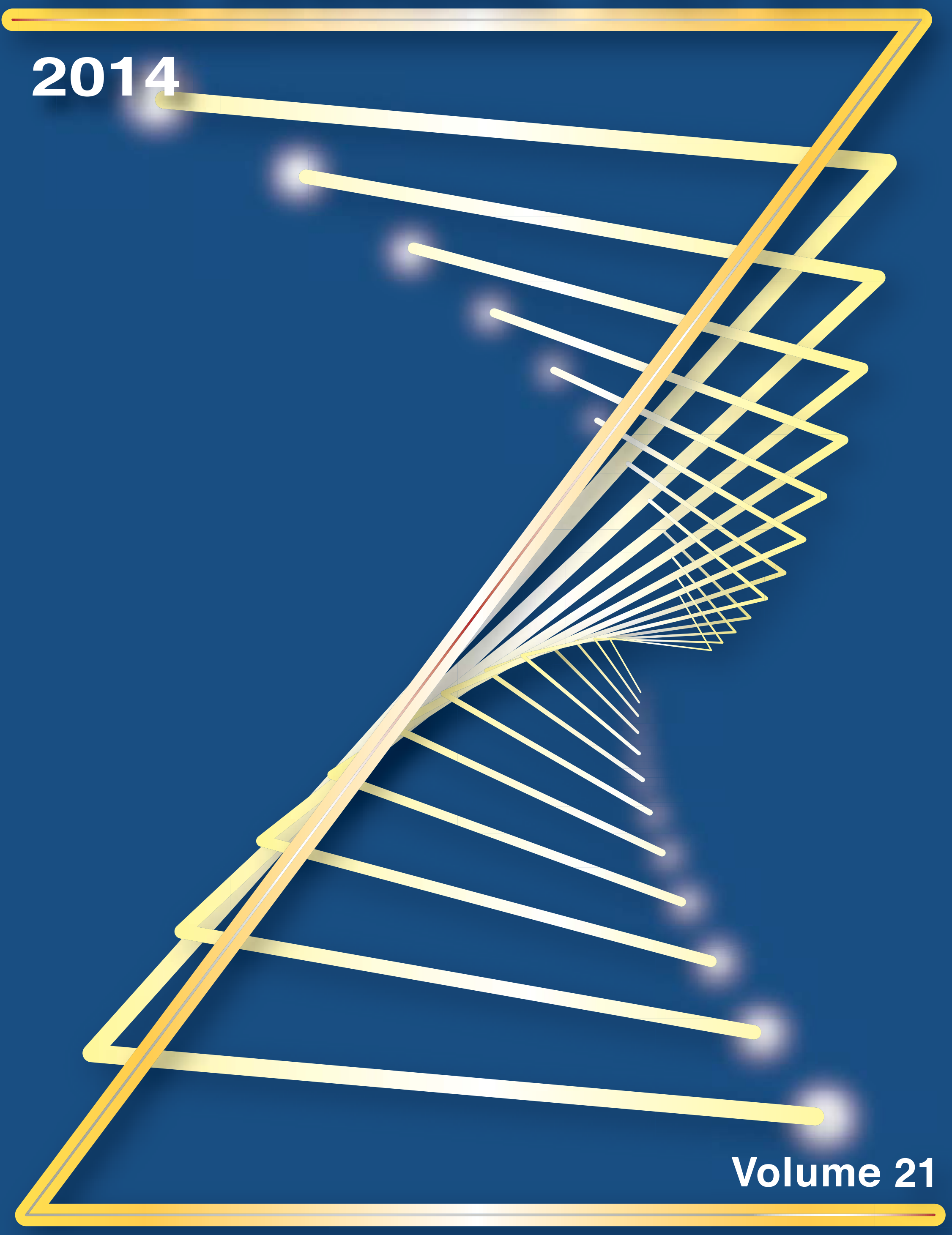
ISSN 1342-0321
IAREFM

ICR ANNUAL REPORT

2014



Volume 21

Institute for Chemical Research
Kyoto University

ICR ANNUAL REPORT 2014 (Volume 21) - ISSN 1342-0321 -
This Annual Report covers from 1 January to 31 December 2014

Editors:
Professor: KURIHARA, Tatsuo
Professor: TERANISHI, Toshiharu
Associate Professor: MASUBUCHI, Yuichi
Assistant Professor: INOUE, Shunsuke

Editorial Staff:
Public Relations Section: TANIMURA, Michiko
HAMAOKA, Meri
INOUE, Junko
TAKEHIRA, Tokiyo

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@kulib.kyoto-u.ac.jp
URL http://lib.kuicr.kyoto-u.ac.jp/homepage/japanese/index.htm

Printed by:
MARUZEN Co., Ltd.
1-9-18, Kaigan, Minato-ku, Tokyo 105-0022, Japan
TEL:+81-(0)3-6367-6099 FAX:+81-(0)3-6367-6208

ICR ANNUAL REPORT 2014

Institute for Chemical Research
Kyoto University
Volume 21

Preface

Institute for Chemical Research (ICR), Kyoto University was launched in 1926 as the first research institute at Kyoto University. The philosophy at the time of its foundation was to “Excel in the Investigation of Basic Principles of Chemistry and Their Applications,” and then the studies on special medicinal substances, organometallic chemistry, incendiary reagents, and so on were undertaken at nine research laboratories. The ICR has continuously produced outstanding research achievements so far. Now, we have reached the current large-scale organization of 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. Currently, about 120 faculty members, 210 graduate students and 60 researchers are engaged in research activities in 31 laboratories in total supervised by full-time professors. Further, we have 5 laboratories supervised by visiting professors and also an endowed laboratory.

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 to which our laboratories belong as cooperative ones accepting graduate students cover diverse fields of science, engineering, pharmaceutical sciences, agriculture, medicine, informatics, and human/environmental studies. These laboratories are spearheading leading-edge research, and yielding outstanding results in their own and/or correlated research areas; as examples, 1) the successful synthesis of the most strained “carbon nano ring”, [5]cycloparaphenylene, 2) novel quadruple perovskite oxide with large magnetization and a high transition temperature, 3) development of new organic semiconducting materials containing quasiplanar skeleton, and 4) photocarrier recombination dynamics in perovskite for solar cell applications, all achieved in all of last year. The legacy of our founding philosophy above 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. Whether or not the human race maintain sustained growth is a key issue of this century, when we must reform our country from various perspectives in Japan. Hence, the ICR encourages its members to be actively involved in research projects with bottom-up approach in mind, and to value the development of unique interdisciplinary research projects, in order to contribute to the future of our society from materials-related fields.

Besides, the ICR is collaborating with domestic/oversea universities and research organizations (with 64 official international collaboration agreements as of 1 January 2015) and is functioning 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, 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. Further, we also fully strive to fostering and securing of 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 also with outside ensures the Institute to serve as the core of global research propellers in chemistry-oriented fields. Finally, we would appreciate your continued encouragement and support.

January 2015

N. Tokitoh

TOKITOH, Norihiro
Director

ICR News 2014

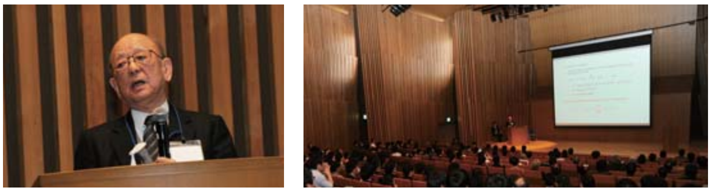
The ICR International Symposium 2014 (ICRIS'14) "The Science and Technology of Smart Materials"

■ Prof TSUJII, Yoshinobu

10—12 March 2014, Uji, Japan, organized by the Institute for Chemical Research (ICR), and co-organized by ICR Joint Usage/Research Center, Institute of Advanced Energy (IAE), and Research Institute for Sustainable Humanosphere (RISH) of Kyoto University

The Institute for Chemical Research (ICR) planned at the 70th anniversary in 1996 and since then has been organizing a series of international symposia as ICRIS covering various chemistry-related fields with selected topics. The symposium in 2014 targeted the field of multidisciplinary science under the title including three main topics, bio-inspired systems, green innovation, and advanced analysis/design. This symposium was supported by the "Zengaku-keihi" project of Kyoto University especially from the viewpoint of international exchange of young researchers. On the basis of a special lecture by the 2010 Nobel Prize Laureate in Chemistry, Emeritus Professor Akira Suzuki (Hokkaido University, Japan), 21 keynote/invited lectures, and 91 poster presentations, high-quality and fruitful discussions on the selected topics were engaged in. The Mayor of Uji, Mr. Tadashi Yamada, and the Executive Vice President of Kyoto University, Professor Nobuyoshi Esaki, kindly joined the symposium banquet, giving a very inspiring speech. 381 participants, much more than expected, got together, clearly indicating deep interest in this field. One of keys to success of this symposium is the joint-research activity organized by the ICR Joint Usage/Research Center. Many of joint researchers gave poster presentations and actively participated in discussions. This symposium must have provided an opportunity of exchanging up-to-date information and having dense scientific discussion in the multidisciplinary science, thereby greatly accelerating the international cooperation.

Poster Session



SUZUKI, Akira, Special Guest Speaker's Lecture

Banquet

The 2nd Kyoto University & National Taiwan University Joint Symposium
Nanoscience and Technology Session @ Uji Campus

Prof TOKITOH, Norihiro

The 2nd Kyoto University and National Taiwan University Symposium (1-2 September 2014) was held at Kyoto University with the objective to promote international research between the two schools. Under the witness of the more than one hundred academic and administrative representatives, the two schools officially signed the agreements to implement faculty exchange and dual degree projects. After the opening session at the Clock Tower Centennial Hall, Nanoscience and Technology Session was held at Uji Obaku Plaza for two days. This session was successfully co-coordinated by Prof. Li-Chyong Chen (NTU) and Prof. Norihiro Tokitoh (KU) and consists of 11 speakers from NTU (Dept. of Chem., Dept. of Mat. Sci. and Eng., Dept. of Phys., and Center for Condensed Matter Sciences (CCMC)) and 7 speakers from KU (ICR). The participants of this session from NTU and KU have fully enjoyed the discussion on the latest results and new techniques in the fields of Nanoscience and Technology, which will be of great interest and importance from the viewpoints of not only fundamental science but also near future application. In 2014, Institute for Chemical Research (ICR) has concluded MOUs individually with Dept. of Chem. (18 March), Dept. of Mat. Sci. and Eng. (30 May), and CCMC (4 April). We are now on the way of discussion to exchange the researchers and students each other based on these MOUs to develop our longtime mutual research exchange and friendship.

The commemorative photo of the Symposium

CHEN, Chun-Wei, representative from National Taiwan University

ICR and iCeMS Provided the First edX Lecture from Japan

Prof UESUGI, Motonari

Kyoto University has started providing Massive Open Online Courses (MOOCs) on a U.S-based nonprofit online learning platform, edX, for the first time from Japan. As the very first KyotoUx-series course, Prof. Uesugi of ICR and iCeMS taught "Chemistry of Life," a 15-week full lecture broadcasted from April thru July 2014. The goal of this course is to develop skills for generating new ideas at the interface between chemistry and biology by analyzing pioneering studies. By bringing together knowledge from multidisciplinary fields, we are empowered with the ability to generate new ideas. A total of 20,269 students participated in this course from the world. Among them, 6 top performing students were invited to visit Kyoto University for a week in July 2014. The students from U.S., Peru, Vietnam, Serbia, Latvia, and the Philippines made a short visit to ICR and its state-of-art facilities and gave a presentation at Prof. Uesugi's real course. Their Kyoto visits were highlighted by major newspapers and broadcasted by NHK.

edX - Kyoto Ux
http://ocw.kyoto-u.ac.jp/ja/edxkyotoux

6 top performing students invited to visit Kyoto University took a look at ICR on 9 July.

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

Endowed Research Section

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
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
  - Interdisciplinary Chemistry for Innovation

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
- Endowed Research Section
  - Nano-Interface Photonics (SEI Group CSR Foundation)
- 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
NESTEROV, Vitaly
(Ph D)


PD
MIYAKE, Hideaki
(D Sc)

Students

MIYAMOTO, Hisashi (D3)
EGAWA, Yasunobu (D3)
WASANO, Tatsuya (D3)
NAGATA, Koichi (D2)
AWANE, Hiroyuki (D1)
HIRANO, Kohki (D1)
SUZUKI, Yuko (M2)
FUJIMORI, Shiori (M1)
SUGAHARA, Tomohiro (M1)

Guest Scholars

KYRI, Andreas	University of Bonn, Germany, 30 April-30 June
HEURICH, Tobias	University of Bonn, Germany, 25 July-25 September

Scope of Research

Organic chemistry has been developed as that of second-row elements such as carbon, oxygen, and nitrogen so far, while the synthesis and isolation of the heavier congeners of typical organic molecules as stable compounds have been one of "dreams" 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 not only fundamental chemistry but also opening the way to more extensive application of main group chemistry.

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

Selected Publications

Wasano, T.; Agou, T.; Sasamori, T.; Tokitoh, N., Synthesis, Structure and Reactivity of a 1-Bromoalumole, *Chem. Commun.*, **50,** 8148-8150 (2014).

Agou, T.; Nagata, K.; Sasamori, T.; Tokitoh, N., Reaction of a Dialumene-Benzene Adduct with Diphenylacetylene: Formation of 3,4-Dialuminacyclobutene and 5,6-Dialuminabicyclo[2.1.1]hex-2-ene Derivatives, *Chem. Asian. J.*, **9,** 3099-3101 (2014).

Agou, T.; Hayakawa, N.; Sasamori, T.; Matsuo, T.; Hashizume, D.; Tokitoh, N., Reactions of Diaryldibromodisilenes with *N*-Heterocyclic Carbenes: Formation of Formal Bis-NHC Adducts of Silyliumylidene Cations, *Chem. Eur. J.*, **20,** 9246-9249 (2014).

Nagata, K.; Agou, T.; Tokitoh, N., Syntheses and Structures of Terminal Arylalumylene Complexes, *Angew. Chem. Int. Ed.*, **53,** 3881-3884 (2014).

Tsurusaki, A.; Sasamori, T.; Tokitoh, N., Synthesis and Structure of a 1-Phospha-2-boraacenaphthene Derivative and Its Chalcogenation Reactions, *Chem. Eur. J.*, **20,** 3752-3758 (2014).

Matsumoto, T.; Sasamori, T.; Miyake, H.; Tokitoh, N., Synthesis of a Rhodium Carbonyl Phosphaalkenyl-Phosphido Complex: A Phosphorus Congener of Schiff Base Type *N,N'*-Chelating Monoanionic Ligands, *Organometallics*, **33,** 1341-1344 (2014).

Terminal Arylalumylene Complexes

Group 13 element (B, Al, Ga, In, and Tl) compounds have less than an octet and have tendency to form an octet by accepting an electron pair from a Lewis base. Therefore, it is difficult to construct π-electron systems (multiple bond, π-conjugated system, and so on) containing a Group 13 element with keeping the vacant p-orbital. Especially, there had been few reports on the Al-containing π-electron systems. We have already succeeded in the synthesis of a benzene-adduct of dialumene (an Al–Al double-bond compound) and revealed its synthetic equivalency to dialumene. During the course of our studies on the reactivity of dialumene-benzene adducts, we have succeeded in the synthesis of novel platinum complexes of terminal alumylenes (monovalent aluminum species).

Terminal arylalumylene complexes of platinum [ArAl–Pt(PCy_3)$_2$] [Ar = 2,6-[CH($SiMe_3$)$_2$]$_2C_6H_3$ (Bbp) or 2,6-[CH($SiMe_3$)$_2$]$_2$-4-(*t*-Bu)C_6H_2 (Tbb)] have been synthesized either by the reaction of a dialumene-benzene adduct with [Pt(PCy_3)$_2$]. X-Ray crystallographic analysis (Figure 1) revealed that the Al–Pt bond lengths of these arylalumylene complexes are shorter than the shortest Al–Pt distance reported previously. DFT calculations suggest that the Al–Pt bonds in the arylalumylene complexes have a significantly high electrostatic character.

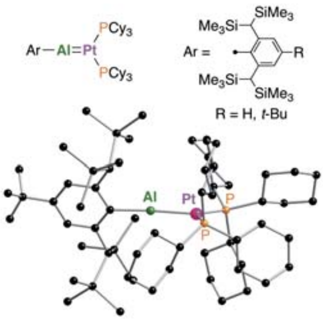


Figure 1. Terminal alumylene complexes.

1-Bromoalumole

Heteroles of electron-deficient group 13 elements are expected to have low-lying LUMOs owing to the orbital interactions between the empty p orbital of group 13 elements and the π* orbitals. Quite recently, we have succeeded in the synthesis of the first Lewis base-free alumole by the introduction of bulky substituent, Mes* [Mes* = 2,4,6-(*t*-Bu)$_3C_6H_2$]. DFT calculations revealed that the 3p(Al)-π* conjugation effectively lowers the LUMO energy level of the alumole. In order to elucidate the properties of alumoles extensively and to utilize them as the key components of functional materials, facile and versatile synthetic methods of alumoles bearing various functional groups should be of importance. Therefore, we examined the synthesis of alumoles bearing halogen-substituent on the aluminum atom.

A stable 1-bromoalumole has been synthesized by the reaction of a 1,4-dilithio-1,3-butadiene derivative with $AlBr_3$. The 1-bromoalumole was found to exist as a dimeric structure in the crystalline state (Figure 2). Reaction of the 1-bromoalumole with Mes*Li afforded the corresponding Mes*-substituted alumole, demonstrating the potential of the 1-bromoalumole for the functionalization of alumoles.

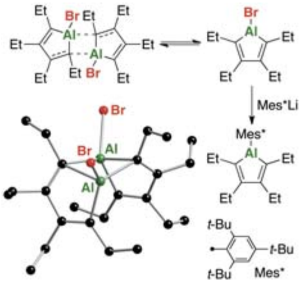


Figure 2. Reactivity of the 1-bromoalumole and its dimeric structure in the crystalline state.

Bis-NHC Adducts of Silyliumylidene Cations

Silyliumylidene cation (RSi:$^+$) is highly coordinatively-unsaturated silicon species and is one of the most challenging intermediates in silicon chemistry. Although several examples of Lewis base-coordinated silyliumylidene have been reported, we have found a novel method to access silyliumylidene stabilized by *N*-heterocyclic carbenes (NHC) by using 1,2-dibromodisilenes as starting materials.

Reactions of stable 1,2-dibromodisilenes [(*E*)-Ar(Br)Si=Si(Br)Ar] with NHC afforded NHC-arylbromosilylene [Ar(Br)Si:] adducts or bromide salts of the corresponding bis-NHC adducts of the formal arylsilyliumylidene cations ([ArSi:]$^+$) (Figure 3). In some cases, an NHC was able to replace a bromide anion in the coordination sphere of the arylbromosilylene-NHC adduct. X-Ray crystallographic analysis revealed that the silicon centers of the bis-NHC adducts of the silyliumylidene cations possess pyramidal geometries, indicating that the lone pair electrons are substantially localized on the silicon atoms.

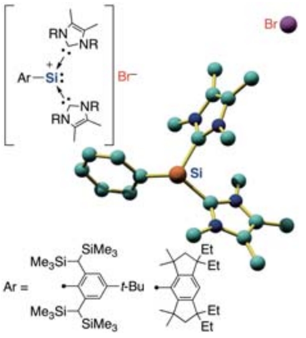


Figure 3. Bis-NHC adducts of silyliumylidene cations.

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
ENDO, Masaru
(D Eng)

PD
ARAMAKI, Yoshitaka
(D Eng)

Assist Techn Staffs

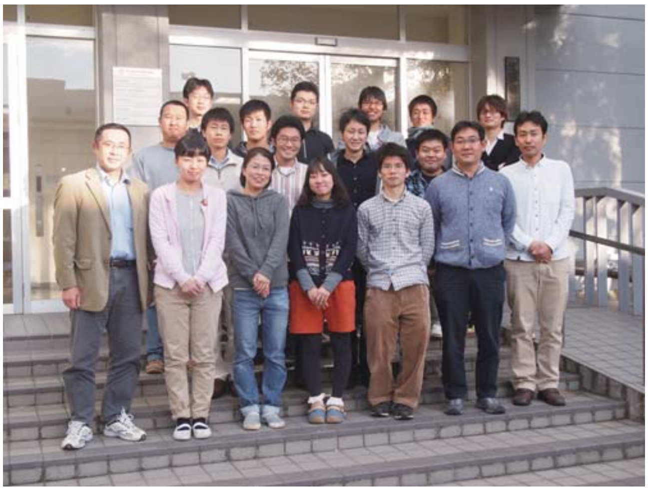
NAKAIKE, Yumi (D Eng)
HORI, Megumi
SHIMAZAKI, Ai

Students

NISHIMURA, Hidetaka (D2)
CHAOLUMEN (D2)
FUTAGOISHI, Tsukasa (D1)
SHIMOGAWA, Hiroyuki (D1)
ZHANG, Rui (D1)
SATO, Motoi (M2)
HASHIKAWA, Yoshifumi (M2)
FUNAKOSHI, Miho (M1)
MARUYAMA, Naoki (M1)
KAJI, Shoji (UG)
MIURA, Tsutomu (UG)

Scope of Research

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



KEYWORDS
π-Conjugated Systems
Endohedral Fullerenes
Functional Materials
Perovskite-based Solar Cells
Organic Solar Cells

Selected Publications

Zhang, R.; Futagoishi, T.; Murata, M.; Wakamiya, A.; Murata, Y., Synthesis and Structure of an Open-Cage Thiafullerene $C_{69}S$: Reactivity Differences of an Open-Cage C_{70} Tetraketone Relative to Its C_{60} Analogue, *J. Am. Chem. Soc.*, **136,** 8193-8196 (2014).

Hashikawa, Y.; Murata, M.; Wakamiya, A.; Murata, Y., Synthesis of Open-Cage Ketolactam Derivatives of Fullerene C_{60} Encapsulating a Hydrogen Molecule, *Org. Lett.*, **16,** 2970-2973 (2014).

Wakamiya, A.; Nishimura, H.; Fukushima, T.; Suzuki, F.; Saeki, A.; Seki, S.; Osaka, I.; Sasamori, T.; Murata, M.; Murata, Y.; Kaji, H., On-Top π-Stacking of Quasiplanar Molecules in Hole-Transporting Materials: Inducing Anisotropic Carrier Mobility in Amorphous Films, *Angew. Chem., Int. Ed.*, **53,** 5800-5804 (2014).

Wakamiya, A.; Endo, M.; Sasamori, T.; Tokitoh, N.; Ogomi, Y.; Hayase, S.; Murata, Y., Reproducible Fabrication of Efficient Perovskite-based Solar Cells: X-ray Crystallographic Studies on the Formation of $CH_3NH_3PbI_3$ Layers, *Chem. Lett.*, **43,** 711-713 (2014).

Chaolumen; Enno, H.; Murata, M.; Wakamiya, A.; Murata, Y., Dibenzo[*a*,*f*]perylene Bisimide: Effects of Introducing Two Fused Rings, *Chem. Asian J.*, **9,** 3136-3140 (2014).

Development of New Organic Semiconducting Materials Containing Quasiplanar Skeleton

The development of excellent charge-transporting materials with high charge carrier mobility is a crucial issue to achieve high performance in organic-device applications. In order to achieve the high charge carrier mobility using small organic molecules, it is important to control their molecular orientation in the solid state. In this work, we have designed and synthesized partially bridged triphenylamine derivatives with a quasiplanar structure. These compounds form one-dimensional on-top π-stacking aggregates in the crystalline state and showed high levels of anisotropic charge transport in the direction of the π-stacking. Furthermore, even in the vacuum deposited amorphous films, these compounds retained some of the face-on π-stacking, thus facilitating an out-of-plane carrier mobility (Figure 1). These results would provide new guideline for molecular design of organic semiconducting materials used in the amorphous state.

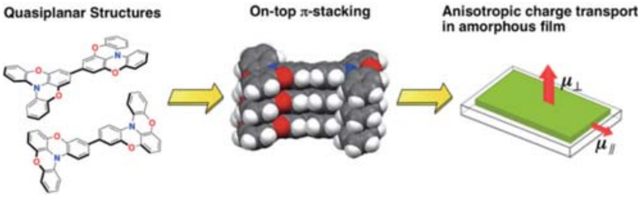


Figure 1. The structures of oxygen-bridged triphenylamine derivatives and their one-dimensional on-top π-stacking structure in the crystalline state. Anisotropic charge carrier mobility in the amorphous films of these compounds is also shown.

X-Ray Crystallographic Studies on the Formation of $CH_3NH_3PbI_3$ Layers

Perovskite-based solar cells with $CH_3NH_3PbX_3$ (X= halogen) as light absorbers have attracted much attention, mostly because the perovskite layer can be easily processed in solution. Although promising PCEs of over 15% have been reported, the cells often suffer from large PCE variations, which severely hamper systematic studies on further improvements. In this work, we examined the influence of water and oxygen as well as the purity of the starting materials on the formation of the perovskite layers. Moreover, the single-crystal X-ray diffraction analyses were conducted on lead halide complexes, which potentially form during the production process. Based on these results, we have established a reproducible fabrication method for highly efficient solar cells (Figure 2).

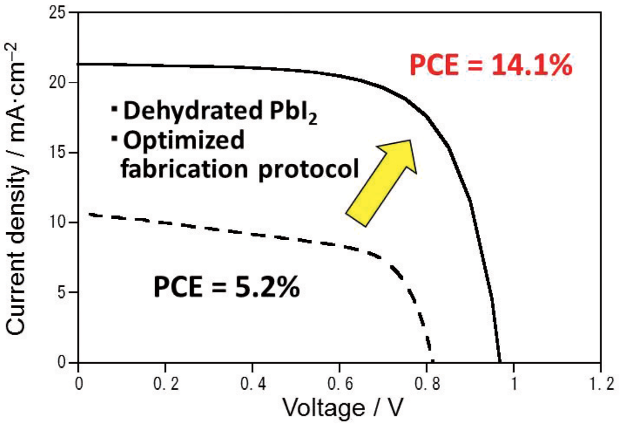


Figure 2. Photocurrent density-voltage curves of perovskite-based solar cell.

Synthesis, Structure, and Properties of Dibenzo[*a*, *f*]perylene Bisimide Derivatives

Perylene bisimides (PBIs) **1** are fascinating dyes with various potential applications. In order to study the effects of introducing dibenzo-fused structure in the perylene moiety, we synthesized π-extended PBI derivative **2** with a dibenzo-fused structure at both of the *a* and *f* bonds (Figure 3). The twisted structure was characterized by X-ray crystal structure analysis. Cyclic voltammetry (CV) measurements demonstrated that two ring fusions at both sides of a naphthalene moiety, which construct a tetracene core, effectively raise the HOMO level with reference to one ring fusion at each naphthalene moiety (two anthracene cores). In particular, [*a*,*f*]-fused PBI **2** showed a broad absorption band at 735 nm with a shoulder band at 780 nm, which was markedly red-shifted by 83 nm compared to that of dibenzo[*a*,*o*]-fused PBI **3** (λ_{max} = 697 nm).

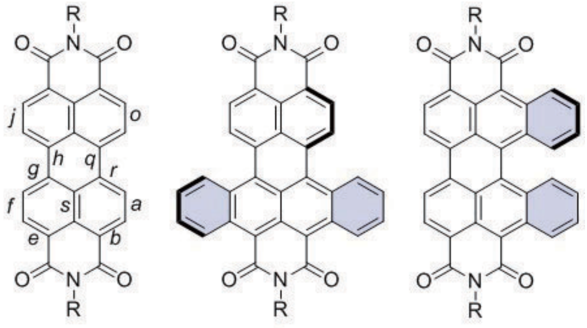


Figure 3. Structures of PBI **1** and dibenzo-fused PBIs **2** and **3**.

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)


Program-Specific 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

SHIGETA, Takashi (D3)
YANG, Pan (D3)
BABA, Tomonori (D3)
YANAGI, Masanori (D3)
TAKEUCHI, Hironori (D2)
LU, Wenjie (D2)
TSUDA, Ayumi (D2)
HYAKUTAKE, Ryuichi (D2)
HIRATA, Atsushi (D2)
KASAMATSU, Koji (D1)
KURIBAYASHI, Toshifumi (D1)
NAKAGAWA, Akihiro (D1)
HAYASAKA, Manami (D1)
OTSUKI, Haruka (M2)
XU, Pei (M2)
WADA, Yoshiyuki (M2)
TANAKA, Yuya (M1)
FUJIMORI, Yusuke (M1)
NISHIJIMA, Hideyuki (M1)
MATAYOSHI, Aki (UG)
YAMAMOTO, Satoru (UG)

Scope of Research

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

KEYWORDS
Organocatalysis
Regioselective Functionalization
Dynamic Chirality
Unusual Amino Acid
Molecular Recognition

Selected Publications

Kawabata, T.; Muramatsu, W.; Nishio, T.; Shibata,T.; Schedel, H., A Catalytic One-Step Process for the Chemo- and Regiocelective Acylation of Monosaccharides, *J. Am. Chem. Soc.*, **129,** 12890-12895 (2007).

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).

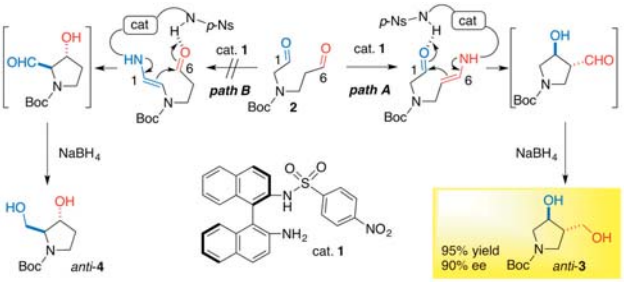
Yoshimura, T.; Tomohara, K.; Kawabata, T., Asymmetric Induction via Short-Lived Chiral Enolates with Chiral C-O Axis, *J. Am. Chem. Soc.*, **135,** 7102-7105 (2013).

Topics

Regio- and Stereoselective Intramolecular Cross-Aldol Reaction of Dials Promoted by Catalysts with “Low” Reactivity

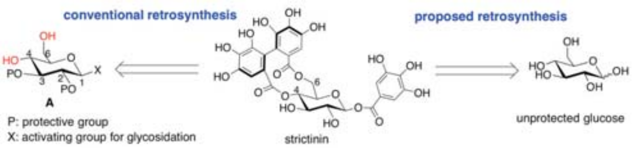
Intramolecular direct cross-aldol reactions of 1,n-alkanedials have high potential in preparing bioactive natural products and pharmaceuticals such as prostaglandins and nucleic acid medicines. To achieve this reaction selectively, not only stereochemistry but also regiochemistry of the products has to be controlled (Figure 1, path A *vs*. path B). In amine-catalyzed reactions based on the enamine mechanism, high regioselectivity is expected only under the conditions that the amine catalyst precisely discriminates two enolizable formyl groups and convert them individually to the aldol donor (enamine component) as well as the aldol acceptor (carbonyl component), selectively.

Axially chiral catalyst **1** having aniline-type amine was employed under the postulation that catalysts with intrinsic low reactivity could readily discriminate the formyl groups and control the regioselectivity during the cross-aldol reaction. As expected, catalyst **1** could distinguish the formyl groups of **2** efficiently to realize the reaction through the enamine of C(6)-formyl group (path A). *Anti*-**3** was obtained as a sole product in high regio- and stereoselectivities, while *anti*-**4** via the enamine of C(1)-formyl group (path B) was not detected.

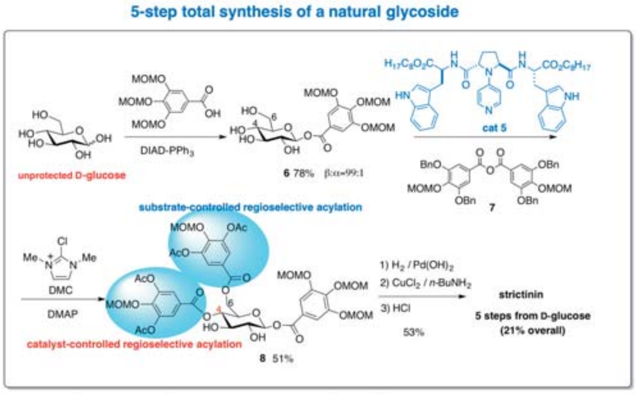


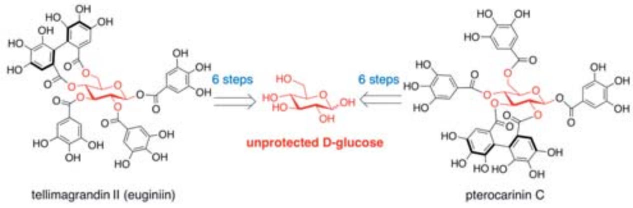
A New Retrosynthetic Approach towards Total Synthesis of Natural Glycosides via Catalyst-Controlled Regioselective Acylation

Natural glycosides have attracted considerable interests as synthetic targets due to the pharmaceutical potentials based on their significant biological activities including anti-HSV, anti-influenza virus, anti-tumor, and neuroprotective activities. Total synthesis of strictinin, a biologically active natural glycoside, is shown here. A conventional retrosynthetic analysis should lead to suitably protected precursor **A**, possessing free C(4)-OH and C(6)-OH (shown in red) and C(1)-X (X : activating group for glycosidation), C(2)-OP (P : protective group), and C(3)-OP to introduce a hexahydroxy diphenoyl (HHDP) group at C(4)-O and C(6)-O of the glucopyranose skeleton. In contrast, we propose a new retrosynthetic approach towards the total synthesis employing unprotected glucose as a direct precursor.



We found that glycosidation of a gallic acid derivative using unprotected glucose as a glycosyl donor took place in a highly β-selective manner under Mitsunobu conditions to give glycoside **6** in 78% yield. Treatment of **6** with anhydride **7** in the presence of catalyst **5** followed by a condensation agent (DMC, DMAP) gave 4, 6-digallate **8** in 51% yield. The first introduction of a galloyl group at the inherently less reactive C(4)-OH was assumed to proceed via catalyst-controlled regioselective acylation, and the second introduction of a galloyl group at the most reactive primary C(6)-OH proceeded via substrate-controlled regioselective acylation. Thus, overall 5-step total synthesis of natural glycoside, strictinin, was achieved from naturally abundant glucose without using any protective groups for glucose. The overall number of the steps for the total synthesis is much less than those previously reported (11 or 13 steps from glucose). Similarly, total syntheses of natural glycosides, tellimagrandin II (eugeniin), and pterocarinin C have been performed in six steps from glucose.





Division of Synthetic Chemistry
– Advanced Inorganic Synthesis –

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

Prof
TERANISHI, Toshiharu
(D Eng)

Assist Prof
SAKAMOTO, Masanori
(D Eng)

Assist Prof *
SATO, Ryota
(D Sc)

PD
TRINH, Thang Thuy
(Ph D)

PD
YOSHIZUMI, Toshihiro
(D Eng)

PD
WU, Hsin-Lun
(D Sc)

*Division of Synthetic Chemistry, Laboratory for Energy Quantum Manipulation

Students

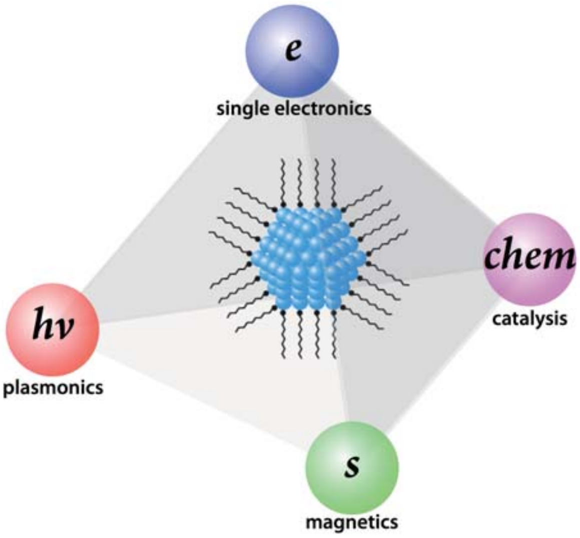
CHEN, Lihui (D2)
KIM, Sungwon (D2)
EGUCHI, Daichi (D1)
YAMAOKA, Satoshi (M2)
TABUCHI, Michimasa (M1)
KIMURA, Masato (M1)
MATSUMOTO, Kenshi (M1)

Scope of Research

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

KEYWORDS

Inorganic Nanoparticles
Single Electronics
Plasmonics
Nanocomposite Magnet
Photocatalysts



Selected Publications

Sakamoto, M.; Inoue, K.; Saruyama, M.; So, Y.-G.; Kimoto, K.; Okano, M.; Kanemitsu, Y.; Teranishi, T., Investigation on Photo-Induced Charge Separation in CdS/CdTe Nanopencils, *Chem. Sci.*, **5,** 3831-3835 (2014).

Ihara, T.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Delocalized and Localized Charged Excitons Single CdSe/CdS Dot-in-Rods Revealed by Polarized Photoluminescence Blinking, *Phys. Rev. B*, **90,** [035309-1]-[035309-5] (2014).

Tanaka, D.; Inuta, Y.; Sakamoto, M.; Furube, A.; Haruta, M.; So, Y.-G.; Kimoto, K.; Hamada, I.; Teranishi, T., Strongest π-Metal Orbital Coupling in a Porphyrin/Gold Cluster System, *Chem. Sci.*, **5,** 2007-2010 (2014).

Okano, M.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Assessment of Hot-carrier Effects on Charge Separation in Type-II CdS/CdTe Heterostructured Nanorods, *J. Phys. Chem. Lett.*, **5,** 2951-2956 (2014).

Xiong, A.; Yoshinaga, T.; Ikeda, T.; Takashima, M.; Hisatomi, T.; Maeda, K.; Setoyama, T.; Teranishi, T.; Domen, K., Effect of Hydrogen and Oxygen Evolution Cocatalysts on Photocatalytic Activity of GaN:ZnO, *Eur. J. Inorg. Chem.*, **2014,** 767-772 (2014).

Visible to Near-Infrared Plasmon-Enhanced Catalytic Activity of Pd Hexagonal Nanoplates for the Suzuki Coupling Reaction

The photocatalytic conversion of solar energy to chemical energy is a sustainable and efficient process for chemical reactions because solar light is an abundant resource and it can facilitate room-temperature chemical transformations by generating electronically excited states in photocatalysts. Pd hexagonal nanoplates with a well-defined and tunable longitudinal local surface plasmon resonance (LSPR) peak enabled the direct harvesting of visible to near-infrared light for chemical reactions. Upon plasmon excitation, the catalytic Suzuki coupling reaction between iodobenzene and phenylboronic acid was accelerated by the plasmonic photocatalytic effect with plasmon induced hot-electrons. The turnover frequency (TOF) of the Pd hexagonal nanoplates in a reaction illuminated with a $\lambda = 300 - 1000$ nm Xenon lamp at 176 mWcm^{-2} was 2.5 and 2.7 times higher than that of non-plasmonic {111}-enclosed Pd nanooctahedra and {100}-enclosed Pd nanocubes, respectively. It was also 1.7 times higher than that of a reaction that was thermally heated to the same temperature.

