya, A.
Development of Organic Dyes Based on Fine Tuning of π-Orbitals using DFT Calculations
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2010−31 March 2016

Wakamiya, A.
Creation of Wireless Electric Power Supply
Center of Innovation Program (COI)
1 October 2013−31 March 2022

Wakamiya, A.
High Dimensional Structural Control of π-Conjugated Systems and Their Functionalization
Grant-in-Aid for Scientific Research (B)
1 April 2014−31 March 2017

Murata, M.
Synthesis of Electron-Accepting π-Systems Containing Fulvalene as a Key Structural Unit
Grant-in-Aid for Scientific Research (B)
1 April 2012−31 March 2015

Murata, M.
Organization of Nanocarbon Molecules Based on Metal Coordination
Grant-in-Aid for Challenging Exploratory Research
1 April 2014−31 March 2016

— Synthetic Organic Chemistry —

Kawabata, T.
Regioselective Molecular Transformation Based on Organocatalytic Molecular Recognition
Grant-in Aid for Scientific Research on Innovative Area
1 October 2011−31 March 2015

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

Yoshimura, T.
Asymmetric Syntheses of Bioactive Natural Products via Chiral Enolate Intermediate with Dynamic Chirality
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

— Advanced Inorganic Synthesis —

Teranishi, T.
Establishment of Deeply Penetrating Photoacoustic Imaging Technology Based on Fucntional Probes: Design and Synthesis of Activatable Probes and Development of in vivo Imaging Technology
Industry-Academia Collaborative R&D Programs, Japan Agency for Medical Research and Development
1 December 2011−31 March 2017

Teranishi, T.
Research on Hydrogen Storage Properties of Polyhedral Palladium Nanoparticles
Grant-in-Aid for Challenging Exploratory Research
1 April 2014−31 March 2016

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

Teranishi, T.
Research on Nanoscale Phase-Controlled Nanocomposite Magnets
Mirai Kaitaku Research Project, NEDO
1 October 2012−31 March 2022

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

Sakamoto, M.
Research for the Photochemical Functions of Porphyrin Face-coordinated Metal Nanoparticles
Grant-in-Aid for Scientific Research (C)
1 April 2013−31 March 2016

Sato, R.
Development of The Novel and Versatile Alloying Process via Nanosized Phosphorus Compounds
Grant-in-Aid for Challenging Exploratory Research
1 April 2015−31March 2017

Saruyama, M.
Orientational Control and Structure-specific Properties of Heterostructural Nanoparticles
Grant-in-Aid for Research Activity Start-up
1 October 2015−31March 2017

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, JST
1 September 2015−31 March 2019

Tsujii, Y.
Development of Novel Nanosystem by Hierarchically Assembling Concentrated Polymer Brushes
Core Research for Evolutional Science and Technology (CREST), JST
1 October 2009−31 March 2015

Tsujii, Y.
Super Lubrication of Novel Nano-Brushes
Advanced Environmental Materials of Green Network of Excellence (GRENE) Program, MEXT
6 December 2011−31 March 2016

Tsujii, Y.
Development of High-Performance Li-ion Batteries using High-capacity, Low-cost Oxide Electrodes
NEDO Project for Development of Novel Technology in Li-ion Batteries
1 October 2012−31 March 2017

Ohno, K.
Development of Molecular Targeted MRI Contrast Agent
A-STEP (Adaptable and Seamless Technology Transfer Program through Target-Driven R&D), JST
1 October 2012−30 September 2015

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

Sakakibara, K.
Construction of Photoresponsive Cellulosic Nanostructures via Polysaccharide-Based Hierarchic Assembly
Grants-in-Aid for Young Scientist (B)
1 April 2012−31 March 2015

— Polymer Controlled Synthesis —

Yamago, S.
Creation of Hoop-shaped π-conjugated Molecules through the Supramolecular Chemical Approach and Elucidation of their Properties
Core Research for Evolutional Science and Technology (CREST), JST
1 October 2010−31 March 2016

Yamago, S.
Highly Value-added Polymer Material Created by New Living Radical Polymerization Agent
Next Generation Technology Transfer Program (NexTEP), JST
1 April 2014−31 March 2020

— Inorganic Photonics Materials —

Masai, H.
Control of the Local Structure and the Luminescent Properties of Glass Phosphor Containing ns^2 Type Emission Center
Grant-in-Aid for Young Scientists (A)
1 April 2014−31 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 Science Research (A)
1 April 2015−31 March 2018

Imanishi, M.
Construction of Artificial Input Systems of the Circadian Clock
Grants-in-Aid for Scientific Research on Innovative Areas “Synthetic Biology”
1 April 2014−31 March 2016

Takeuchi, T.
Therapeutic Drug Development for Treatment of Polyglutamine Diseases by Reverse Drug Design Strategy
Grants-in-Aid for Young Scientists (A)
1 April 2014−31 March 2017

— Chemistry of Molecular Biocatalysts —

Watanabe, B.
Synthesis of γ-Glutamyl Transpeptidase-Specific Chemical Probes and Their Application to Cancer Immunotherapy
Grant-in-Aid for Young Scientists (B)
1 April 2015−31 March 2017

— Molecular Biology —

Aoyama, T.
Development of an Artificial Gene Expression Responding to UV-B Light
Grant-in-Aid for Challenging Exploratory Research
1 April 2013−31 March 2016

Tsuge, T.
Regulatory Mechanism of Plant Morphogenesis by Regulators of mRNA Metabolism
Grant-in-Aid for Scientific Research (C)
1 April 2013−31 March 2016

DIVISION OF ENVIRONMENTAL CHEMISTRY

— Molecular Materials Chemistry —

Kaji, H.
Structure and Function of Organic Thin-Film Solar Cells: Specially-Shaped Polymers and Hierarchical Structure Analysis
Grant-in-Aid for Scientific Research (A)
1 April 2013−31 March 2016

Fukushima, T.
Solid-State NMR Analysis of Bulk Heterostructures toward High-efficiency Organic Solar Cells
Grant-in-Aid for Young Scientists (B)
1 April 2014−31 March 2016

Fukushima, T.
Study on Weather Resistance of Solution-Processable Organic Solar Cells
Suga Weathering Technology Foundation
1 April 2015−31 March 2016

Shizu, K.
Molecular Design for Deep-Blue Electroluminescent Materials by Visualizing Radiative and Nonradiative Decays
Grant-in-Aid for Young Scientists (B)
1 April 2015−31 March 2017

— Hydrospheric Environment Analytical Chemistry —

Sohrin, Y.
Ocean Section Study in the Pacific Ocean, Indian Ocean and Japan Sea Using Multielemental Analysis of Trace Metals
Grant-in-Aid for Scientific Research (A)
1 April 2012−31 March 2015

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

Takano, S.
Biogeochemical Cycling of Nickel, Copper, and Zinc Isotopes in the Ocean
Sasakawa Scientific Research Grant
1 April 2014−28 February 2015

— Solution and Interface Chemistry —

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 Novel Analytical Techniques for Revealing Molecular Orientation of Adsorbed Molecules on a Rough Surface or on Nano Particles
Grant-in-Aid for challenging Exploratory Research
1 April 2014−31 March 2016

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

— 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 of Cold-Adapted Microorganisms to Develop Low-Temperature Bioprocessing Systems
Grant-in-Aid for Scientific Research (B)
1 April 2013−31 March 2016

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.
Application of Polyunsaturated Fatty Acid-Containing Phospholipids as a Lipophilic Molecular Chaperone
Grant-in-Aid for Challenging Exploratory Research
1 April 2014−31 March 2016

Ogawa, T.
Research on Acyltransferases that Create Heterogeneity of Bacterial Biomembranes
Grant-in-Aid for Research Activity Start-up
23 August 2015−31 March 2017

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

— Polymer Materials Science —

Kanaya, T.
Non-equilibrium Intermediate States and Polymer Crystrallization-Towards Establishment of Basis for Industrial Application
Grant-in-Aid for Scientific Research (A)
1 April 2012−31 March 2017

Ogawa, H.
Development of GISAXS-CT Measurement for Visualizing Functional Polymer Thin Films
Grant-in-Aid for Young Scientist (B)
1 April 2015−31 March 2017

— 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.
An Ion Source Using Direct Injection of Short-pulse Laser Plasma to RF Bucket
Grant-in-Aid for Challenging Exploratory Research
1 April 2012–31 March 2015

Iwashita, Y.
Quantum Improvement of the Superconducting Acceleration Cavity Performance by the Laminated Film Structure
Grant-in-Aid for Challenging Exploratory Research
1 April 2014–31 March 2016

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

— Laser Matter Interaction Science —

Sakabe, S.
Demonstration of Ultra-fast Electron Diffraction Using Fast Wlectrons Accelerated in Plasmas by an Intense Femtosecond Laser
Grant-in-Aid for Scientific Research (S)
1 April 2011–31 March 2016

Hashida, M.
New Functionality on Metal Surface Induced by Femtosecond Laser Ablation
Grant-in-Aid for Scientific Research (C)
1 April 2013–31 March 2016

Inoue, S.
Increasing the Brightness of the Laser-accelerated Electron Source by Controlling the Peripheral Plasma and the Electromagnetic Field
Grant-in-Aid for Young Scientists (B)
1 April 2014–31 March 2016

Inoue, S.
A New Technology for Controlling Laser Accelerated Electron Pulse with Laser Produced Plasma
Grant-in-Aid for MATSUO FOUNDATION
29 October 2014–28 October 2015

— Electron Microscopy and Crystal Chemistry —

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

Haruta, M.
Electronic State Mapping Using Oxygen
Grant-in-Aid for Young Scientist (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

— Organic Main Group Chemistry —

Nakamura, M.
Synthesis of Nitrogen-Containing Polycyclic Aromatic Compounds via Iron-catalyzed C-H Amination
Grant-in-Aid for challenging Exploratory Research
1 April 2015–31 March 2016

Takaya, H.
Solution-Phase Characterization of Paramagnetic Metal Complex by X-ray Absorption Spectroscopy
Grant-in-Aid for challenging Exploratory Research
1 April 2015–31 March, 2017

Isozaki, K.
Development of Catalytic Multi-photon-excited Photoreactions in the Reaction Field Localizing Substrates and Excitation Sources
Grant-in-Aid for Scientific Research on Innovative Areas "Application of Cooperative Excitation into Innovative Molecular Systems with High-Order Photofunctions"
1 April 2015–31 March 2017

Iwamoto, T.
Development of Aromatic C-H Functionalization Base on Cation-π Interaction
Grant-in-Aid for Young Scientists (B)
1 April 2015–31 March 2017

— Advanced Solid State Chemistry —

Shimakawa, Y.
Exploring for New Functional Materials with Unusual Ionic States and Coordinations
Creation of Innovative Functions of Intelligent Materials on the Basis of the Element Strategy
1 April 2011–31 March 2016

— Organotransition Metal Chemistry —

Ozawa, F.
Synthesis and Catalytic Properties of Stimulus-responsible Transition Metal Complexes Bearing Low-coordinate Phosphorus Ligands
Grant-in-Aid for Scientific Research on Innovative Areas "Stimuli-responsive Chemical Species for the Creation of Functional Molecules"
1 April 2012–31 March 2017