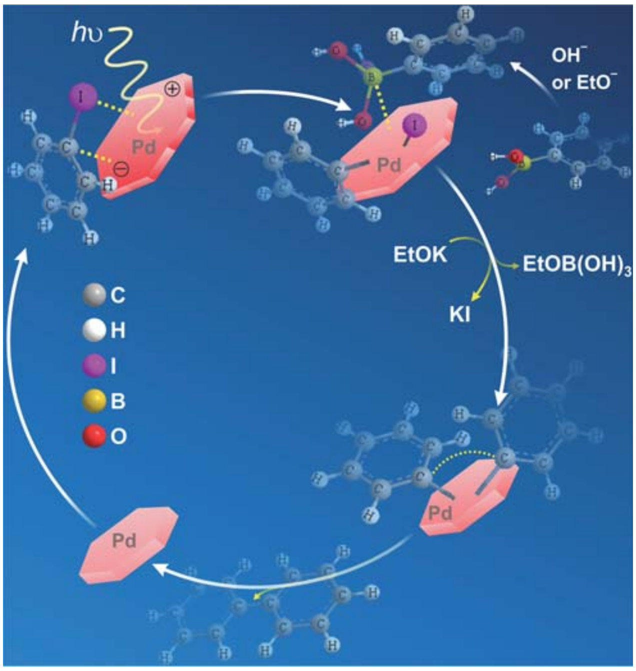


Figure 1. Proposed mechanism for the Suzuki coupling reaction catalyzed by heterogeneous plasmonic Pd hexagonal nanoplates.

Determination of a Localized Surface Plasmon Resonance Mode of Cu_7S_4 Nanodisks by Plasmon Coupling

Plasmon properties such as peak position, extinction cross-section, and local electric field intensity, are strongly dependent on excited, localized surface plasmon resonance (LSPR) modes. In non-spherical copper chalcogenide nanoparticles, assignment of the LSPR peaks to the corresponding oscillation modes has been controversial and requires experimental verification. We determined the transversal LSPR mode of roxbyite Cu_7S_4 nanodisks from the plasmon coupling effect of nanodisks in solution. Compared with individual Cu_7S_4 nanodisks, self-assembled Cu_7S_4 nanodisk arrays in chloroform exhibited a blue-shifted LSPR peak with weaker optical density. This strongly suggests that the singular LSPR peak in the near-infrared region mainly originates from the in-plane oscillation mode. In addition, we demonstrate that the same LSPR peak can be readily tuned by controlling the number of disks in the array.

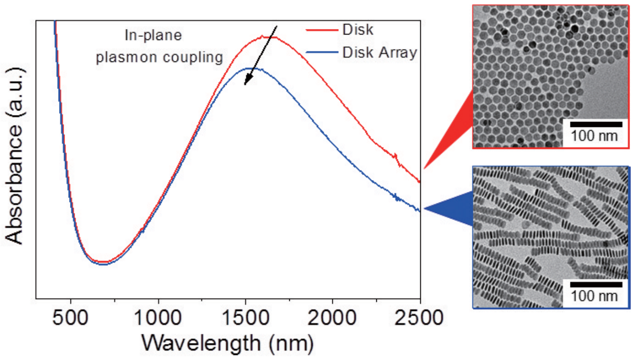


Figure 2. Spectral shift through the formation of Cu_7S_4 nanodisk array.

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)

Program-Specific Assist Prof
ISHIGE, Ryohei
(D Eng)

PD
BAEK, Sung Chul
(Ph D)

Researchers(pt)

HSU, Shu-Yao
HUANG, Yun (D Eng)
KAGATA, Hideki (D Environmental Earth Sc)
KAWANO, Yuko
KONISHI, Kyoko
MORIKI, Yoshito
NAKAMICHI, Kimiyo
SAKAUE, Motokazu
SEO, Haruna

Students

NAKANISHI, Yohei (D3)
YAHATA, Yoshikazu (D2)
AKIMOTO, Shuhei (M2)
KINOSE, Yuji (M2)
SHIKURI, Ryuji (M2)
TAKAHASHI, Kenichi (M2)
NOGAMI, Naotsugu (M1)
MASUDA, Shota (M1)
WADA, Ryota (M1)
ZHAO, Chenzhou (RS)
ISHIBASHI, Daigo (UG)
EGI, Kohki (UG)
YAMASHITA, Kohei (UG)

Guest Research Associates

EJAZ, Muhammad (D Eng)	Tulane University, U.S.A., 10 July–9 September
IOCOZZIA, James Arthur	Georgia Institute of Technology, U.S.A., 17 June–19 August

Scope of Research

Kinetic and mechanistic analyses are made for better understandings of the chemical and physicochemical reactions occurring in polymerization systems and for better routes to the synthesis of well-defined polymers. By various polymerization techniques, in particular, living polymerizations, new well-defined polymers or polymer assemblies are prepared, 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. (3) Synthesis, properties, and applications of concentrated polymer brushes (CPB).

KEYWORDS

Precision Polymerization
Hybrid Materials
Living Radical Polymerization
Biointerface
Polymer Brush

Selected Publications

Tsujii, Y.; Nomura, Y.; Okayasu, K.; Gao, W.; Ohno, K.; Fukuda, T., AFM Studies on Microtribology of Concentrated Polymer Brushes in Solvents, *J. Phys.: Conf. Ser.*, **184,** no. 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).

Controlled Synthesis of High-molecular-weight Triblock Copolymers and Their Gel Formation in Ionic Liquid

Well-defined and high-molecular-weight triblock copolymers containing poly(styrene) (PS) and poly(methyl methacrylate) (PMMA) as A- and B-segments, respectively, were prepared by atom transfer radical polymerization techniques using a bi-functional initiator under a high pressure and/or in an ionic-liquid solvent. The optimization of polymerization conditions enabled us to achieve a block efficiency higher than 90% and a total molecular weight over one million. The tirblock copolymer efficiently gelled an ionic liquid, *N,N*-diethyl-*N*-methyl-*N*-(2-methoxyethyl) ammonium bis(trifluoromethanesulfonyl)imide (DEME-TFSI), which is a good solvent for PMMA but a non-solvent for PS, even at a concentration as low as 0.5 wt% simply by casting using volatile solvent. Thus obtained gels were rheologically and electrochemically characterized, demonstrating a conductivity as high as 0.1 mS/cm at a polymer concentration of 10 wt %. The structure of cross-linking point, as was expected to be a microphase-separated domain of PS, was dependent especially on the molecular weight of PS block. The figure compares two samples with almost the same molecular weight of PMMA but different molecular weights of PS. Interestingly, the sample of higher molecular weight PS gave a blue color, that is a kind of structural colors. The SAXS measurement estimated the size and its distribution of PS domain to be 21.4 nm in R_0 and 1.7 in standard deviation. The correlation between PS domains is still under investigation.

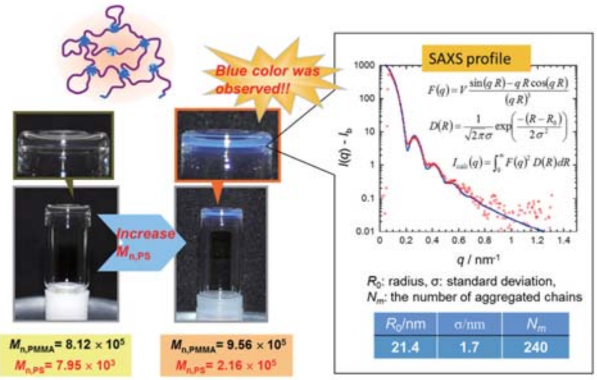


Figure 1. Gellation of ionic liquid by ABA-triblock copolymers and SAXS profile determining the structure of crosslinking PS-domain.

Design of Diblock Copolymer Dispersants for Cellulose Nanofiber Reinforced Resin Nanocomposite Materials

Among mechanically strong and lightweight materials, cellulose nanofibers (CNFs) have a range of promising properties leading to fiber-reinforced thermoplastic composites. Owing to the hydrophilic nature on surface, CNFs can only be stable in the form of aqueous suspensions and are compatible with hydrophilic resins, so that the development of CNF-reinforced hydrophobic matrices such as polyolefin is most challenging. One of promising strategies is the modification of CNF surface to make it hydrophobic. We have successfully fabricated CNF-reinforced nanocomposite materials of high-density polyethylene (HDPE) using a diblock copolymer as a dispersant, which relies on the multiple and concerted interaction via strong hydrogen bonding between a cellulose-interactive segment of the block copolymer and CNF surface (Figure 2a). In fact, simple addition of a designed block copolymer resulted in much reduced aggregation of CNFs in HDPE matrices (Figure 2b) and hence significant increase in Young's modulus (over twice) and tensile strength (about 1.5 times) (Figure 2c). This study represents a potential approach to mediate CNF-CNF and CNF-resin interactions and to significantly improve the dispersibility of CNF without chemical functionalization, which can be a low-cost and environmentally green process especially suitable for an industrial application.

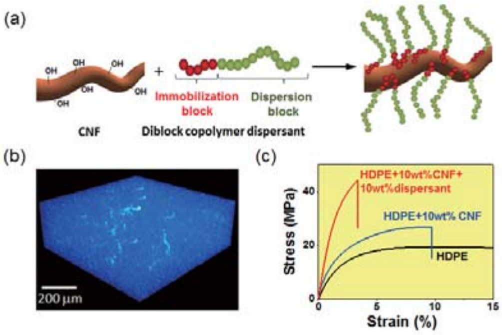


Figure 2. (a) Schematic illustration of adsorption of polymer dispersant onto cellulose nanofiber (CNF). (b) Reconstructed 3D X-ray CT image of CNF-reinforced HDPE nanocomposite with dispersant. (c) Representative stress-strain curves.

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)

Students

FUJITA, Takehiro (D3)
LU, Yangtian (D1)
FUJII, Akira (M2)
NOGUCHI, Naoki (M2)
MAEDA, Yuuki (M2)
YAMAZOE, Ryota (M2)
OHNISHI, Hiroaki (M1)
OGIHARA, Tasuku (M1)
KONO, Taro (M1)
FAN, Weijia (M1)
QU, Rui (M1)
HUA, Shen Zhiren (RS)
OSUKA, Kyoko (UG)
MIYOSHI, Syunichiro (UG)
YAMAMOTO, Yuuki (UG)

Guest Research Associates

AROUA, Safwan	Eidgenössische Technische Hochschule Zürich, Switzerland, 16 September–15 October
GROS, Alice Yukiko	Ecole Centrale de Nantes, France, 30 October–25 November

Scope of Research

Our research focuses on creation of new organic molecules which would become 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. One such topic is the development of new living radical polymerization method utilizing heavier heteroatom compounds as controlling agents. The other topic is the synthesis of cycloparaphenylenes, hoop-shaped π-conjugated molecules, based on new synthetic strategy. We also study various polymer condensed states by both static and dynamic methods to understand the relation of physical properties and structures.

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

Selected Publications

Iwamoto, T.; Kayahara, E.; Yasuda, N.; Suzuki, T.; Yamago, S., “Synthesis, Characterization, and Properties of [4]Cyclo-2,7-pyrenylene: Effect of Cyclic Structure on the Electronic Properties of Pyrene Oligomers”, *Angew. Chem. Int. Ed.*, **53,** 6430-6434 (2014).

Kayahara, E.; Patel, V. K.; Yamago, S., “Synthesis and Characterization of [5]Cycloparaphenylene”, *J. Am. Chem. Soc.*, **136,** 2284-2287 (2014).

Nakamura, Y.; Arima, T.; Yamago, S., “Modular Synthesis of Mid-Chain Functionalized Polymers by Photoinduced Diene- and Styrene-Assisted Radical Coupling Reaction of Polymer-End Radicals”, *Macromolecules*, **47,** 582-588 (2014).

Nakamura, Y.; Nakanishi, K.; Yamago, S.; Tsujii, Y.; Takahashi, K.; Morinaga, T.; Sato, T., “Controlled Polymerization of a Protic Ionic Liquid Monomer by ARGET ATRP and TERP”, *Macromol. Rapid Commun.*, **35,** 642-648 (2014).

Kayahara, E.; Iwamoto, T.; Takaya, H.; Suzuki, T.; Fujitsuka, M.; Majima, T.; Yasuda, N.; Matsuyama, N.; Seki, S.; Yamago, S., Synthesis and Physical Properties of a Ball-like Three-dimensional π-conjugated Molecule, *Nature Commun.*, **4,** 2694 (2013).

Synthesis and Characterization of [5]Cycloparaphenylene

Considerable interest has recently been focused on hoop-shaped π-conjugated molecules because of their great potential in molecular electronics. In particular, cycloparaphenylenes (CPPs) which consist of phenylene units that are para-linked in a cyclic manner, have attracted increasing attention in this area for not only their aesthetic structure having radially extended unique π orbitals originating from the curvature but also their applications in electronic and optoelectronic materials. However, the synthesis of CPPs has been a significant challenge because of the difficulty in constructing the highly strained cyclic structure. We achieved the synthesis of highly strained [5]CPP, a structural unit of the periphery of C_{60} and the shortest possible structural constituent of the sidewall of a (5,5) carbon nanotube, in nine steps in 17% overall yield. The synthesis relied on metal-mediated ring closure of a triethylsilyl (TES)-protected masked precursor followed by removal of the TES groups and subsequent reductive aromatization. UV−vis and electrochemical studies revealed that the HOMO−LUMO gap of [5]CPP is narrow and is comparable to that of C_{60}, as predicted by theoretical calculations. The results suggest that [5]CPP should be an excellent lead compound for molecular electronics.

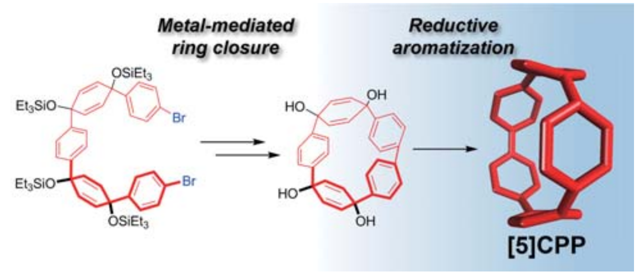


Figure 1. Synthesis of [5]CPP.

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 polymer-end 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.

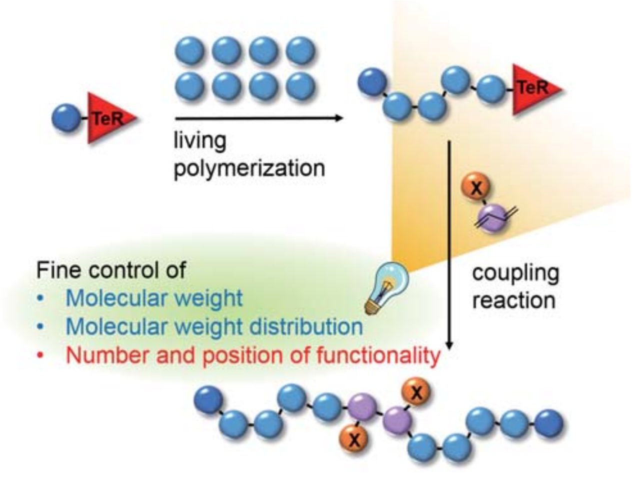


Figure 2. Novel synthetic strategy for mid-chain-functionalized polymers.

Division of Materials Chemistry
– Inorganic Photonics Materials –

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


Assoc Prof
TOKUDA, Yomei
(D Eng)


Assist Prof
MASAI, Hirokazu
(D Eng)

Students

OKUMURA, Shun (M2)
MATSUKI, Hiroaki (M2)
TOKUNAGA, Yuta (M2)
TAKAHASHI, Yuya (M1)
UEDA, Yuki (M1)
USUI, Takaaki (M1)
NORIKAWA, Yutaro (UG)

Scope of Research

In the laboratory, the main subject is to create novel functional amorphous materials such as organic-inorganic hybrids, polycrystalline and amorphous inorganic oxides. For obtaining such materials, the amorphous structure and the property 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 proton conducting membrane, optical biosensor, and amorphous phosphor.

KEYWORDS
Glass
Photonics
Remediation
Organic-inorganic Hybrid

Selected Publications

Minami, T.; Tokuda, Y.; Masai, H.; Ueda, Y.; Ono, Y.; Fujimura, S.; Yoko, T., Structural Analysis of Alkali Cations in Mixed Alkali Silicate Glasses by 23Na and 133Cs MAS NMR", *J. Asian Ceram. Soc*., doi:10.1016/j.jascer.2014.07.001 (2014).

Ueda, Y.; Tokuda, Y.; Goto, H.; Kobayashi, T.; Ono Y., Removal of Radioactive Cs from Nonwoven Cloth with Less Waste Solution Using Aqueous Sodium Metasilicate, *J. Soc. Remed. Radioact. Contam. Environ*., **1,** 191-195 (2013).

Masai, H.; Takahashi, Y.; Fujiwara, T.; Matsumoto, S.; Yoko, T., High Photoluminescent Property of Low-Melting Sn-Doped Phosphate Glass, *Applied Physics Express*, **3,** [082102-1]-[082102-3] (2010).

Masai, H.; Fujiwara, T.; Matsumoto, S.; Takahashi, Y.; Iwasaki, K.; Tokuda, Y.; Yoko, T., White Light Emission of Mn-Doped SnO-ZnO-P_2O_5 Glass Containing No Rare Earth Cation., *Optics Letters*, **36,** 2868-2870 (2011).

Masai, H.; Yamada, Y.; Suzuki, Y.; Tearamura, K.; Kanemitsu, Y.; Yoko, T., Narrow Energy Gap between Triplet and Singlet Excited States of Sn^{2+} in Borate Glass, *Scientific Reports*, **3,** 3541 (2013).

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 originates 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, electrodynamic, and other factors.

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) NMR studies. The results were also supported by the 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 mechanism underlying the MAE, analyses of the local structure of both alkali ions are required.

Here, we report the structural analysis of Na^+ and Cs^+ in sodium cesium silicate glasses by using ^{23}Na and ^{133}Cs magic-angle spinning nuclear magnetic resonance (MAS NMR) spectroscopy. In the NMR spectra of cesium silicate crystals, the peak position shifted to 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, 1.0; $x+y = 1$) glass reveal that the average coordination number of both the alkali cations decreases with 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 of the mixed alkali effect.

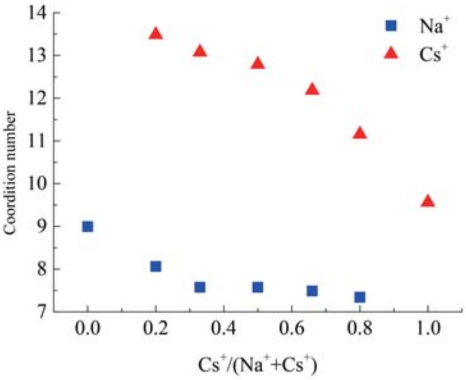


Figure 1. Average coordination number of Na^+, Cs^+ in xNa_2O-yCs_2O-$2SiO_2$ glasses ($x = 1.0, 0.8, 0.66, 0.5, 0.33, 0.2$; $x+y = 1$).

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 bring a random network that allows diversity in local structure. The diversity is the origin of various functionalities of inorganic glass.

Phosphate glass is one of important oxide glass materials and P_2O_5 is generally classified into a network former (NWF) group from the viewpoint of glass forming ability. However, P_2O_5 is indeed different from other NWF oxides, such as SiO_2, and B_2O_3, because of P=O bond, which allows to take non-bridging ortho- or pyro-phosphate units by delocalized electrons. Although it is predicted that the connectivity of PO_4 units in the glasses have strong influence on the network formation (in other words, the chemical composition of the glass), there is no universal understanding of atomistic and electronic structure in phosphate glasses even for simple binary phosphate glasses due to the lack of detailed information on the behavior of P=O bond.

Recently, we have examined the 3-dimentional (3D) atomistic and electronic structures in a combination with synchrotron X-ray total scattering, Extended X-ray Absorption Fine Structure (EXAFS), and solid state NMR. Furthermore, we construct 3-D structure model by reverse Monte Carlo (RMC)-modelling method on the basis of total scattering and XAFS data, and try to understand not only atomic ordering in the glasses. It has found that the ZnOx network is formed instead of phosphate chains with increasing ZnO amount in binary ZnO-P_2O_5 glass (Figure 2). (This work has done by collaboration with Dr. S. Kohara, Spring-8).

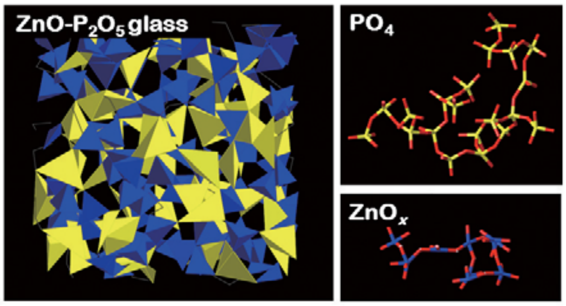


Figure 2. 3D modeling of a ZnO-P_2O_5 glass obtained by RMC modelling. (blue pyramid: PO_4 tetrahedron, yellow pyramid: ZnO_x tetrahedron). The connectivity of PO_4 and ZnO_x tetrahedra in the ZnO-P_2O_5 glass is also shown.

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
(Ph D)


Techn Staff *
KUSUDA, Toshiyuki


PD
UEDA, Kohei
(D Sc)

* Re-employed Staff


PD
KIM, Sanghoon
(Ph D)

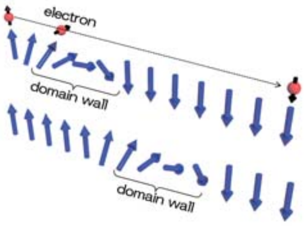
Students

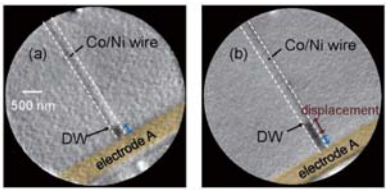
NISHIHARA, Yoshitaka (D3)
HIRAMATSU, Ryo (D3)
NAGATA, Masaki (D3)
HATA, Hiroshi (D3)
KAWAGUCHI, Masashi (D2)
YOSHIMURA, Yoko (D2)
KAKIZAKAI, Haruka (D1)
YAMADA, Kihiro (D1)
TANAKA, Kensho (M2)
TANIGUCHI, Takuya (M2)
KAMIYA, Michinari (M2)
MATSUZAKI, Noriko (M1)
MIZUNO, Hayato (M1)
TONO, Takayuki (M1)

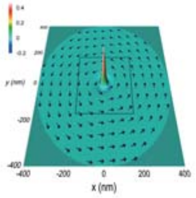
Scope of Research

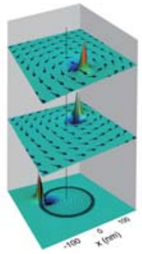
The conventional electronics utilizes only the “charge” of electrons, while the traditional magnetic devices use only “spin” degree of freedom of electrons. Aiming at the complete control of both charge and spin in single solid-state devices, an emerging field called *spintronics* is rapidly developing and impacting 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

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).

Yamauchi, Y.; Sekiguchi, K.; Chida, K.; Arakawa, T.; Nakamura, S.; Kobayashi, K.; Ono, T.; Fujii, T.; Sakano, R., Evolution of the Kondo Effect in a Quantum Dot Probed by Shot Noise, *Phys. Rev. Lett.*, **106,** [176601-1]-[176601-4] (2011).

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).

Tanabe, K.; Chiba, D.; Ohe, J.; Kasai, S.; Kohno, H.; Barnes, S. E.; Maekawa, S.; Kobayashi, K.; Ono, T., Spin-motive Force Due to a Gyrating Magnetic Vortex, *Nature Communications*, **3,** 845 (2012).

Im, M-Y.; Fischer, P.; Yamada, K.; Sato, T.; Kasai, S.; Nakatani, Y.; Ono, T., Symmetry Breaking in the Formation of Magnetic Vortex States in a Permalloy Nanodisk, *Nature Communications*, **3,** 983-988 (2012).

Koyama, T.; Ueda, K.; Kim, K.-J.; Yoshimura, Y.; Chiba, D.; Yamada, K.; Jamet, J.-P.; Mougin, A.; Thiaville, A.; Mizukami, S.; Fukami, S.; Ishiwata, N.; Nakatani, Y.; Kohno, H.; Kobayashi, K.; Ono, T., Current-induced Magnetic Domain Wall Motion Below Intrinsic Threshold Triggered by Walker Breakdown, *Nature Nanotechnology*, **7,** 635 (2012).

Kim, K.-J.; Hiramatsu, R.; Koyama, T.; Ueda, K.; Yoshimura, Y.; Chiba, D.; Kobayashi, K.; Nakatani, Y.; Fukami, S.; Yamanouchi, M.; Ohno, H.; Kohno, H.; Tatara, G.; Ono, T., Two-barrier Stability That Allows Low-power Operation in Current-induced Domain-wall Motion, *Nature Communications*, **4,** 2011 (2013).

Two-barrier Stability That Allows Low Power Operation in Current-induced Domain Wall Motion

Energy barriers appear in diverse systems and its determination has long been a debatable issue because it determines the thermal stability of devices as well as the threshold force triggering their dynamics. In general, there is a severe dilemma between the thermal stability of bit data and the operation power of devices, because larger energy barrier for higher thermal stability inevitably leads to larger magnetic field (or current) for operation. Here we show that this is not the case for the current-induced magnetic domain wall motion induced by the adiabatic spin transfer torque. By quantifying domain wall depinning energy barriers by magnetic field and current, we have found that there exist two different pinning barriers, extrinsic and intrinsic energy barriers, which govern the thermal stability and threshold current, respectively. This unique two-barrier system allows the low power operation with high thermal stability, which is impossible in conventional single-barrier systems.

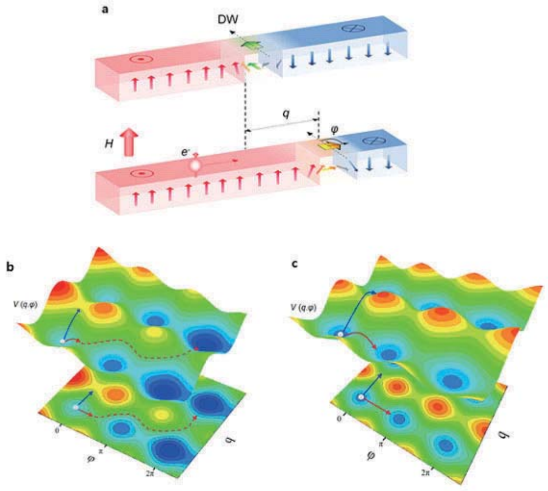


Figure 1. Schematic illustration of DW motion and energy landscape. (a) A magnetic DW in a nanowire and its collective coordinates, the position q and the tilting angle φ. (b,c) Energy landscape for the DW motion in the presence (b) and absence (c) of d.c. current.

Real-time Observation of Snell’s Law for Spin Waves in Thin Ferromagnetic Films

Magnon, a quasiparticle of the spin wave, can potentially be used for information processing and storage technology. We report the real-time observation of spin-wave propagation across a step inserted between two ferromagnetic films with different thicknesses. Because the dispersion relation of the spin wave depends on the thickness of the film, the step works as a junction to affect the spin wave propagation. When the spin wave transmits through the junction, the wavenumber undergoes modulation as per Snell’s law, which states that the refraction index is proportional to the wavenumber. From the viewpoint of “magnonics”, the present achievement opens up new possibilities of controlling the wavenumber of spin waves.

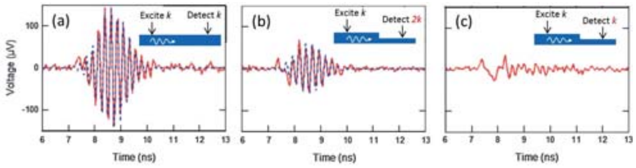


Figure 2. Time-domain wave packet transmission measurements for (a) film with no thickness difference (b) and (c) film with a thickness step at which the film thickness becomes a half. One can see the wavevector k is doubled when the wave is transmitted through the step.

Division of Biochemistry
– Biofunctional Design-Chemistry –

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

Prof
FUTAKI, Shiroh
(D Pharm Sc)

Assist Prof
IMANISHI, Miki
(D Pharm Sc)

Assist Prof
TAKEUCHI, Toshihide
(D Pharm Sc)

Students

KAWAGUCHI, Yoshimasa (D2)
OKU, Akihiko (D2)
MURAYAMA, Tomo (D1)
TSUJI, Shogo (D1)
NAKAHASHI, Takahiro (M2)
AKISHIBA, Misao (M1)
SASAKI, Yuichiro (M1)
SHINODA, Kouki (M1)
MASUDA, Toshihiro (UG)
TAKAGI, Shun (UG)
WATANABE, Kensuke (UG)

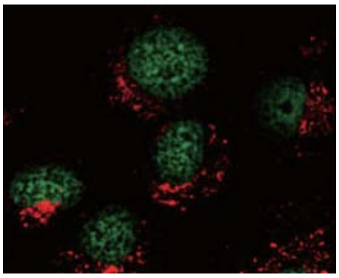
Guest Research Associate

BACKLUND, Coralie	University of Massachusetts, U.S.A., 17 June–19 August

Scope of Research

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

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



Selected Publications

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).
Nakase, I.; Osaki, K.; Tanaka, G.; Utani, A.; Futaki, S., 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, *Biochem. Biophys. Res. Commun.*, **446,** 857-862 (2014).
Takeuchi, T.; Popiel, H. A.; Futaki, S.; Wada, K.; Nagai, Y., Peptide-Based Therapeutic Approaches for Treatment of the Polyglutamine Diseases, *Curr. Med. Chem.*, **21,** 2575-2582 (2014).
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).
Nakase, I.; Tanaka, G.; Futaki, S., Cell-Penetrating Peptides (CPPs) as a Vector for the Delivery of siRNAs into Cells, *Mol Biosyst.*, **9,** 855-861 (2013).

Controlling Leucine-Zipper Partner Recognition in Cells through Modification of *a–g* Interactions

The establishment of peptides that specifically inhibit protein interactions has been one of the major challenges in chemical biology. Selection of peptides from sophisticatedly designed libraries is one of the promising approaches in order to obtain peptides that strongly bind the target proteins. We have focused on the inhibition of a protein from the human T-lymphotropic virus type I (HTLV-1) known to cause adult T-cell leukemia (ATL). ATL is a peripheral T-cell neoplasm associated with infection by HTLV-1. The viral genome encodes the HTLV-1 bZIP factor (HBZ) known to promote T-cell proliferation and systemic inflammation. HBZ has a cFos-like leucine-zipper segment, which confers interaction of HBZ with cJun and related leucine-zipper proteins. Peptides that specifically block the interaction of HBZ with Jun related proteins could be powerful tools to elucidate the role of the interaction in the onset of ATL. By focusing on the *a–g* interactions, we successfully obtained a leucine-zipper segment that discriminates the appropriate partner over another that provides very similar patterns of electrostatic interactions (Figure 1).

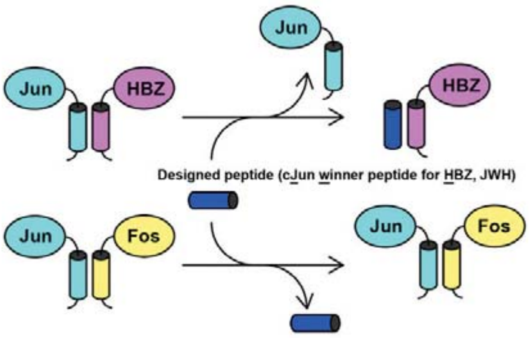


Figure 1. Designing an HBZ specific peptide without interfering with Jun–Fos recognition in cell.

Creating a TALE Protein with Unbiased 5’-T Binding

Artificial DNA binding proteins binding to desired DNA sequences are useful to control transcription of various genes and/or gene editing. So, they can be powerful tools for synthetic biology. Transcription activator-like effectors (TALEs) are sequence-specific DNA binding proteins secreted by the bacterial pathogen *Xanthomonas*. Though TALEs have the target sequence versatility determined by tandem repeats regions, almost all TALE binding sites are preceded by a highly conserved 5’ terminal T nucleotide. An N-terminal noncanonical repeat (Repeat -1) has been thought to interact specifically with the 5’-T. We performed directed evolution of the repeat to bind to non 5’-T sequences using a bacterial 1-hybrid assay (Figure 2). The selected mutants showed significantly strong DNA binding activity to the binding sites starting from non 5’-T.

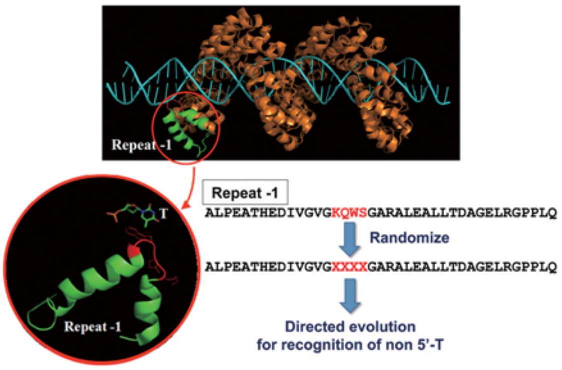


Figure2. Directed evolution of TALE repeat-1 for recognition of non 5’-T.

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

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.

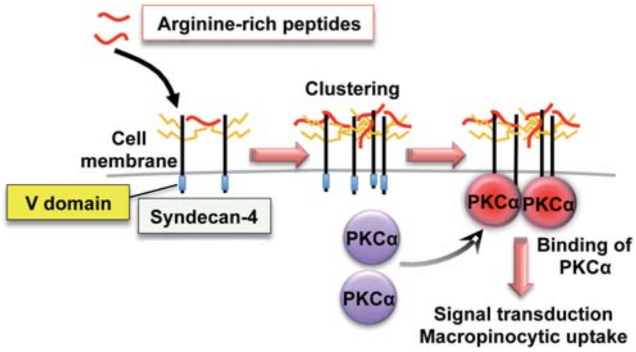


Figure 3. Schematic diagram of Syn-4 clustering and binding to PKCα inside cells induced by arginine-rich peptides.

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

OZAKI, Ayane (M2)
AKASHI, Takuya (M1)
KURODA, Kou (M1)
YIN, Ziwei (M1)
LI, Xian (RS)

Scope of Research

Our research focuses on the molecular design and synthesis of specific inhibitors of physiologically important enzymes (biocatalysts). The enzyme inhibitors are used for probing the reaction mechanisms, three-dimensional structures and identifying the physiological roles of the enzymes. The finely designed inhibitors are further elaborated to develop useful bioactive substances that could knockout the specific enzyme *in vivo* to develop lead compounds for novel pharmaceuticals, agrochemicals and cosmetic ingredients. Our current research includes the design, synthesis and applications of transition-state analogue 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 that plays a pivotal role in the biosynthesis of a vast array of phenylpropanoid 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 the physiological function of the biosynthetic enzymes in 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).

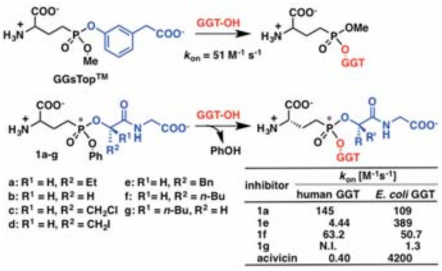
Kodan, A.; Yamaguchi, T.; Nakatsu, T.; Sakiyama, K.; Hipolito, C. J.; Fujioka, A.; Hirokane, R.; Ikeguchi, K.; Watanabe, B.; Hiratake, J.; Kimura, Y.; Suga, H.; Ueda, K.; Kato, H., Structural Basis for Gating Mechanisms of a Eukaryotic P-Glycoprotein Homolog, Proc. *Natl. Acad. Sci. U.S.A*., **111,**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

Topics

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 cellular defense system. γ-Glutamyltranspeptidase (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 phosphonate-based mechanism-based inhibitor, GGsTop^{TM}, 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).



inhibitor	k_{on} [M^{-1}s^{-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^{TM} and peptidyl phosphonate inhibitors **1a**-**g**.

Interestingly, GGsTop^{TM}, a highly efficient inhibitor of human GGT, induces 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^{TM} to serve as a novel active ingredient for anti-ageing cosmetics. This compound are now marketed under a trade name of "Nahlsgen®" and has attracted significant interests from the cosmetic market.

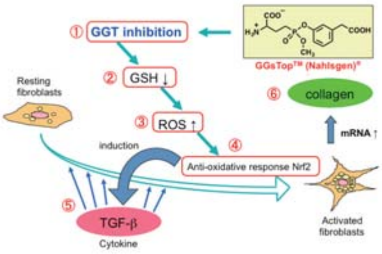
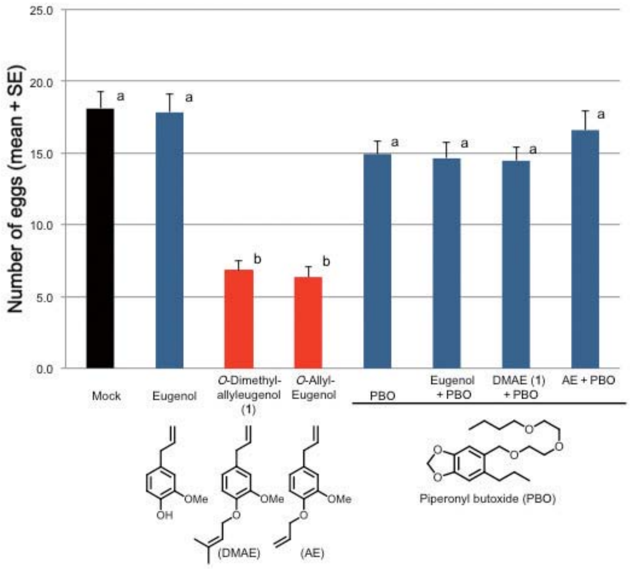


Figure 2. Mechanism for activation of human fibroblasts by GGT inhibitor, GGsTop^{TM}.

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, anti-oxidative and anti-tumor activities. Eugenol and its derivatives such as estragole, *O*-methyleugenol, 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 amount in leaves of Japanese star anise (*Illicium anisatum*) and exhibits unique activity of suppression of oviposition of mites, whereas its parent compound eugenol does not. We therefore are interested in the mode of action of DMAE and performed structure-activity relationship studies.

O-alkyled eugenol such as estragole, methyleugenol and safrole did not show any oviposition suppression activity at 2 mM, whereas *O*-allyl-based alkenyl derivatives include DMAE solely 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 and the formation of *p*-quinone methide is inferred as an active entity.



Division of Biochemistry
– Molecular Biology –

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

Prof
AOYAMA, Takashi
(D Sc)

Assoc Prof
TSUGE, Tomohiko
(D Sc)

Assist Prof
FUJIWARA-KATO, Mariko
(D Agr)

Techn Staff
YASUDA, Keiko

Students

NAKAI, Hideto (RF)
GOTO, Kakeru (D1)
ZHANG, Xiao-Juan (D1)
SAITO, Ryo (M2)
SHIMAMURA, Ryota (M2)
WATARI, Machiko (M1)

Guest Research Associate

LIN, Qing	Peking University, China, P.R., 25 September 2014–18 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 phospholipid signalings in cell morphogenesis, the transcriptional network for cytokinin responses, COP9 signalosome modulating signal transduction in the nuclei, and the endoreduplication cell cycle in cell differentiation.

KEYWORDS

Morphogenesis
Signal Transduction
Phospholipid
COP9 Signalosome
Cytokinin

Selected Publications

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

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

Lin, Q.; Aoyama, T., Pathways for Epidermal Cell Differentiation *via* the Homeobox Gene *GLABLA2*: Update on the Roles of the Classic Regulator, *J. Integr. Plant Biol.*, **54,** 729-737 (2012).

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).

Taniguchi, Y. Y.; Taniguchi, M.; Tsuge, T.; Oka, A.; Aoyama, T., Involvement of *Arabidopsis thaliana* Phospholipase Dζ2 in Root Hydrotropism through the Suppression of Root Gravitropism, *Planta*, **231,** 491-497 (2010).

Phosphatidylinositol Phosphate 5-Kinase Genes Mediate a Phosphate-Deficiency Signal to Root Hair Elongation in *Arabidopsis thaliana*

Root system architecture is highly plastic and responsive to the surrounding growth conditions, ensuring that plants adapt to variegated underground environments. Soil phosphate (Pi) deficiency is a challenging growth condition that land-based plants encounter frequently. To cope with this difficulty, plants drastically alter their root system architecture by modifying the length and branching patterns of roots, and the length and density of root hairs, as well as their metabolic state throughout the whole plant. During Pi deficiency, most accessions of *Arabidopsis thaliana* suppress primary root growth *via* root apical meristem (RAM) exhaustion and impaired root cell elongation and enhance lateral root development, resulting in a short and bushy root system. These macro-scale responses in root system architecture enable exploration of the upper soil layers, where Pi tends to accumulate. In addition, in the micro-scale architecture of roots, Pi deficiency remarkably enhances root hair development and elongation for effective Pi absorption from soil (Figure 1).

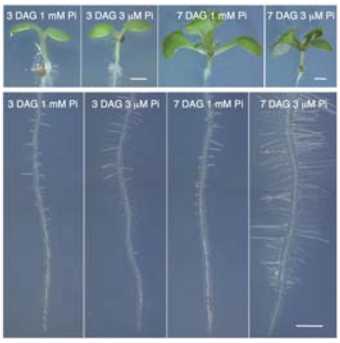


Figure 1. Wild-type seedlings grown for 3 and 7 days after germination (DAG) under the Pi-sufficient and deficient conditions.
Areal parts (upper row), and roots (lower row) of 3- and 7-DAG wild-type seedlings grown under the 1 mM and 3 μM Pi conditions are shown. Bar = 1 mm (upper row), and 0.5 mm (lower row).

To elucidate the regulatory pathways specific to the root hair elongation response to Pi deficiency, we investigated the expression of type-B phosphatidylinositol phosphate 5-kinase (*PIP5K*) genes, as putative regulators of root hair elongation in *Arabidopsis*. Of the nine *Arabidopsis* B-type *PIP5K* genes, the *PIP5K3* and *PIP5K4* genes responded to Pi deficiency in steady-state transcript levels *via* PHR1-binding sequences (P1BSs) in their upstream regions at young seedling stages. Both *pip5k3* and *pip5k4* single mutants, which exhibit short-root-hair phenotypes, remained responsive to Pi deficiency for root hair elongation. However, the *pip5k3pip5k4* double mutant exhibited shorter root hairs than the single mutants, and lost responsiveness to Pi deficiency at young seedling stages. In the tactical complementation line in which modified *PIP5K3* and *PIP5K4* genes with base substitutions in their P1BSs were co-introduced into the double mutant, root hairs of young seedlings had normal lengths under Pi-sufficient conditions, but were not responsive to Pi deficiency. From these results, we conclude that *PIP5K* genes connect a Pi-deficiency signal to the regulatory pathway for root hair elongation *via* their P1BSs.

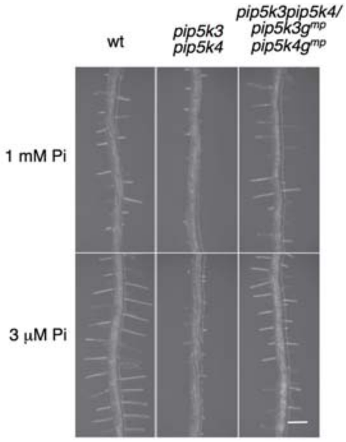


Figure 2. Root hair of 3-DAG wild-type, *pip5k3pip5k4* double mutant, and its tactical complementation seedlings grown under Pi-sufficient and deficient conditions.
Roots of 3-DAG seedlings of the indicated lines grown under the 1 mM and 3 μM Pi conditions are shown. Bar = 0.2 mm.

Interestingly, the P1BS and sequences similar to the root hair cell-specific *cis*-element (RHE) in the *PIP5K3* upstream intergenic region are conserved in *Brassicaceae*, the family to which *Arabidopsis* belongs. It has been proposed that *Brassicaceae* plants take advantage of rapid root growth and root hair formation rather than mycorrhizal symbiosis as a strategy for nutrition uptake. *PIP5K3* might play a crucial role in enhancing the root hair elongation response to Pi deficiency in *Brassicaceae*, especially at young seedling stages, when macro-scale architectures of the root system are still immature.

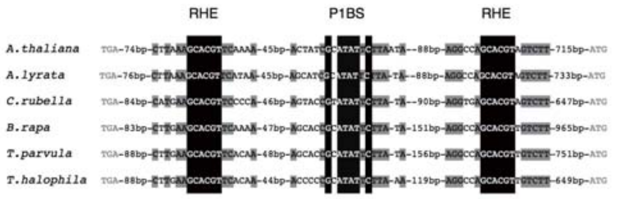


Figure 3. Conserved cis-elements in the upstream intergenic regions of *Brassicaceae PIP5K3* orthologs.
Upstream intergenic sequences of *Arabidopsis thliana*, *Arabidopsis lyrata*, *Capsella rubella*, *Brassica rapa*, *Thellungiella parvula*, and *Thellungiella halophila* are aligned. Conserved nucleotides and *cis*-elements (RHE: 5'-GCACGT-3' and P1BS: 5'-GNATATNC-3') are marked in grey and black, respectively.

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)


Assist Prof
WATANABE, Mizuki
(D Pharm Sc)


Program-Specific Senior Lect
PERRON, Amelie
(Ph D)


Proj Res*
SATO, Shinichi
(D Eng)


Proj Res**
KATSUDA, Yousuke
(D Sc)


Proj Res**
TAKENOYA, Mihoko
(D Eng)


Guest Res Assoc
PARVATKAR, Prakash Tukaram
(Ph D)

Researchers

IWATA, Jun***
FURUTA, Tomoyuki***

Researchers(pt)

WATANABE, Haruhi
QIN, Ying***

* Assist Prof of iCeMS
** PD of iCeMS
*** iCeMS

Assist Techn Staff

FRISCO, Heidie Laya***

Assist Res Staff

NAKASHIMA, Mitsue***

Students

MAO, Di (D3)
TAKAYA, Junichiro (D3)
ASANO, Risa (D1)
LIAO, Youqi (D1)
MBENZA, Mbambi Naasson (M1)
CHUNG, Watson Xie Khim (RS)
PUNZALAN, Louvy Lynn (RS)
ITO, Megumi (RS)

Scope of Research

KEYWORDS
Cell Therapy
Chemical Biology
Small Molecules
Chemical Library
Chemical Genetics

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 by 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 activity permits small-molecule initiated exploration of complex cellular events. Our mission is to create a new world of bioactive synthetic molecules: their new way to use, their new shapes, and their 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.

Selected Publications

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.*, accepted (in press).

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).

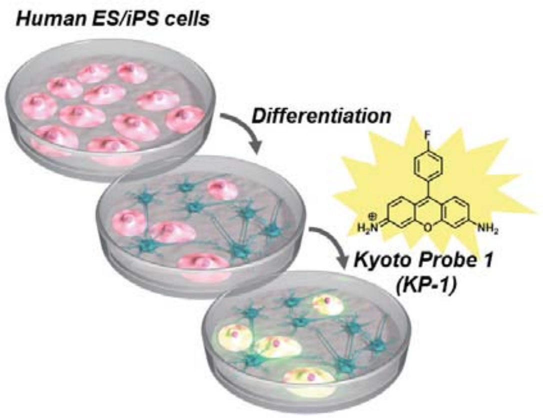
Hirata, N.; Nakagawa, M.; Fujibayashi, Y.; Yamauchi, K.; Murata, A.; Minami, I.; Tomioka, M.; Kondo, T.; Kuo, T. F.; Endo, H.; Inoue, H.; Sato, S.; Ando, S.; Kawazoe, Y.; Aiba, K.; Nagata, K.; Kawase, E.; Chang, Y. T.; Suemori, H.; Eto, K.; Nakauchi, H.; Yamanaka, S.; Nakatsuji, N.; Ueda, K.; Uesugi, M., A Chemical Probe That Labels Human Pluripotent Stem Cells, *Cell Reports*, **6,** 1165-1174 (2014).

Sakano, D.; Shiraki, N.; Kikawa, K.; Yamazoe, T.; Kataoka, M.; Umeda, K.; Araki, K.; Mao, D.; Matsumoto, S.; Nakagata, N.; Andersson, O.; Stainier, D.; Endo, F.; Kume, K.; Uesugi, M.; Kume, S., VMAT2 Identified as a Regulator of Late-stage β Cell Differentiation, *Nat. Chem. Biol.*, **10,** 141-148 (2014).

Topics

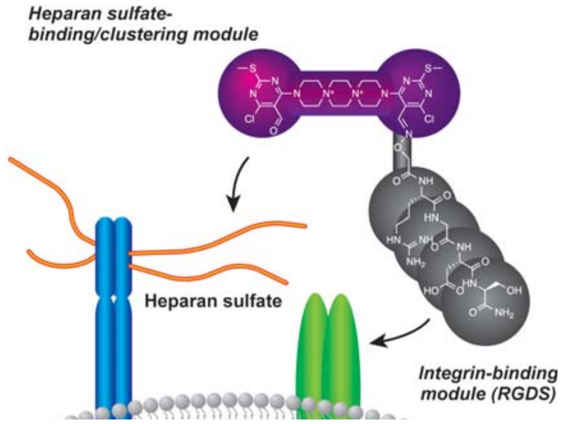
A Chemical Probe That Labels Human Pluripotent Stem Cells

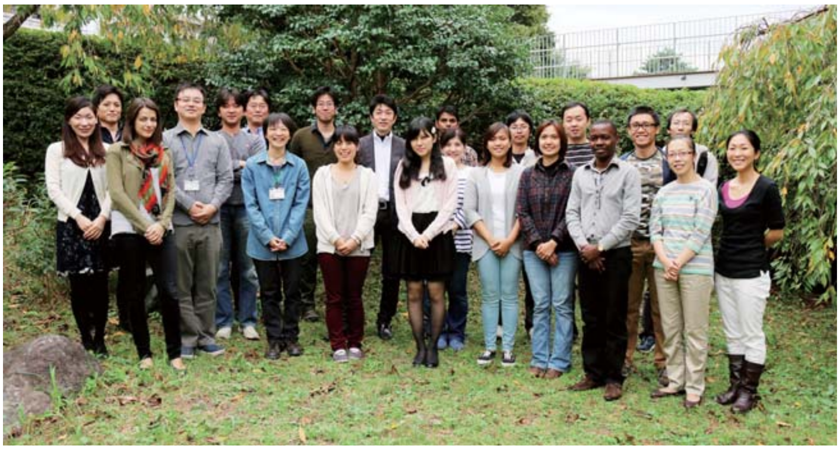
A small-molecule fluorescent probe specific for human pluripotent stem cells would serve as a useful tool for basic cell biology research and stem cell therapy. Screening of fluorescent chemical libraries with human induced pluripotent stem cells (iPSCs) and subsequent evaluation of hit molecules identified a fluorescent compound (Kyoto probe 1 [KP-1]) that selectively labels human pluripotent stem cells. Our analyses indicated that the selectivity results primarily from a distinct expression pattern of ABC transporters in human pluripotent stem cells and from the transporter selectivity of KP-1. Expression of ABCB1 (MDR1) and ABCG2 (BCRP), both of which cause the efflux of KP-1, is repressed in human pluripotent stem cells. Although KP-1, like other pluripotent markers, is not absolutely specific for pluripotent stem cells, the identified chemical probe may be used in conjunction with other reagents.



Synthetic Molecules That Protect Cells from Anoikis and Their Use in Cell Transplantation

One of the major problems encountered in cell transplantation is the low level of survival of transplanted cells due to detachment-induced apoptosis, called anoikis. The present study reports on the chemical synthesis and biological evaluation of water-soluble molecules that protect suspended cells from anoikis. The synthetic molecules bind to and induce clusters of integrins and heparan-sulfate-bound syndecans, two classes of receptors that are important for extracellular matrix-mediated cell survival. Molecular biological analysis indicates that such molecules prolong the survival of suspended NIH3T3 cells, at least in part, by promoting clustering of syndecan-4 and integrin β1 on the cell surface, leading to the activation of small GTPase Rac-1 and Akt. In vivo experiments using animal disease models demonstrated the ability of the molecules to improve cell engraftment. The cluster-inducing molecules may provide a starting point for the design of new synthetic tools for cell-based therapy.





Division of Environmental Chemistry
– Molecular Materials Chemistry –

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


Prof
KAJI, Hironori
(D Eng)


Assoc Prof
GOTO, Atsushi
(D Eng)


Assist Prof
FUKUSHIMA, Tatsuya
(D Eng)


Techn Staff
OHMINE, Kyoko


Techn Staff
MAENO, Ayaka


PD
SUZUKI, Katsuaki
(D Human&Envirnmtl. Studies)


PD
SHIZU, Katsuyuki
(D Eng)


PD
LEI, Lin
(D Eng)

Researchers

TANISHIMA, Miho
NAKAJIMA, Yuuki

Lect (pt)

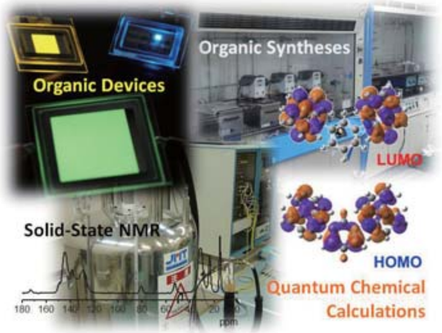
NISHIYAMA, Yusuke (D Sc)
JEOL Resonance

Students

ITO, Kyohei (M2)
KURODA, Risako(M2)
TANAKA, Fumiya (M2)
ISHIBASHI, Hirotaka (M1)
KUBO, Shosei (M1)
MIWA, Takuya (M1)
OGATA, Isamu (UG)
WADA, Yoshimasa (UG)

Scope of Research

Our research target is to develop high-performance organic electroluminescence devices, organic solar cells, and polymer materials. For the purpose, we have carried 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, detailed analyses of structures and dynamics are performed mainly by sophisticated solid-state NMR spectroscopy in order to obtain structure-dynamics-property relationships.



KEYWORDS
Solid-State NMR
Amorphous Materials
Organic Solar Cells
Organic Light-Emitting Diodes
Living Radical Polymerization

Selected Publications

Suzuki, F.; Nishiyama, Y.; Kaji, H., Clarification of Isomeric Structures and the Effect of Intermolecular Interactions in Blue-emitting Aluminum Complex Alq$_3$ Using First-principles ^{27}Al NMR Calculations, *Chemical Physics Letters*, **605-606,** 1-4 (2014).
Uejima, M.; Sato, T.; Detani, M.; Wakamiya, A.; Suzuki, F.; Suzuki, H.; Fukushima, T.; Tanaka, K.; Murata, Y.; Adachi, C.; Kaji, H., A Designed Fluorescent Anthracene Derivative: Theory, Calculation, Synthesis, and Characterization, *Chemical Physics Letters*, **602,** 80-83 (2014).
Lei, L.; Tanishima, M.; Goto, A.; Kaji, H.; Yamaguchi, Y.; Komatsu, H.; Jitsukawa, T.; Miyamoto, M., Systematic Study on Alkyl Iodide Initiators in Living Radical Polymerization with Organic Catalysts, *Macromolecules*, **47,** 6610-6618 (2014).
Lei, L.; Tanishima, M.; Goto, A.; Kaji, H., Living Radical Polymerization via Organic Superbase Catalysis, *Polymers*, **6,** 860-872 (2014).

Clarification of Isomeric Structures and the Effect of Intermolecular Interactions in Blue-emitting Aluminum Complex, Alq_3, Using First-principles ^{27}Al NMR Calculations

Tris(8-hydroxyquinoline) aluminum(III) (Alq_3) has been a widely used light-emitting and electron-transporting material in organic light-emitting diodes. Conventionally, the emission color of Alq_3 has been observed as green; however, recently, blue-emitting Alq_3 have been found. The blue-emitting Alq_3 exhibits photoluminescence quantum yield of ~50%, approximately twofold greater than that of conventional Alq_3. To understand the different luminescent properties, we have performed structure analysis on the blue-emitting Alq_3 using ^{27}Al NMR and first-principles gauge-including projector-augmented wave calculations. From the analysis, we obtained clear evidence that the difference of the luminescent properties originates from the isomeric state of Alq_3 molecules.

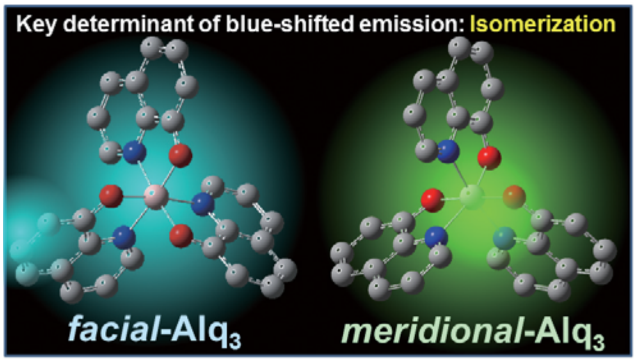


Figure 1. Emission color of Alq_3 is determined by the isomeric state.

Living Radical Polymerization via Organic Superbase Catalysis

Organic superbases reacted with alkyl iodides (R–I) to reversibly generate the corresponding alkyl radicals ($R^{\bullet}$). Via this reaction, organic superbases were utilized as new and highly efficient organic catalysts in living radical polymerization. The superbase catalysts included guanidines, aminophosphines and phosphazenes. Low-polydispersity polymers (M_w/M_n = 1.1–1.4) were obtained up to high conversions (e.g., 80%) in reasonably short times (3–12 h) at mild temperatures (60–80 °C) for methyl methacrylate, styrene and several functional methacrylates. The high polymerization rate and good monomer versatility are attractive features of these superbase catalysts.

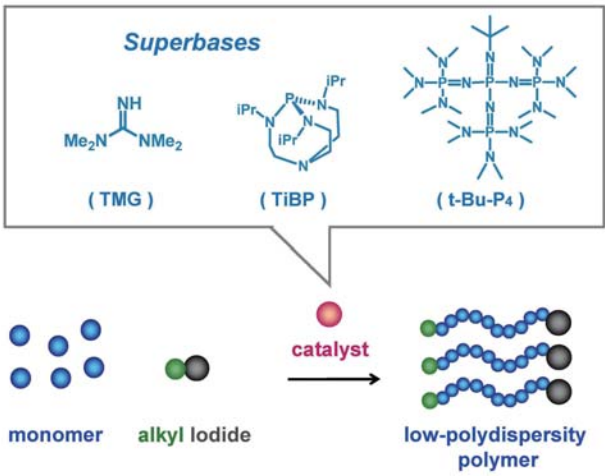
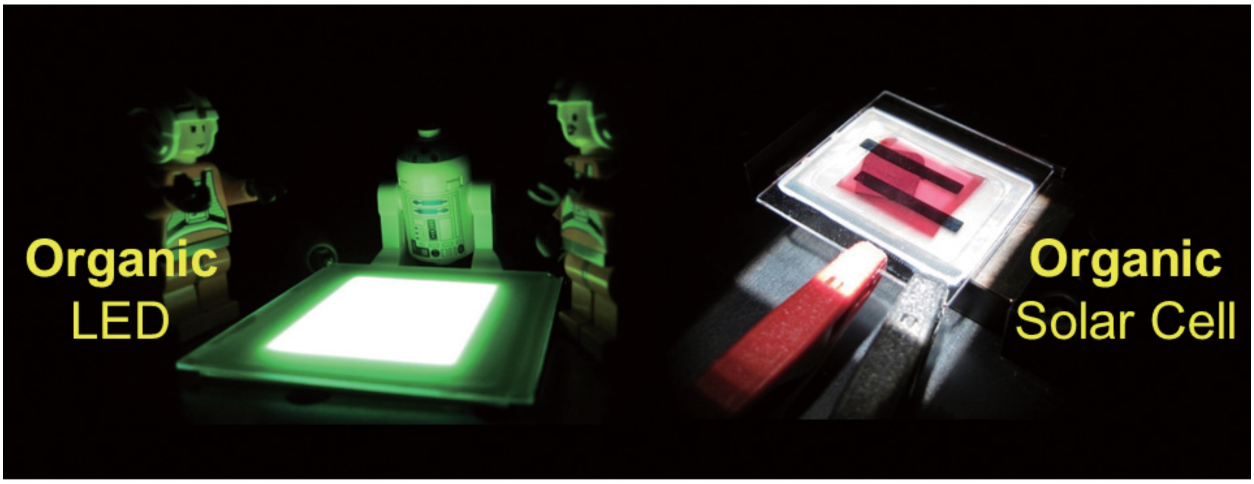


Figure 2. Living Radical Polymerization via Organic Superbase Catalysis.



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)

Techn Staff
MINAMI, Tomoharu
(D Eng)

Students

TAKANO, Shotaro (D3)
ZHENG, Linjie (M2)
MURATA, Rena (M1)
SASAKI, Masanobu (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 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

Takano, S.; Tanimizu, M.; Hirata, T.; Sohrin, Y., Isotopic Constraints on Biogeochemical Cycling of Copper in the Ocean, *Nat. Commun.*, **5,** doi:10.1038/ncomms6663 (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,** doi: 10.1038/srep01745 (2013).

Cid, A. P.; Nakatsuka, S.; Sohrin, Y., Stoichiometry among Bioactive Trace Metals in the Chukchi and Beaufort Seas, *J. Oceanogr.*, **68,** 985-1001 (2012).

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).

Biogeochemical Cycling of Copper Isotopes in the Ocean

Copper plays an important role as a micronutrient for organisms, but it is also toxic at high concentrations of the free Cu^{2+}. In the ocean, Cu is subjected to various biogeochemical processes, such as atmospheric input, biological uptake, and adsorption onto sinking particles. Precise isotopic measurement of Cu has become possible since the advent of multiple collector inductively coupled plasma mass spectrometry. To elucidate the biogeochemical cycling of Cu in the oceans, it is important to determine the profiles of Cu isotopes in the ocean, because Cu isotopes are fractionated during various biogeochemical processes. We have determined dissolved Cu concentration and the isotopic composition of seawater samples collected from the western/eastern North Pacific, the central South Indian, and the North Atlantic. The isotopic composition is reported as $\delta^{65}Cu=[(^{65}Cu/^{63}Cu)_{sample}/(^{65}Cu/^{63}Cu)_{NIST\ SRM\ 976\ standard}-1]\times10^3$. Observed $\delta^{65}Cu$ is from +0.41 to +0.48‰ in the surface seawater and becomes heavier in the depths. In the deep seawater, $\delta^{65}Cu$ ranges from +0.41 to +0.85‰ and correlates with AOU that is a measure of the age of deep seawater. We propose that $\delta^{65}Cu$ in surface seawater is a mixture of rain water, river water, and deep seawater, and $\delta^{65}Cu$ in deep seawater becomes heavier with the age of deep seawater because of preferential removal of light Cu isotopes. Also, we build a new box model for Cu in the ocean based on the combination of Cu concentration and $\delta^{65}Cu$, which successfully constrains marine biogeochemical cycling of Cu (Figure 1).

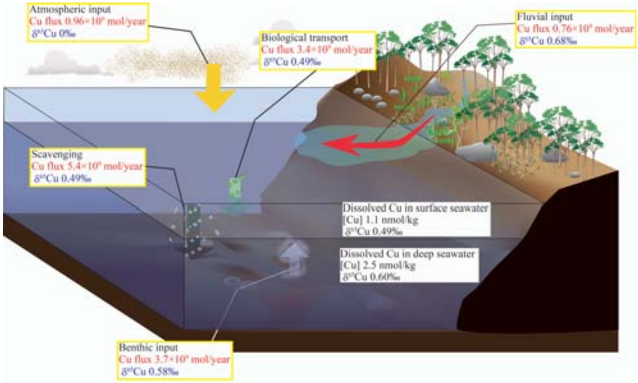


Figure 1. Box model for Cu cycling in the ocean based on both elemental concentration and isotopic ratio.

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

Trace elements and their isotopes (TEIs) in the ocean are important as tracers in oceanography, micronutrients and/or toxins in biogeochemistry, and proxies in paleoceanography. Recently, an international research program of the marine biogeochemical cycles of TEIs, referred to as GEOTRACES, was commenced to determine the distributions of key TEIs (such as Al, Mn, Fe, Cu, Zn, Cd, and Pb) and to clarify their sensitivity toward changing environmental conditions. While high-resolution inductively coupled plasma mass spectrometry (HR-ICP-MS) is a powerful technique in the multi-elemental determination of trace metals, major constituents of seawater interfere with the precise determination. A novel automated off-line preconcentration system for trace metals (Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb) in seawater was developed by improving a commercially available solid-phase extraction system SPE-100 (Hiranuma Sangyo). The utilized chelating resin was NOBIAS Chelate-PA1 (Hitachi High-Technologies) with ethylenediaminetriacetic acid and iminodiacetic acid functional groups. Parts of an 8-way valve made of alumina and zirconia in the original SPE-100 system were replaced with parts made of polychlorotrifluoroethylene in order to reduce contamination of trace metals. The eluent pass was altered for the back flush elution of trace metals. We optimized the cleaning procedures for the chelating resin column and flow lines of the preconcentration system, and developed a preconcentration procedure, which required less labor and led to a superior performance compared to manual preconcentration. The nine trace metals were simultaneously and quantitatively preconcentrated from ~120 g of seawater, eluted with ~15 g of 1 M HNO_3, and determined by HR-ICP-MS using the calibration curve method. The single-step preconcentration removed more than 99.998% of Na, K, Mg, Ca, and Sr from seawater. The procedural blanks and detection limits were lower than the lowest concentrations in seawater for Mn, Ni, Cu, and Pb, while they were as low as the lowest concentrations in seawater for Al, Fe, Co, Zn, and Cd. The accuracy and precision of this method were confirmed by the analysis of reference seawater samples and seawater samples for vertical distribution in the western North Pacific Ocean.

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

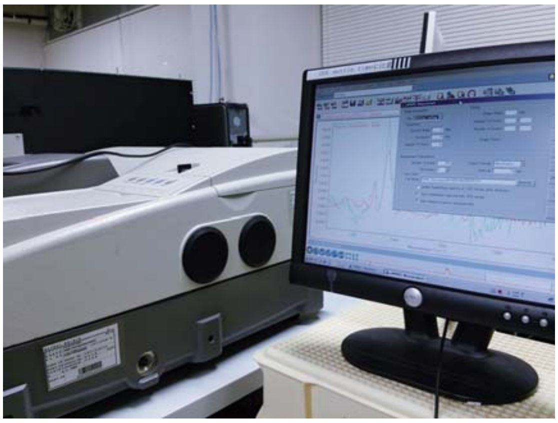
TU, Kai-min (D3)
SHIOYA, Nobutaka (M2)
TANAKA, Yuki (M2)

Scope of Research

To understand the chemical structure, property and reactions in a two-dimensional molecular aggregate, the keywords of molecular interactions and orientation are focused on, and the fluctuated molecular aggregates are investigated by using originally developed spectroscopic and theoretical techniques. The current major topics are: (1) a new chemical model accounting for bulk properties specific to perfluoroalkyl compounds; (2) analysis of molecular orientation and conformation in a thin film of organic semiconductor polymer; (3) study on a novel surface selection rule for discussing the molecular orientation in a thin film adsorbed on a rough surface.

KEYWORDS

Infrared and Raman Spectroscopy
Surface and Interface Chemistry
Perfluoroalkyl Compounds
Organic Semiconductor
Polymer Electrolyte Membrane
Nano Particle and Fibril Analysis



Selected Publications

Hasegawa, T.; Shimoaka, T.; Shioya, N.; Morita, K.; Sonoyama, M.; Takagi, T.; Kanamori, T., Stratified Dipole-Arrays Model Accounting for Bulk Properties Specific to Perfluoroalkyl Compounds, *ChemPlusChem*, **79,** 1421-1425 (2014).

Nakata, S.; Ueda, T.; Miyaji, T.; Matsuda, Y.; Katsumoto, Y.; Kitahata, H.; Shimoaka, T.; Hasegawa, T., Transient Reciprocating Motion of a Self-Propelled Object Controlled by a Molecular Layer of a *N*-Stearoyl-*p*-nitroaniline: Dependence on the Temperature of an Aqueous Phase, *J. Phys. Chem. C*, **118(27),** 14888-14893 (2014).

Shioya, N.; Shimoaka, T.; Hasegawa, T., Analysis of Molecular Orientation and Conformation of Poly(3-hexylthiophene) Thin Films on Silicon by Infrared p-Polarized Multiple-Angle Incidence Resolution Spectrometry, *Chem. Lett*., **43(8),** 1198-1200 (2014).

Morimine, S.; Norimoto, S.; Shimoaka, T.; Hasegawa, T., Surface Selection Rule of Infrared Diffuse Reflection Spectrometry for Analysis of Molecular Adsorbates on a Rough Surface of a NonAbsorbing Medium, *Anal. Chem*., **86,** 4202-4208 (2014).

Tu, K.-M.; Ishizuka, R.; Matubayasi, N., Spatial-decomposition Analysis of Electrical Conductivity in Concentrated Electrolyte Solution, *J. Chem. Phys*., **141,** [044126-1]- [044126-9] (2014).

Topics

Stratified Dipole-Arrays Model Accounting for Bulk Properties Specific to Perfluoroalkyl Compounds

Perfluoroalkyl compounds are known to exhibit a hydrophobic character on the surface of the material, although the C-F bond has a large dipole, which should make the molecular surface polar and hydrophilic. This inconsistency has long been a chemical matter to be solved. Herein, a stratified dipole-arrays model is proposed: the molecular polar surface can be fully hidden by forming a two-dimensional aggregate of perfluoroalkyl (Rf) groups; this aggregate is spontaneously induced by dipole–dipole interaction arrays owing to the helical structure of the Rf group. In this model, a ‘short’ Rf group should play the role of a single Rf group with a hydrophilic character, whereas a ‘long’ Rf group should spontaneously form a hexagonal aggregate. To examine this model, Rf-containing myristic acids with various Rf lengths have been synthesized and their aggregation properties are analyzed by using the Langmuir monolayer technique aided by precise IR spectroscopic analysis.

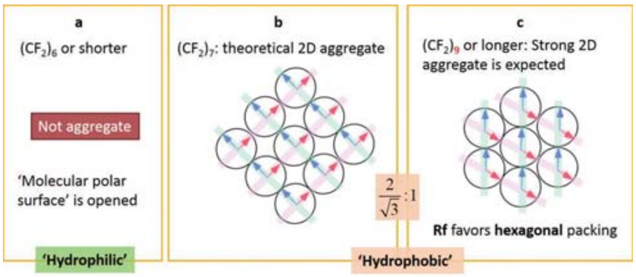


Figure 1. Top views of the 2D molecular aggregates as a function of the Rf length.

Analysis of Molecular Orientation and Conformation of Poly(3-hexylthiophene) Thin Films on Silicon by Infrared p-Polarized Multiple-angle Incidence Resolution Spectrometry

Infrared (IR) p-polarized multiple-angle incidence resolution spectrometry (p-MAIRS) has been employed for the first time to reveal the molecular orientation in two different poly(3-hexylthiophene) (P3HT) thin films having face-on and edge-on orientations. The CH out-of-plane deformation vibration mode (ca. 820 cm^{-1}) of the thiophene ring is found to be highly localized on the ring, which is quite useful for molecular orientation analysis coupled with IR p-MAIRS. On the other hand, the CH stretching vibration region is useful for determining the molecular order, conformation, and folding of the hexyl chain via MAIRS dichroism.

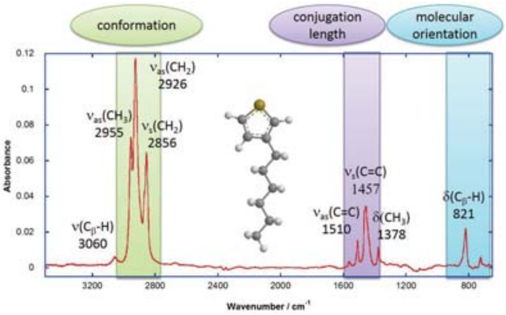


Figure 2. IR p-MAIRS spectra of a P3HT thin film deposited on a Si substrate prepared by using a chloroform.

Surface Selection Rule of Infrared Diffuse Reflection Spectrometry for Analysis of Molecular Adsorbates on a Rough Surface of a Nonabsorbing Medium

The surface selection rule (SSR) for discussing the molecular orientation in a thin film adsorbed on a rough surface is determined by analyzing a surface monolayer by defining the angle of incidence and polarizations. As the standard sample, a highly organized self-assembled monolayer (SAM) on a rough alumina surface is employed. By introducing crossed-Nicol polarizers in the incident and detection paths, the specular reflection and diffuse reflection components are readily separated. To fully understand the spectra of the SAM, a new idea is proposed that the incidental light can be excluded from the discussion when the angle of incidence is small, which is named the pseudotransmission (pd-Tr) model. Another important idea is that a part of a spectrum is degraded in the signal-to-noise ratio by the suppression of incidental light on the rough surface via a deconstructive interference, which can experimentally be revealed by the crossed-Nicol measurements of single-beam spectra depending on the angle of incidence. Through the experiments of all the combinations of polarizations and angles of incidence, the pd-Tr model and the light suppression are found to be important base to fully understand the SSR of molecular adsorbates on a rough surface of a nonabsorbing medium.

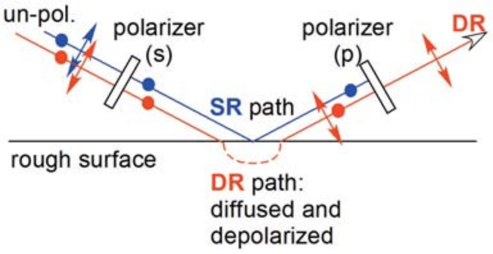


Figure 3. A schematic of the DR filter consisted of two mutually orthogonal (crossed-Nicol) polarizers. The incidental and detection angles are set to be equal to each other. The solid circle (●) and the two-direction arrow (↔) indicate the s- and p-polarizations, respectively. Only the DR component passes through the second polarizer.

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)

PD
CHO, Hyun-Nam
(D Agr)

Assist Techn Staff

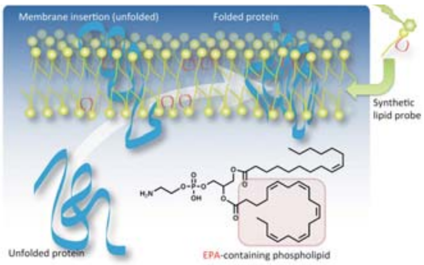
KITAYAMA, Kaori

Students

HIGA, Mariko (D2)
SUGIURA, Miwa (D2)
KAWAI, Soichiro (D1)
OHKE, Yoshie (D1)
ASAI, Azusa (M2)
IWANO, Yuriko (M2)
OHASHI, Sayaka (M2)
OGURA, Ryutaro (M2)
SUMIDA, Yukie (M2)
TOKUNAGA, Tomohisa (M2)
MARUYAMA, Saori (M2)
NINOMIYA, Takemasa (M1)
TOYOTAKE, Yosuke (M1)
CHEN, Chen (RS)

Scope of Research

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



KEYWORDS
Microbiology
Extremophiles
Long-Chain Polyunsaturated Fatty Acid
Membrane Proteins
Microbial Metal Respiration

Selected Publications

Fukuyama, S.; Mihara, H.; Miyake, R.; Ueda, M.; Esaki, N.; Kurihara, T., Characterization of a Thermostable 2,4-diaminopentanoate Dehydrogenase from *Fervidobacterium nodosum* Rt17-B1, *Journal of Bioscience and Bioengineering*, **117,** 551-556 (2014).

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,** e85045 (2014).

Imai, T.; Kurihara, T.; Esaki, N.; Mihara, H., Glutathione Contributes to the Efflux of Selenium from Hepatoma Cells, *Bioscience, Biotechnology, and Biochemistry*, **78,** 1376-1380 (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 : Journal of the Pharmaceutical Society of Japan*, **134,** 507-513 (2014).

Studies of the Microdomian Formation in Biological Membranes of an Antarctic Bacterium

A cold-adapted microorganism, *Shewanella livingstonensis* Ac10, was isolated from Antarctic seawater. This bacterium produces a kind of long-chain polyunsaturated fatty acid, eicosapentaenoic acid (EPA), which is introduced to *sn*-2 position of membrane phospholipids. By using a fluorescence-labeled phospholipid containing eicosapentaenyl group, we found that this strain forms membrane microdomain structure composed of EPA-containing phospholipids, which might regulate the function of cell division proteins at low temperatures. To analyze the mechanism of the microdomain formation, we developed monoclonal antibodies raised against EPA-biosynthesis enzymes of *S. livingstonensis* Ac10 through hybridoma technology and analyzed their subcellular localization at low temperatures by immunofluorescence staining. Orf5, a scaffold protein for EPA synthesis, was localized at the cell division site and cell pole of *S. livingstonensis* Ac10 grown at 4 ˚C. When Orf8, a putative enoyl reductase, was analyzed, we observed the same localization as Orf5. These results suggest that Orf5 and Orf8 colocalize at the cell division site and act as protein complex to contribute to the formation of EPA-containing microdomain at cell division site.

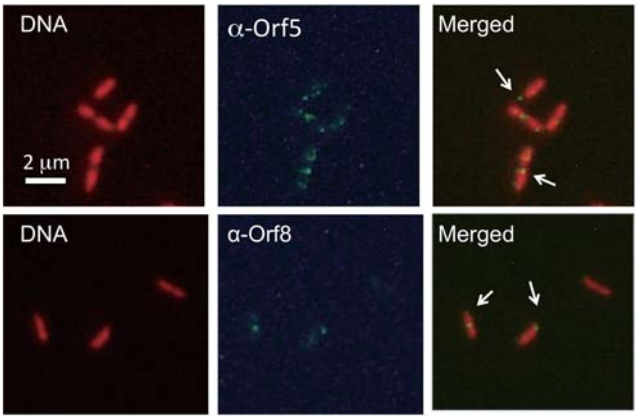


Figure 1. Subcellular localization of EPA-biosynthesis enzymes, Orf5 and Orf8. Fluorescence microscopic images of the cells stained with Hoechst 33342 (false-colored red) (left), immunostained with anti-Orf5 and Orf8 monoclonal antibody as a primary antibody and visualized with a secondary Alexa-488 conjugated anti-mouse antibody (center), and merged images (right). Arrows indicate the position of Orf5 and Orf8, respectively.