Ozawa, F.
Synthesis and Catalytic Applications of Non-innocent Phosphaalkene Ligands
Grants-in-Aid for Scientific Research (B)
1 April 2014–31 March 2017

Wakioka, M.
Development of Living Polymerization based on Direct Arylation
Grants-in-Aid for Young Scientists (B)
1 April 2012–31 March 2015

Wakioka, M.
Development of highly efficient catalytic systems for direct arylation polymerization based on equilibrium between active and dormant species
Grants-in-Aid for Young Scientists (B)
1 April 2015–31 March 2017

Ozawa, F.
Development of Highly Efficient Catalysts for Synthesizing of π-Conjugated Polymers via Direct Arylation
ACT-C, JST
1 October 2012–31 March 2018

Takeuchi, K.
Development of Novel Phosphaalkene-NHC Multidentate Ligands and Their Application for Metal Complexes and Catalytic Reactions
The Kyoto University Research Funds for Young Scientists (Step-up) FY2014
1 April 2014–31 March 2015

— Photonic Elements Science —

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

BIOINFORMATICS CENTER

— Chemical Life Science —

Goto, S.
Development of Integrated Proteome Database jPOST
Grant-in-Aid for Scientific Research (B), MEXT
1 April 2015–31 March 2018

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

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

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), MEXT
1 April 2014–31 March 2018

— 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 (JST)
1 September 2015–31 March 2017

Mamitsuka, H.
Estimating Data Structures from Various Semi-Structured Data
Grants-in-Aid for Scientific Research (B)
1 April 2012–31 March 2016

THESES

EGAWA, Yasunobu
D Sc, Kyoto University
“Studies on the Synthesis of (*Z*)-Dialkynyldisilenes”
Supervisor: Prof TOKITOH, Norihiro
23 March 2015

FRISCO, Heidie Laya
D Med Sc, Kyoto University
“Synthetic Molecules That Protect Cells from Anoikis and Their Use in Cell Transplantation”
Supervisor: Prof UESUGI, Motonari
23 March 2015

HASEGAWA, Takanori
D Inf, Kyoto University
“Reconstructing Biological Systems Incorporating Multi-Source Biological Data via Data Assimilation Techniques”
Supervisor: Prof AKUTSU, Tatsuya
23 January 2015

HATA, Takushi
D Sc, Kyoto University
“Spin Wave Propagation in Nano-structured Devices”
Supervisor: Prof ONO, Teruo
13 January 2015

HIRAI, Kei
D Sc, Kyoto University
“Physical Property Control of Oxygen-deficient Transition-metal-oxide Heterostructures”
Supervisor: Prof SHIMAKAWA, Yuichi
23 March 2015

HIRAMATSU, Ryo
D Sc, Kyoto University
“Current Induced Spin Precession in Magnetic Domain Wall”
Supervisor: Prof ONO, Teruo
13 January 2015

LU, Wei
D Inf, Kyoto University
“Integer Programming-based Methods for Computing Minimum Reaction Modifications of Metabolic Networks for Constraint Satisfaction”
Supervisor: Prof AKUTSU, Tatsuya
23 March 2015

MIZUTANI, Sayaka
D Sc, Kyoto University
“Inferring Drug Side Effect Mechanisms Based on Associations between Drugs, Target Proteins, and Side Effects”
Supervisor: Assoc Prof GOTO, Susumu
23 March 2015

MORI, Tomoya
D Inf, Kyoto University
“Methods for Analyzing Tree-Structured Data and Their Applications to Computational Biology”
Supervisor: Prof AKUTSU, Tatsuya
24 September 2015

NAGATA, Masaki
D Sc, Kyoto University
“Spin Motive Force in Ferrimagnetic Fe_3O_4”
Supervisor: Prof ONO, Teruo
13 January 2015

NAKAGAWA, Naohisa
D Eng, Kyoto University
“Selective Synthesis of Alkynes and Alkenes using Iron-Catalyzed Cross-coupling and Organometallic Addition Reactions”
Supervisor: Prof NAKAMURA, Masaharu
25 May 2015

NAKAJIMA, Natsu
D Inf, Kyoto University
“Genetic Network Completion Using Dynamic Programming and Least-Squares Fitting”
Supervisor: Prof AKUTSU, Tatsuya
23 January 2015

NISHIHARA, Yoshitaka
D Sc, Kyoto University
“Non-equilibrium Current Fluctuation in Semiconductor Quantum Wire”
Supervisor: Prof ONO, Teruo
13 January 2015

RUAN, Peiying
D Inf, Kyoto University
“Computational Methods for Analyzing Protein Complexes and Protein-Protein Interactions”
Supervisor: Prof AKUTSU, Tatsuya
26 March 2015

SHIGETA, Takashi
D Pharm Sc, Kyoto University
“Remote Asymmetric Induction by Organocatalysis”
Supervisor: Prof KAWABATA, Takeo
23 March 2015

SUZUKI, Shinya
D Eng, Kyoto University
“Rheological Properties of Telechelic Associative Polymer in Aqueous Solution”
Supervisor: Prof WATANABE, Hiroshi
23 July 2015

TAKANO, Shotaro
D Sc, Kyoto University
“Biogeochemical Cycling of Copper Isotopes in the Ocean”
Supervisor: Prof SOHRIN, Yoshiki
23 March 2015

TU, Kai-Min
D Sc, Kyoto University
“Spatial-Decomposition Analysis of Electrical Conductivity in Concentrated Ionic Systems”
Supervisor: Assoc Prof MATUBAYASI, Nobuyuki
22 March 2015

UECHI, Lisa
D Inf, Kyoto University
“Modeling of Biological and Economical Phenomena Based on Analysis of Nonlinear Competitive Systems”
Supervisor: Prof AKUTSU, Tatsuya
23 March 2015