Development of a Novel Lipophilic Probe for Functional Analysis of Bioactive Fatty Acids in Human Vein Endothelial Cells

Oleic acid, a kind of monounsaturated fatty acids, is commonly found in olive oil and fish oil and is known to be a bioactive compound that decreases risk of hypertension and various vascular disease of human. However, it remains unclear how oleic acid exerts its physiological function at molecular level in biological membrane. In this study, we synthesized a novel fatty acid probe, oleic acid containing an ω-ethynyl group (click18:1), which is applicable to *in vivo* postlabeling by click chemistry with azide compounds containing fluorescent group and crosslinking reagent. Here, we used human umbilical vein endothelial cells (HUVEC) as a model and attempted to identify the proteins covalently modified with oleic acid in human vascular cells. The crude extracts from HUVEC cultivated with click18:1 were applied to click chemistry with azide biotin. Biotinylated proteins via click18:1 were purified with streptavidin-conjugated beads. Purified proteins were identified by MALDI-TOF MS and following PMF analysis. As the result, three proteins were identified as novel proteins modified with oleic acid.

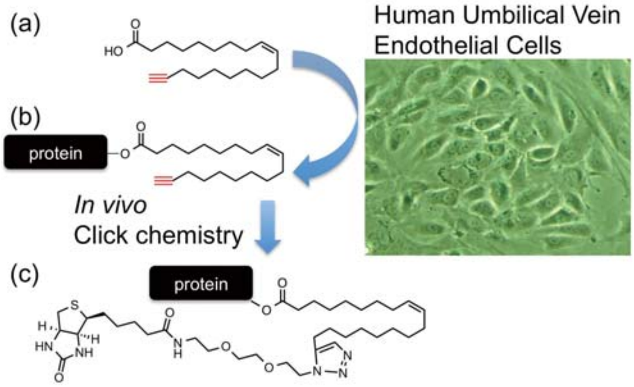


Figure 2. Exploration of oleic acid-modified proteins in human vascular endothelial cells by click chemistry. Oleic acid containing an ω-ethynyl group (click18:1 (a)) was incorporated into HUVEC and recruited to protein lipidation (b). By click chemistry with azide biotin, lipidated proteins were biotinylated and applied to affinity purification with streptavidin-conjugated beads (c).

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)


Program-Specific Res
TAKAHASHI, Nobuaki
(D Eng)

Students

MASHITA, Ryo (D1)
SHIRAISHI, Yasuhiro (M2)
TAKEDA, Kazuki (M2)
MAEDE, Tadahiko (M2)
KISHIMOTO, Mizuki (M1)
FUJISHIMA, Yudai (M1)
MURAKAMI, Momoko (M1)
OKIHARA, Tetsuya (UG)
MIYATAKE, Yuki (UG)
MURAMOTO, Haruka (UG)

Scope of Research

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

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

Selected Publications

Kanaya, T.; Inoue, R.; Saito, M.; Seto, M.; Yoda, Y., Relaxation Transition in Glass-forming Polybutadiene as Revealed by Nuclear Resonance X-ray Scattering, *J. Chem. Phys.*, **140,** [144906-1]-[144906-5] (2014).

Tanaka, K.; Nishida K.; Gabrys, B. J.; Lawrence, M. J.; Kanaya T., Critical Dissolution Ionic Strength of Aqueous Solution of Chitosan Hydrochloride Salt, *Sen'i Gakkaishi* (*J. Soc. Fiber Sci. Technol., Jpn.*), **70,** 225-231 (2014).

Inoue, R.; Kanaya, T.; Hu, Y.; Masuda, T.; Nishida, K.; Yamamuro, O., Relationship between the Local Dynamics and Gas Permeability of Polyacetylenes Containing Polymethylated Indan/tetrahydronaphtalene Moieties, *Polymer*, **55,** 182-186 (2014).

Hara, A.; Inoue, R.; Takahashi, N.; Nishida, K.; Kanaya, T., Trajectory of Critical Point in Polymerization-Induced Phase Separation of Epoxy/Oligoethylene Glycol Solutions, *Macromolecules*, **47,** 4453-4459 (2014).

Wernecke, J.; Okuda, H.; Ogawa, H.; Siewer, F.; Krumrey, M., Depth-Dependent Structural Changes in PS-b-P2VP Thin Films Induced by Annealing, *Macromolecules*, **47,** 5719-5727 (2014).

Trajectory of Critical Point in Polymerization-induced Phase Separation of Epoxy/oligoethylene Glycol Solutions

In this work, we have studied kinetics of polymerization-induced phase separation of epoxy solution in oligoethylene glycol using light scattering (LS) and optical microscope (OM). It was found that special double droplet morphology was observed only in a very narrow range of epoxy fraction (φ~0.35), which depended on the reaction temperature. In the narrow range the phase separation rate was very fast and the bicontinuous structure which was typical in spinodal decomposition-type phase separation was observed only in the very early stage (see Figure 1), suggesting that the solutions in the narrow fraction range entered directly the spinodal decomposition region without crossing the bimodal region. It is therefore considered that the temperature dependent narrow fraction range corresponds to the trajectory of the critical point of the phase separation curve in the fraction-temperature diagram.

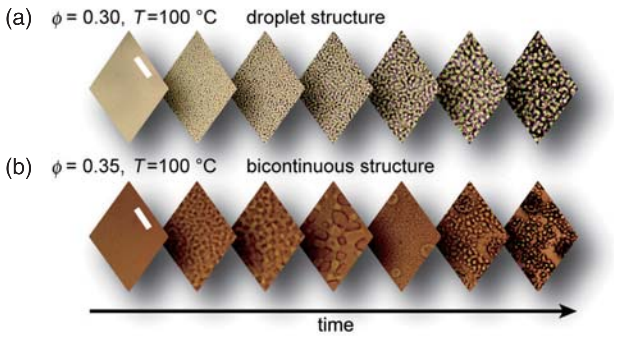


Figure 1. Time evolutions of OM images for φ = 0.30 (a) and 0.35 (b) after the phase separation starts at T_r = 100 °C.

Spin-coating Process of PS-b-P2VP through the *in-situ* Fast GISAXS Measurements

Block copolymer thin films has been recently noticed considerable attention because the self-assembly of the periodic nanoscale has potential in highly density data storage, solar cells and nanostructured membranes. In order to optimize the physical properties by controlling the long-range order and the orientation of the microdomains, various processes have been accordingly utilized in recent years. It is well known that the structure of microdomains as well as the physical properties of thin films is decisively affected by the interactions from the surface and interface. Besides the interactions, the solvent selectivity, film thickness and the solvent evaporation rate also affect the structural development of the microdomains. In this work, ordering transition mechanism of nanostructures in spin-coated poly(styrene-b-2vinylpyridine) (PS-b-P2VP) films has been investigated. In contrast to the lamellar structure observed in the bulk as a thermodynamically stable structure, a cylindrical structure forms in bot PS-b-P2VP thin films. From the in-situ grazing small angle X-ray scattering (GISAXS) measurements on thin film fabricated by spin-coating, the oriented cylindrical structure along perpendicular to the film surface formed: after the successive transitions from micelles in solution to the BCC lattice of micelles, oriented cylindrical structures are observed in thin film (Figure 2). In this transition, undergoing vitrification of PS and P2VP prohibited further this transition from the cylinder to lamellar structure. The cylinder perpendicularly aligned on the substrate grown in thin films fabricated by spin-coating is found to be a new non-equilibrium structure caused by the rapid solvent evaporation and the convection effect that solvent could efficiently evaporate from inside the thin films.

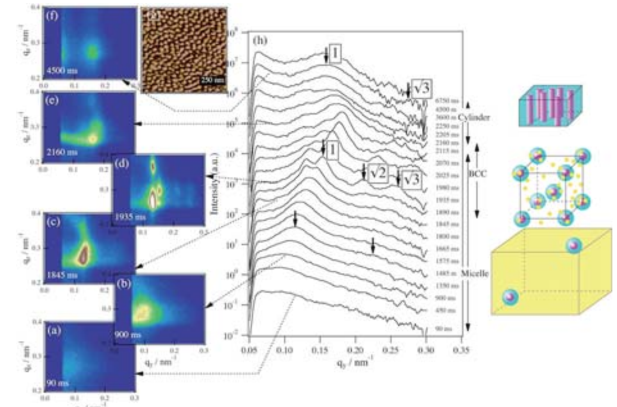


Figure 2. Time-resolved two dimensional GISAXS images (a) - (f) at the incident angle of 0.14o, the surface AFM image (g) and time-resolved in-plane profiles at $q_z = 0.298$ nm^{-1} (h) of PS-*b*-P2VP during spin-coating.

Division of Multidisciplinary Chemistry
– Molecular Rheology –

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


Prof
WATANABE, Hiroshi
(D Sc)


Assoc Prof
MASUBUCHI, Yuichi
(D Eng)


Assist Prof
MATSUMIYA, Yumi
(D Eng)


Techn Staff *
OKADA, Shinichi

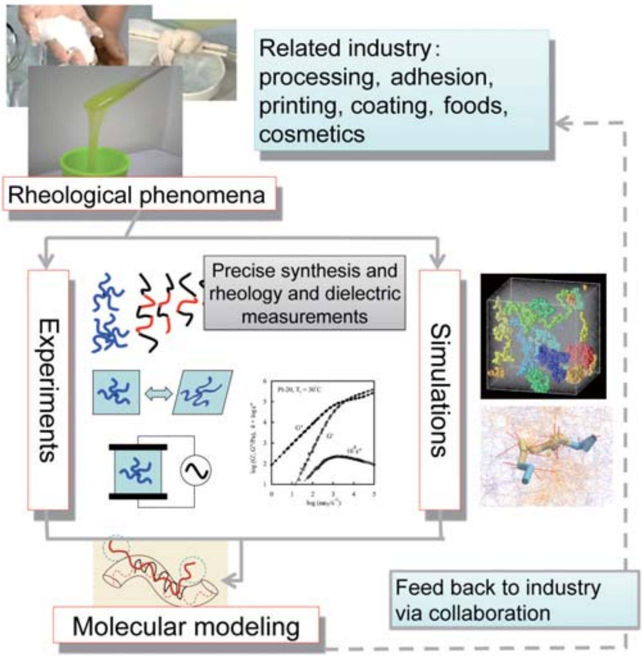
*Re-employed Staff

Students

KAWASAKI, Yohji (D3)
KUMAZAWA, Kazuki (M2)
EGAMI, Ryoma (M2)
HIROTSU, Soichiro (M1)
TANAKA, Takeya (M1)
ICHIHARA, Kentaro (UG)
MIYATAKE, Hiroyuki (UG)

Scope of Research

The molecular origin of various rheological properties of material is studied. 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 a basic understanding of the features, the molecular motion and structures of various scales are studied for polymeric systems in deformed state. Measurements are performed of rheological properties with various rheometers, of isochronal molecular orientation with flow birefringence, and of auto-correlation of the orientation with dynamic dielectric spectroscopy. Direct observation of molecular-motion is also carried out with fluorescent microscopy and molecular simulations.



KEYWORDS

Rheology
Dielectric Spectroscopy
Softmatter
Primitive Chain Network Simulation

Selected Publications

Masubuchi, Y.; Watanabe, H., Origin of Stress Overshoot under Start-up Shear in Primitive Chain Network Simulation, *ACS Macro Letters*, **3,** 1183-1186 (2014).

Matsumiya, Y.; Masubuchi, Y.; Inoue, T.; Urakawa, O.; Liu, C.-Y.; van Ruymbeke, E.; Watanabe, H., Dielectric and Viscoelastic Behavior of Star-Branched Polyisoprene: Two Coarse-Grained Length Scales in Dynamic Tube Dilation, *Macromolecules*, article ASAP DOI: 10.1021/ma501561y.

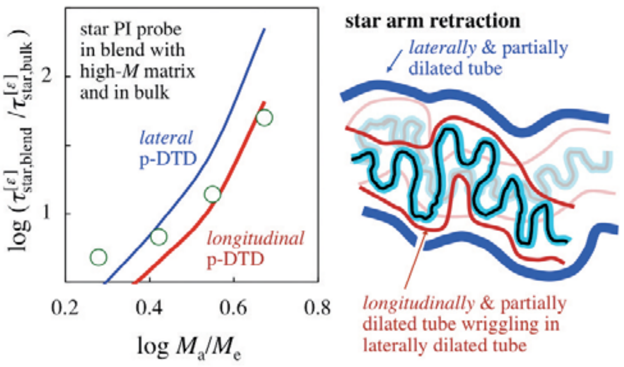
van Ruymbeke, E.; Shchetnikava, V.; Matsumiya, Y.; Watanabe, H., Dynamic Dilution Effect in Binary Blends of Linear Polymers with Well-Separated Molecular Weights, *Macromolecules*, article ASAP DOI: 10.1021/ma501566w.

Masubuchi, Y.; Matsumiya, Y.; Watanabe, H., Test of Orientation/Stretch-Induced Reduction of Friction via Primitive Chain Network Simulations for Polystyrene, Polyisoprene, and Poly (n-butyl acrylate), *Macromolecules*, **47(19),** 6768-6775 (2014).

Masubuchi Y.; Matsumiya, Y.; Watanabe, H.; Marrucci, G.; Ianniruberto, G., Primitive Chain Network Simulations for Pom-Pom Polymers in Uniaxial Elongational Flows, *Macromolesules*, **47(10),** 3511-3519 (2014).

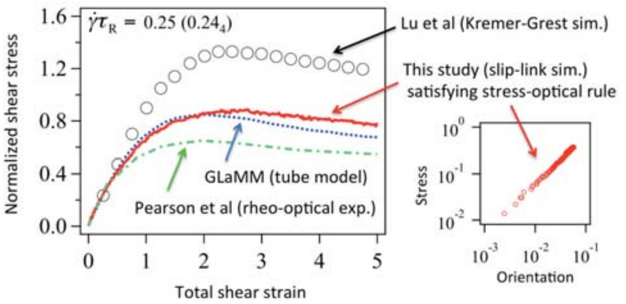
Dielectric and Viscoelastic Behavior of Star-Branched Polyisoprene: Two Coarse-Grained Length Scales in Dynamic Tube Dilation

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, we examined dielectric and viscoelastic behavior of star PI probe chains (arm molecular weight $10^{-3}M_\mathrm{a}$ = 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 $\mu(t)$, $\mu(t) = \varphi'(t)/\beta(t)$ 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,** 6067-6080 (2013).].



Origin of Stress Overshoot under Start-up Shear in Primitive Chain Network Simulation

Birefringence measurement demonstrates that the segment orientation of entangled polymers overshoots on start-up of fast shear [Pearson et al., *J. Rheol.*, **33,** 517-536 (1989).]. The stress-optical rule holds for those polymers, so that the overshoot of orientation results in the overshoot of shear stress. On the other hand, an opposite result was deduced from the recent molecular dynamics simulation for bead–spring chain [Lu et al., *ACS Macro Lett.*, **3,** 569-573 (2014).]: the evolution of segment orientation does not overshoot but the chain stretch induces the stress overshoot, even at the shear rate $\dot\gamma$ smaller than the reciprocal Rouse time, $1/\tau_\mathrm{R}$. In this study, we performed the primitive chain network simulation to find that our simulation reproduces the overshoot of both stress and orientation and the chain stretch exhibits a slight, monotonic increase but no overshoot. Our result is thus fully consistent with the experiment.



Division of Multidisciplinary Chemistry
– Molecular Aggregation Analysis –

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


Prof
SATO, Naoki
(D Sc)


Assoc Prof
ASAMI, Koji
(D Sc)


Assist Prof
YOSHIDA, Hiroyuki
(D Sc)


Assist Prof
MURDEY, Richard James
(Ph D)

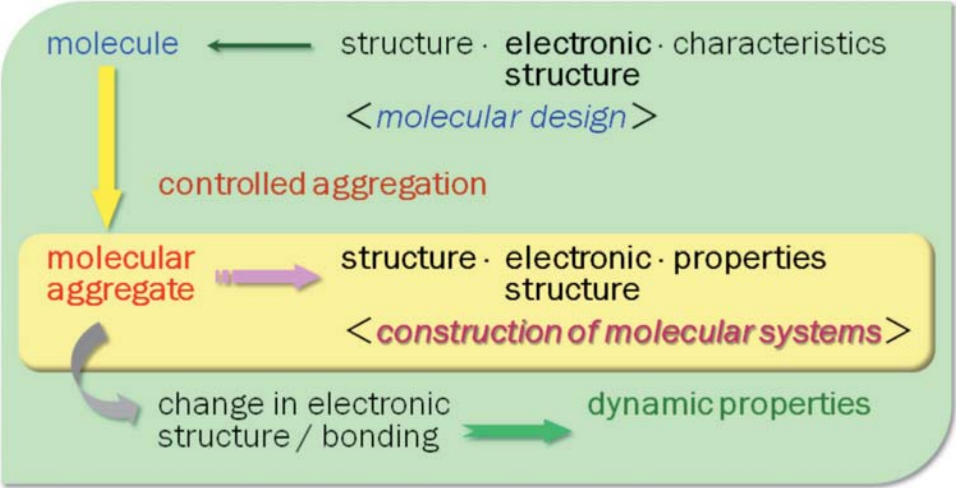
Students

SHINTAKU, Naoto (M2)
YAMADA, Kazuto (M2)
NAKAO, Kazuto (M1)

Scope of Research

The research at this subdivision is devoted to correlation studies on structures and properties of both natural and artificial molecular aggregates from two main standpoints: photoelectric and dielectric properties. The electronic structure of organic thin films is studied using photoemission and inverse photoemission spectrosocpies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with heterogeneous sturcutres in mocrocapsules, boipolymers, biological membranes and biological cells, and the nonlinearity in their dielectric properties is also studied in relation to molecular motions.

KEYWORDS
Activation Energy
Bilayer Lipid Membrane
Dielectric Spectroscopy
Organic Semiconductor
Trap State



Selected Publications

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

Yoshida, H., Low-energy Inverse Photoemission Study on the Electron Affinities of Fullerene Derivatives for Organic Photovoltaic Cells, *J. Phys. Chem. C*, **118,** 24377-24382 (2014).

Hidaka, Y.; Asami, K., Measurement of Dipole Potential in Bilayer Lipid Membranes by Dielectric Spectroscopy, *J. Membrane Biol*., **247,** 721-727 (2014).

Asami, K., Low-Frequency Dielectric Dispersion of Bacterial Cell Suspensions, *Colloids Surf. B*, **119,** 1-5 (2014).

Interpretation of the Thermal Activation Energy of Conduction for Organic Semiconductor Thin Films with Blocking Contacts

A two-terminal lead phthalocyanine (PbPc) thin film device exhibited reversible rectification *in situ* when a high bias stress potential was applied to the electrodes, as shown in Figure 1. The current rectification was associated with a shift of the thermal activation energy of conductance by about –0.1 eV (forward bias) and +0.1 eV (reverse bias) from the pre-bias value of 0.67 eV as the equilibrium one. The rectification ratio of the conductance was changed less than that predicted from the observed change in activation energy, indicating that the system obeyed the Meyer–Neldel rule normally associated with charge carriers in thermal equilibrium with a logarithmic tail of trap states. Annealing the sample at 175 °C removed the rectification behavior, providing further indication that trap states play a significant role in the transport mechanism. Rectification implies blocking electrodes and injection limited current at both electrodes, under which conditions the activation energy is expected to correlate with the energy barrier for charge injection—the energy separation between the Fermi level of the electrode and the mobility edge of the organic semiconductor (see Figure 2). Neither of these energy levels, however, depends explicitly on an excess of trapped charge in the logarithmic density of trail states induced by the bias stress. A change in the trap filling level induced by the space charge injection during the bias stress should not, therefore, influence either state in a way that satisfactorily explains the observed rectification. The most likely interpretation that explains our results is that the metal Fermi level is pinned to the trap filling level in the organic thin film.

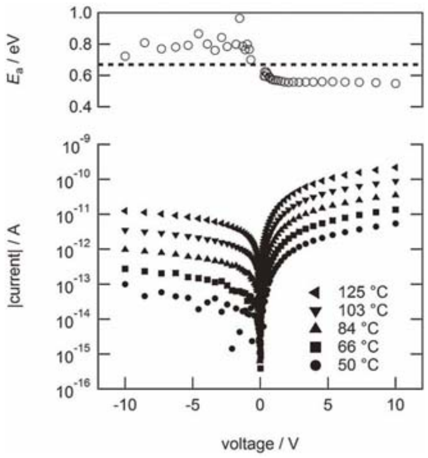


Figure 1. *In situ I–V* curves and activation energies obtained for an 8 nm-thick PbPc film deposited at 50 °C and annealed at 125 °C for 48 h. The forward rectification was observed when a +500 V bias applied for 2–3 h at 125 °C. The dotted line indicates the pre-stress activation energy of 0.67 eV.

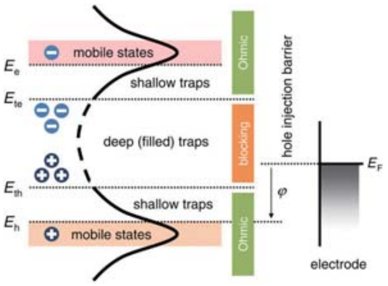


Figure 2. A schematic energy diagram for the interface between an organic semiconductor and a metal electrode. The organic semiconductor has trap states distributed throughout the transport energy gap, $E_e - E_h$. An electrode Fermi level falling within the trap filling states is expected to result in blocking contacts, whereas Fermi levels falling closer to either mobility edge are likely to form an Ohmic contact for either holes or electrons.

Measurement of Dipole Potential in Bilayer Lipid Membranes by Dielectric Spectroscopy

It is known that there is a positive electrostatic potential within a bilayer lipid membrane (BLM) originating from alignment of dipolar residues of lipids and water molecules. The potential is termed the dipole potential (DP) and is thought to be important in regulating the functions of membrane proteins and the interactions of various bioactive compounds with the membranes. To understand the DP, we studied dielectric properties of planar BLMs using dipicrylamine (DPA) (hydrophobic anion) as a probe for the DP. The BLMs doped with DPA showed dielectric relaxation due to the translocation of DPA between the membrane interfaces (Figure 3). Incorporating either cholesterol (CL) or 6-ketocholestanol (KC) into the membranes increased the characteristic frequency of the dielectric relaxation, which is proportional to the translocation rate constant of DPA. The results suggested that the sterol dipoles induced positive potential changes within the membrane interior. The changes of the DP were 70 mV for CL and 150 mV for KC when the sterol mole fraction was 0.67. The opposite effect was caused by phloretin added to the aqueous media, and the maximum DP change was –90 mV at 100 µM.

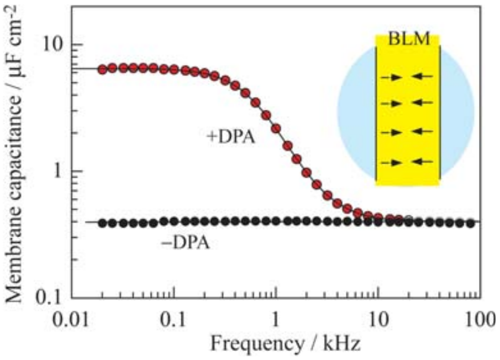


Figure 3. Dielectric relaxation of bilayer lipid membranes in the absence and presence of DPA. Inset: sterol dipoles in the membrane are illustrated.

Division of Multidisciplinary Chemistry
– Interdisciplinary Chemistry for Innovation –

http://www.probe.abe.kyoto-u.ac.jp/toshimitsu/index.html

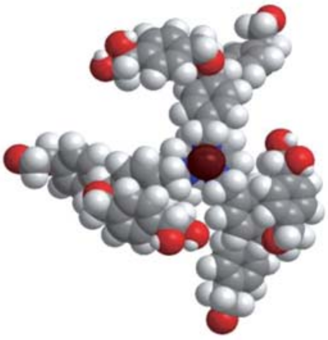
Prof
TOSHIMITSU, Akio
(D Eng)

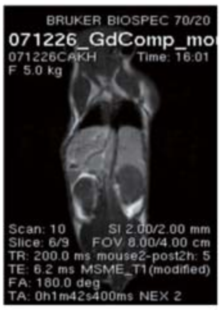
Students

IURA, Yoshihito (M2)	IMAI, Yuta (UG)
KAMEDA, Tetsuro (M2)	ORITO, Naomi (UG)
SUZUKI, Yuki (M1)	

Scope of Research

Organic chemistry can contribute to the innovation through the design and synthesis of molecules those are valuable to human society. Our methodology possesses advantage in heteroatom chemistry, transition metalcatalyzed reactions, and asymmetric synthesis. As for the synthetic procedure, we take note to develop atomeconomic as well as environment-benign reactions. We recognize the importance of the collaboration with various fields of technology of industry and academia. Recent examples of our projects include design, synthesis, and evaluation of aromatic compounds used in light-emitting field-effect transistors, sugar-fullerene linked compounds used in photodynamic therapy of cancers, and gadolinium complex of chiral dendrimers used in magnetic resonance imaging of cancers (shown in the figure).





KEYWORDS
Innovation
Organic Synthesis
Heteroatom Chemistry
Transition Metal Catalyst
Asymmetric Synthesis

Selected Publications

Miyake, Y.; Kimura, Y.; Ishikawa, S.; Tsujita, H.; Miura, H.; Narazaki, M.; Matsuda, T.; Tabata, Y.; Yano, T.; Toshimitsu, A.; Kondo, T., Synthesis and Functional Evaluation of Chiral Dendrimer-Triamine-Coordinated Gd Complexes as Highly Sensitive MRI Contrast Agents, *Tetrahedron Lett*., **53,** 4580-4583(2012).

Kondo, T.; Kimura, Y.; Kanda, T.; Takagi, D.; Wada, K.; Toshimitsu, A., Simple and Practical Aerobic Oxidation of Alcohols Catalyzed by a (μ-Oxo)tetraruthenium Cluster, *Green Sus. Chem*., **1,** 149-154 (2011).

Kondo, T.; Niimi, M.; Yoshida, Y.; Wada, K.; Mitsudo, T.; Kimira, Y.; Toshimitsu, A., Rhodium-catalyzed Linear Codimerization and Cycloaddition of Ketenes with Alkynes, *Molecules*, **15,** 4189-4200 (2010).

Sakanoue, T.; Yahiro, M.; Adachi, C.; Takimiya, K.; Toshimitsu, A., Electrical Characteristics of Single-component Ambipolar Organic Field-effect Transistors and Effects of Air Exposure of Them, *J. Appl. Phys*., **103,** [094509-1]-[094509-6] (2008).

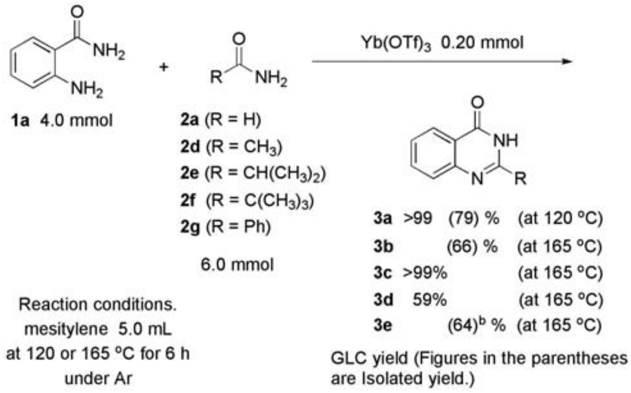
Sakanoue, T.; Yahiro, M.; Adachi, C.; Uchiuzou, H.; Takahashi, T.; Toshimitsu, A., Ambipolar Light-emitting Organic Field-effect Transistors Using a Wide-band-gap Blue-emitting Small Molecule, *Appl. Phys. Lett*., **90,** [171118-1]- [171118-3] (2007).

Simple, Selective, and Practical Synthesis of 2-Substituted 4(3*H*)-Quinazolinones by Yb(OTf)$_3$-Catalyzed Condensation of 2-Aminobenzamide with Carboxamides

4(3*H*)-Quinazolinones belong to one of the most important classes of fused heterocyclic compounds with a wide range of biological activities; *e.g.*, protein tyrosine kinase inhibitor, cholecystokinin inhibitor, antimalarial, antibacterial, antifungal, antiviral, anti-HIV, anticancer, antiinflammatory, antiallergy, anticonvulsant, antihypertensive, and antidiabetic. In addition, the 4(3*H*)-quinazolinone nucleus is also the key component of chromophoric, thermochromic, and fluorescent materials.

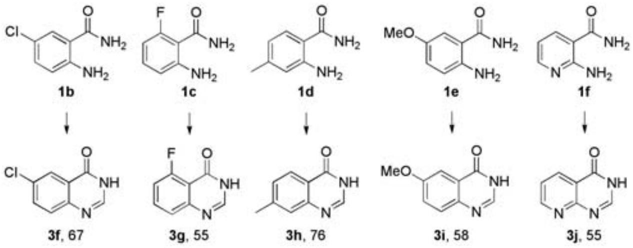
We found that the reaction of 2-aminobenzamide **1a** (4.0 mmol) with formamide **2a** (6.0 mmol) in the presence of a catalytic amount of Yb(OTf)$_3$ (0.20 mmol) in mesitylene (5 ml) at 120 ºC for 6 h affords 4(3*H*)-quinazolinone **3a** in quantitative yield (Scheme 1).

Formamide **2a** is the most effective C1 source in the construction of 4(3*H*)-quinazolinone **3a**, while methyl formate **2b** or paraformaldehyde, $(CH_2O)_n$ **2c**, instead of formamide **2a**, gave **3a** in 39% and 12% yield, respectively, even under reflux in mesitylene (bath temp. 165 ºC). Besides formamide **2a**, carboxamides, such as acetamide **2d**, 2-methylpropanamide **2e**, pivalamide **2f**, and benzamide **2g**, can be used in the present reaction to give 2-methyl-, 2-isopropyl-, 2-(*tert*-butyl)-, and 2-phenyl-4(3*H*)-quinozolinone (**3b-e**) in good to high yields as also shown in Scheme 1.



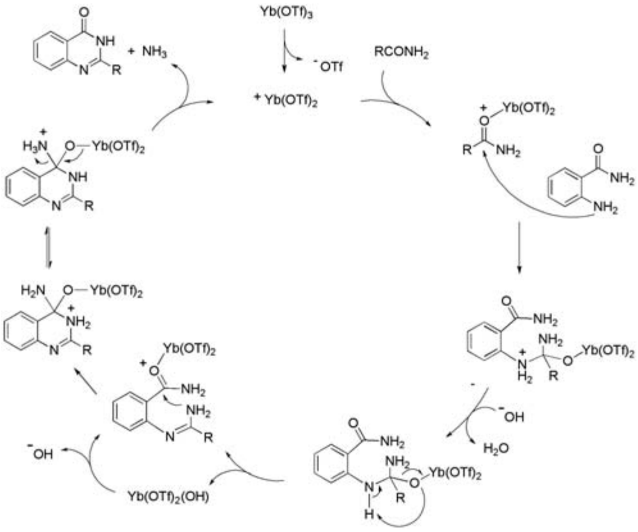
Scheme 1. Yb(OTf)$_3$-catalyzed synthesis of 4(3*H*)-quinazolinones **3** from 2-aminobenzamide **1a** and carboxamides **2**.

Condensation of several 2-aminobenzamides (**1b-e**) with formamide (**2a**) proceeded smoothly, by Yb(OTf)$_3$ catalyst, to give the corresponding 4(3*H*)-quinazolinones (**3f-i**) in moderate to high isolated yields (Scheme 2). In addition, the related 2-aminonicotinamide (**1f**) also reacted with **2a** under the present catalytic reaction conditions to give pyrido[2,3-*d*]pyrimidin-4(3*H*)-one (**3j**) in an isolated yield of 55%.



Scheme 2. Synthesis of 4(3*H*)-quinazolinones **3f-j** by Yb(OTf)$_3$-catalyzed condensation of 2-aminobenzamides **1b-e** and the related **1f** with formamide **2a**. Reaction conditions; **1** (4.0 mmol), $HCONH_2$ **2a** (6.0 mmol), Yb(OTf)$_3$ (0.20 mmol) in mesitylene (5.0 mL) at 165 °C (bath temp.) for 6 h under an Ar atmosphere.

Considering the results obtained above, the most plausible mechanism is illustrated in Scheme 3. We believe that the dissociation of a triflate anion (OTf^-) from Yb(OTf)$_3$ first occurred to generate catalytically active $Yb(OTf)_2^+$, which immediately coordinates to a carbonyl oxygen in carboxamide. Subsequent nucleophilic attack of an amino group in 2-aminobenzamide to the activated carbonyl carbon in carboxamide proceeded to give an amidine intermediate and Yb(OTf)$_2$(OH), followed by dissociation of OH^- to regenerate $Yb(OTf)_2^+$. $Yb(OTf)_2^+$ again coordinates to a carbonyl oxygen in benzamide to promote the intramolecular nucleophilic attack of an amino group to the activated carbonyl carbon. Isomerization of the intermediate, followed by elimination of NH_3 give 4(3*H*)-quinazolinone and $Yb(OTf)_2^+$.



Scheme 3. The most plausible mechanism of this reaction.

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)

KAZAMA, Ichiro
CENNI, Enrico (Ph D)

Lect (pt)

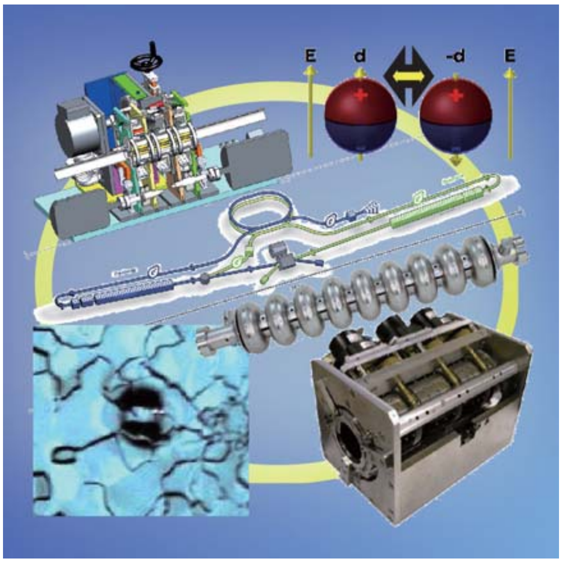
SHIMIZU, M. Hirohiko (D Sc)	Laboratory for Particle Properties, Department of Physics, Nagoya University

Students

IMAJO, Sohei	(D3)	KITAHARA, Ryunosuke	(D1)
FUWA, Yasuhiro	(D2)	IKEDA, Hideki	(M2)

Scope of Research

Particle accelerators have been contributing on progress of science in a variety of fields. Among these fields, our current activity covers neutron science and participation in International Linear Collider (ILC) project. Including subsidiary subjects, the following subjects are being studied: neutron beam focusing by modulating sextupole magnets, neutron acceleration/deceleration, compact neutron source including ion source, permanent quadrupole magnets for final focusing of ILC, nondestructive inspections for superconducting accelerating tube towards higher yield and performance and multi layered film structure for RF.



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

Selected Publications

Arimoto, Y.; Geltenbort, P.; Imajo, S.; Iwashita, Y.; Kitaguchi, M.; Seki, Y.; Shimizu, H. M.; Yoshioka, T., Demonstration of Focusing by a Neutron Accelerator, *Phys. Rev. A*, **86,** 023843 (2012).
Yamada, M.; Iwashita, Y.; Kanaya, T.; Yamada, N. L.; Shimizu, H. M.; Mishima, K.; Hino, M.; Kitaguchi, M.; Hirota, K.; Geltenbort, P.; Guerard, B.; Manzin, G.; Andersen, K.; Lal, J.; Carpenter, J. M.; Bleuel, M.; Kennedy, S. J., A Compact TOF-SANS Using Focusing Lens and Very Cold Neutrons, *Physica B: Condensed Matter*, **406(12),** 2453-2457 (2011).
Arimoto, Y.; Yoshioka, T.; Shimizu, H. M.; Mishima, K.; Ino, T.; Taketani, K.; Muto, S.; Kitaguchi, M.; Imajo, S.; Iwashita, Y.; Yamashita, S.; Kamiya, Y.; Yoshimi, A.; Asahi, K.; Shima, T.; Sakai, K., Longitudinal-gradient Magnet for Time Focusing of Ultra-cold Neutrons, *Physics Procedia*, **17,** 20-29 (2011).
Iwashita, Y.; Ichikawa, M.; Yamada, M.; Sugimoto, T.; Tongu, H.; Fujisawa, H.; Masuzawa, M.; Tauchi, T.; Oku, T.; Hirota, K.; Shimizu, H. M.; Zhu, C.; Shi, Y., Practical Applications of Permanent Magnet Multipoles, *IEEE Trans. on Applied Supercond.*, **20(3),** 842-845 (2010).
Iwashita, Y.; Tajima, Y.; Hayano, H., Development of High Resolution Camera for Observations of Superconducting Cavities, *Phys. Rev. S.T. -Accel. Beams*, **11,** [093501-1]-[093501-6] (2008).

Production of Pulsed UCN in J-PARC MLF

Ultracold neutrons (UCNs) are neutrons whose kinetic energies are lower than 240 neV. The de Broglie wavelength of UCN is longer than 58 nm. UCN interacts with a spatially averaged step-like potential of millions of nuclei. Therefore UCN can be stored in a vessel with interior surface made of the materials whose averaged potential is higher than the kinetic energy of UCN. UCN is used for longtime storage experiments such as searches of the neutron electric dipole moment (nEDM) or measurements of the neutron lifetime.

UCNs can be produced with a neutron Doppler shifter, which reflects neutrons by a neutron mirror rotating with the half tangential velocity of the target neutrons and decelerates them into the UCN region by the Doppler effect. We have developed the Doppler shifter in order to carry out the R&D of the apparatus for our nEDM searches or other UCN experiments in Japan. It is installed in the BL05 of Materials and Life Science Experimental Facility (MLF) at J-PARC (Figure 1).

We have succeeded in producing pulsed UCNs by decelerating the neutrons of 136 m/s in 2010 and have obtained the UCNs of 0.17 cps at 113.2 kW beampower. The repetition frequency of UCN production is 8.33 Hz. However, this output of UCNs was too weak for the R&D. Hence we tried to improve the output of UCNs by increasing the flux of the neutrons injected into the Doppler shifter.

We newly installed the supermirror guides and focusing guides in a neutron beamline and inserted the nickel-coated UCN extracting guide in the Doppler shifter. As a result, the UCN count rate became 48 cps at the beam power of 300 kW. Their count rate increased about 34 times and the count rate of UCNs increased about 80 times in the same beampower and detection efficiency. Considering the beampower increase of J-PARC, the count rate of UCNs increased to about 250 times (Figure 2).

By using the Doppler shifter, we have already started the R & D of the apparatuses for our nEDM searches, for example, the UCN transport experiment with nickel-coated UCN guides, whose length is 5.6 m and the mean reflectivity at one reflection is evaluated to be 97 % (Figure 3). At present we are developing the UCN accelerator, which produces high density UCNs by time focus, and planning the experiment of the performance evaluation of the accelerator by using the Doppler shifter and the UCN guides (Figure 4).

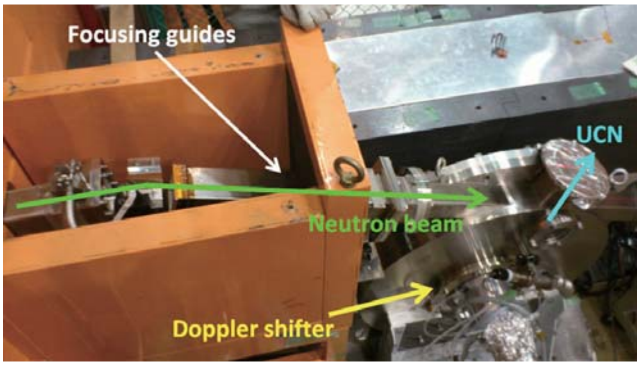


Figure 1. Layout of the Doppler shifter and the focusing guides.

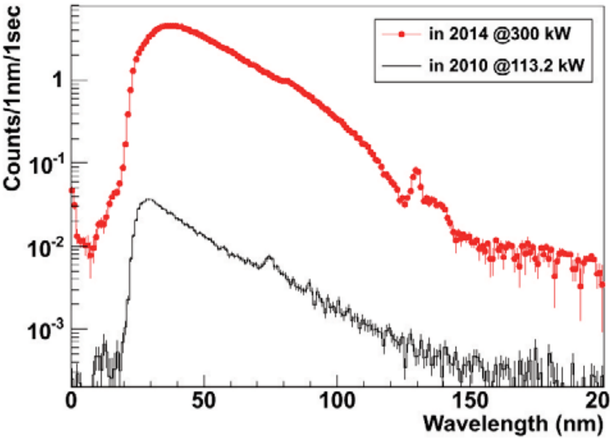


Figure 2. UCN spectra from the Doppler shifter before and after improvement.

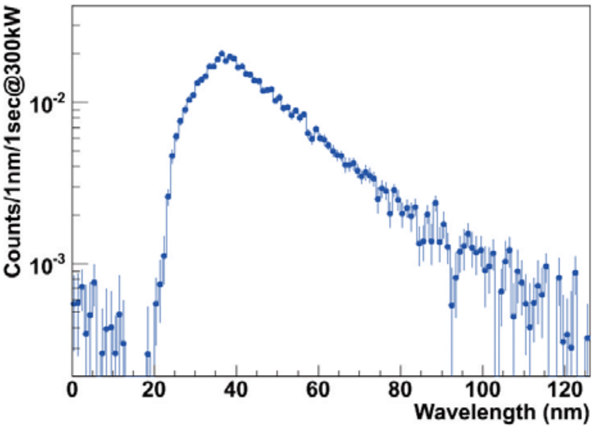


Figure 3. Result of the UCN transport experiment. We succeeded in measuring the UCN spectrum through the UCN guides of 5.6 m length.

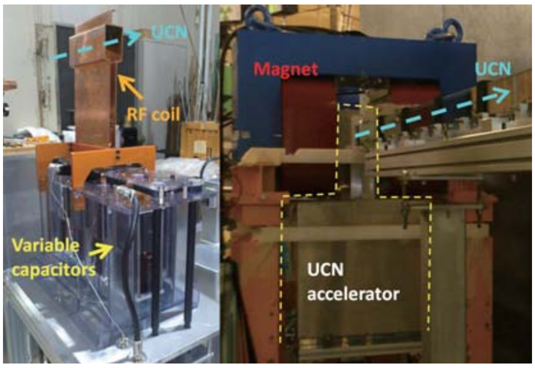


Figure 4. Photograph of the inner machinery of UCN accelerator (left) and experimental setup (right).

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)

PD
MIYASAKA, Yasuhiro
(D Sc)

Lect (pt)

TOKITA, Shigeki (D Eng) Institute of Laser Engineering, Osaka University

Students

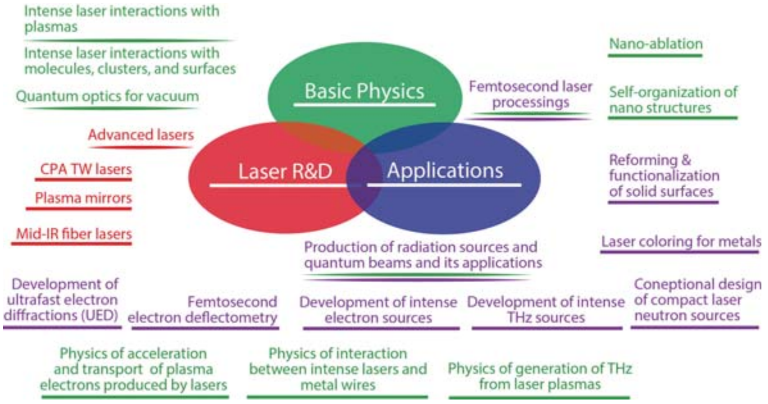
MORI, Kazuaki (D1)
TERAMOTO, Kensuke (M2)
NAKASHIMA, Yuto (M2)
NISHII, Takaya (M2)
MAEDA, Kazuya (M2)
WATANABE, Kota (M1)

Scope of Research

The interaction of femtosecond laser pulses with matters involves interesting physics, which does not appear in that of nanosecond laser pulses. Investigating the interaction physics, potential of intense femtosecond lasers for new applications is being developed (such as laser produced radiations and laser processing). Ultra-intense lasers can produce intense radiations (electrons, ions, THz, and so on), which can be expected as the next-generation radiation sources. Ultra-short lasers are available to process any matters without thermal dissociation. The femtosecond laser processing is also the next-generation laser processing. In our laboratory ultra intense femtosecond laser named T^6-laser is equipped, and the physics of intense laser matter interactions and its applications are researched.

KEYWORDS

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



Selected Publications

Gemini, L.; Hashida, M.; Shimizu, M.; Miyasaka, Y.; Inoue, S.; Tokita S.; Limpouch, J.; Mocek T.; Sakabe, S., Periodic Nanostructures Self-formed on Silicon and Silicon Carbide by Femtosecond Laser Irradiation, *Appl. Phys. A*, **117,** 49-54 (2014).

Hashida, M.; Gemini, L.; Nishii, T.; Miyasaka, Y.; Sakagami, H.; Shimizu, M.; Inoue, S.; Limpouch, J.; Mocek T.; Sakabe S., Periodic Grating Structures on Metal Self-organized by Double-pulse Irradiation, *J. Laser Micro/Nanoeng*., (in press).

Nakajima, H.; Tokita, S.; Inoue, S.; Hashida, M.; Sakabe, S., Divergence-Free Transport of Laser-Produced Fast Electrons Along a Meter-Long Wire Target, *Phys. Rev. Lett*., **110,** 155001 (2013).

Hashida M.; Ikuta Y.; Miyasaka Y.; Tokita S.; Sakabe S., Simple Formula for the Interspaces of Periodic Grating Structures Self-organized on Metal Surfaces by Femtosecond Laser Ablation, *Appl. Phys. Lett*., **102,** 174106 (2013).

Jahangiri, F.; Hashida, M.; Tokita, S.; Nagashima, T.; Hangyo, M.; Sakabe, S., Enhancing the Energy of Terahertz Radiation from Plasma Produced by Intense Femtosecond Laser Pulses, *Appl. Phys. Lett*., **102,** 191106 (2013).

Topics

Transient Changes in Electric Fields Induced by Interaction of Ultra-intense Laser Pulses with Insulator/Metal Foils: Sustainable Fields Spanning Several Millimeters

The generation and transport of fast electrons during and after the interaction of ultra-short high-intensity laser pulses with a target play a crucial role in the consequent emission of energetic radiation, such as ions, X-rays, gamma rays, and terahertz waves. Studies have demonstrated that the dynamics of fast electrons is influenced by the shape and material of the laser-irradiated target. Many shapes and materials for irradiation targets have been studied in order to achieve better control over the dynamics of fast electrons. Most recently, some reports have indicated that the shape and material of the target outside the laser-induced plasma can influence the dynamics of fast electrons, and consequently the characteristics of other types of radiation. Therefore, it is important to observe and understand the dynamics of fast electrons, and the electromagnetic fields that they induce, over a large region (on the order of several millimeters) outside the laser-irradiated region for various materials. This could aid the development of efficient laser-induced plasma radiation sources for many attractive applications, including fast ignition for inertial confinement fusion, ultrafast electron diffraction measurements, time-resolved X-ray probes, laser-driven nuclear physics, and tumor therapy using ion beams.

We report measurements of electromagnetic fields at a distance of several millimeters from the position irradiated with an intense laser for three types of targets: insulating foil, conductive foil, and insulating foil onto which a metal disk was deposited. The measurements were performed by femtosecond electron deflectometry. We observed distinct differences in the direction and temporal evolution of the fields depending on the target material. We also measured the electromagnetic fields for different laser intensities (1.3×10^{18} and 8.2×10^{18} W/cm^2) and found that the transport of fast electrons also depended on laser intensity for each target material.

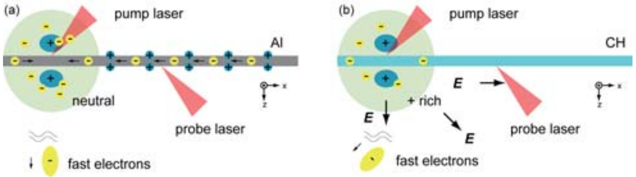


Figure 1. Schematic illustrations of the reduction of electric field along the target surface due to the influx of the surrounding free electrons (a) and the generation of the electric fields by the large resistivity of the insulating target (b).

Periodic Grating Structures on Metal Self-organized by Double-pulse Irradiation

The formation of periodic grating structures has been demonstrated on a titanium surface irradiated by a double-pulse beam with a time delay of 160 fs. The first-pulse fluence F_{PP} was varied and always kept below the threshold $F_{\mathrm{TH}} = 60$ mJ/cm^2 for forming periodic grating structures on Ti and the delayed pulse fluence F_{LP} was kept above F_{TH}. The grating structure interspaces were $0.5\lambda_{\mathrm{L}}$ to $0.85\lambda_{\mathrm{L}}$ and decreased with F_{PP} for all values of F_{LP}. This tendency suggests that variation in surface plasma density, which is associated with the fluence of the first pulse, led to variation of the grating interspaces. We found that the interspaces produced by double-pulse irradiation agreed relatively well with those produced by single-pulse irradiation and those predicted by a parametric decay model. To visualize the surface plasma wave induced by the femtosecond laser, two-dimensional particle-in-cell simulation was conducted for a pre-formed plasma on a metal. The simulation results suggest that the preformed plasma density led to the variation in the grating interspaces.

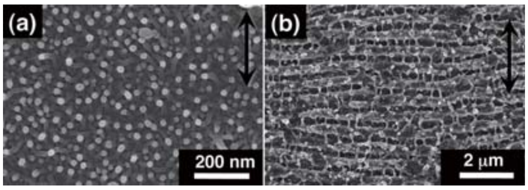


Figure 2. SEM images of surface structures on titanium produced by (a) 1 pulse and (b) 25 pulses, for double-pulse irradiation with a time delay of 160 fs. The laser fluence of the first pulse was $F_{\mathrm{PP}} = 45$ mJ/cm^2 and that of the delayed pulse was $F_{\mathrm{LP}} = 100$ mJ/cm^2. Black arrows indicate the laser polarization direction for the double-pulse beam.

Intense THz Emission from Laser Produced Cluster Plasma

Intense terahertz (THz) radiations have a possibility of being used in great variety of applications. To generate intense THz waves, the schemes using nonlinear crystal or photoconductive antenna have been studied. However incident laser energy is limited by the damage threshold of the crystal. Laser plasmas have benefit of 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 proposed the cluster plasma as the target, which combines both the advantages of the solid and the gas plasmas. The properties of generated THz waves have been measured for various laser pulse duration. It has been found that the energy and spectrum of THz pulse generating from argon cluster plasmas depend on laser pulse duration.

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

Res
MORIGUCHI, Sakumi
(D Sc)

*Nanotechnology Platform

Assist Techn Staff

HIRAIZUMI, Yuri

Students

FUJIYOSHI, Yoshifumi (D3)
YAMAGUCHI, Atsushi (D1)
MITSUTA, Itaru (M2)
TOMISAKI, Yuriko (M1)

Scope of Research

Crystallographic and electronic structures of materials and their transformations are studied 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, the following subjects are urging: direct structure analysis, electron crystallographic analysis, epitaxial growth of molecules, structure formation in solutions, and fabrication of low-dimensional functional assemblies.

KEYWORDS
Surface Plasmon
EELS
Dispersion Curve
STEM
Transition-Metal Oxide

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).

Dispersion Relations for Coupled Surface Plasmon-polariton Modes Excited in Multilayer Structures

The coupled surface plasmon-polariton (SPP) modes excited in an Al/SiO_2/Al multilayer structure were analyzed using angle-resolved electron energy-loss spectroscopy (AREELS) with a relativistic electron probe. Three dispersion curves for coupled antisymmetric short range (AC-SR), symmetric short range (SC-SR) and antisymmetric long rang (AC-LR) modes were observed, but the symmetric long range (SC-LR) mode could not be detected because of its low excitation probability. The obtained dispersion curves agreed well with the calculated curves when an aluminum oxide layer was present on the surfaces, which indicates that the dispersion relations are very sensitive to multilayer surface conditions. In the multilayer structures, the dispersion relation for the coupled SPP modes was found to be sensitive to the thickness of each film, which could be interpreted qualitatively by the electron energy-loss probability calculated for thin aluminum (Al) films and narrow Al gaps using Kröger's formula. It was demonstrated that significant differences in the excitation probability for SPPs could be observed depending on the coupling modes.

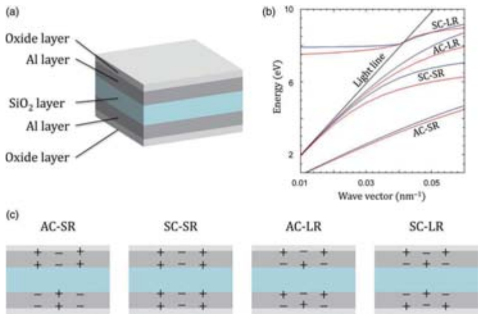


Figure 1. (a) Model of the multilayer structure for the dispersion calculation. (b) Examples of dispersion calculations. The red curves were calculated for the multilayer structure of AlO_x(3 nm)/Al(13 nm)/SiO_2(23 nm)/Al(13 nm)/AlO_x(3 nm). The blue curves were calculated for the multilayer without aluminum oxide layers of Al(16 nm)/SiO_2(23 nm)/Al(16 nm). (c) Schematic diagram of the charge distribution for each of the coupled SPP modes.

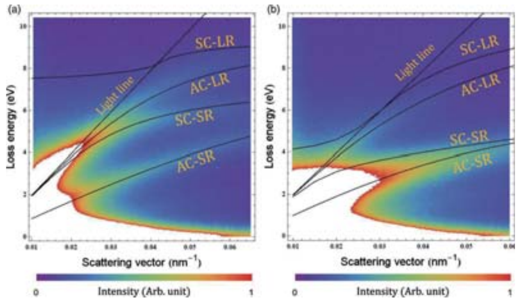


Figure 2. E–q maps obtained from (a) sample A and (b) sample B. The black curves are the dispersion curves for the coupled SPP modes calculated. The assumed structures of multilayer are AlO_x(3 nm)/Al(13 nm)/SiO_2(23 nm)/Al(13 nm)/AlO_x(3 nm) for (a) sample A and AlO_x(3 nm)/Al(7 nm)/SiO_2(61 nm)/Al(7 nm)/AlO_x(3 nm) for (b) sample B.

Control of Structural Distortions in Transition-metal Oxide Films through Oxygen Displacement at the Heterointerface

Structural distortions in the oxygen octahedral network in transition-metal oxides play crucial roles in yielding a broad spectrum of functional properties, and precise control of such distortions is a key for developing future oxide-based electronics. Here, it is shown that the displacement of apical oxygen atom shared between the octahedra at the heterointerface is a determining parameter for these distortions and consequently for control of structural and electronic phases of a strained oxide film. The present analysis by complementary annular dark- (HAADF) and bright-field (ABF) imaging in aberration-corrected scanning transmission electron microscopy (STEM) reveals that structural phase differences in strained monoclinic and tetragonal $SrRuO_3$ (SRO) films grown on $GdScO_3$ (GSO) substrates result from relaxation of the octahedral tilt, associated with changes in the in-plane displacement of the apical oxygen atom at the heterointerface. It is further demonstrated that octahedral distortions and magnetrotransport properties of the $SrRuO_3$ films can be controlled by interface engineering of the oxygen displacement. This provides a further degree of freedom for manipulating structural and electronic properties in strained films, allowing the design of novel oxide-based heterostructures.

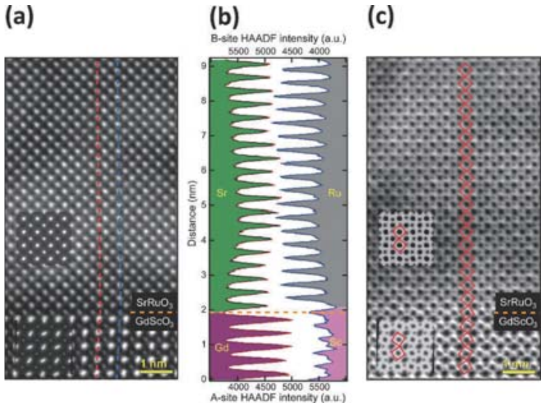


Figure 3. High-resolution cross-sectional HAADF- and ABF-STEM images of SRO/GSO heterostructure and element characterization. (a) High-resolution HAADF image of the 23 nm-thick tetragonal SRO thin film grown on the GSO substrate taken along the [001] ortho direction. Simulated HAADF images of bulk SRO and GSO with orthorhombic structures are also inserted in the image. (b) HAADF intensity profiles of A-site (left side) and B-site (right side) cations across the heterointerface. The data were collected along the red and blue dashed lines for A- and B-site cationic rows in (a), respectively. In the profiles, Sr (Z = 38), Gd (Z = 64), Ru (Z = 44), and Sc (Z = 21) atomic columns are colored in green, purple, gray, and pink, respectively. The interface position is denoted by the orange dashed line. (c) ABF image taken from the same region as the HAADF image (a). In the image, oxygen atoms are clearly visible as dark contrast, revealing the projected shape of each oxygen octahedron and the octahedral connection across the interface as indicated with red solid rectangles. The simulated ABF images of bulk SRO and GSO are also included.

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)

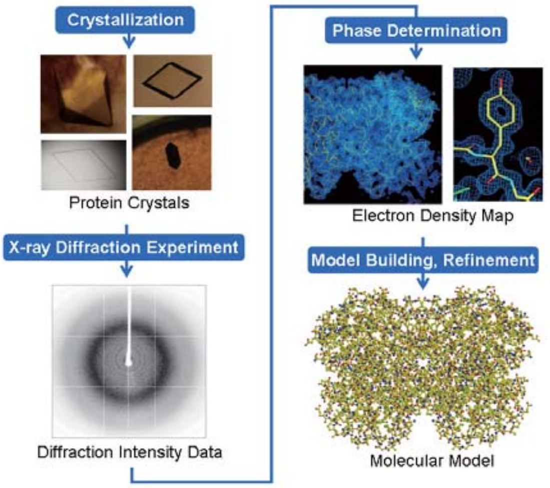
Assist Prof *
YAMAUCHI, Takae
(D Agr)

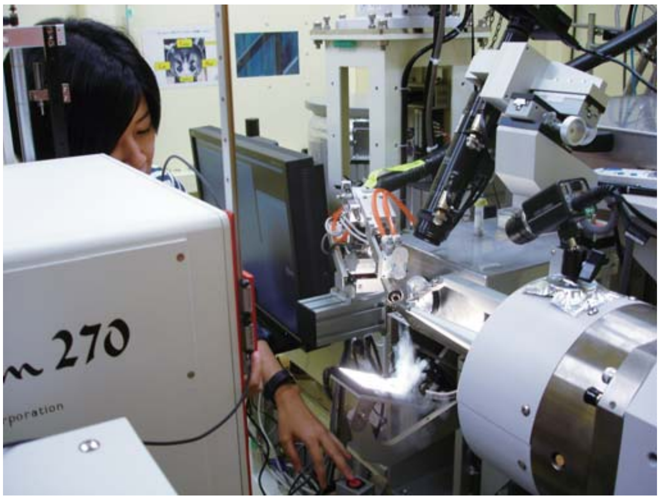
*Advanced Research Center for Beam Science, Laboratory for Structural Proteomics

Scope of Research

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

The research activities in this laboratory are performed for X-ray structural analyses of biological macromolecules and the investigation of the electronic state in materials as follows: The main subjects of the biomacromolecular crystallography are crystallographic studies on the reaction mechanism of enzymes, the relationship between the multiform conformation and the functional variety of proteins, and the mechanism of 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 spectromator with a 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 new typed X-ray spectrometer with ultra high-resolution have also been carried out.





Selected Publications

Fujii, T.; Maeda, M.; Mihara, H.; Kurihara, T.; Esaki, N.; Hata, Y., Structure of a Nif S Homologue: X-ray Structure Analysis of CsdB, an *Escherichia coli* Counterpart of Mammalian Selenocysteine Lyase, *Biochemistry*, **39,** 1263-1273 (2000).

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).

Crystal Structure Analysis of the Reductase Component of a Resorcinol Hydroxylase (GraD) in Complex with FAD

The resorcinol hydroxylase is involved in the first step of the resorcinol catabolic pathway and catalyzes hydroxylation of resorcinol to hydroxyquinol. The enzyme belongs to the two-component flavin-diffusible monooxygenase (TC-FDM) family and consists of two components: an oxygenase and a flavin reductase. It uses molecular oxygen and reduced flavin for hydroxylation and NAD(P)H for flavin reduction. The small component, flavin reductase, generates reduced flavin for the oxygenase component to oxygenate the substrate. Thus, the enzymatic reaction is separated into two steps. However, hydroxylation activity is exhibited in the cooperative presence of both the components. To understand the structural basis for the catalytic mechanism, we performed the crystal structure analysis of the reductase component (GraD) from *Rhizobium* sp. strain MTP-10005 in complex with FAD. GraD is a dimer and its subunit consists of 179 amino acid residues with the mass of 19,429 Da.

The N-terminal His-tagged GraD was used for crystallization. The protein solution consisted of 2.0 mg/ml GraD, 0.1 mM FAD and 50 mM Tris-HCl pH 8.0. Crystals with size of 0.15 mm × 0.1 mm × 0.1 mm were obtained in about 6 days by a sitting drop vapor diffusion method with a reservoir solution consisting of 100 mM sodium citrate pH 5.6, 13–16% (w/v) PEG2000, 6–9 % (v/v) 2-propanol, 10 mM dithiothreitol and 0.2 mM FAD (Figure 1). The crystals of GraD were deep yellow in color, indicated that GraD crystals contain oxidized FAD cofactor. Diffraction data were collected up to 1.8 Å resolution under cryogenic conditions at beamline NW12A, Photon Factory PF-AR, Tsukuba, Japan. The GraD crystal belongs to the tetragonal space group $P4_12_12$ with unit cell dimensions of $a = b = 77.8$ Å and $c = 124.2$ Å. Assuming that the crystal contains two subunits in the asymmetric unit, the V_M value is 2.17 Å^3/Da and a solvent content is 43%, which is acceptable for a protein crystal. The structure was determined by molecular replacement and refined at 1.8 Å resolution.

In the crystal, one homodimer exists in the asymmetric unit and each subunit binds an FAD molecule (Figure 2). The subunit consists of twelve β-strands, three α-helices and two 3_{10} helices. The core of the GraD subunit is a seven-stranded anti-parallel β-barrel capped by one α-helix. The subunit adopts a FMN-binding split barrel fold (Greek key architecture), related to the ferredoxin reductase like FAD-binding domains. The FAD molecule is located in the groove in the surface of the enzyme. The N5-atom of the isoalloxazine ring is hydrogen bonded to the hydroxyl group of the side chain of Thr50. The dimethyl benzene moiety of isoalloxazine ring is located in a hydrophobic pocket formed by hydrophobic amino acid residues which are highly conserved in flavin reductases. The O2, O4 and N3 atoms of the pyrimidine moiety of isoalloxazine ring are hydrogen bonded to backbone atoms of protein (Figure 3).

Figure 1. Crystals of the reductase component of a resorcinol hydroxylase (GraD) from *Rhizobium* sp. strain MTP-10005 in complex with FAD.

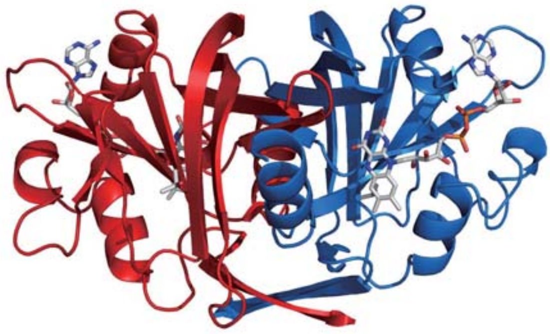


Figure 2. Dimeric molecular structure of the reductase component of a resorcinol hydroxylase (GraD) from *Rhizobium* sp. strain MTP-10005 in complex with FAD.

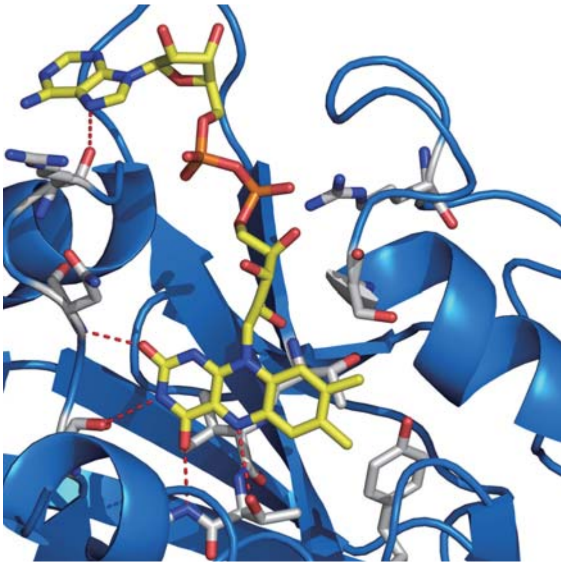


Figure 3. Structure of FAD-binding site of the reductase component of a resorcinol hydroxylase (GraD) from *Rhizobium* sp. strain MTP-10005 in complex with FAD.

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)

PD (JSPS)
ADAK, Laksmikanta
(Ph D)

Assist Techn Staff

MINAGAWA, Toshie

Assist Res Staff

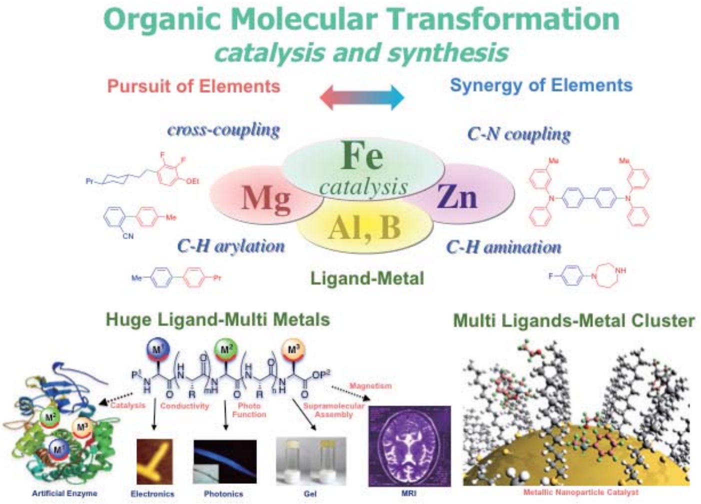
NAKAGAWA, Naohisa

Students

NAKAJIMA, Sho (D1)
YOSHIDA, Ryota (D1)
AGATA, Ryosuke (M2)
AOKI, Yuma (M2)
NISHIKORI, Tatsushi (M2)
ISHIBASHI, Kosuke (M1)
SAITO, Shota (M1)
ITO, Ran (UG)
MONDEN, Taihei (UG)

Scope of Research

Our research activity focuses on the development of new molecular transformations, which can contribute to better or ideal synthesis of functional molecules as well as to exploitation of new chemical (metal and carbon) resources. The present research subjects are (1) metal-catalyzed carbon–carbon and carbon–heteroatom bond forming reactions by using universal metals such as iron (2) development of smart materials based on synergistic effect of various metals on artificial peptides (3) development of smart metallic nanoparticle catalysts based on supramolecular approaches (4) understanding of synergistic effects of multi-element center interactions for the catalysis 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

Hashimoto, S.; Ikuta, T.; Shiren, K.; Nakatsuka, S.; Nakamura, M.; Hatakeyama, T., Triplet-Energy Control of Polycyclic Aromatic Hydrocarbons by BN Replacement: Development of Ambipolar Host Materials for Phosphorescent OLEDs, *Chem. Mater*., (in press).

Hashimoto, S.; Nakatsuka, S.; Nakamura, M.; Hatakeyama, T., Construction of a Highly Distorted Benzene Ring in a Double Helicene, Angew. *Chem. Int. Ed*., **53,** 14074-14076 (2014).

Aoki, Y.; Imayoshi, R.; Hatakeyama, T.; Takaya, H.; Nakamura, M., Synthesis of 2,7-Disubstituted 5,10-Diaryl-5,10-dihydrophenazines via Iron-catalyzed Intramolecular Ring-Closing C–H Amination, *Heterocycles*, **90,** 893-900 (2014).

Takaya, H.; Isozaki, K.; Haga, Y.; Ogata, K.; Naota, T., Synthesis and Self-Assembling Properties of Pt-Complex-Bound Oligoglutamic Acids, *Chem. Lett*., **43,** 1167-1169 (2014).

Iron-Catalyzed Intermolecular and Intramolecular C-H Amination of Diarylamines

Transition-metal-catalyzed aromatic amination is of great importance in the field of organic synthesis, pharmaceuticals, and materials science. Recently we developed an iron-catalyzed aromatic amination giving various triaryamines. Further investigation for novel reactivities of iron-catalyst in amination reactions has led us to discover the unprecedented intermolecular C-H amination of diarylamines that provides various *o*-phenylene diamines. In addition, subsequent intramolecular C–H amination of the diamine products under iron catalysis was found to furnish 5,10-diaryl-5,10-dihydrophenazine derivatives, which are highly attractive compounds in material science.

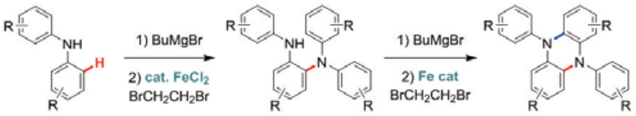


Figure 1. Iron-catalyzed intermolecular and intramolecular C-H amination of diarylamines.

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

In the past a few decades, iron-catalysts have regained much attention in cross-coupling chemistry due to their unprecedented reactivity and the practical advantages. However the mechanistic understanding remains limited because characterization of organoiron intermediates in solution has been hampered by their paramagnetic nature and instability toward air and moisture. We have succeeded in determining the solution-phase structure of organoiron species in FeBr$_2$(SciOPP)-catalyzed coupling reaction between ArMgBr and alkyl halides by using synchrotron X-ray absorption spectroscopies. XANES and EXAFS spectra demonstrated the reactions of FeBr$_2$(SciOPP) with 1.0 or 2.0 equivalents of MesMgBr in THF afforded tetrahedral FeBrMes(SciOPP) and square-planer FeMes$_2$(SciOPP), respectively. By consideration of these results with examination of their reactivities, i.e., FeMes$_2$(SciOPP) was found to react with an alkyl halide to give the corresponding coupling product and FeBrMes(SciOPP), the intermediacy of the mesityliron complexes in the FeBr$_2$SciOPP-catalyzed cross-coupling reaction.

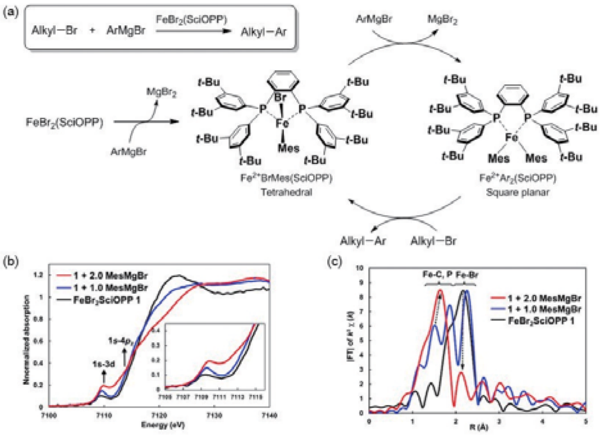


Figure 2. (a) FeBr$_2$(SciOPP)-catalyzed KTC-coupling of an arylmagnesium halide with a alkylhalide and the reaction mechanism. (b) The Fe K-edge XANES spectra and (c) the Fe K-edge EXAFS spectra: THF solutions of FeBr$_2$(SciOPP) and reaction mixtures of FeBr$_2$(SciOPP) with 1.0 and 2.0 equivalents of MesMgBr.

Supramolecular Approach for Creating Enhanced Catalysis of Metallic Nanoparticles

This project focuses on the development of highly active and selective metallic nanoparticle catalysts based on supramolecular approaches. To achieve this purpose, four key methodologies act considerably important roles: 1) creation of reaction field with advanced self-assembly, 2) design of selective molecular transformation with multi-points intermolecular interaction, 3) size selective synthesis of metallic nanoparticles, and 4) plasmonic resonance with light. We aim to create a new class of catalyst system using a range of transition metallic nanoparticles.

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)

Students

HIRAI, Kei (D3)
SEKI, Hayato (D2)
HOSAKA, Yoshiteru (D1)
GUO, Haichuan (D1)
KUROSAKI, Ryo (M2)
SATO, Riko (M2)
MANABE, Keisuke (M2)
SASAKI, Takahiro (M1)
BABA, Erina (M1)
PENG, Xiong (RS)

Scope of Research

Transition metal oxides display a wide variety of interesting and useful functional properties, including electronic conduction, superconductivity, ferroelectricity, and ferromagnetism. In fact, some of these oxides have been 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. With advanced oxide-synthesis techniques such as high-pressure synthesis and epitaxial thin film growth, we are currently exploring such functional oxides.

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

Selected Publications

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, *Nature 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. Reprts*, **1,** [27-1]-[27-4] (2011).

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

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

A Half-metallic A- and B-site-ordered Quadruple Perovskite Oxide $CaCu_3Fe_2Re_2O_{12}$ with Large Magnetization and a High Transition Temperature

Materials with spin-polarized conduction electrons are of considerable interest in magnetic and electronic materials' research and for technological applications such as spin-polarized field emission and spin-polarized tunneling devices. Transition metal oxides with an ordered double-perovskite structure $A_2BB'O_6$, where the transition metal ions B and B´ are arranged alternately in a rock-salt manner, are useful materials for spintronic applications. An important example is Sr_2FeMoO_6, which is half-metallic and shows substantial TMR at room temperature. The B-site Fe^{3+} ($3d^5$, S=5/2) and the B´-site Mo^{5+} ($4d^1$, S=1/2) spins couple antiferromagnetically, leading to ferrimagnetism.

In this study, we have explored a strategy for enhancing spintronic properties relative to double perovskites by introducing further magnetic cations that can participate in a 1:3 order at the A sites, leading to the discovery of a new A- and B-site ordered quadruple perovskite oxide with large magnetization and a high magnetic ordering temperature. We have successfully synthesized a new A- and B-site-ordered quadruple perovskite oxide, $CaCu_3Fe_2Re_2O_{12}$ (Figure 1) by a solid-state reaction at a high temperature (1400 K) and high pressure (10 GPa). The magnetic and transport property measurements and electronic structure calculation reveal that the material has spin-polarized conduction electrons and is ferrimagnetic up to 560 K. The couplings between the three magnetic cations lead to the high Curie temperature, a large saturation magnetization of 8.7 μ_B and a half-metallic electronic structure, in which only minority-spin bands cross the Fermi level, producing highly spin-polarized conduction electrons. Spin polarization is confirmed by an observed low-field magnetoresistance effect in a polycrystalline sample. Optimization of $CaCu_3Fe_2Re_2O_{12}$ and related quadruple perovskite phases is expected to produce a new family of useful spintronic materials.

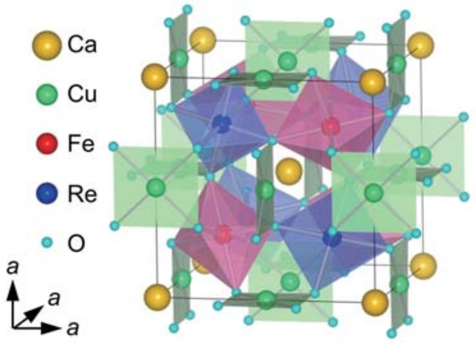


Figure 1. Crystal structure of A- and B-site ordered quadruple perovskite oxide $CaCu_3Fe_2Re_2O_{12}$.

Low-temperature Reduction in Oxide Heterostructures

Transition-metal ions in oxides can modify their oxidation states and oxygen coordinations. In iron oxides like $CaFeO_x$ the oxidation state of the Fe ions in the perovskite-structure framework changes from Fe^{2+} to Fe^{4+} when the oxygen content x changes from 2 to 3. Because oxygen ions are incorporated into and released from the perovskite structure framework during oxidation and reduction reactions, tracking structural phase associated with the change in the oxygen contents provides us an excellent platform to see oxygen-ion migration in the oxides.

Given that a topotactic reaction between $CaFeO_2$ (CFO2) and $CaFeO_{2.5}$ (CFO2.5) takes place at low temperatures below 300 °C, the low-temperature reduction and oxidation of artificial oxide heterostructures would provide us interesting information on oxygen-ion migrations. In this study we have investigated low-temperature reduction of $LaAlO_3$(LAO)/CFO2.5 heterostructures made on $SrTiO_3$ substrates by pulsed laser deposition. We found that the CFO2.5 layer in the heterostructures were reduced to a layer of CFO2 with an infinite-layer by the low-temperature CaH_2 treatment while the structure of the LAO layer remains unchanged. A key observation is that the time needed to reduce the CFO2.5 in the heterostructures to CFO2 depended on the lattice matching of the capping layer LAO to the CFO2.5 one (Figure 2). This suggests that the oxygen ions migrate through the coherently-grown strained LAO layer of the heterostructures predominantly in the out-of-plane direction and that the kinetics of the oxygen-ion migration is determined by the LAO/CFO2.5 interface. The present experimental results revealed the importance of lattice relaxation at the interface in the oxide heterostructure with regard to oxygen-ion migration behavior.

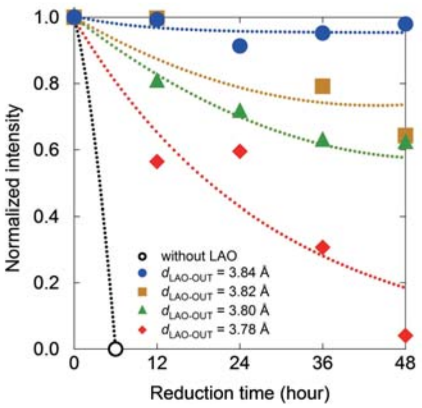


Figure 2. CFO2.5 (080) x-ray diffraction intensity as a function of reduction time for the LAO/CFO2.5 heterostructures with different lattices of the LAO capping layer. The plotted intensities are normalized by the intensity for the as-prepared heterostructure. The result without a capping layer (black) is also plotted for comparison.

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)


PD
CHANG, Yung-Hung
(D Eng)

Assist Res Staff

NAKAMURA-OGATA, Yuki

Researcher(pt)

ICHIHARA, Nobuko

Students

ISHIKI, Satoru (M2)
TAGUCHI, Hiro-omi (M2)
IIZUKA, Eisuke (M1)
TANIGAWA, Ippei (M1)
SASAKI, Daichi (UG)
TAKAHASHI, Rina (UG)

Scope of Research

This laboratory aims at establishment of 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 by using direct arylation.