WADA, Yukika
D Sc, Kyoto University
“Function of *Arabidopsis PIP5K3* Gene in the Root Hair Elongation Responding Phosphate Starvation”
Supervisor: Prof AOYAMA, Takashi
23 March 2015

WASANO, Tatsuya
D Sc, Kyoto University
“Syntheses and Properties of Stable Alumoles”
Supervisor: Prof TOKITOH, Norihiro
23 March 2015

YANG, Pan
D Pharm Sc, Kyoto University
“Asymmetric Synthesis of Highly Strained β-Lactams with Contiguous Multi-substituted Carbon Centers Based on Memory of Chirality”
Supervisor: Prof KAWABATA, Takeo
23 March 2015

THE 115TH
ICR ANNUAL
SYMPOSIUM

SEMINARS

MEETINGS AND
SYMPOSIA

THE 115TH ICR ANNUAL SYMPOSIUM

(11 December 2015)

ORAL PRESENTATIONS

SHIZU, Katsuyuki (Molecular Materials Chemistry)
"Theoretical and Computational Chemistry toward Organic Materials and Devices"

NGUYEN, Hao Canh (Bio-knowledge Engineering)
"Machine Learning on Graphs for Biological Network Analysis"

UMETANI, Shigeo (Hydrospheric Environment Analytical Chemistry)
"Development of Functional Separation Materials Selective for Rare Metals"

TAKEUCHI, Toshihide (Biofunctional Design-Chemistry)
"Intercellular Chaperone Transmission via Exosomes Contributes to Maintenance of Organismal Proteostasis"

MATSUMIYA, Yumi (Molecular Rheology)
"Dynamics of Associative Polymer System"

— ICR Award for Young Scientists —
MURATA, Michihisa (Structural Organic Chemistry)
"Electron-deficient Tetrabenzo-fused Pyracylene and Conversions into Curved and Planar π-Systems Having Distinct Emission Behaviors"

— ICR Award for Young Scientists —
UEDA, Yoshihiro (Synthetic Organic Chemistry)
"Final-stage Site-selective Acylation for the Total Syntheses of Multifidosides A-C"

— ICR Award for Young Scientists (Foreign Researchers' Category) —
PATEL, Vijay Kumar (Polymer Controlled Synthesis)
"Practical Synthesis of [n]Cycloparaphenylenes (n=5, 7-12) by H_2SnCl_4-Mediated Aromatization of 1,4-Dihydroxycyclo-2,5-diene Precursors"

— ICR Award for Graduate Students —
TAKEUCHI, Hironori (Synthetic Organic Chemistry)
"Total Synthesis of Ellagitannins via Regioselective Sequential Functionalization of Unprotected Glucose"

— ICR Award for Graduate Students —
SHIOYA, Nobutaka (Solution and Interface Chemistry)
"A New Schematic for Poly(3-alkylthiophene) in an Amorphous Film Studied Using a Novel Structural Index in Infrared Spectroscopy"

— ICR Grants for Promoting Integrated Research —
NAKANISHI, Yohei
"Orientation Process of Brush-modified Nanoparticles by Synchrotrom Small Angle X-ray Scattering"

ISOZAKI, Katsuhiro
"Unprecedented Acceleration of Silane Alcoholysis Reaction in Self-assembled Monolayer on Gold Nanoparticle Catalysts"

POSTER PRESENTATIONS

LW : Laboratory Whole Presentation
LT : Laboratory Topic
GE : General Presentation

— Organoelement Chemistry —

LW "Research Topics in Organoelement Chemistry"

— Structural Organic Chemistry —

LW "Research Activities in Structural Organic Chemistry Laboratory"

GE KAJI, Shoji; MURATA, Michihisa; WAKAMIYA, Atsushi; MURATA, Yasujiro
"Synthesis and Structure of Gold Complexes Having Thianthrene Dithiolate Ligands"

GE SHIMOGAWA, Hiroyuki; WAKAMIYA, Atsushi; MURATA, Yasujiro
"D-A Type Organic Dyes with Bis(Difluoroboron) Dipyrrolylethanedione as a New Electron-Accepting Unit"

— Synthetic Organic Chemistry —

LW "Recent Advances of Research in Synthetic Chemistry Laboratory"

GE YELLA, Ramesh; BABA, Tomonori; TANAKA, Yuya; YAMAMOTO, Satoru; FURUTA, Takumi; KAWABATA, Takeo
"Stereoselective Intramolecular Cross-aldol and Desymmetrization of Aliphatic Dials Enabled by Axially Chiral Aniline-type Catalyst"

— Advanced Inorganic Synthesis —

LW "Research Activity of Advanced Inorganic Synthesis"

GE EGUCHI, Daichi; SAKAMOTO, Masanori; TERANISHI, Toshiharu
"Structural Control of Porphyrin Face-coordinated Gold Clusters for Constructing Suprastructures"

GE MATSUMOTO Kenshi; SATO Ryota; TRINH, T. Thuy; SAKUMA Noritsugu; TERANISHI Toshiharu
"High-Performance $L1_0$-FePd/α-Fe Nanocomposite Magnets with Controlled Crystal Grain Size"

GE KIMURA, Masato; SAKAMOTO, Masanori; FURUBE, Akihiro; ADACHI, Hiroyuki; SUGIMOTO, Toshiki; WATANABE, Kazuya; MATSUMOTO, Yoshiyasu; TERANISHI, Toshiharu
"Synthesis and Visible Light-induced Charge Separation of Heterostructured Au/ZnS Nanoparticles"

— Chemistry of Polymer Materials —

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

GE YAHATA, Yoshikazu; OHNO, Kohji; TSUJII, Yoshinobu
"Polymer-brush-grafted Particles for Control of Phase Separation in Polymer/ionic-liquid Blend Films"

— Polymer Controlled Synthesis —

LW "Research Topics of Polymer Controlled Synthesis Laboratory"

GE ONISHI, Hiroaki; KAYAHARA, Eiichi; YAMAGO, Shigeru
"Synthesis and Physical Property of Oxigenated [10] Cycloparaphenylene"

GE QU, Rui; KAYAHARA, Eiichi; YAMAGO, Shigeru
"Synthetic Studies of CPP Derivatives via Bromination of CPPs"

GE FAN, Weijia; NAKAMURA, Yasuyuki; YAMAGO, Shigeru
"Controlled Polymer Synthesis Based on Multi-functional TERP Initiators"

GE OGIHARA, Tasuku; NAKAMURA, Yasuyuki; YAMAGO, Shigeru
"Elucidation of the Effect of Reaction Media in the Radical-radical Reaction"

— Inorganic Photonics Materials —

LT UEDA, Yuki; MASAI, Hirokazu; TOKUDA, Yomei
"Structural Analysis of Lithium Silicate Glasses"

GE USUI, Takaaki; MASAI, Hirokazu; TOKUDA, Yomei
"Optical Properties of Ce^{3+}-doped Li_2O-B_2O_3-SiO_2 Glasses"

— Nano Spintronics —

LT "Development of Novel Spintronic Devices"

GE KAKIZAKAI, Haruka; YAMADA, Kihiro; KAWAGUCHI, Masashi; KOYAMA, Tomohiro; CHIBA, Daichi; Ono, Teruo
"Approach to Electric Field Induced Domain Wall Motion in MgO/Co/Pt System"

GE YAMADA, Kihiro; KAKIZAKAI, Haruka; KOYAMA, Tomohiro; ONO, Shimpei; MIWA, Kazumoto; KAWAGUCHI, Masashi; CHIBA, Daichi; ONO, Teruo
"Electric Field Control of Superpamagnetic Ni/Cu Structure"

— Biofunctional Design-Chemistry —

LW "Research Activity at Biofunctional Design Chemistry"

GE WATANABE, Kensuke; TAKEUCHI, Toshihide; NAKASE, Ikuhiko; FUTAKI, Shiroh
"Analyzing Cellular Functions of Syndecan-4 Using Method for Controlling Dimer Formation of Membrane Proteins"

— Chemistry of Molecular Biocatalysts —

LW "Research Activities in the Laboratory of Chemistry of Molecular Biocatalysts"

— Molecular Biology —

LW "Research Activity in Laboratory of Molecular Biology"

— Chemical Biology —

LW "Create New World of Bioactive Synthetic Small Molecules"

— Molecular Materials Chemistry —

LT FUKUSHIMA, Tatsuya; SUZUKI, Hajime; SHIZU, Katsuyuki; SUZUKI, Katsuaki; KUBO, Shosei; KOMINO, Takeshi; OIWA, Hajime; SUZUKI, Furitsu; WAKAMIYA, Atsushi; MURATA, Yasujiro; ADACHI, Chihaya; KAJI, Hironori
"Purely Organic Emitter for Organic Light-emitting Diodes with External Quantum Efficiency above 40%"

— Hydrospheric Environment Analytical Chemistry —

LT MINAMI, Tomoharu; KONAGAYA, Wataru; Zheng, Linjie; SOHRIN, Yoshiki
"Sectional Distributions of Bioactive Trace Metals in the Pacific Sector of the Southern Ocean and the Western Pacific"

GE UEHARA, Wataru; TAKANO, Shotaro; ZHENG, Linjie; MINAMI, Tomoharu; SOHRIN, Yoshiki
"Development of Analytical Method for Nickel, Copper and Zinc Stable Isotopes in Seawater with an Off-line Automated Preconcentration System"

— Solution and Interface Chemistry —

GE IZUMI, Naoki; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
"IR Spectroscopic Analysis of Polymer Thin Films of Fluoroacrylates Having an Rf Side Chain with Various Lengths"

GE UKAI, Hironori; SHIMOAKA, Takafumi; NODA, Takumu; YAMADA, Norihiro; HASEGAWA, Takeshii
"Study on the Long-distance Interaction of Perfluoroalkyl Compounds Involving a Bulky Substituent"

LT HADA, Miyako; SHIOYA, Nobutaka; SHIMOAKA, Takafumi; EDA, Kazuo; HASEGAWA, Takeshi
"Structure Analysis of a Semiconductor Thin Film of a Porphyrin Derivative Using IR pMAIRS and GIXD"

— Molecular Microbial Science —

LW "Research of Molecular Microbial Science Laboratory"

GE TOKUNAGA, Tomohisa; WATANABE, Bunta; KAWAMOTO, Jun; KURIHARA, Tatsuo
"Synthesis of ω-terminal Modified Polyunsaturated Fatty Acid and Its Application to Physiological Studies"

— Polymer Materials Science —

LW "Polymer Material Science"

GE MURAKAMI, Momoko; MAEDE, Tadahiko; OGAWA, Hiroki; NISHIDA, Koji; KANAYA, Toshiji
"Structure Formation of Polyethylene Films during Uniaxial Drawing"

GE KISHIMOTO, Mizuki; INOUE, Riontaro; OGAWA, Hiroki; NISHIDA, Koji; KANAYA, Toshiji
"Effect of Substrate Surface Modification on the Glass Transition Temperature and Its Distribution of Polymer Thin Films"

— Molecular Rheology —

LW “Research Activities in Molecular Rheology Laboratory”