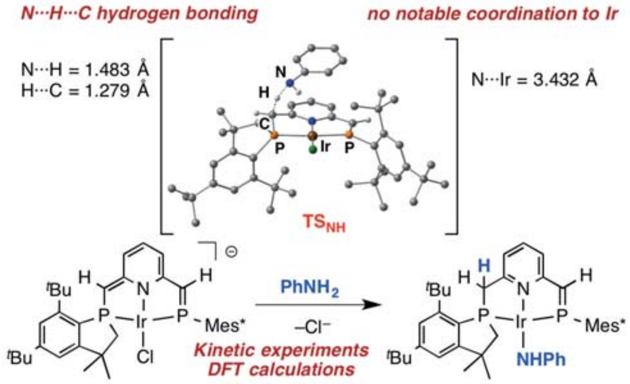
KEYWORDS
Transition Metal Complex
Homogeneous Catalyst
Reaction Mechanism
Low-coordinate Phosphorus Ligand
π-Conjugated Polymer

Selected Publications

Lin, Y.-F.; Ichihara, N.; Nakajima, Y.; Ozawa, F., Disproportionation of Bis(phosphaethenyl)pyridine Iron(I) Bromide Induced by tBuNC, *Organometallics*, (in press).
Wakioka, M.; Nakamura, Y.; Hihara, Y.; Ozawa, F.; Sakaki, S., Effects of PAr3 Ligands on Direct Arylation of Heteroarenes with Isolated $[\mathrm{Pd}(2,6\text{-}\mathrm{Me_2C_6H_3})(\mu\text{-}\mathrm{O_2CMe})(\mathrm{PAr_3})]_4$ Complexes, *Organometallics*, **33,** 6247-6252 (2014).
Takeuchi, K.; Minami, A.; Nakajima, Y.; Ozawa, F., Synthesis and Structures of Nickel Complexes with a PN-Chelate Phosphaalkene Ligand, *Organometallics*, **33,** 5365-5370 (2014).
Lin, Y.-F.; Nakajima, Y.; Ozawa, F., Reduction of an Fe(I) Mesityl Complex Induced by π-Acid Ligands, *Dalton Trans*., **43,** 9032-9037 (2014).
Chang, Y.-H.; Nakajima, Y.; Tanaka, H.; Yoshizawa, K.; Ozawa, F., Mechanism of N–H Bond Cleavage of Aniline by a Dearomatized PNP-Pincer Type Phosphaalkene Complex of Iridium(I), *Organometallics*, **33,** 715-721 (2014).
Wakioka, M.; Ichihara, N.; Kitano, Y.; Ozawa, F., A Highly Efficient Catalyst for the Synthesis of Alternating Copolymers with Thieno[3,4-c]pyrrole-4,6-dione Units via Direct Arylation Polymerization, *Macromolecules*, **47,** 626-631 (2014).

Mechanism of N–H Bond Cleavage of Aniline by a Dearomatized PNP-Pincer Type Phosphaalkene Complex of Iridium(I)

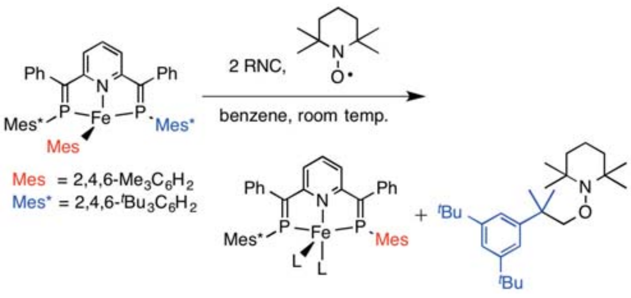
Detailed mechanistic investigations using kinetic and theoretical methods have been conducted for deprotonative N–H bond cleavage of *p*-YC$_6$H$_4$NH$_2$ (Y = H, MeO, Me, Cl, Br, NO$_2$) by [K(18-crown-6)][Ir(Cl)(PPEP*)] (**1a**) bearing a dearomatized PNP-pincer type phosphaalkene ligand (PPEP*) to afford [Ir(NHC$_6$H$_4$Y)(PPEP)] (**2**) with an aromatized ligand (PPEP). While 1a is in equilibrium with [K(18-crown-6)]Cl (**3**) and [Ir(PPEP*)] (**4**) in solution, the N–H bond cleavage proceeds via association of **1a** with aniline, where the coordination of aniline to iridium is insignificant; instead, aniline is associated with PPEP* by hydrogen bonding. In contrast, the N–H bond cleavage of ammonia proceeds via the pentacoordinate intermediate [Ir(Cl)(NH$_3$)(PPEP*)]. The difference between the N–H bond cleavage processes of aniline and ammonia is examined by DFT calculations.



Scheme 1. Mechanism of N–H bond cleavage of aniline by [Ir(Cl)(PPEP*)]–.

Reduction of an Fe(I) Mesityl Complex Induced by π-Acid Ligands

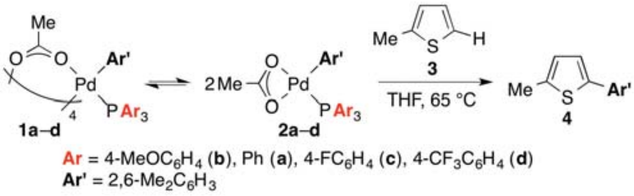
Treatment of the Fe(I) mesityl complex [Fe(Mes)(BPEP-Ph)] (BPEP-Ph = 2,6-bis[1-phenyl-2-(2,4,6-tri-*tert*-butylphenyl)-2-phosphaethenyl]pyridine) with π-acid ligands (L = CO, RNC) leads to one-electron reduction via Mes group migration from Fe to P, followed by homolytic elimination of the 2,4,6-*t*Bu$_3$C$_6$H$_2$ group, to afford Fe(0) complexes of the formula [Fe(L)$_2$(BPEP-Ph*)] (BPEP-Ph* =2-[1-phenyl-2-mesityl-2-phosphaethenyl]-6-[1-phenyl-2-(2,4,6-tri-*tert*-butylphenyl)-2-phosphaethenyl]pyridine). This reduction process is supported by radical trapping experiments and theoretical studies. The 2,4,6-*t*Bu3C$_6$H$_2$• radical is captured by 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) in high yield. DFT calculations reveal the mechanism of Mes group migration with a reasonable energy profile.



Scheme 2. One-election reduction process of [Fe(Mes)(BPEP-Ph)] induced by isocyanides.

Effects of PAr$_3$ Ligands on Direct Arylation of Heteroarenes with Isolated [Pd(2,6-Me$_2$C$_6$H$_3$)(μ-O$_2$CMe)(PAr$_3$)]$_4$ Complexes

The palladium-catalyzed direct arylation of heteroarenes with aryl halides has attracted considerable attention as a simple cross-coupling process. It is generally accepted that this catalysis proceeds via an arylpalladium carboxylate intermediate. In this study, we investigated the ligand effects on reactivity of arylpalladium acetates (**1a–d**) (Scheme 3). While **1a–d** have a tetrameric form in the solid state, they are in rapid equilibrium with the monomeric species [Pd(2,6-Me$_2$C$_6$H$_3$)(O$_2$CMe-κ^2*O*)(PAr$_3$)] (**2a–d**) in solution. Complexes **1a–d** react with thiophene **3** in THF at 65 °C to give the direct arylation product (4) in high yields. The reaction is accelerated by electron-deficient PAr$_3$ (**1b** < **1a** < **1c** < **1d**). The ligand effects are also examined by DFT calculations. Unlike the general assumption, the C–H bond cleavage process is relatively insensitive to electronic properties of PAr$_3$ ligands. Instead, the reaction of **2** invokes the C–C reductive elimination process as the rate-determining step, and the activation energy is significantly reduced by electron-deficient ligands.



Scheme 3. Ligand effects on direct arylation of 2-methylthiophene with arylpalladium acetate complexes.

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)

Assoc Prof
TAYAGAKI, Takeshi
(D Sc)

Assist Prof
IHARA, Toshiyuki
(D Sc)

PD
TEX, David Michael
(D Eng)

PD
LE, Phuong Quang
(D Eng)

PD (JSPS)
TAHARA, Hirokazu
(D Sc)

Students

OHNO, Kai (M2)
IBUKI, Hiroto (M1)
YAMADA, Takumi (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. Optical properties of semiconductor quantum nanostructures and strongly-correlated electron systems in lowdimensional materials are studied by means of space- and time-resolved laser spectroscopy. The main subjects are as follows: (1) Investigation of optical properties of single nanostructures through the development of 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

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).

Yamada, Y.; Yasuda, H.; Tayagaki, T.; Kanemitsu, Y., Temperature Dependence of Photoluminescence Spectra of Undoped and Electrondoped $SrTiO_3$: Crossover from Auger Recombination to Single-carrier Trapping, *Phys. Rev. Lett.*, **102,** [247401-1]-[247401-4] (2009).

Matsunaga, R.; Matsuda, K.; Kanemitsu, Y., Evidence for Dark Excitons in a Single Carbon Nanotube Due to the Aharonov-Bohm Effect, *Phys. Rev. Lett.*, **101,** [147404-1]-[147404-4] (2008).

Hosoki, K.; Tayagaki, T.; Yamamoto, S.; Matsuda, K.; Kanemitsu, Y., Direct and Stepwise Energy Transfer from Excitons to Plasmons in Close-packed Metal and Semiconductor Nanoparticle Monolayer Films, *Phys. Rev. Lett.*, **100,** [207404-1]-[207404-4] (2008).

Photoluminescence Blinking in CdSe/CdS Dot-in-rods

Semiconductor nanostructures have been extensively studied owing to their interest both in the fundamental physics and potential applications in optoelectronic devices. CdSe/CdS heterostructure nanocrystals with quasi-type-II band alignment provide a platform for studying the photoluminescence (PL) blinking associated with their morphologies. By using simultaneous measurements of the PL intensity, lifetime, and polarization anisotropy, we reveal the role of the electron delocalization during the blinking of single CdSe/CdS dot-in-rods. We found that a significant change in the PL polarization anisotropy distinguishes between two kinds of charged excitons with different electron delocalizations. We observed polarized PL blinking governed by the band alignments and the Coulomb interactions between the charges inside and outside the dot-in-rod.

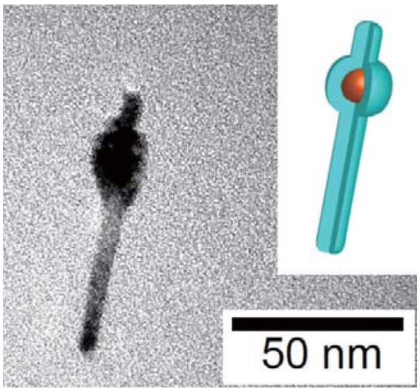


Figure 1. Transmission electron microscope image of a CdSe/CdS dot-in-rod and a schematic of its structure.

Photoluminescence and Photocurrent Imaging Spectroscopy of InAs Nanostructures

Quantum dots (QDs) have attracted attention because of their interesting physical properties and potential applications in optoelectronic devices such as light emitters and solar cells. We performed microscopic imaging of photoluminescence (PL) and photocurrent (PC) on InAs nanostructures including disklike structures (nanodisks) and QDs. The correlation between PL and PC images indicates that the major fraction of upconverted carriers originates from nanodisks. By analyzing the excitation spectra, we find evidence that nanodisks and QDs need to be spatially separated to enhance PC generation via upconversion. The simultaneous use of both QDs and nanodisks is an alternative approach to intermediate-band solar cells, where low-energy photons are upconverted in the QDs and high-energy photons are efficiently upconverted in the nanodisks, resulting in enhanced carrier generation yields. With spatially resolved upconverted PL, we show that PC generation in nanodisks is due to ejection of both electrons and holes.

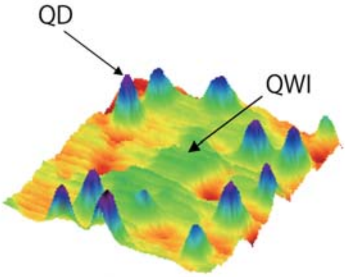


Figure 2. 3D AFM image with quantum dots (QDs) and a quantum well island (QWI) on the wetting layer of an InAs/AlGaAs layer without capping.

Optical Properties in Photonic Nanostructure Fabricated from Quantum Dot Arrays

With the reduced optical thickness of the absorber material, electromagnetic phenomena such as propagating surface plasmons, nano-optic cavities, and photonic crystals have been pursued to enhance the absorption. We demonstrated enhanced photocarrier generation using photonic nanostructures fabricated by a wet etching technique with vertically aligned quantum dots (QDs). Using photoluminescence excitation spectroscopy, we found that the photocarrier generation in Ge/Si QDs placed close to the surface is enhanced below the band gap energy of crystalline silicon. The enhancement is explained by light trapping owing to the photonic nanostructures. Electromagnetic wave simulations also indicate that the photonic nanostructure will be available to light trapping for efficient photocarrier generation.

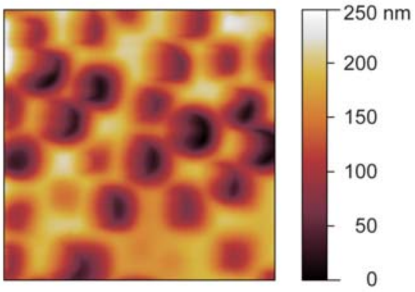


Figure 3. Atomic force microscope images of the photonic nanostructures formed by HF/HNO$_3$ etching. Images are ~1 × 1 μm in size.

Bioinformatics Center
– Chemical Life Science –

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

Prof
OGATA, Hiroyuki
(D Sc)

Assoc Prof
GOTO, Susumu
(D Eng)

Program-Specific Assist Professors

TOKIMATSU, Toshiaki (D Agr)
KOTERA, Masaaki (D Sc)

Program-Specific Researchers

MORIYA, Yuki
NAKAGAWA, Zenichi

Researcher(pt)

SHIMIZU, Yugo

Students

MIZUTANI, Sayaka (D3)
FUJITA, Megumi (D3)
NISHIMURA, Yosuke (D3)
MIHARA, Tomoko (D3)

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 integrated bioinformatics approaches. We currently focus on 1) the evolution of giant DNA viruses and their links to the origin of life, 2) the ecological and evolutionary significance of microorganisms in the oceanic ecosystem, and 3) the development of new bioinformatics methods and biological knowledge resources for biomedical and industrial applications. To fuel these research activities, we take part in several environmental sampling campaigns such as the *Tara* Oceans project. Our resource and methodological developments are accessible from the GenomeNet service to scientific communities and public.

KEYWORDS
GenomeNet
Bioinformatics
(Meta)genomics
Evolutionary Biology
Pharmacoinformatics

Selected Publications

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.*, doi: 10.1038/ismej.2014.221. (2014).

Wilson, W. H.; Gilg, I. C.; Duarte, A.; Ogata, H., Development of DNA Mismatch Repair Gene, MutS, as a Diagnostic Marker for Detection and Phylogenetic Analysis of Algal Megaviruses, *Virology*, doi, 10.1016/j.virol.2014.07.001. (2014).

Kotera, M.; Tabei, Y.; Yamanishi, Y.; Muto, A.; Moriya, Y.; Tokimatsu, T.; Goto, S., Metabolome-scale Prediction of Intermediate Compounds in Multistep Metabolic Pathways with a Recursive Supervised Approach, *Bioinformatics*, **30,** i165-i174 (2014).

Yamanishi, Y.; Kotera, M.; Moriya, Y.; Sawada, R.; Kanehisa, M.; Goto, S., DINIES: Drug-target Interaction Network Inference Engine Based on Supervised Analysis, *Nucleic Acids Res*., **42,** W39-W45 (2014).

Mizutani, S.; Noro, Y.; Kotera, M.; Goto, S., Pharmacoepidemiological Characterization of Drug-induced Adverse Reaction Clusters towards Understanding of Their Mechanisms, *Comput. Biol. Chem*., **50,** 50-59 (2014).

Functional and Evolutionary Analysis of Intragenic miRNAs in Animals

MicroRNAs (miRNAs) are short single-stranded non-coding RNAs present in diverse organisms and suppress the expression of several target genes by binding to the 3'UTR of their mRNAs. They are key regulators in gene expression networks and have influence on various genetic pathway and pathologic states in multiple diseases. Expanding repertoire of miRNAs and variation of their target sites in animal evolution are associated with major body-plan innovations. However, individual functions of most miRNAs still remain unclear.

In animal genomes, miRNAs are enriched in protein coding regions (genes), several of which are evolutionary conserved. The overlapping miRNA and gene are called as an intragenic miRNA and its host gene, respectively, and not a small number of them are transcribed as the same transcription unit, which is also indicated by a correlation of their expression levels. Thus, we hypothesized that each intragenic miRNA has a functional association with its host gene. In this study, we first collected miRNA data from a database and predicted their targets, and then performed statistical tests on two types of regulation model (Figure 1); *A. direct regulation model*, where a miRNA regulates its host gene directly, and *B. functional regulation model*, where a miRNA regulates a set of genes with the related function to its host gene. As a result, 34.9% of intragenic miRNAs in animals turned out to follow these two models.

Emergence of widely conserved miRNAs and their conserved target sites is important events in animal evolution. We detected 12 intragenic miRNA families that are specifically conserved among mammals to reveal evolutionary origin of conserved target sites (on-going, Figure 2).

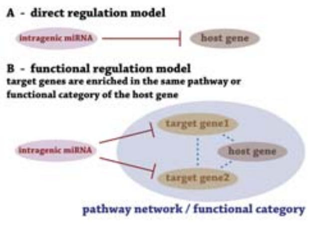


Figure 1. Two regulation models of intragenic miRNAs.

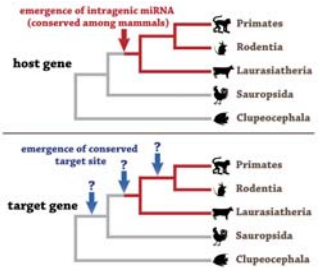


Figure 2. Emergence period of conserved target site of intragenic miRNAs that are specifically conserved among mammals.

Phylogenomics of Virus-encoded Amino Acid Metabolic Enzymes

Viruses do not encode their own translation machinery and thus depend on their hosts regarding the metabolism for protein synthesis. However, certain viruses are known to encode a few amino acid (AA) biosynthetic enzymes in their genomes. Curiously, these viral enzymes correspond to only a part of entire AA metabolic pathways, while many other enzymes are likely to be required (and supplied by their hosts) for a complete metabolism. To better understand why these viruses encode such specific AA enzymatic reactions and to clarify their evolutionary origins, we systematically identified virus-encoded AA enzymes in complete viral genomes and performed comparative genomics and phylogenetic analyses.

We searched complete viral genomes (200 bp to 2.5 Mbp) for AA metabolic genes using KAAS (KEGG Automatic Annotation Server) with cellular homologs as queries and identified 147 viral genes (32 KEGG orthologs involved in nine KEGG AA pathways) in 69 viral genomes. These viral genomes were relatively large (32 kbp to 2.5 Mbp), and the encoded viral enzymes were more widely distributed across different cellular organisms than other AA enzymes (p<0.007). Phylogenetic analyses of one of the viral ortholog groups indicate that viral homologs are distributed in two clades, being relatively similar to eukaryotic homologs than to prokaryotic ones with no clear phylogenetic affinity to the homologs from their hosts (Figure 3). We are currently undertaking network analyses and metagenomic (virome) data mining to investigate the role of these viral enzymes and to characterize the extent of this phenomenon in natural samples, eventually to get better insight into viral strategies in the control of amino acid metabolisms for their survival.

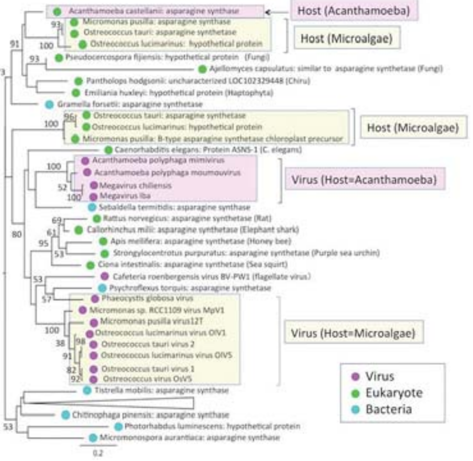


Figure 3. Maximum likelihood phylogenetic tree of viral asparagine synthases and their homologs. Thirteen viruses infecting eukaryotes including Mimivirus encode an asparagine synthase. Bootstrap values greater than 50% are shown along the branches.

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)

PD (JSPS)
ZHAO, Yang
(D Inf)

Students

NAKAJIMA, Natsu (D3)
LU, Wei (D3)
UECHI, Risa (D3)
RUAN, Peiying (D3)
HASEGAWA, Takanori (D3)
MORI, Tomoya (D3)
JIRA, Jindalertudomdee (D2)
BAO, Yu (D1)
HWANG, Jaewook (M2)
CAO, Yue (M1)
NGOUV, Hayliang (M1)

Guest Scholar

CHENG, Xiaoqing	The University of Hong Kong, China P.R., 20 May-15 August

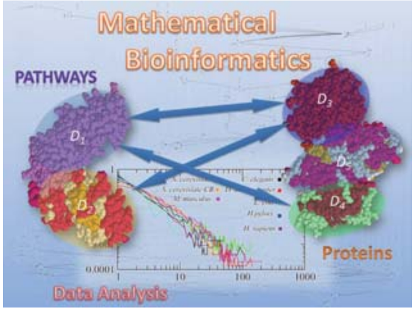
Guest Res Assoc

LIU, Liwei (Ph D)	Dalian University of Thechnology, China P.R., 1 April-31 March

Scope of Research

Due to rapid progress of the genome projects, 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 recently studying the following topics: systems biology, scalefree networks, protein structure prediction, inference of biological networks, chemo-informatics, 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.; Fukagawa, D.; Takasu, A., Efficient Exponential-Time Algorithms for Edit Distance between Unordered Trees, *Journal of Discrete Algorithms*, **25,** 79-93 (2014).
Hayashida, M.; Ruan, P.; Akutsu, T., Proteome Compression via Protein Domain Compositions, *Methods*, **67,** 380-385 (2014).
Lu, W.; Tamura, T.; Song, J.; Akutsu, T., Integer Programming-based Method for Designing Synthetic Metabolic Networks by Minimum Reaction Insertion in a Boolean Model, *PLoS ONE*, **9,** e92637 (2014).
Suzuki, M.; Nagamochi, H.; Akutsu, T., Efficient Enumeration of Monocyclic Chemical Graphs with Given Path Frequencies, *Journal of Cheminformatics*, **6,** 31 (2014).
Wang, M.; Zhao, X.-M.; Tan, H.; Akutsu, T.; Whisstock J. C.; Song, J., Cascleave 2.0, A New Approach for Predicting Caspase and Granzyme Cleavage Targets, *Bioinformatics*, **30,** 71-80 (2014).

Proteome Compression via Protein Domain Compositions

We focus on the entropy that the individual contains, and analyze domain compositions of proteins through compression of whole proteins in an organism. We suppose that a protein is a multiset of domains. Since gene duplication and fusion have occurred through evolutionary processes, the same domains and the same compositions of domains appear in multiple proteins, which enables us to compress a proteome by using references to proteins for duplicated and fused proteins. Such a network with references to at most two proteins is modeled as a directed hypergraph.

We propose a heuristic approach by combining the Edmonds algorithm with an integer linear programming, and apply our procedure to fourteen proteomes of *D. discoideum, E. coli, S. cerevisiae, S. pombe, C. elegans, D. melanogaster, A. thaliana, O. sativa, D. rerio, X. laevis, G. gallus, M. musculus, P. troglodytes, and H. sapiens*.

The compressed size using both of duplication and fusion was smaller than that using only duplication, which suggests the importance of fusion events in evolution of a proteome. In addition, we observed the difference of gene duplication rates between organisms. It is considered that gene duplication in *M. musculus and H. sapiens* tends to occur more frequently than other organisms examined in this study. Furthermore, we observed the phenomenon in several organisms that a fused gene was used in another gene fusion event again. For correlation between the compression ratio of each proteome and the phylogenetic tree, further analysis is needed. The proteome compression using domain compositions in this study can be applied to compression of protein amino acid sequences and DNA base sequences, and the compression ratio may be improved by making use of sequences included in domains as reference.

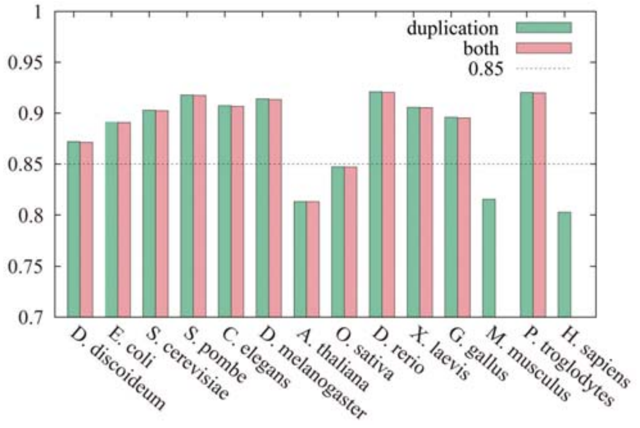


Figure 1. Results on the compression ratio by duplication rules and by both duplication and fusion rules.

Integer Programming-Based Method for Designing Synthetic Metabolic Networks by Minimum Reaction Insertion in a Boolean Model

In this study, we consider the Minimum Reaction Insertion (MRI) problem for finding the minimum number of additional reactions from a reference metabolic network to a host metabolic network so that a target compound becomes producible in the revised host metabolic network in a Boolean model. Although a similar problem for larger networks is solvable in a flux balance analysis (FBA)-based model, the solution of the FBA-based model tends to include more reactions than that of the Boolean model. However, solving MRI using the Boolean model is computationally more expensive than using the FBA-based model since the Boolean model needs more integer variables. Therefore, in this study, to solve MRI for larger networks in the Boolean model, we have developed an efficient Integer Programming formalization method in which the number of integer variables is reduced by the notion of feedback vertex set and minimal valid assignment. As a result of computer experiments conducted using the data of metabolic networks of E. coli and reference networks downloaded from the Kyoto Encyclopedia of Genes and Genomes (KEGG) database, we have found that the developed method can appropriately solve MRI in the Boolean model and is applicable to large scale-networks for which an exhaustive search does not work. We have also compared the developed method with the existing connectivity-based methods and FBA-based methods, and show the difference between the solutions of our method and the existing methods. A theoretical analysis of MRI is also conducted, and the NP-completeness of MRI is proved in the Boolean model. Our developed software is available at "http://sunflower.kuicr.kyoto-u.ac.jp/~rogi/minRect/minRect.html."

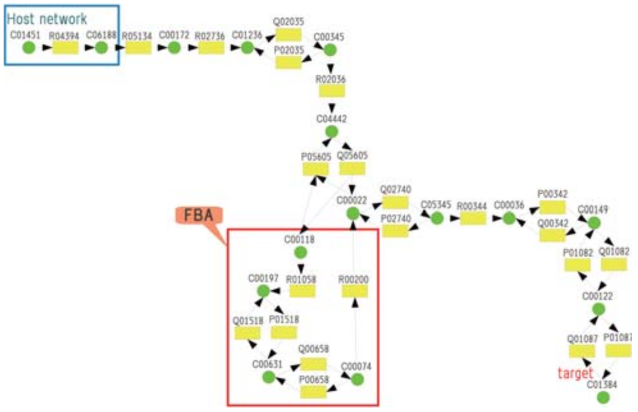


Figure 2. The result of the computer experiment where the host network is E.coli and the target compound is butanol.

Bioinformatics Center
– Bio-knowledge Engineering –

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

Prof
MAMITSUKA, Hiroshi
(D Sc)

Assist Prof
KARASUYAMA, Masayuki
(D Eng)

Assist Prof
NGUYEN, Hao Canh
(Ph D)

Proj Res
NATSUME, Yayoi
(D Agr)

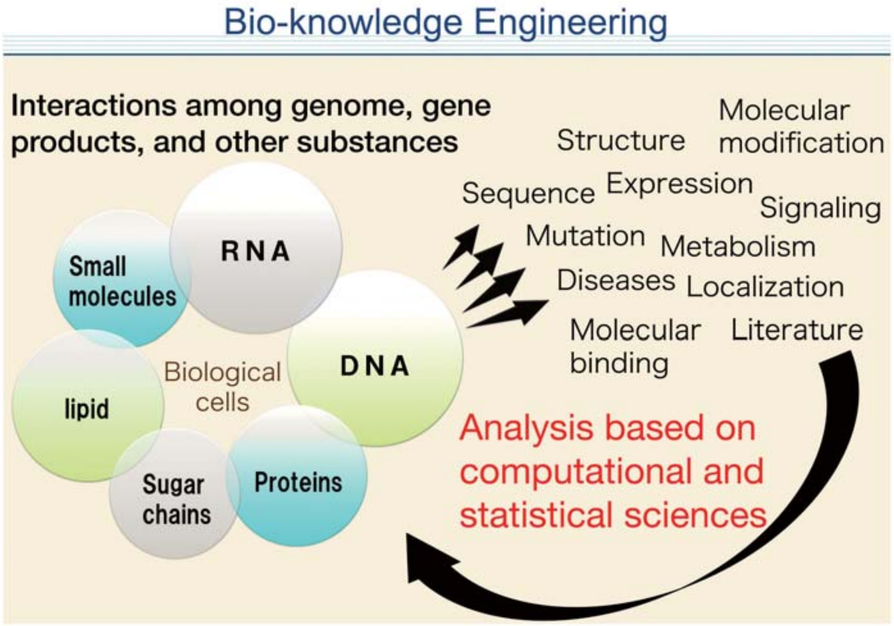
Students

MOHAMED, Ahmed Mohmed (D3)
YAMAGUCHI, Shigeru (D2)
YOTSUKURA, Sohiya (D2)

Scope of Research

We are interested in graphs and networks in biology, chemistry and medical sciences, which include 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 developed techniques to real data to demonstrate the performance of the methods and further to find new scientific insights.

KEYWORDS
Bioinformatics
Computational Genomics
Data Mining
Machine Learning
Systems Biology



Selected Publications

Karasuyama, M.; Mamitsuka, H., Manifold-based Similarity Adaptation for Label Propagation, *Proceedings of the Twenty-Seventh Annual Conference on Neural Information Processing Systems (NIPS 2013)*, 1547-1555 (2013).

Karasuyama, M.; Mamitsuka, H., Multiple Graph Label Propagation by Sparse Integration, *IEEE Transactions on Neural Networks and Learning Systems*, **24 (12),** 1999-2012 (2013).

Nguyen, C. H.; Wicker, N.; Mamitsuka, H., Selecting Graph Cut Solutions via Global Graph Similarity, *IEEE Transactions on Neural Networks and Learning Systems*, **25 (7),** 1407-1412 (2014).

Mohamed, A.; Hancock, T.; Nguyen, C. H.; Mamitsuka, H., NetPathMiner:R/Bioconductor Package for Network Path Mining through Gene Expression, *Bioinformatics*, **30 (21),** 3139-3141 (2014).

Sparse Multiple Graph Integration for Label Propagation

Predicting labels on a network is an important topic in systems biology and other fields of structured data analysis. For example, the connectivity structure of protein-protein interaction networks (Figure 1) is informative for function category estimation of proteins. A common approach is to propagate information of known function categories to other proteins, of which function categories are unknown, through network connections. In machine learning, this is a problem called *graph-based semi-supervised learning*, because a network can be represented as a "graph" mathematically, and the propagation approach is called "label propagation".

The usefulness of the label propagation algorithms has been demonstrated so far, but their performance highly depends on the way of generating the input graph. For example, in the protein function prediction, various information sources are available such as gene expression, gene sequences and subcellular localization, which can be all given as graphs. We however cannot see the most important graph for prediction. We propose a new approach for the issue of integrating multiple graphs under the label propagation framework.

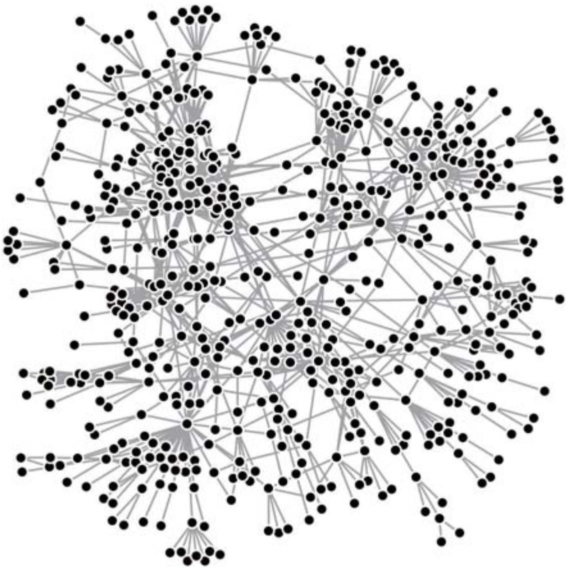


Figure 1. The example of a protein-protein interaction network. Each node corresponds to a protein, and connected protein pairs interact each other.

As already done by the most existing methods, our approach also combines multiple graphs linearly and estimates their weight coefficients. However, our unique property is the sparsity of graph weights. That is, graph weights of our approach can be sparse, meaning that only a part of weights has non-zero values and the rest are equal to exactly 0. This important property provides two advantages. The first advantage is that eliminating irrelevant or noisy graphs in integrating multiple graphs can improve the classification performance. Conventional approaches however have cases of assigning non-zero weights to graphs which are irrelevant to classification (we define such graphs as irrelevant graphs), by which prediction performance can be deteriorated, since irrelevant graphs are kept as the input. On the other hand, our sparseness property allows us to eliminate irrelevant graphs completely because their weights are estimated at zero. The second advantage is that sparse weight coefficients allow to identify the graphs which are important (or not needed) for classification easily. Furthermore, our formulation can provide a clear interpretation of the mechanism of sparsity, and it also offers a kind of grouping effect, which is similar to that given by the standard sparse statistical model called elastic net.

We verified the effectiveness of our approach through synthetic and real-world datasets compared to some other existing approaches (e.g., Figure 2).

Reference

[1] Karasuyama, M.; Mamitsuka, H., Multiple Graph Label Propagation by Sparse Integration, *IEEE Transactions on Neural Networks and Learning Systems*, **24(11),** 1999-2012 (2013).

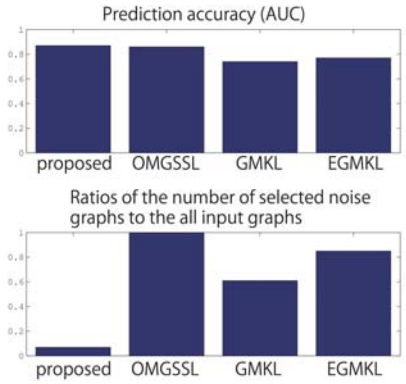


Figure 2. Performance comparison on a protein function prediction. (Top) Prediction accuracy (AUC) of our proposed method and other existing methods. We see that our approach has the highest AUC value in this case. (Bottom) Ratios of the number of selected noise graphs to the all input graphs. In this experiment, we added artificial noise graphs as input graphs. Our approach appropriately removes those noise graphs compared to the other methods.

Endowed Research Section
– Nano-Interface Photonics –
(SEI Group CSR Foundation)

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

Program-Specific Assoc Prof
YAMADA, Yasuhiro
(D Sc)

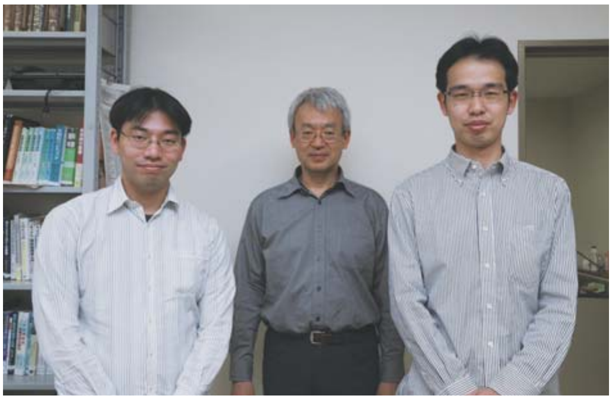
Program-Specific Assist Prof
OKANO, Makoto
(D Sc)

Prof (Supporting Factulty Member)
KANEMITSU, Yoshihiko
(D Eng)

Scope of Research

Nanostructured materials are one class of the most promising candidates for future device materials because of their unique electronic and optical properties beyond the bulk crystals. Our research aim is to open up new research fields of nanomaterials science, by focusing on nano-interface as a platform to develop novel optical functionalities. We study optical properties of semiconductor nanomaterials by means of time- and spaceresolved spectroscopy, leading to new solar energy conversion technologies. The main subjects are (1) photocarrier dynamics and photovoltaic effects in transition metal oxides and (2) ultrafast carrier dynamics and unique optical properties of one-dimensional materials.

KEYWORDS
Nano-interface
Photovoltaic Science
Solar Energy Conversion
Laser Spectroscopy



Selected Publications

Okano, M.; Sakamoto, M.; Teranishi T.; Kanemitsu, Y., Assessment of Hot-Carrier Effects on Charge Separation in Type-II CdS/CdTe Heterostructured Nanorods, *J. Phys. Chem. Lett.*, **5,** 2951-2956 (2014).

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).

Okano, M.; Takabayashi, Y.; Sakurai, T.; Akimoto, K.; Shibata, H.; Niki, S.; Kanemitsu, Y., Slow Intraband Relaxation and Localization of Photogenerated Carriers in $CuIn_{1-x}GaxSe_2$ Thin Films: Evidence for the Existence of Long-lived High-energy Carriers, *Phys. Rev. B*, **89,** [195203-1]-[195203-6] (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]-[047403-4] (2013).

Yamada, Y.; Kanemitsu, Y., Determination of Electron and Hole Lifetimes of Rutile and Anatase TiO_2 Single Crystals, *Appl. Phys. Lett.*, **101,** [133907-1]-[133907-4] (2012).

Topics

Nanointerface as a Platform to Develop Novel Optical Functionalities

Solar energy conversion is a key technology to solve the world-wide and emergent energy problems, such as fossil fuel exhaustion and global warming. However, the conversion efficiency of practically used solar cell is still less than 30%, and thus there is a compelling need for the development of highly-efficient and cost-effective solar cells.

Nanostructured materials, such as nanoparticles, nanotubes, and nanowires, are the most promising candidates for the next-generation solar cells because of their unique electronic and optical properties beyond the bulk crystals. For example, plasmon resonance in metal nanoparticles enhances the light absorption efficiency, and carrier multiplication due to strong carrier confinement and Coulomb interactions in the semiconductor nanoparticles can improve the light conversion efficiencies.

To take more advantages of nanomaterials, it is significant to understand the role of their surface and interface. Nanomaterials have large surface-to-volume ratios, and thus their optoelectronic properties are strongly affected by the surrounding materials and interface states. This indicates that the novel optoelectronic properties can be developed by controlling the nano-interface. Moreover, in the practical nanomaterial-based devices, the energy and carrier transport processes are dominated by the characteristics of the interface between nanomaterials.