— Molecular Aggregation Analysis —

LT MURDEY, Richard; NAKAO, Kazuto; SATO, Naoki
“*In Situ* Electrical Measurements on Donor-Acceptor Thin Film Interfaces”

— Particle Beam Science —

LW “Status of Accelerator Laboratory, Advanced Research Center for Beam Science”

GE FUWA, Yasuhiro; IWASHITA, Yoshihisa; TONGU, Hiromu
“Development of RF-Synchronized Short Pulse Laser Ion Source”

GE KITAHARA, Ryunosuke; IWASHITA, Yoshihisa; NOP Group
“A Report of the Neutron Life Time Measurement at J-PARC/BL05”

GE IMAJO, Sohei
“Ultracold Neutron Production with Doppler Shifter at J-PARC/BL05”

— Laser Matter Interaction Science —

LW “Research Activities in Laboratory of Laser Matter Interaction Science”

GE WATANABE, Kota; INOUE, Shunsuke; TERAMOTO, Kensuke; NEMOTO, Takashi; NAKAMIYA, Yoshihide; KURATA, Hiroki; HASHIDA, Masaki; SAKABE, Shuji
“Development of the Ultrafast Electron Diffraction Instrument Using Laser-accelerated Electron Beams”

GE TERAMOTO, Kensuke; INOUE, Shunsuke; TOKITA, Shigeki; YASUHARA, Ryo; MORI, Kazuaki; WATANABE, Kota; NAKAMIYA, Yoshihide; HASHIDA, Masaki; SAKABE, Shuji
“Transmission of Electromagnetic Waves Emitted from Intense Laser Plasma Using a Metal Wire”

GE MORI, Kazuaki; HASHIDA, Masaki; NAGASHIMA, Takeshi; INOUE, Shunsuke; SAKABE, Shuji
“Terahertz Wave Generation in the Interaction of Two-pulse Laser with Clusters”

GE NAKAJI, Ryosuke; INOUE, Shunsuke; TERAMOTO, Kensuke; FUJITA, Kazuhisa; MIMA, Kunioki; KATO, Yoshiaki; NAKAMIYA, Yoshihide; HASHIDA, Masaki; SAKABE, Shuji
“Development of Diagnostics for Li-ion Batteries by Using Laser-driven Proton Beams”

— Electron Microscopy and Crystal Chemistry —

LW “Research Activities in Laboratory of Electron Microscopy and Crystal Chemistry”

LT KURATA, Hiroki; HARUTA, Mitsutaka; FUJIYOSHI, Yoshifumi; TOMISAKI, Yuriko; NEMOTO, Takashi
“High Energy Resolution EELS of Organic Thin Films”

— Structural Molecular Biology —

LW “Introduction of Structural Molecular Biology Laboratory”

— Organic Main Group Chemistry —

LW “Research of Organic Main Group Chemistry”

GE ADAK, Laksmikanta; JIN, Masayoshi; NAKAMURA, Masaharu
“Iron-Catalyzed Enantioselective Cross-Coupling Reaction of Racemic α-Haroesters”

GE NAKAJIMA, Sho; ISOZAKI, Katsuhiro; NAKAGAWA, Naohisa; IMAYOSHI, Ryuji; HASHIMOTO, Toru; GOWER, Nicholas, J.; ADAK, Laksmikanta; HONMA, Tetsuo; TAKAGAKI, Masafumi; SUNADA, Yusuke; NAGASHIMA, Hideo; HASHIZUME, Daisuke; IWAMOTO, Takahiro; HATAKEYAMA, Takuji; TAKAYA, Hikaru; NAKAMURA, Masaharu
“Mechanistic Study of Iron-Catalyzed Cross-Coupling Reaction Using Synchrotron X-Ray Absorption Spectroscopy”

GE AGATA, Ryosuke; IWAMOTO, Takahiro; NAKAGAWA, Naohisa; ISOZAKI, Katsuhiro; HATAKEYAMA, Takuji; TAKAYA, Hikaru; NAKAMURA, Masaharu
“Development of Iron Fluoride-NHC Catalyzed Alkylation of Aryl Chlorides and XAFS Study on the Mechanism”

— Advanced Solid State Chemistry —

LW “Introduction of Advanced Solid State Chemistry Laboratory”

GE GUO, Haichuan; HOSAKA, Yoshiteru; SEKI, Hayato; SAITO, Takashi; ICHIKAWA, Noriya; SHIMAKAWA, Yuichi
“The Synthesis and Peculiar Charge Disproportionation of the Novel A-site Layered Perovskite Oxide $LaCa_2Fe_3O_9$ with Unusual High Valence Fe Ion”

— Organotransition Metal Chemistry —

LW “Activity Report: Organotransition Metal Chemistry Laboratory”

GE TAGUCHI, Hiroomi; SASAKI, Daichi; CHANG, Yung-Hung; TAKEUCHI, Katsuhiko; TSUJIMOTO, Shota; MATSUO, Tsukasa; TANAKA, Hiromasa; YOSHIZAWA, Kazunari; OZAWA, Fumiyuki
“Synthesis and Reaction of Transition Metal Complexes with a Noninnocent PNP-Pincer Type Phosphaalkene Ligand Eind-PPEP”

GE IIZUKA, Eisuke; WAKIOKA, Masayuki; OZAWA, Fumiyuki
“Development of A Mixed-Ligand Approach to Highly Selective Direct Arylation Polymerization”

— Photonic Elements Science —

LW “Recent Research Topics of Photonic Elements Science Group”

— Chemical Life Science —

LW “Research Topics in Laboratory of Chemical Life Science”

GE NISHIYAMA, Hiroki; OGATA, Hiroyuki; AOYAMA, Takashi
“Characterization of Arabidopsis thaliana ARR1 Binding Sites Based on ChIP-Seq Data”

GE KHAIRIL ANUAR, Mohammad Fahmi Arieef; ABDUL HALIM, Arhaime Hamezze; MUHAMAD, Rafidah; MOHD HASRI, Nurul Nadzirah; BLANC-MATHIEU, Romain; OGATA, Hiroyuki; GOTO, Susumu
“GenomeNet Service and a New Computational Tool for Gene Function Annotation”

— Mathematical Bioinformatics —

LT “Predicting Heterodimeric Protein Complexes Using Novel Kernel Functions”

— Bio-knowledge Engineering —

LT NGUYEN, Hao Canh; MAMITSUKA, Hiroshi
“Global Graph Comparison for Graph Cut-based Clustering”

— Research Center for Low Temperature and Materials Sciences —

LT TERASHIMA, Takahito
“Hybrid Superlattices of Heavy Fermion Compounds”

SEMINARS

Prof Em AKASAKA, Takeshi
Foundation for Advancement of International Science, Ibaraki, Japan
"New Vistas in the Fullerene World: Endohedral Metallofullerenes"
18 November 2015

Dr BARILLOT, Emmanuel
Computational Systems Biology of Cancer Department at Institut Curie, Paris, France
"Exploiting Synthetic Interactions and Signaling Network Modeling to Combat Cancer"
7 May 2015

Prof CHANG, Young-Tae
Department of Chemistry, National University of Singapore, Singapore
"Universal Fluorescent Probe platform for Almost Everything"
23 April 2015

Dr DOUAT, Céline
CNRS, IECB & Université de Bordeaux, France
"Urea-Based Foldamers: from Structure to Function"
19 November 2015

Prof FISCHER, Felix R.
University of California Berkeley, U.S.A.
"Teaching Polymers the Meaning of Life… and Quantum Confinement in Graphene Nanostructures"
13 November 2015

Prof GLOE, Karsten
Department of Chemistry and Food Chemistry, Technische Universität Dresden, Germany
"Supramolecular Chemistry in Solvent Extraction: Principles and Applications"
24 July 2015

Prof HAMILTON, Andrew
Chemistry Research Laboratory, University of Oxford, U.K.
"Synthetic Mimics of Protein Structure and Function"
11 November 2015

Associate Prof HASHIMOTO, Hisako
Faculty of Science and Graduate School of Science, Tohoku University, Miyagi, Japan
"Synthesis and property of transition metal–silicon/germanium multiple bond complexes"
23 January 2015

Prof HIRANO, Masafumi
Department of Applied Chemistry, Graduate School of Engineering, Tokyo University of Agriculture and Technology, Tokyo, Japan
"Synthesis and Catalytic Application of Low-Valent Ruthenium and Palladium Complexes : A Breakthrough Came with Mechanistic Study"
21 May 2015

Prof HYVARINEN, Aapo
University of Helsinki, Finland
"Independent Component Analysis: Recent Advances"
23 October 2015

Prof IMAI, Yumiko
Graduate School of Medicine, Akita University, Akita, Japan
"Potential of Anti-influenza Drug Development Targeting Host Nuclear Network"
27 May 2015

Prof IMAMOTO, Tsuneo
Organic R&D Department, Nippon Chemical Industrial Co., Ltd., Tokyo, Japan
Department of Chemistry, Graduate School of Science, Chiba University, Chiba, Japan
"Chemistry of Chiral Phosphine Ligands"
16 July 2015

Dr IWATA, Tomoharu
NTT Communication Science Laboratries, Kyoto, Japan
"Unsupervised Cluster Matching for Relational Data"
24 November 2015

Prof JOHNSON, Jeremiah, A.
Department of Chemistry & Program for Polymers and Soft Matter, Massachusetts Institute of Technology, U.S.A.
"Closing the Loop: Chemistry for Controlling Primary Structure in Polymers and Polymer Networks"
27 November 2015

Dr KANDO, Masaki
Kansai Photon Science Institute, Kyoto, Japan
"Research Results and Future Development Using the JKAREN Laser"
16 January 2015

Prof KASKI, Samuel
Aalto University, Finland
"Bayesian Factorization of Multiple Data Sources"
20 October 2015

Prof Em KAWASHIMA, Takayuki
School of Science and Technology, Gunma University, Gunma, Japan
"The Chemistry of Hypervalent Compounds of Main Group Element"
18 November 2015

Dr KIRIYAMA, Hiromitu
Kansai Photon Science Institute, Kyoto, Japan
"Current Status and Future Development of the JKAREN Laser System"
16 January 2015

Prof KUCHEROV, Gregory
CNRS/LIGM Marne-la-Vallee, France
"Efficient Index-baced Filtering for NGS Read Processing"
17 May 2015

Dr KUPERSTEIN, Inna
Computational Systems Biology of Cancer Department at Institut Curie, Paris, France
“Atlas of Cancer Signaling Network and NaviCell: Comprehensive Resource and Web Tool for Data Analysis and Interpretation”
7 May 2015

Prof LEBLANC, Roger M.
Department of Chemistry, University of Miami, FL, U.S.A.
“Carbon Nanomaterials at the Biointerface”
1 December 2015

Assoc Prof MAGMIN, Morgan
National Institute of Informatics, Tokyo, Japan
“Analyzing Regulation Thanks to a Concurrent Dynamic Framework: the Process Hitting”
6 February 2015

Assist Prof MOGUSHI, Kaoru
Juntendo University, Tokyo, Japan
“Gene Expression Analysis by R”
16-17 November 2015

Prof Em NAGASE, Shigeru
Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan
“Multiple Bond of Heavier Main Group Elements”
18 November 2015