In our research group, we focus on such nano-interface as a platform to develop novel optical functionalities. Using advanced time- and space-resolved spectroscopy, we study the optical properties of unique nanomaterials and their nanocomposites. Through the studies on the nano-interface photonics, we aim to open up new research fields of nanomaterials science, leading to new solar energy conversion technology.

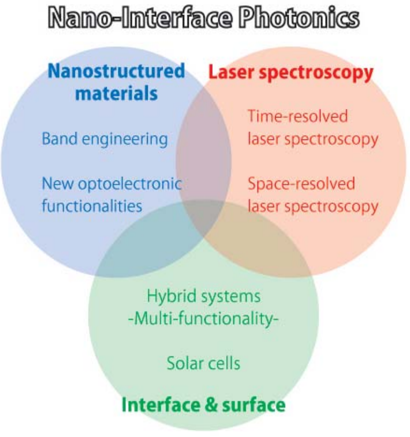


Figure 1.

Assessment of Hot-carrier Effects on Charge Separation in Type-II CdS/CdTe Heterostructured Nanorods

Recently, hot carrier effects on charge separation at heterointerfaces have been of great interest from the viewpoints of fundamental physics and potential device applications. Semiconducting heterostructured nanocrystals provide an excellent platform for studying the influence of hot-carriers on charge separation because of their long lifetimes. We studied the charge-separation dynamics in type-II CdS/CdTe heterostructured nanorods (HNRs) revealed by femtosecond transient-absorption (TA) measurements with a broad-band white-light probe. Under selective excitation of the CdTe segment, bleaching signals at the band gap energy of CdS were clearly observed with a rise component on a subpicosecond time scale, which indicates efficient electron transfer from CdTe to CdS. The TA spectra and dynamics due to CdS bleaching in CdS/CdTe HNRs were insensitive to the pump energy, in stark contrast to those in directly photoexcited CdS NRs. Based on the dynamical analysis and the TA spectral change, we conclude that a major portion of hot electrons rapidly thermalizes to the bottom of the conduction band, after which electron transfer from CdTe to CdS takes place.

Photocarrier Recombination Dynamics in Halide Perovskite Semiconductor $CH_3NH_3PbI_3$

Lead halide-based perovskite semiconductor $CH_3NH_3PbX_3$ (X=Cl, Br, and I) recently attracts growing interests because of its high performance as a solar-cell material. The power conversion efficiency of perovskite solar cells currently attains nearly 20 %. We studied the photocarrier recombination processes in $CH_3NH_3PbX_3$ thin films by means of time-resolved photoluminescence and transient absorption measurements at room temperature. The photocarrier dynamics are well described by considering single-carrier trapping and electron–hole radiative recombination. This result provides clear evidence that the photoexcited electrons and holes behave as free carriers and do not form exciton at room temperature. Our findings provide useful information about the dynamical behaviors of photoexcited carriers, which is needed for developing high-efficiency perovskite solar cells.

HAKUBI RESEARCHERS' ACTIVITIES IN ICR

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

Research Topic

Algorithmic Graph Theory with Applications to Bioinformatics

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

Host Laboratory Laboratory of Mathematical Bioinformatics

Host Professor AKUTSU, Tatsuya

Outline of Research

One of my research topics this year is fast matrix multiplication.Given two square matrices A and B of size (n x n) with nonnegative integer entries, the naive algorithm for computing the matrix product AB runs in O(n^{3}) time. There exist algorithms that run in substantially subcubic time, e.g., a very recent one due to F. Le Gall uses O(n^{2.3728639}) time, and a major open question in Theoretical Computer Science is whether it can be done in quadratic time. We have developed a new technique based on interpreting matrices as 3D histograms. To multiply A and B, we decompose their 3D histograms into 3D blocks which are then manipulated in a pairwise manner using the interval tree data structure. This leads to an O*(n^{2} + rs)-time algorithm for matrix multiplication, where r and s denote the minimum number of 3D blocks into which A and B can be partitioned, respectively. In other words, whenever A and B admit a partition into a small number of 3D blocks, our algorithm is very efficient.

ACTIVITIES OF JOINT USAGE/RESEARCH CENTER

JURC Cooperative Research Subjects 2014

(1 April 2014 ~ 31 March 2015)

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

Neutron Imaging with Small Pulse Neutron Source
OTAKE, Yoshie, Riken Center for Advanced Photonics
Host in JURC IWASHITA, Yoshihisa

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

Mechanistic Study for Homogeneous Catalytic Hydrogenation of Unsaturated Hydrocarbons by Fe and Ru Complexes Having Disilametallacycle Fragments: The Role of Silane–Ligand toward H_2 Activation
TAHARA, Atsushi, Institute for Materials Chemistry and Engineering (IMCE), Kyushu University
Host in JURC OZAWA, Fumiyuki

Development of Transition-Metal Catalysts Ligated by Silyl-Perturbed Low-Coordinated Phosphines
ITO, Shigekazu, Graduate School of Science and Engineering, Tokyo Institute of Technology
Host in JURC OZAWA, Fumiyuki

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

Study for Dynamical Screening in Carbon Nanotubes and Quantum Wires
SUZUURA, Hidekatsu, Graduate School of Engineering, Hokkaido University
Host in JURC KANEMITSU, Yoshihiko

Development of Gold Nanoparticle 2D-Arrays for Plasmon-Enhanced Photochemical Reactions
MIKI, Kazushi, Polymer Materials Unit, National Institute for Materials Science
Host in JURC ISOZAKI, Katsuhiro

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

Probabilistic Methods for Analysis on Protein Interaction Networks
MARUYAMA, Osamu, Institute of Mathematics for Industry, Kyushu University
Host in JURC AKUTSU, Tatsuya

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

Bioinformatics with Auxiliary Biological Knowledge
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

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

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

Synthesis of Novel Photoacoustic Contrast Agent Using Functional Metal Nanoparticles
ISHIHARA, Miya, National Defense Medical College
Host in JURC TERANISHI,Toshiharu

Chitin Nanofiber Polymer Brush for Novel Soft Materials via Self-assemble Approach
IFUKU, Shinsuke, Graduate School of Engineering, Tottori University
Host in JURC TSUJII, Yoshinobu

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

Novel Scaffold Using Short Fibers Coated with Concentrated Polymer Brushes
YOSHIKAWA, Chiaki, World Premier International (WPI) Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS)
Host in JURC TSUJII, Yoshinobu

Development of Novel Linear π-Extended Molecules Exhibiting Fluorescence Directed toward Electronic Materials
SUGA, Seiji, Graduate School of Natural Science and Technology, Okayama University
Host in JURC MURATA, Yasujiro

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

Studies on Highly Efficient and Colorful Dye-sensitized Solar Cell Device Using Designed Anthocyanin
YOSHIDA, Kumi, Department of Complex Systems Science, Guraduate School of Information Science, Nagoya University
Host in JURC MURATA, Yasujiro

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

Study on Size- and Shape-dependent Hydrogen Storage in Pd Nanoparticles by Time-resolved Synchrotron XRD Technique
YAMAUCHI, Miho, International Institute for Carbon-Neutral Energy Research, Kyushu University
Host in JURC TERANISHI,Toshiharu

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

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

Device Developments for Fundamental Physics with Neutrons
KITAGUCHI, Masaaki, Graduate School of Science, Nagoya University
Host in JURC IWASHITA, Yoshihisa

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

X-ray Analysis of Structure-Function Relationship of Resorcinol Monooxygenase
OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai 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 HATA, Yasuo

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

Spin Dynamics in Group-IV Semiconductor Nanostructures
FUKATSU, Susumu, Graduate School of Arts and Science, The University of Tokyo
Host in JURC TAYAGAKI, Takeshi

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

Construction of Functional Molecular Organization by Supramolecular Chemistry
HAINO, Takeharu, Graduate School of Science, Hiroshima University
Host in JURC YAMAGO, Shigeru

Mechanistic Studies on the Iron-catalyzed Carbon-carbon Bond Forming Reactions: Exploring Comprehensive Approach for Solution Phase Determination of Catalytic Intermediates
NAGASHIMA, Hideo, Institute for Materials Chemistry and Engineering, Kyushu University
Host in JURC NAKAMURA, Masaharu

Synthesis of Sugar-Phenyleneethynylene Conjugates and Their Application to Fluorescent Probe
ORITA, Akihiro, Department of Applied Chemistry, Okayama University
Host in JURC NAKAMURA, Masaharu

Development of Ruthenium-Complex-Bound Amino Acids and Peptides for Oxidative Degradation of Wooden Biomasses
WATANABE, Takashi, Research Institute for Sustainable Humanosphere, Kyoto University
Host in JURC NAKAMURA, Masaharu

Development of Fluorescent Organosilicon Compounds and Elucidation of Emission Mechanism
MAEDA, Hajime, School of Chemistry, College of Science and Engineering, Kanazawa University
Host in JURC TOSHIMITSU, Akio

Synthesis of Polysubsitututed Carbon Frameworks via Selenation of Various Compounds Using Elemental Selenium
SHIBAHARA, Fumitoshi, Faculty of Engineering, Gifu University
Host in JURC TOSHIMITSU, Akio

Improvement of Metabolic and Physiological Potential Evaluator (MAPLE)
TAKAMI, Hideto, Institute of Biogeoscience, Japan Agency for Marine-Earth Science and Technology
Host in JURC GOTO, Susumu

Development of Organic-Inorganic Hybrid Polymers for Ambipolar Solar Cells
OKUBO, Takashi, Department of Chemistry, Kinki University
Host in JURC WAKAMIYA, Atsushi

Fabrication of Oxide Glass Phosphor Exhibiting Radiosensitivity
YANAGIDA, Takayuki, Kyushu Institute of Technology
Host in JURC MASAI, Hirokazu

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

Synthesis, Structure, Photophysical, and Electronic Properties of Partially Overlapped Carbazolophane-Polymers
TANI, Keita, Division of Natural Science, Osaka Kyoiku University
Host in JURC TSUJII, Yoshinobu

Extensional Rheology and Self-Healing of Dynamic Network
NORO, Atsushi, Graduate School of Engineering, Nagoya University
Host in JURC MATSUMIYA, Yumi

Constraint Release Mechanism in Monodisperse Entangled Systems of Star Polymers
INOUE, Tadashi, Graduate School of Science, Osaka University
Host in JURC MATSUMIYA, Yumi

Theoretical Analysis of Dielectric Relaxation of Polymer Melts Under Fast Flow
UNEYAMA, Takashi, Division of Natural Sciences, Graduate School of Natural Science and Technology, Kanazawa University
Host in JURC MATSUMIYA, Yumi

Colloidal Crystallization and Glass Transition 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 Carbxylic Acid
KAWAGUCHI, Tatsuya, Graduate School of Science, Osaka University
Host in JURC KANAYA, Toshiji

A Formation Process of the Polymer Blend Ultra Thin Films during the Spin-coating with Using the Time-resolved Grazing Incidence Small Angle X-ray Measurement
KAWAI, Takahiko, School of Science and Technology, Gunma University
Host in JURC KANAYA, Toshiji

A Study on Intermolecular Atomic Contacts Involving Chalcogen Atoms in Organic Crystals
TSUZUKI, Seiji, Nanosystem Research Institute, The National Institute of Advanced Industrial Science and Technology (AIST)
Host in JURC SATO, Naoki

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

Multinuclear-NMR-study for Morphology Control of Alternating Metal-oxo Oligomers
TAKAHASHI, Masahide, Graduate School of Engineering, Osaka Prefecture University
Host in JURC KAJI, Hironori

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

Characterization of Amphiphilic Compounds Involving Gluconic Acid and Perfluoroalkyl Groups
YAMADA, Norihiro, Graduate School of Education, Chiba University
Host in JURC HASEGAWA, Takeshi

Correlation between Structure of Periodic Metal Nanoparticle Arrays and Intensity of Raman Scattering from Adsorbed Molecules
SHIMADA, Toru, Faculty of Education, Hirosaki University
Host in JURC HASEGAWA, Takeshi

Development of Artificial Proteins That Target Metastable DNA Structures in Trinucleotide Repeats
HAGIHARA, Masaki, Graduate School of Science and Technology, Hirosaki University
Host in JURC IMANISHI, Miki

Delivery of Therapeutic Peptide for Hyperuricemia Using Octa-arginine Peptide
TANAKA, Gen, School of Medicine, Kyorin University
Host in JURC FUTAKI, Shiroh

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 Novel Gene Therapy Using Zinc Finger Proteins
NOMURA, Wataru, Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University
Host in JURC IMANISHI, Miki

Electrical Property of the Fine Bubbles and Ion Uptake Efficiency of Agricultural Crops
NIHEI, Naoto, Graduate School of Agricultural and Life Sciences, The University of Tokyo
Host in JURC TOKUDA, Yomei

Complementary Analyses of Water Structures in Biological Systems by Broadband Dielectric Spectroscopy with Other Observation Techniques
YAGIHARA, Shin, Department of Physics, School of Science, Tokai University
Host in JURC ASAMI, Koji

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

Development of Methods to Measure Four Wave-mixing Process in Vacuum
HONMA, Kensuke, Graduate School of Science, Hiroshima University
Host in JURC SAKABE, Shuji

Fabrication and Properties of Room Temperature-driven Nanocluster Single-Electron Transistor
MAJIMA, Yutaka, Materials & Structures Laboratory, Tokyo Institute of Technology
Host in JURC TERANISHI,Toshiharu

Study for Tunnel Magnetoresistive Effect and Local Magnetism of Magnetic Tunnel Junctions Using Co_2MnSn Heusler Alloy Electrodes Prepared by Atomically-controlled Alternate Deposition
TANAKA, Masaaki, Department of Engineering Physics, Electronics and Mechanics, Nagoya Institute of Technology
Host in JURC ONO, Teruo

Metastable Bound State between Domain Walls in Asymmetric Co/Ni Nanowire
NAKATANI, Yoshinobu, Department of Communication Engineering and Informatics, The University of Electro-Comuunications
Host in JURC ONO, Teruo

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

Dynamics of the Transcription Factor ARR1 Responding to Cytokinin
KIM, Jong-Myong, Plant Science Center, RIKEN
Host in JURC AOYAMA, Takashi

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

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

Chemical Biology on Novel Lipid Modification Control
YOSHIDA, Minoru, RIKEN
Host in JURC UESUGI, Motonari

Exploration of Pyroelectricity in Charge-ordered Perovskite
TAKAHASHI, Ryota, Institute for Solid State Physics, The University of Tokyo
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

Bulk Heterojunction 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

Fusion of Structural Control and Dynamics Evaluation Aiming at Revealing Electrical Property of Organo-Metal Perovskite Single Crystal
SAEKI, Akinori, Graduate School of Engineering, Osaka University
Host in JURC WAKAMIYA, Atsushi

Analysis on the Dynamic Behavior of Cesium Ions in Soils Using Solid State NMR
FUJIMURA, Shigeto, NARO Tohoku Agricultural Research Center
Host in JURC TOKUDA, Yomei

Enzymatic Production of Chiral Amine Compounds
MIHARA, Hisaaki, Department of Biotechnology, College of LifeSciences, Ritsumeikan University
Host in JURC KURIHARA,Tatsuo

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

Intense THz Emission for Nonlinear Interaction Physics
NAGASHIMA, Takeshi, Institute of Laser Engineering, Osaka University
Host in JURC HASHIDA, Masaki

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

Control of Magnetism in Metals
CHIBA, Daichi, Department of Engineering, The University of Tokyo
Host in JURC ONO, Teruo

Development of Cystine/Glutamate Antiporter xCT Inhibitors
SATO, Hideyo, Faculty of Agriculture, Yamagata University
Host in JURC HIRATAKE, Jun

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

SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

Structural Elucidation of Extracellular Matrices Using Mass Spectrometry
NOMIZU, Motoyoshi, The School of Pharmacy, Tokyo University of Pharmacy and Life Sciences
Host in JURC FUTAKI, Shiroh

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

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

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

Study on the Chemical Bonding of Hypervalent Organotelluriums Using Precise X-Ray Analysis
MINOURA, Mao, Department of Chemistry, Rikkyo University
Host in JURC TOKITOH, Norihiro

Analysis of Bonding State of High Coordinate Compounds of Main Group Elements by X-Ray Diffraction Method
HASHIZUME, Daisuke, Center for Emergent Matter Science, RIKEN
Host in JURC TOKITOH, Norihiro

Synthesis of Heteroatom Compounds with Exotic Structures and Their Structures and Properties
SAITO, Masaichi, Department of Chemistry, Graduate School of Science and Engineering, Saitama University
Host in JURC TOKITOH, Norihiro

Synthesis and Structure of Main Group Element-Protected Metal Nanoparticles
FUJIHARA, Hisashi, Department of Chemistry, Fuculty of Science and Engineering, Kinki University
Host in JURC TOKITOH, Norihiro

Study of High Photonic Density Nano-Cavity by Electron Probe Spectroscopy
YAMAMOTO, Naoki, Quantum Nanoelectronics Research Center, Tokyo Institute of Technology
Host in JURC KURATA, Hiroki

The Mechanism of Chain Polymerization of a Diacetylene Compound 10,12-Pentacosadiyn-1-ol Molecular Layers Adsorbed on Graphite Studied by STM
TAKAJO, Daisuke, Graduate School of Science, Osaka University
Host in JURC KURATA, Hiroki

Fabrication of Metal Nano-ring by Soft-template Method
KAWAI, Takeshi, Faculty of Engineering, Tokyo University of Science
Host in JURC KURATA, Hiroki

Crystal Structures of *Peri*-aroylnaphthalene Compounds with Restricted Molecular Alignment of Aroyl Groups
OKAMOTO, Akiko, Department of Organic and Polymer Materials Chemistry, Tokyo University of Agriculture and Technology
Host in JURC ISOZAKI, Katsuhiro

High-resolution Mass Spectrometry of Magic Metal Clusters
NEGISHI, Yuichi, Department of Applied Chemistry, Tokyo University of Science
Host in JURC TAKAYA, Hikaru

SUBJECTS ENCOURAGING JOINT PROGRAM

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

The 10th International Workshop for East Asian Young Rheologists
TAKAHASHI, Yoshiaki, Institute for Materials Chemistry and Engineering, Kyushu University
Host in JURC WATANABE, Hiroshi

JURC Publications (Selected Examples)

(until 31 May 2014)

Development of a Novel Nanoparticle by Dual Modification with the Pluripotential Cell-Penetrating Peptide PepFect6 for Cellular Uptake, Endosomal Escape, and Decondensation of an siRNA Core Complex

Mitsueda, A.; Shimatani, Y.; Ito, M.; Ohgita, T.; Yamada, A.; Hama, S.; Gräslund, A.; Lindberg, S.; Langel, Ü.; Harashima, H.; Nakase, I.; Futaki, S.; Kogure, K., *Biopolymers*, **100,** 698-704 (2013).

Abstract

Development of novel devices for effective nucleotide release from nanoparticles is required to improve the functionality of nonviral delivery systems, because decondensation of nucleotide/polycation complexes is considered as a key step for cytoplasmic delivery of nucleotides. Previously, PepFect6 (PF6) comprised chloroquine analog moieties and a stearylated cell-penetrating peptide to facilitate endosomal escape and cellular uptake, respectively, was developed as a device for efficient siRNA delivery. As PF6 contains bulky chloroquine analog moieties, the polyplexes are expected to be loose structure, which facilitates decondensation. In the present study, siRNA was electrostatically condensed by PF6, and the PF6/siRNA complexes were coated with lipid membranes. The surface of the nanoparticles encapsulating the PF6/siRNA core (PF6-NP) was modified with PF6 for endosomal escape (PF6/PF6-NP). The RNAi effect of PF6/PF6-NP was compared with those of stearylated cell-penetrating peptide octaarginine (R8)-modified PF6-NP, R8-modified nanoparticles encapsulating the R8/siRNA core (R8-NP) and PF6-modified R8-NP. Nanoparticles encapsulating the PF6 polyplex, especially PF/PF-NP, showed a significant knockdown effect on luciferase activity of B16-F1 cells stably expressing luciferase. siRNA was widely distributed within the cytoplasm after transfection of the nanoparticles encapsulating the PF6 polyplex, while siRNA encapsulated in the R8-presenting nanoparticles was localized within the nuclei. Thus, the siRNA distribution was dependent on the manner of peptide-modification. In conclusion, we have successfully developed PF6/PF6-NP exhibiting a potent RNAi effect resulting from high cellular uptake, efficient endosomal escape and decondensation of the polyplexes based on the multifunctional cell penetrating peptide PF6. PF6 is therefore a useful pluripotential device for siRNA delivery.

Infrared Spectroscopic Study of Stereo-controlled Poly(*N*-isopropylacrylamide) with an Extended Chain Conformation Induced by Adsorption on a Gold Surface

Shimoaka, T.; Rikiyama, K.; Katsumoto, Y.; Hasegawa, T., *Anal. Bioanal. Chem.*, **405,** 9411-9418 (2013).

Abstract

Poly(*N*-isopropylacrylamide) (PNiPAM) compounds with various diad tacticities were prepared, and the molecular interaction properties in a thin film deposited on a gold surface were analyzed using infrared spectroscopy. The intramolecular and intermolecular interactions were found to depend on the tacticity, and only atactic (diad ratio 46 %) PNiPAM exhibits poor molecular interaction even in the bulk sample. On the other hand, the same series of compounds dissolved in an acetone solution were spread on a gold surface to form a thin film. In the dissolution process, the polymer molecules are relaxed via solvation, and they are bound to the gold surface by a molecular interaction to form a submonolayer thin film. In the thin film, the molecular interaction with the gold surface via the N−H group was monitored in the infrared spectra only for a nearly isotactic ($m=90$) PNiPAM by an apparent shift of the N−H stretching vibration band. This shift was confirmed by changing the degree of hydrophilicity of the gold surface: a larger shift is found on a gold surface with stronger hydrophilicity. As a result, the conformation of a nearly isotactic molecule is found to be extended by the interaction with the gold surface, which works to immobilize the molecule.

Synthesis and Physical Properties of a Ball-like Three-dimensional π-Conjugated Molecule

Kayahara, E.; Iwamoto, T.; Takaya, H.; Suzuki, T.; Fujitsuka, M.; Majima, T.; Yasuda, N.; Matsuyama, N.; Seki, S.; Yamago, S., *Nature Commun.*, **4,** 2694 (2013).

Abstract

Curved π-conjugated molecules with closed and three-dimensional (3D) structures, such as fullerenes and carbon nanotubes, have been the subject of intensive research due to their potential applications in molecular electronics. However, basic molecular skeletons of 3D molecules are limited because of the lack of a rational and selective synthetic method by organic synthesis. Here we report the synthesis of a 3D π-conjugated molecule based on the platinum-mediated assembly of four molecules of a stannylated trisubstituted benzene derivative forming a hexanuclear platinum complex with an octahedral shape, from which reductive elimination of platinum gave the target molecule. As many supramolecular transition metal–ligand complexes with 3D cages and polyhedral structures have been synthesized by self-assembly of ligands and metals, the current assembly/reductive elimination strategy could provide a variety of new 3D π-conjugated molecules with different structures and topologies, which are challenging to obtain using conventional synthetic methods.

VMAT2 Identified as a Regulator of Late-stage β Cell Differentiation

Sakano, D.; Shiraki, N.; Kikawa, K.; Yamazoe, T.; Kataoka, M.; Umeda, K.; Araki, K.; Mao, D.; Matsumoto, S.; Nakagata, N.; Andersson, O.; Stainier, D.; Endo, F.; Kume, K.; Uesugi, M.; Kume, S., *Nat. Chem. Biol.*, **10,** 141-148 (2014).

Abstract

Cell replacement therapy for diabetes mellitus requires cost-effective generation of high-quality, insulin-producing, pancreatic β cells from pluripotent stem cells. Development of this technique has been hampered by a lack of knowledge of the molecular mechanisms underlying β-cell differentiation. The present study identified reserpine and tetrabenazine (TBZ), both vesicular monoamine transporter 2 (VMAT2) inhibitors, as promoters of late-stage differentiation of *Pdx1*-positive pancreatic progenitor cells into *Neurog3* (referred to henceforth as *Ngn3*)-positive endocrine precursors. VMAT2-controlled monoamines, such as dopamine, histamine and serotonin, negatively regulated β-cell differentiation. Reserpine or TBZ acted additively with dibutyryl adenosine 3',5'-cyclic AMP, a cell-permeable cAMP analog, to potentiate differentiation of embryonic stem (ES) cells into β cells that exhibited glucose-stimulated insulin secretion. When ES cell–derived β cells were transplanted into AKITA diabetic mice, the cells reversed hyperglycemia. Our protocol provides a basis for the understanding of β-cell differentiation and its application to a cost-effective production of functional β cells for cell therapy.

Measurement of Transient Photoabsorption and Photocurrent of $BiFeO_3$ Thin Films: Evidence for Long-lived Trapped Photocarriers

Yamada, Y.; Nakamura, T.; Yasui, S.; Funakubo, H.; Kanemitsu, Y., *Phys. Rev. B*, **89,** [035133-1]-[035133-5] (2014).

Abstract

We have studied the optical response and dynamical behavior of photocarriers in $BiFeO_3$ thin films by means of transient absorption (TA) and photocurrent (PC) measurements. PC and absorption spectroscopy indicate that $BiFeO_3$ thin films have an indirect band gap energy of ～2.4 eV. The TA and PC decay dynamics have fast (～1 ns) and slow

(～100 ns) components that are attributed to the localization of free carriers to shallow trap states and the recombination of trapped carriers, respectively. The long decay time of the PC is caused by the thermal activation of trapped carriers into the conduction band. Long-lived trapped photocarriers can be linked to the ferroelectricity and give rise to unique photoinduced phenomena in $BiFeO_3$.

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
MATSUKAWA, Kimihiro
(D Eng)

Laboratory of Chemistry of Polymer Materials

Director, Electronic Materials Research Division, Osaka Municipal Technical Research Institute
(Morinomiya, Joto-ku, Osaka 536-8553)

Lecture at *ICR*
Development of Epoxy Monolith for Functional Materials
Fabrication of Organic-Inorganic Hybrid Materials with Controlled Refractive Index

Vis Prof
KOBAYASHI, Toshihide
(D Pharm Sc)

Laboratory of Molecular Microbial Science

Chief Scientist, Lipid Biology Laboratory, RIKEN
(2-1 Hirosawa, Wako, Saitama 351-0198)

Lecture at *ICR*
Imaging of Lipid Domain

Vis Prof
SUENAGA, Kazutomo
(D Eng)

Laboratory of Electron Microscopy and Crystal Chemistry

Prime Senior Researcher, Nanotube Research Center, National Institute of Advanced Industrial Science and Technology(AIST)
(AIST Central 5, Tsukuba 305-8565)

Lecture at *ICR*
Low Voltage TEM/STEM for Atomic Resolution Imaging and Spectroscopy

Vis Prof
MORISHITA, Shinichi
(D Sc)

Laboratory of Bio-knowledge Engineering

Professor, Graduate School of Frontier Sciences, The University of Tokyo
(5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8561)

Lecture at *ICR*
Novel Insights into Mid-sized Heterozygous Structural Variations and DNA Methylome in a Diploid Human Genome through SMRT Sequencing

Vis Prof
LI, Zhiping
(Ph D)

Laboratory of Organic Main Group Chemistry

Professor, Renmin University of China
(Beijing 100872, China)

Lecture at *ICR*
Iron-catalyzed C-H Functionalization
Iron-catalyzed Carbonylation-Peroxidation of Alkene

Vis Assoc Prof
YOKOSHIMA, Satoshi
(D Pharm Sc)

Laboratory of Synthetic Organic Chemistry

Associate Professor, Graduate School of Pharmaceutical Sciences , Nagoya University
(Furo-cho, Chikusa-ku, Nagoya 464-8601, Japan)

Lecture at *ICR*
Synthetic Studies of Natural Products Having Highly Fused Ring Systems

Vis Assoc Prof
MIZUTANI, Masaharu
(D Agr)

Laboratory of Chemistry of Molecular Biocatalysts

Associate Professor, Graduate School of Agricultural Science, Kobe University
(1-1 Rokkodai, Nada-ku, Kobe 657-8501)

Lecture at *ICR*
Biosynthesis of Plant Steroidal SaponinsF

Vis Assoc Prof
HAYASHI, Naoto
(D Sc)

Laboratory of Molecular Aggregation Analysis

Associate Professor, Graduate School of Science and Engineering for Research, University of Toyama
(3190 Gofuku, Toyama 930-8555)

Lecture at *ICR*
Effects of the Condensation Form of Furan Rings in Furanoid Polycyclic Aromatic Compounds on Their Crystal Structures and Solid-State Fluorescence Properties

Vis Assoc Prof
HASHIMOTO, Hisako
(D Sc)

Laboratory of Organotransition Metal Chemistry

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

Lecture at *ICR*
Syntheses and Peculiar Properties of Transition-metal Complexes Having a Metal-Silicon/Germanium Multiple Bond

Vis Assoc Prof
ALEZRA , Valerie
(Ph D)

Laboratory of Synthetic Organic Chemistry

Associate Professor, Institute for Molecular Chemistry and Materials of Orsay (ICMMO), University Paris Sud
(15, Rue Georges Clemenceau, 91405 Orsay Cedex, FRANCE)

Prof Em KANEHISA, Minoru (D Sc)

Appointed as Res (pt) at ICR,
1 April 2012–31 March 2015

PERSONAL

Retirement

Professor TOSHIMITSU, Akio
Division of Multidisciplinary Chemistry
– Interdisciplinary Chemistry for Innovation –

On March 31, 2015, Dr. Akio Toshimittsu retired from Kyoto University after 36 years of service and was honored with the title of Professor Emeritus of Kyoto University.

Dr. Toshimitsu was born in Tokyo on September 12, 1949. He graduated from Faculty of Engineering, Kyoto University in 1973 and studied organic chemistry under the supervision of Professor Emeritus Masaya Okano in the Department of Hydrocarbon Chemistry, Graduate School of Engineering. In 1979, he received the doctoral degree of engineering, Kyoto University, for the thesis "Preparation of Some Organo-thallium and -selenium Compounds and their Utilization in Organic Synthesis". After one year experiment as a post-doctoral fellow of Japan Promotion of Science, he continued his research activity at the Institute for Chemical Research as Educational Staff (from 1979) and was promoted to Assistant Professor in 1982 and Associate Professor in 1993. He was appointed Professor at the International Innovation Center, Kyoto University, in 2002. The center was re-organized as Innovative Collaboration Center in 2007 and he served as the Director of this Center from 2009. In 2010, the Center was again re-organized as Office of Society-Academia Collaboration for Innovation. In 2011, he returned to ICR directing the Laboratory of Interdisciplinary Chemistry for Innovation in Division of Multidisciplinary Chemistry.

Throughout his academic career, Dr. Toshimitsu devoted himself to the investigation of novel reactions in organic synthesis based on heteroatom chemistry. He succeeded in the control of the stereochemistry in the reactions through anchimecric assistance of sulphur or selenium to introduce versatile oxygen, nitrogen, and carbon nucleophiles. Notably, he clarified that the chiral carbon in the three-membered cationic intermediate containing selenium atom racemizes through bimolecular attack of nucleophile on the selenium atom. By the steric protection of the selenium atom, both the racemization of the chiral carbon and the selenophilic attack of the carbon nucleophile were suppressed to realize the construction of chiral carbon center by the formation of new C-O, C-N, or C-C bond. He also clarified that divalent silicon species, silylene, behaves as nucleophile by the intramolecular coordination of base. He provided experimental proof to the conformational dependence of conjugation of Si-Si bonds. Thus, he controlled the configuration of tetrasilane to *anti* or *syn* by the introduction of bicyclic carbon unit to the central Si-Si bond. Using the oligosilanes prepared by these units, it was clearly shown that only the *anti* unit contributes to the elongation of conjugation and the *syn* unit interrupts the conjugation.

It should be noted that he has opened new aspect of academic activity in the industry-academia collaboration. He pointed out that it is not impossible to fulfill the requirement of companies by the investigation which is also important in the academic society. Actually, his investigation on anticancer reagents and organic light-emitting transistor provided good patents as well as scientific papers of high quality.

Dr. Toshimitsu's educational contribution is also notable. In these years, he has supervised 25 graduate students including 4 doctor theses as a chief examiner. His students gained valuable experience in the field of organic syntheses through his supervision and assume important roles in various fields of industry and academia.

His contribution to the administration of Kyoto University in the days of collaboration centers should also be noted. He recognized the importance of coordinator who can understand the essence of academic as well as industrial activities. He has learned the know-how of the coordinator for the success of the collaboration from his experience and established the system of "on the job training" of young staffs. As for the intellectual properties, he established the system to discriminate the wrights which should be owned by Kyoto University and how to utilize them in the license to the industry. Recent remarkable increases in the funds for the collaborations and license fee in Kyoto University should be attributed to these foundations.

Dr. Toshimitsu's contribution to Kyoto University and the Institute through his scientific, educational, and administrative activities is greatly acknowledged. His perpetual quest of the rule of nature will be remembered for a long time to come.

Awards

SASAMORI, Takahiro

Friedrich Wilhelm Bessel Research Award

Alexander von Humboldt Foundation

6 May 2014

AGOU, Tomohiro

Ube Industries, Ltd. Award in Synthetic Organic Chemistry

"Development of Activation of Aromatic π-Bonds Utilizing the Low-valent Organoaluminum Compounds Bearing a Metal-metal Bond"

The Society of Synthetic Organic Chemistry, Japan

20 February 2014

NAGATA, Koichi

ICR Award for Graduate Students

"Syntheses and Structures of Terminal Arylalumylene Complexes"

Institute for Chemical Research, Kyoto University

12 December 2014

NISHIMURA, Hidetaka

ICR Award for Graduate Students

"On-top π-Stacking of Quasiplanar Molecules in Hole-Transporting Materials: Inducing Anisotropic Carrier Mobility in Amorphous Films"

Institute for Chemical Research, Kyoto University

12 December 2014

FURUTA, Takumi

The Society of Synthetic Organic Chemistry, Japan, Kansai Branch Award

"Development of Biaryl Amino Acids with Molecular Recognition Ability"

The Society of Synthetic Organic Chemistry, Japan, Kansai Branch

2 December 2014

YANAGI, Masanori

Best Presentation Award

The 134th Annual Meeting of the Pharmaceutical Society of Japan

"Organocatalytic Regioselective Functionalization of Sugars with Acid Chloride as Acylating Reagent"

The Pharmaceutical Society of Japan

31 March 2014

KASAMATSU, Koji

Best Presentation Award

The 134th Annual Meeting of the Pharmaceutical Society of Japan

"Intermolecular Asymmetric α-Arylation of Amino Acid Derivatives via Memory of Chirality (MOC)"

The Pharmaceutical Society of Japan

31 March 2014

WADA, Yoshiyuki

Best Presentation Award

The 134th Annual Meeting of the Pharmaceutical Society of Japan

"A Hydride-transfer Mechanism in the Nitroxyl Radical-promoted Oxidation Reactions"

The Pharmaceutical Society of Japan

31 March 2014

NISHIJIMA, Hideyuki

Best Presentation Award

The 134th Annual Meeting of the Pharmaceutical Society of Japan

“Organocatalytic Parallel Kinetic Resolution of Diols”

The Pharmaceutical Society of Japan

31 March 2014

SATO, Ryota

CSJ Presentation Award 2014

The 94th Annual Meeting of the Chemical Society of Japan

“Amorphous Pd-P Seed-mediated Synthesis of Highly Monodisperse Pd-based Alloy Nanoparticles”

The Chemical Society of Japan

10 April 2014

KAYAHARA, Eiichi

ICR Award for Young Scientists

“Synthesis and Physical Properties of a Ball-like Three-dimensional π-Conjugated Molecule”

Institute for Chemical Research, Kyoto University

12 December 2014

ONO, Teruo

DOCOMO Mobile Science Award

“Development of Novel Spin Devices Using Nano-magnets”

Mobile Communication Fund

17 October 2014

FUTAKI, Shiroh

Best Reviewer Award of 2013, JSPS's Screening Committee for Young Researcher Fellowships

Japan Society for the Promotion of Science

31 July 2014

TSUJI, Shogo

Excellent Presentation Award

The 134th Annual Meeting of the Pharmaceutical Society Japan

“Creating a TALE Protein with Unbiased 5'-T Binding”

The Pharmaceutical Society of Japan

31 March 2014

AKISHIBA, Misao

Young Investigator Award

The 51st Japanese Peptide Symposium

“A Novel Peptide Sequence for Endosome Disruption Derived from Natural Hemolytic Peptide”
The Japanese Peptide Society

23 October 2014

Best Discussion Award
Bioorganic Research Institute Symposium
Suntory Foundation for Life Sciences

17 November 2014

MURAYAMA, Tomo

Best Discussion Award

Bioorganic Research Institute Symposium

Suntory Foundation for Life Sciences

17 November 2014

KAJI, Hironori

7th Outstanding Achievement Award of the Organic LED Forum

“Theoretical Study of Organic Electronics Materials Using Quantum Chemical Calculations”

The Organic LED Forum

18 July 2014

KURIHARA, Tatsuo

Nagase Foundation Award

“Analysis of Functions of Polyunsaturated Fatty Acids in Folding and Post-translational Modification of Membrane Proteins”

NAGASE Science Technology Foundation

25 April 2014

OGURA, Ryutaro

The Best Presentation Award

The 486th Annual Meeting of the Kansai Branch of Japan Society for Bioscience, Biotechnology, and Agrochemistry

"Analysis of Eicosapentaenoic Acid-Biosynthesis Enzymes Localized at the Cell Division Site of a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10"

Japan Society for Bioscience, Biotechnology, and Agrochemistry

20 September 2014

YOSHIDA, Hiroyuki

Grand Renewable Energy 2014, Best Oral Presentation Award

"Low Energy Inverse Photoemission Study of the LUMO Levels of Acceptors for Organic Photovoltaic Cells"

The Organizer of Grand Renewable Energy 2014 International Conference

1 August 2014

IWASHITA, Yoshihisa

PASJ Award for Technical Contributions

11th Annal Meeting of Particle Accelerator Society of Japan

"Development of the Repair Technique Using by the Local Polishing System with High Quality Optical Inspection Camera for the L-band Superconducting RF Cavity"

Particle Accelerator Society of Japan

10 August 2014

INOUE, Shunsuke

Young Scientist Award of the Physical Society of Japan

"Femtosecond Electron Deflectometry for Measuring Ultrafast Transient Field Induced by Intense Laser Pulses"

The Physical Society of Japan

29 March 2014

Young Scientist Oral Presentation Award

PLASMA CONFERENCE 2014

"Characteristics of the Electron Beam Generated by Irradiation of Foil Target with Femtosecond Laser Plasma"

21 November 2014

MIYASAKA, Yasuhiro

Young Researcher Presentation Award

The 9th Asia Pacific Laser Symposium

"Ablation Rate Dependence on Incident Angle and Polarization for Copper Irradiated by Femtosecond Laser Pulses"

24 April 2014

The ICPEPA-9 Outstanding Student Paper Award

The 9th International Conference on Photo-Excited Processes and Applications

"Dependence of Ablation Rate on Laser Fluence for Metals by Oblique Femtosecond Laser Irradiation"

3 October 2014

HARUTA, Mitsutaka

JSAP Young Scientist Oral Presentation Award

The 74th JSAP Autumn Meeting

"Electronic State Mapping of Oxygen in Metal Oxide"