Prof NORBERT, Krause
Dortmund University of Technology, Organic Chemistry, Dortmund, Germany
“Sustainable Gold Catalysis”
4 November 2015

Assist Prof OKAJIMA, Koji
Graduate School of Science, Osaka Prefecture University, Osaka, Japan
“Signal Transduction Mechanism for Blue Light by Phototropin; Blue-Light Sensor of Plants”
5 February 2015

Dr OHTA, Yukari
Japan Agency for Marine-Earth Science and Technology, R&D Center for Marine Biosciences, Kanagawa, Japan
“Lignin-Degrading Enzymes from Marine Bacterium”
13 October 2015

Prof PATEL, Bhisma K.
Indian Institute of Technology Guwahati, India
“Unconventional Ways to Ester Synthesis”
7 April 2015

Prof PRASAD, B. L. V.
National Chemical Laboratory, India
“Molecular Tools for the Manipulation of Size, Surface Chemistry and Assemblies of Metal Nanoparticles”
19 November 2015

Prof RIVARD, Eric
University of Alberta, Alberta, Canada
“Phosphorescence and Parent Inorganic Hydride Chemistry in the Main Group”
18 September 2015

Prof SAGAN, Sandrine
Laboratoire des Biomolécules, UMR7203 CNRS–University Pierre et Marie Curie –École Normale Supérieure, Paris, France
“Molecular and Structural Aspects for Efficient Internalisation of Cell-Penetrating Peptides in Cells: Arginine Magic or Tryptophan Power ?”
19 November 2015

Assoc Prof SAITO, Koh
Nagoya University Eco Topia Science Institute, Aich, Japan
“Development of Spin-polarized and Pulsed Transmission Electron Microscope with Semiconductor Photocathode”
10 March 2015

Dr SETO, Keita
Extreme Light Infrastructure Nuclear Physics, Romania
“Current Status and Future Development of ELI-NP”
7 April 2015

Prof SHIMIZU, Hirohiko, M.
Laboratory for Particle Properties, Department of Physics, Nagoya University, Aichi, Japan
“Application of epithermal neutron”
1 July 2015

Prof SMERALDI, Fabrizio
Queen Mary University of London, London, England
“Handing Missing Features with Boosting Algorithms for Protein-protein Interaction Prediction”
18 May 2015

Sinior Research Fellow SONG, Jiangning
Monash University, Australia
“The Predictive Power of Machine Learning Techniques in Data-driven Biomedical Knowledge Discovery: My Structural Bioinformatics Journey”
9 September 2015

Assoc Prof TAIRA, Takunori
National Institute of NaturalSciences, Aich, Japan
“Theoretical Foundations, Applications and Future Developments of Giant Micro-photonics”
9 March 2015

Prof TAYLOR, Mark S.
University of Toronto, Canada
“Noncovalent and Reversible Covalent Interactions: Fundamental Studies and New Application”
21 May 2015

Prof XAVIER, Franck
Research Director, CNRS & University of Rouen, France
“New Protein Stain Derived from Natural Product: Proteomics and Chemical Biology Applications”
6 November 2015

Dr YAMADA, Makoto
Yahoo! Labs, U.S.A.
“Minimum Redundancy Maximum Relevance Feature Selection for Large and High-dimensional Data”
7 January 2015

Prof ZHANG, Qichun
Nanyang Technological University, Singapore
“Some Novel Strategies to Prepare New Exotic Material”
3 March 2015

Prof ZHANG, Yan
School of Chemistry & Chemical Engineering, Nanjing University, China, P.R.
“Chemical Biological Applications of Photo-Induced Reactions”
25 March 2015

Prof ZHIQUN, Lin
Georgia Institute of Technology, U.S.A.
“Nonlinear Block Copolymer-Enabled Monodisperse Nanoparticles and Nanorods with Precisely Controlled Dimensions, Compositions and Architectures”
12 June 2015

MEETINGS AND SYMPOSIA

The 10th International Workshop for East Asian Young Rheologists (IWEAYR-10)
Co-organized by WATANABE, Hiroshi
4-7 February 2015 (Fukuoka, Japan)

Stimuli-responsive Chemical Species for the Creation of Functional Molecules
“The 4th symposium”
Organized by OZAWA, Fumiyuki
22 May 2015

The 10th Organoelement Chemistry Seminar
Organized by TOKITOH, Norihiro; SASAMORI, Takahiro; MIZUHATA, Yoshiyuki; AGOU, Tomohiro
8 June 2015 (Uji, Japan)

Information in Biology, Medicine and Pharmacology 2015
(The 2015 Annual Conference of the Japanese Society for Bioinformatics)
Organized by Bioinformatics Center,
29-31 October 2015 (Uji, Japan)

“Frontiers in Data-Driven Science and Technology: Recent Advances in Machine Learning and Applications”
Organized by MAMITSUKA, Hiroshi
5-6 November 2015 (Nagoya, Japan)

Stimulating Meeting for Young Researchers in Chemistry on Stimuli-responsive Chemical Species
Organized by TOKITOH, Norihiro; SASAMORI, Takahiro; MIZUHATA, Yoshiyuki; AGOU, Tomohiro
12 November 2015 (Uji, Japan)

Pacifichem 2015 (Topic Area: Macromolecular, Session Title: Advances in Precision Polymer Synthesis Using Reversible Deactivation Radical Polymerization)
Organized by KEDDIE, Daniel; MOAD, Graeme; TSAREVSKY, Nicolay; YAMAGO, Shigeru
17-18 December 2015 (Honolulu, U.S.A)

INDEX

NAME INDEX

KEYWORD INDEX

Institute for
Chemical
Research

Kyoto University

2015

ICR ANNUAL REPORT

Volume 22