The Japan Society of Applied Physics

17 March 2014

SAITO, Takashi; SHIMAKAWA, Yuichi

The 38th JSPM Award for Inovatory Research

The 113th Spring Meeting of Japan Society of Powder and Powder Metallurgy

"Synthesis of Novel Functional Oxide Materials under High Pressures"

Japan Society of Powder and Powder Metallurgy

3 June 2014

KUROSAKI, Ryo

JSPM Award for Best Presentation by Student

The 113th Spring Meeting of Japan Society of Powder and Powder Metallurgy

"Catalytic Activities of Perovskite-Mn Oxide Thin Films for Oxygen-reduction Reaction"

Japan Society of Powder and Powder Metallurgy

5 June 2014

MURAKAMI, Noriaki

Young Scientist Oral Presentation Award

The 36th Spring Meeting of the Japan Society of Applied Physics

“Oxygen-ion Diffusion in $LaAlO_3/CaFeO_{2.5}/SrTiO_3$ Heterostructure during Low-temperature Reduction”

The Japan Society of Applied Physics

17 September 2014

TAKEUCHI, Katsuhiko

The 30th Inoue Research Award for Young Scientists

“Reactivity of a Silicon–Silicon Triply Bonded Compound, a Disilyne, toward Small Organic Molecules Containing Oxygen, Nitrogen, and Boron Atoms”

Inoue Foundation for Science

4 February 2014

TEX, David Michael

ICR Award for Young Scientists

“Control of Hot-carrier Relaxation for Realizing Ideal Quantum-dot Intermediate-band Solar Cells”

Institute for Chemical Research, Kyoto University

12 December 2014

GOTO, Susumu

2014 Thomson Reuters Highly Cited Researchers

Thomson Reuters

18 June 2014

SIGBIO (Special Interest Group on Bioinformatics) Contribution Award

“Contribution to Development of SIGBIO as a chair of SIGBIO”

SIGBIO (Special Interest Group on Bioinformatics), Information Processing Society of Japan

18 December 2014

AKUTSU, Tatsuya

Forum on Information Technology Encouragement Award

Forum on Information Technology 2014

“On Observability of Steady States in a Boolean Network”

FIT Organizing Committee

5 September 2014

SIGBIO (Special Interest Group on Bioinformatics) Contribution Award

“Contribution to Establishment of IPSJ Transactions on Bioinformatics and Development of SIGBIO as a Chair of SIGBIO”

SIGBIO (Special Interest Group on Bioinformatics), Information Processing Society of Japan

18 December 2014

TOMITA, Etsuji[1]; AKUTSU, Tatsuya; MATSUNAGA, Tsutomu[2]

InTech Award Diploma

“Efficient Algorithms for Finding Maximum and Maximal Cliques: Effective Tools for Bioinformatics”

InTech (Open Access Publisher)

26 October 2014

[1] University of Electro-Communications

[2] NTT DATA Corporation

HAYASHIDA, Morihiro

IPSJ Yamashita SIG Research Award

“Predicting Protein-RNA Residue-base Contacts Using Two-dimensional Conditional Random Field”

Information Processing Society of Japan

11 March 2014

KARASUYAMA, Masayuki; MAMITSUKA, Hiroshi

Best Performer in the DREAM 9

DREAM Challenges and Cytoscape Workshops 2014

“Broad-DREAM Gene Essentiality Prediction Challenge Sub-Challenge 1”

The DREAM Challenges

11 November 2014

MOHAMED, Ahmed Mohmed

ICR Award for Graduate Students

"NetPathMiner: R/Bioconductor Package for Network Path Mining through Gene Expression"

Institute for Chemical Research, Kyoto University

12 December 2014

Paper Awards

YOSHIDA, Hiroyuki

The 12th Publication Award of M&BE, Japanese Society of Applied Physics

"Near-Ultraviolet Inverse Photoemission Spectroscopy Using Ultra-Low Energy Electrons"

Division of Molecular Electronics and Bioelectronics, Japanese Society of Applied Physics

18 September 2014

Poster Awards

NAGATA, Koichi

Student Poster Prize

XXVI International Conference on Organometallic Chemistry (ICOMC2014)

"Synthese and Structures of Alumlene-Platinum Complexes"

18 July 2014

ZHANG, Rui

Poster Award

25th Symposium on Physical Organic Chemistry

"Synthesis and X-ray Structure of an Open-Cage Thiafullerene $C_{69}S$ Derivative"

The Society of Physical Organic Chemistry

9 September 2014

Poster Award

4th CSJ Chemistry Festa 2014

"Synthesis and X-ray Structure of an Open-Cage Thiafullerene $C_{69}S$ Derivative"

The Chemical Society of Japan

10 November 2014

CHAOLUMEN

Poster Award

25th Symposium on Physical Organic Chemistry

"Synthesis and Properties of Dibenzo[*a*,*f*]perylene Bisimide Derivatives"

The Society of Physical Organic Chemistry

9 September 2014

MARUYAMA, Naoki

Best Poster Presentation Award

6th Thin-Film Solar Cell Seminar 2014

"Development of Fabrication Method for Efficient Organic-Inorganic Hybrid Solar Cells"

Organizing Committee of 6th Thin-Film Solar Cells Seminar

16 October 2014

HASHIKAWA, Yoshifumi

Poster Award

4th CSJ Chemistry Festa 2014

"Synthesis of Azafullerene Encapsulating Molecular Hydrogen"

The Chemical Society of Japan

10 November 2014

BABA, Tomonori

Best Poster Award

Symposium on Molecular Chirality 2014

"Intramolecular Asymmetric Cross-aldol Reaction Catalyzed by Axially Chiral Acid-base Catalysts Bearing Aniline-type Amine"

Molecular Chirality Research Organization (MCRO)

7 June 2014

Chemical and Pharmaceutical Bulletin Poster Award

The 44th Congress of Heterocyclic Chemistry

"Intramolecular Asymmetric Cross-aldol Reaction Catalyzed by Axially Chiral Acid-base Catalysts Bearing Aniline Type Amine"

Organizing Committee of 44th Congress of Heterocyclic Chemistry

12 September 2014

TAKEUCHI, Hironori

Best Poster Award

The 32nd Japanese Carbohydrate Symposium

"Advanced Synthesis of Natural Saccharides via Regioselective Sequential Functionalization of Glucose"

Organizing Committee of the 32nd Japanese Carbohydrate Symposium

10 August 2014

FUJIMORI, Yusuke

Poster Award

The XXVIIth International Conference on Polyphenols & the 8th Tannin Conference

"Total Synthesis of Ellagitannins via Regioselective Acylation of Glucose"

Organizing Committee of The XXVIIth International Conference on Polyphenols & The 8th Tannin Conference

6 September 2014

SATO, Ryota

Excellent Poster Award for Young Scientists

The 12th Annual Meeting of Society of Nano Science and Technology

"High-Performance $L1_0$-FePd/α-Fe Nanocomposite Magnets with Precisely Controlled Nano-Interfaces"

The Society of Nano Science and Technology

23 May 2014

WU, Hsin-Lun

Excellent Poster Award for Young Scientists

The 12th Annual Meeting of Society of Nano Science and Technology

"Shape Dependent Crystal Structural Control of Semiconductor Nanocages"

The Society of Nano Science and Technology

23 May 2014

KIMURA, Masato

Poster Award

The 65th Divisional Meeting on Colloid and Interface Chemistry

"Synthesis and Optical Properties of Heterostructured Au/ZnS Nanoparticles"

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

4 September 2014

KINOSE, Yuji

The Best Poster Award

The 21st Annual Meeting of the Cellulose Society of Japan

"Synthesis of Amphiphilic Bottle Brushes with Cellulose Backbone via Regioselective Substitution Reaction"

The Cellulose Society of Japan

18 July 2014

KAWAGUCHI, Yoshimasa

The Poster Presentation Award

The 51st Japanese Peptide Symposium

"Identifying Membrane Proteins Involved in Cellular Uptake of Octaarginine Peptide by Photocrosslinking"

The Japanese Peptide Society

24 October 2014

YAMADA, Kazuto

The Best Poster Presentation Award

The 2nd Lecture Meeting of Kansai Chapter, the Japan Society of Applied Physics in 2014 Fiscal Year

"Precise Measurements of Unoccupied Levels in Organic Semiconductor Thin Films Using Low-Energy Inverse Photoemission Spectroscopy to Observe Their Molecular Orientation Dependence"

Kansai Chapter, the Japan Society of Applied Physics

26 June 2014

SEKI, Hayato

Poster Award

The 4th CSJ Chemistry Festa 2014

"Valence States and Magnetic Properties of the Perovskite $SrFe_{1-x}Ni_xO_3$"

The Chemical Society of Japan

10 November 2014

HOSAKA, Yoshiteru

Poster Award

The 4th CSJ Chemistry Festa 2014

"Layered Perovskite with Two Dimensional Arrangement of Unusually High Valent Fe^{4+}"

The Chemical Society of Japan

10 November 2014

IIZUKA, Eisuke

Poster Award

The 61st Symposium on Organometallic Chemistry

"Synthesis of D-A Type π-Conjugated Polymer with Dithienosilole Units via Direct Arylation Polymerization"

Division of Organometallic Chemistry,

The Kinki Chemical Society

15 October 2014

MIHARA, Tomoko;
GOTO, Susumu;
OGATA, Hiroyuki

The Design Award

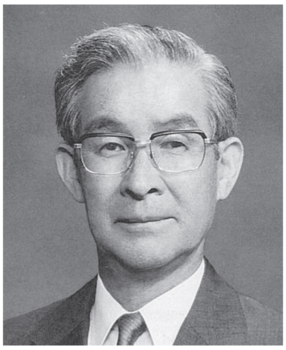
Informatics in Biology, Medicine and Pharmacology 2014

"Why Do Some Viruses Encode Amino Acid Biosynthetic Genes?"

Informatics in Biology, Medicine and Pharmacology 2014

3 October 2014

Obituary



Professor Emeritus

Dr. TAKENAKA, Tohru (1929–2014)

Dr. Tohru Takenaka, Professor Emeritus of Kyoto University, passed away unexpectedly on July 26, 2014, in Kyoto, at the age of 85.

Dr. Tohru Takenaka was born in Tsuyama, Okayama on July 20, 1929. After graduating from Department of Physics, Hiroshima-Bunrika University (present Hiroshima University) in 1952, he immediately became a student of Department of Physics, Graduate School of Science, Kyoto University. He was soon employed as an Assistant Professor in a laboratory under the direction of Professor Renpei Goto in Institute for Chemical Research, Kyoto University in May, 1953. He received his doctoral degree of science from Kyoto University in 1962 for the study on "Inductive Effect of Substituent Groups on the Symmetrical Deformation of Methyl Groups." Dr. Takenaka was promoted to be an Associate Professor of Laboratory of Colloid Chemistry, Institute for Chemical Research, Kyoto University in February, 1967, and he was promoted to be a Full Professor of the same laboratory in April, 1971. After the reorganization of the institute in 1992, he led the laboratory with a new name of 'Laboratory of Chemical Interface I' as a Full Professor. Dr. Takenaka retired from Kyoto University in March, 1993, and he was honored with the title of Professor Emeritus, Kyoto University on April 1, 1993.

After the retirement of Kyoto University, he was immediately invited by Okayama University of Science to be a Professor of Department of Science, and he continued chemical education of about quantum chemistry for eight years. After that, he went to the university from his home in Kyoto every week to have some chemistry classes as a part-time lecturer for additional five years. In 2006, he was invited by Northeast Normal University, China, as a guest Professor. In this manner, he was long engaged in enthusiastic chemistry education.

Dr. Takenaka is globally recognized to be a pioneer of vibrational spectroscopist on surface and interface chemistry. When he was employed as an Assistant Professor, very few research groups are available in Japan for infrared (IR) and Raman spectroscopy, and he was involved in fundamental researches of theory and instrumentation with his good colleagues in 1950's. After receiving his doctoral degree, his research interest was gradually oriented to surface chemistry involving ultrathin films. One of the early successes of his surface chemistry using Raman spectroscopy is a study of a Langmuir monolayer at the air/water interface with an optical geometry of the total reflection. This experimental approach has become a standard technique in this field in nowadays. He was also interested in Fourier transform (FT) IR spectrometer in early days, and he introduced it with some different optical accessories to reveal the molecular structure in Langmuir-Blodgett (LB) films on a solid substrate.

In addition, Dr. Takenaka was also interested in high-sensitivity techniques applicable to IR and Raman spectrometries. In particular, surface-enhanced Raman scattering (SERS) was an important topic in 1980's. He readily used the LB technique to discriminate the charge-transfer and plasmon resonance effects on the SERS phenomena, which had an impact on the research field being still active.

With a progress of the FT-IR technology, the optical geometry of external-reflection for analysis of an LB film deposited on a dielectric substrate was a new target of his study. To quantitatively reveal the surface selection rule of this technique, the analytical theory on electrodynamics was studied, with which the molecular orientation in a thin film was readily revealed with a good analytical quality.

During his career, he played a role of Chair of Division of Colloid and Interface Chemistry, Chemical Society of Japan from 1997 for two years. He had not only Japanese colleagues, but also many international colleagues, and he was actively involved in international scientific activities through his life.

Obituary

Professor Emeritus

Dr. INOUYE, Yuzo (1920–2014)

Dr. Yuzo Inouye, Professor Emeritus of Kyoto University, passed away on November 1, 2014, in Kamakura. Dr. Yuzo Inouye was born in Tottori on March 25, 1920. He graduated from the Department of Agricultural Chemistry, Collage of Agriculture, Kyoto Imperial University in 1946 and continued his research on pyrethrum chemistry as a graduate student at the Department of Agricultural Chemistry, Faculty of Agriculture, Kyoto University under the supervision of Professor Sankiti Takei. After graduation, he became an Assistant Professor of the Department in 1951 and started his academic career, majoring in chemistry of plant products and pesticides. In 1957, he joined the member of the Institute for Chemical Research, Kyoto University. He received a doctoral degree (D. Agr.) from Kyoto University in 1958 for his studies on synthetic pyrethroids under the supervision of Professor Takei. In 1962, Dr. Inouye was promoted to an Associate Professor of the Institute for Chemical Research, Kyoto University. Immediately, on leave from university, he stayed at Florida State University, USA as a visiting professor and worked on asymmetric reactions in co-operation with Professor H. M. Walborsky. In 1973, Dr. Inouye was promoted to a Full Professor of Kyoto University to hold a chair of Laboratory of Plant Products Chemistry, the Institute for Chemical Research, Kyoto University. He retired from Kyoto University on April 1, 1983 and was honored with the title of Professor Emeritus, Kyoto University on that day.

Dr. Inouye performed extensive studies in natural product chemistry, organic stereochemistry and bioorganic chemistry. In particular, he pursued extensive studies as a pioneer in asymmetric synthesis and the biological activities of pyrethrins, an insecticidal principal of Dalmatian pyrethrum, *Tanacetum cinerariifolium*, from a stereochemical point of view. He succeeded in the structural identification of the second chrysanthemic acid (pyrethric acid) and in determining the absolute stereochemistry of pyrethrolones by their total synthesis. His extensive structure-activity relationship studies successfully identified the comprehensive stereochemical requirements of pyrethrins for insecticidal activities. His studies formulated the chemical basis of synthetic pyrethroids that has triggered the revolutionary development of the subsequent synthetic insecticides industry in Japan. For these accomplishments, Dr. Inouye received Agricultural Chemistry Award from the Japan Society for Bioscience, Biotechnology, and Agrochemistry in April, 1959.

Dr. Inouye was also interested in the development of novel methodology and the theoretical background of asymmetric reactions. He pursued extensive studies on the carbanion and carbenoid chemistry for asymmetric cyclopropanation and formulated the dependence of the stereochemical outcome on the solvent polarity. His theoretical consideration of solvent polarity in asymmetric reactions made an epoch to the development of this field. For his excellent achievements, the Prize from Petroleum Research Fund administrated by the American Chemical Society was awarded to him. Dr. Inouye is the first Japanese winner of this award. His research interests also covered the asymmetric reactions with enamines, sigmatropic rearrangement and the stereochemical control of the addition of Grignard reagents. His outstanding academic expertise in asymmetric synthesis came to fruition with his authored book "Asymmetric Organic Synthesis – Comprehensive Interpretation Thereof" (Kagaku Dojin, 1977, ISBN 9784759800463) and his other translated books.

Dr. Inouye's research interest was further extended to enzyme model reactions that mimic asymmetric reduction of ketones by alcohol dehydrogenases. He succeeded in developing novel chiral NADH model compounds that rivaled alcohol dehydrogenases in stereoselectivity and chemical yield.

Dr. Inouye's superiority as a teacher as well as a researcher, deep insight into science and warm hospitality have attracted and stimulated many young and talented students, and have won him the respect and admiration of many friends and colleagues from all over the world. He also served as an executive board of scientific societies such as the Japan Society for Bioscience, Biotechnology, and Agrochemistry.

For his outstanding professional activities in research and education, he received the Third Order of Merit with the Order of the Sacred Treasure from the Japanese government in April, 1994.

Obituary

Professor

Dr. YOKO, Toshinobu (1949–2014)

Dr. Toshinobu Yoko, Professor of Kyoto University, passed away on 25, Feb, 2014 in Kyoto.

Dr. Toshinobu Yoko was born in Hokkaido on 4, November, 1949. He graduated from the Department of Metallurgy, Tohoku University, with the degree of B. Eng. in 1972 and from the graduate course at the same university with the degree of M. Eng. in 1975. In 1979 he received Dr. Eng. from Tohoku University for a thesis entitled "Viscoelastic Behavior of $ZnCl_2$ - MCl (M = Li, Na, K, Cs) Binary Melts".

He worked as a postdoctoral fellow at Rensselaer Polytechnic Institute (Troy, New York, USA) for two years from 1979 to 1981. He got an academic position of research associate at the Department of Industrial Chemistry, Mie University, in 1981. In 1984 he was promoted to Associate professor at the same university. In 1988 he moved to Institute for Chemical Research, Kyoto University and was promoted to a Full Professor there in 1994.

The achievements made by him were mainly concerned with the preparation and the structure- and property-characterization of a variety of functional glasses and sol-gel derived coating thin films. His research was composed of five fields such as (1) structure and properties of glasses, (2) nonlinear optical properties of inorganic glasses and sol-gel derived films, (3) preparation of functional materials by sol-gel method, (4) photoelectrochemistry of sol-gel derived semiconducting oxide films, and (5) high temperature molten salt chemistry. In 1993 he received the Scientific Award of the Ceramic Society of Japan for "Preparation and characterization of functional ceramic coatings by sol-gel process".

He analyzed the glass structure by using X-ray diffraction, neutron diffraction and solid state NMR. He found that the local structure of alkalis in glasses is not homogeneous but heterogeneous. This is because each alkali has the different electrical field; a cation with high field strength was likely to aggregate in mixed silicate glasses. This type of structural inhomogeneity generated site mismatch energy, which was found to be responsible for the mixed alkali effect.

He also proposed the highest quantum efficiency for amorphous phosphate glass. It is notable that the broad emission is brought about by Sn^{2+} center, and that the UV-excited emission efficiency is the largest efficiency of glass material without rare earth (RE) cation ever reported. He has also demonstrated white light emission of RE-free Mn-doped phosphate glass. The transparent glass showed blue ~ white ~ red emission, which depended on the amount of MnO. Because the high value of quantum efficiency is comparable to crystalline phosphor, it suggests that RE-free glass phosphor is very fascinating material from the viewpoint of unique emission mechanisms in a random matrix.

He was also interested in organic-inorganic hybrid materials. He proposed new synthetic method under a solventless, catalyst-free, low-temperature, one-pot condition by metathesis. This reaction provided crack-free monolithic materials easily because of no solvent evaporation. The hybrid material shows low-melting property, as melting temperatures ranged from 50 to 110 °C where the organic dyes do not degrade. The durability of these hybrids was also high, indicating that these materials can be used as highly durable low-melting hybrids for optical host application.

Dr. Yoko's superiority as a teacher, insight into science, and warm hospitality not only have attracted and stimulated many young and talented students but also have won the respect and admiration of many friends and colleagues. Among his numerous professional activities, he has served as executive boards of scientific societies such as Ceramic Society of Japan.

PUBLICATIONS
INTERNATIONAL RESEARCH COLLABORATIONS
SELECTED GRANTS
THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Sugamata, K.; Sasamori, T.; Tokitoh, N., Unique Synthetic Approach toward a Phosphaalkene: Synthesis of a Selenium-substituted Phosphaalkene with Bulky Substituents, *Chem. Lett.*, **43,** 95-96 (2014).

Azuma, T.; Kobayashi, Y.; Sakata, K.; Sasamori, T.; Tokitoh, N.; Takemoto, Y., Synthesis and Characterization of Binary-Complex Models of Ureas and 1,3-Dicarbonyl Compounds: Deeper Insights into Reaction Mechanisms Using Snap-Shot Structural Analysis, *J. Org. Chem.*, **79,** 1805-1817 (2014).

Morisaki, Y.; Gon, M.; Sasamori, T.; Tokitoh, N.; Chujo, Y., Planar Chiral Tetrasubstituted [2.2]Paracyclophane: Optical Resolution and Functionalization, *J. Am. Chem. Soc.*, **136,** 3350-3353 (2014).

Hamada, S.; Wada, Y.; Sasamori, T.; Tokitoh, N.; Furura, T.; Kawabata, T., Oxidative Kinetic Resolution of Racemic Alkyl Aryl Carbinols by an Electronically Tuned Chiral Nitroxyl Radical, *Tetrahedron Lett.*, **55,** 1943-1945 (2014).

Tsuji, T.; Fukazawa, S.; Sugiyama, R.; Kawasaki, K.; Iwasa, T.; Tsunoyama, H.; Tokitoh, N.; Nakajima, A., Physical Properties of Mononuclear Organoeuropium Sandwich Complexes Ligated by Cyclooctatetraene and Bis(trimethylsilyl) Cyclooctatetraene, *Chem. Phys. Lett.*, **595,** 144-150 (2014).

Tsuji, T.; Hosoya, N.; Fukazawa, S.; Sugiyama, R.; Iwasa, T.; Tsunoyama, H.; Hamaki, H.; Tokitoh, N.; Nakajima, A., Liquid-Phase Synthesis of Multidecker Organoeuropium Sandwich Complexes and Their Physical Properties, *J. Phys. Chem. C*, **118,** 5896-5907 (2014).

Nakanishi, K.; Sasamori, T.; Kuramochi, K.; Tokitoh, N.; Kawabata, T.; Tsubaki, K., Synthesis and Properties of Butterfly-Shaped Expanded Naphthofuran Derivatives, *J. Org. Chem.*, **79,** 2625-2631 (2014).

Matsumoto, T.; Sasamori, T.; Miyake, H.; Tokitoh, N., Synthesis of a Rhodium Carbonyl Phosphaalkenyl-Phosphido Complex: A Phosphorus Congener of Schiff Base Type *N,N'*-Chelating Monoanionic Ligands, *Organometallics*, **33,** 1341-1344 (2014).

Tsurusaki, A.; Sasamori, T.; Tokitoh, N., Synthesis and Structure of a 1-Phospha-2-boraacenaphthene Derivative and Its Chalcogenation Reactions, *Chem. Eur. J.*, **20,** 3752-3758 (2014).

Nagata, K.; Agou, T.; Tokitoh, N., Syntheses and Structures of Terminal Arylalumylene Complexes, *Angew. Chem. Int. Ed.*, **53,** 3881-3884 (2014).

Tanifuji, K.; Yamada, N.; Tajima, T.; Sasamori, T.; Tokitoh, N.; Matsuo, T.; Tamao, K.; Ohki, Y.; Tatsumi, K., A Convenient Route to Synthetic Analogues of the Oxidized Form of High-Potential Iron-Sulfur Proteins, *Inorg. Chem.*, **53,** 4000-4009 (2014).

Wakamiya, A.; Endo, M.; Sasamori, T.; Tokitoh, N.; Ogomi, Y.; Hayase, S.; Murata, Y., Reproducible Fabrication of Efficient Perovskite-based Solar Cells: X-ray Crystallographic Studies on the Formation of $CH_3NH_3PbI_3$ Layers, *Chem. Lett.*, **43,** 711-713 (2014).

Wasano, T.; Agou, T.; Sasamori, T.; Tokitoh, N., Synthesis, Structure and Reactivity of a 1-Bromoalumole, *Chem. Commun.*, **50,** 5148-8150 (2014).

Mizuhata, Y.; Inamura, K.; Tokitoh, N., Coordination Chemistry of 9-Sila- and 9-Germa-phenanthrenes — Unique Coordination Modes in Their Metallene Complexes, *Can. J. Chem.*, **92,** 441-446 (2014).

Kuwabara, T.; Ishimura, K.; Sasamori, T.; Tokitoh, N.; Saito, M., Facile Synthesis of Dibenzopentalene Dianions and Their Application as New π-Extended Ligands, *Chem. Eur. J.*, **20,** 7571-7575 (2014).

Agou, T.; Hayakawa, N.; Sasamori, T.; Matsuo, T.; Hashizume, D.; Tokitoh, N., Reactions of Diaryldibromodisilenes with *N*-Heterocyclic Carbenes: Formation of Formal Bis-NHC Adducts of Silyliumylidene Cations, *Chem. Eur. J.*, **20,** 9246-9249 (2014).

Sasamori, T.; Suzuki, Y.; Sakagami, M.; Miyake, H.; Tokitoh, N., Structure of Stable Telluradiphosphirane Bearing Bulky Ferrocenyl Ligands, *Chem. Lett.*, **43,** 1464-1466 (2014).

Kuwabara, T.; Guo, J. D.; Nagase, S.; Sasamori, T.; Tokitoh, N.; Saito, M., Synthesis, Structures, and Electronic Properties of Triple- and Double-Decker Ruthenocenes Incorporated by a Group 14 Metallole Dianion Ligand, *J. Am. Chem. Soc.*, **136,** 13059-13064 (2014).

Agou, T.; Nagata, K.; Sasamori, T.; Tokitoh, N., Reaction of a Dialumene-Benzene Adduct with Diphenylacetylene: Formation of 3,4-Dialuminacyclobutene and 5,6-Dialuminabicyclo[2.1.1]hex-2-ene Derivatives, *Chem. Asian J.*, **9,** 3099-3101 (2014).

Sasamori, T.; Sakagami, M.; Tokitoh, N., Bromination of a Stable 1,2-Bis(ferrocenyl) Dibismuthene: Synthesis of a 1,2-Dibromodibismuthane Derivative, *Heteroatom Chem.*, **25,** 306-312 (2014).

— Structural Organic Chemistry —

Zhang, R.; Futagoishi, T.; Murata, M.; Wakamiya, A.; Murata, Y., Synthesis and Structure of an Open-Cage Thiafullerene $C_{69}S$: Reactivity Differences of an Open-Cage C_{70} Tetraketone Relative to Its C_{60} Analogue, *J. Am. Chem. Soc.*, **136,** 8193-8196 (2014).

Hashikawa, Y.; Murata, M.; Wakamiya, A.; Murata, Y., Synthesis of Open-Cage Ketolactam Derivatives of Fullerene C_{60} Encapsulating a Hydrogen Molecule, *Org. Lett.*, **16,** 2970-2973 (2014).

Wakamiya, A.; Nishimura, H.; Fukushima, T.; Suzuki, F.; Saeki, A.; Seki, S.; Osaka, I.; Sasamori, T.; Murata, M.; Murata, Y.; Kaji, H., On-Top π-Stacking of Quasiplanar Molecules in Hole-Transporting Materials: Inducing Anisotropic Carrier Mobility in Amorphous Films, *Angew. Chem., Int. Ed.*, **53,** 5800-5804 (2014).

Wakamiya, A.; Endo, M.; Sasamori, T.; Tokitoh, N.; Ogomi, Y.; Hayase, S.; Murata, Y., Reproducible Fabrication of Efficient Perovskite-based Solar Cells: X-ray Crystallographic Studies on the Formation of $CH_3NH_3PbI_3$ Layers, *Chem. Lett.*, **43,** 711-713 (2014).

Chaolumen; Enno, H.; Murata, M.; Wakamiya, A.; Murata, Y., Dibenzo[*a*, *f*]perylene Bisimide: Effects of Introducing Two Fused Rings, *Chem. Asian J.*, **9,** 3136-3140 (2014).

Aoyagi, S.; Hoshino, N.; Akutagawa, T.; Sado, Y.; Kitaura, R.; Shinohara, H.; Sugimoto, K.; Zhang, R.; Murata, Y., A Cubic Dipole Lattice of Water Molecules Trapped inside Carbon Cages, *Chem. Commun.*, **50,** 524-526 (2014).

Maroto, E. E.; Izquierdo, M.; Filippone, S.; Murata, M.; Murata, Y.; Komatsu, K.; Martin, N., Catalytic Stereodivergent Functionalization of $H_2@C_{60}$, *Chem. Commun.*, **50,** 740-742 (2014).

Garbuio, L.; Li, Y.; Antonello, S.; Gascon, J. A.; Lawler, R. G.; Lei, X.; Murata, Y.; Turro, N. J.; Maran, F., Interaction of $H_2@C_{60}$ and Nitroxide through Conformationally Constrained Peptide Bridges, *Photochem. Photobiol.*, **90,** 439-447 (2014).

Uejima, M.; Sato, T.; Detani, M.; Wakamiya, A.; Suzuki, F.; Suzuki, H.; Fukushima, T.; Tanaka, K.; Murata, Y.; Adachi, C.; Kaji, H., A Designed Fluorescent Anthracene Derivative: Theory, Calculation, Synthesis, and Characterization, *Chem. Phys. Lett.*, **602,** 80-83 (2014).

Li, L.; Matsuda, R.; Tanaka, I.; Sato, H.; Kanoo, P.; Joen, H. J.; Foo, M. L.; Wakamiya, A.; Murata, Y.; Kitagawa, S., A Crystalline Porous Coordination Polymers Decorated with Nitroxyl Radicals Catalyzes Aerobic Oxidation of Alcohols, *J. Am. Chem. Soc.*, **136,** 7543-7546 (2014).

Goh, K.; Jimenez-Ruiz, M.; Johnson, M. R.; Roles, S.; Ollivier, J.; Denning, M. S.; Mamone, S.; Levitt, M. L.; Lei, X.; Li, Y.; Turro, N. J.; Murata, Y.; Horsewill, A. J., Symmetry-breaking in the Endofullerene $H_2O@C_{60}$ Revealed in the Quantum Dynamics of Ortho and Para-water: a Neutron Scattering Investigation, *Phys. Chem. Chem. Phys.*, **16,** 21330-21339 (2014).

Katayama, T.; Jinno, A.; Takeuchi, E.; Ito, S.; Endo, M.; Wakamiya, A.; Murata, Y.; Ogomi, Y.; Hayase, S.; Miyasaka, H., Inhomogeneous Deactivation Process with UV Excitation in Submicron Grains of Lead Iodide Perovskite-based Solar Cell as Revealed by Femtosecond Transient Absorption Microscopy, *Chem. Lett.*, **43,** 1656-1658 (2014).

Satou, M.; Uchinaga, K.; Wakamiya, A.; Murata, Y., Thiazole-Fused Benzothiaziazole as a Key Skeleton for T-Shaped Electron Accepting Building Blocks, *Chem. Lett.*, **43,** 1386-1388 (2014).

Yamada, Y.; Nakamura, T.; Endo, M.; Wakamiya, A.; Kanemitsu, Y., Near-Band Edge Optical Responsed of Solution-Processed Organic-Inorganic Hybrid Perovskite $CH_3NH_3PbI_3$ on Mesoporous TiO_2 Electrodes, *Appl. Phys. Express*, **7,** [32302-1]-[32302-4] (2014).

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).

Kushida, T.; Camacho, C.; Shuto, A.; Irle, S.; Muramatsu, M.; Katayama, T.; Ito, S.; Nagasawa, Y.; Miyasaka, H.; Sakuda, E.; Kitamura, N.; Zhou, Z.; Wakamiya, A.; Yamaguchi, S., Constraint-Induced Structural Deformation of Planarized Triphenylboranes in the Excited State, *Chem. Sci.*, **5,** 1296-1304 (2014).

Lee, J.; Kim, B.; Kwon, J. E.; Kim, J.; Yokoyama, D.; Suzuki, K.; Nishimura, H.; Wakamiya, A.; Park, S. Y.; Park, J., Excimer Formation in Organic Emitter Films Associated with a Molecular Orientation Promoted by Steric Hindrance, *Chem. Commun.*, **50,** 14145-14148 (2014).

Fuse, S.; Matsumura, K.; Wakamiya, A.; Hisashi, M.; Tanaka, H.; Yoshikawa, S.; Takahashi, T., Elucidation of the Structure-Property Relationship of p-Type Organic Semiconductors through Rapid Library Construction via a One-pot, Suzuki-Miyaura Coupling Reaction, *ACS. Comb. Sci.*, **16,** 494-499 (2014).

[Others]

Murata, Y.; Zhang, R.; Hashikawa, Y., Water-Encapsulating Endofullerene, *Frontier of Fullerene Derivatives and Encapsulation Technique, CMC Publishing Co., LTD.*, 135-142 (2014) (in Japanese).

Wakamiya, A.; Nishimura, H.; Murata, Y., Development of Organic Semiconducting Materials Using Quasiplanar Structure as a Key Scaffold, *Kagaku, Kagaku-Dojin Publishing Co., Inc.*, **69,** 12-17 (2014) (in Japanese).

Yamada, Y.; Wakamiya, A.; Kanemitsu, Y., Perovskite Semiconductor Solar Cells, *Solid State Physics, AGNE Gijutsu Center Inc.*, **49,** 27-35 (2014) (in Japanese).

Wakamiya, A., Single-Crystal X-ray Analyses of Perovskite Materials and Improvement of Power Conversion Efficiency, *Solar Energy, Japan Solar Energy Society*, **40,** 33-37 (2014) (in Japanese).

— Synthetic Organic Chemistry —

Hamada, S.; Wada, Y.; Sasamori, T.; Tokitoh, N.; Furuta, T.; Kawabata, T., Oxidative Kinetic Resolution of Racemic Alkyl Aryl Carbinols by an Electronically Tuned Chiral Nitroxyl Radical, *Tetrahedron Lett.*, **55,** 1943-1945 (2014).

Nakanishi, K.; Fukatsu, D.; Takaishi, K.; Tsuji, T.; Uenaka, K.; Kuramochi, K.; Kawabata, T.; Tsubaki, K., Oligonaphthofurans: Fan-Shaped and Three-Dimensional π-Compounds, *J. Am. Chem. Soc.*, **136,** 7101-7109 (2014).

Yoshimura, T., Catalytic Asymmetric Reactions in Alkaloids and Terpenoids Syntheses, *Tetrahedron Lett.*, **55,** 5109-5118 (2014).

Hirooka, Y.; Ikeuchi, K.; Kawamoto, Y.; Akao, Y.; Furuta, T.; Asakawa, T.; Inai, M.; Wakimoto, T.; Fukuyama, T.; Kan, T., Enantioselective Synthesis of SB-203207, *Org. Lett.*, **16,** 1646-1649 (2014).

Nakanishi, K.; Sasamori, T.; Kuramochi, K.; Tokitoh, N.; Kawabata, T.; Tsubaki, K., Synthesis and Properties of Butterfly-Shaped Expanded Naphthofuran Derivatives, *J. Org. Chem.*, **79,** 2625-2631 (2014).

[Others]

Kawabata, T., Catalytic Acylation, *Fine Chemical*, **63,** 14-23 (2014).

— Advanced Inorganic Synthesis —

Okano, M.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Assessment of Hot-carrier Effects on Charge Separation in Type-II CdS/CdTe Heterostructured Nanorods, *J. Phys. Chem. Lett.*, **5,** 2951-2956 (2014).

Kano, S.; Tanaka, D.; Sakamoto, M.; Teranishi, T.; Majima, Y., Control of Charging Energy in Chemically Assembled Nanoparticle Single-Electron Transistors, *Nanotechnology*, **26,** 045702 (2014).

Ihara, T.; Sato, R.; Teranishi, T.; Kanemitsu, Y., Delocalized and Localized Charged Excitons Single CdSe/CdS Dot-in-Rods Revealed by Polarized Photoluminescence Blinking, *Phys. Rev. B*, **90,** [035309-1]-[035309-5] (2014).

Sakamoto, M.; Inoue, K.; Saruyama, M.; So, Y.-G.; Kimoto, K.; Okano, M.; Kanemitsu, Y.; Teranishi, T., Investigation on Photo-Induced Charge Separation in CdS/CdTe Nanopencils, *Chem. Sci.*, **5,** 3831-3835 (2014).

Tanaka, D.; Inuta, Y.; Sakamoto, M.; Furube, A.; Haruta, M.; So, Y.-G.; Kimoto, K.; Hamada, I.; Teranishi, T., Strongest π-Metal Orbital Coupling in a Porphyrin/Gold Cluster System, *Chem. Sci.*, **5,** 2007-2010 (2014).

Osakada, Y.; Pratx, G.; Sun, C.; Sakamoto, M.; Ahmad, A.; Volotskova, O.; Ong, Q.; Teranishi, T.; Harada, Y.; Xing, L.; Cui, B., Hard X-ray-induced Optical Luminescence via Biomolecule-directed Metal Clusters, *Chem. Commun.*, **50,** 3549-3551 (2014).

Xiong, A.; Yoshinaga, T.; Ikeda, T.; Takashima, M.; Hisatomi, T.; Maeda, K.; Setoyama, T.; Teranishi, T.; Domen, K., Effect of Hydrogen and Oxygen Evolution Cocatalysts on Photocatalytic Activity of GaN: ZnO, *Eur. J. Inorg. Chem.*, **2014,** 767-772 (2014).

[Others]

Sato, R.; Teranishi, T., Fabrication of $L1_0$-FePd/α-Fe Nanocomposite Magnets, *Bull. Soc. Nano. Sci. Tech.*, **13,** 17-23 (2014) (in Japanese).

Wu, H.-L.; Sato, R.; Teranishi, T., Selective Synthesis and Plasmonic Properties of Polyhedral Gold Nanoparticles, *Bull. Soc. Nano. Sci. Tech.*, **13,** 43-47 (2014) (in Japanese).

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

Huang, Y.; Morinaga, T.; Tai, Y.; Tsujii, Y.; Ohno, K., Immobilization of Semisoft Colloidal Crystals Formed by Polymer-Brush-Afforded Hybrid Particles, *Langmuir*, **30,** 7304-7312 (2014).

Tanishima, M.; Goto, A.; Lei, L.; Ohtsuki, A.; Kaji, H.; Nomura, A.; Tsujii, Y.; Yamaguchi, Y.; Komatsu, H.; Miyamoto, M., Macromolecular Architectures Designed by Living Radical Polymerization with Organic Catalysts, *Polymers*, **6,** 311-326 (2014).

Nakamura, Y.; Nakanishi, K.; Yamago, S.; Tsujii, Y.; Takahashi, K.; Morinaga, T.; Sato, T., Controlled Polymerization of Protic Ionic Liquid Monomer by ARGET-ATRP and TERP, *Macromol. Rapid Commun.*, **35,** 642-648 (2014).

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 (2014).

Ohno, K.; Huang, Y.; Okubo, T., Drying Dissipative Structures of Spindle-Shaped Hematite Particles Coated with Polymer Brush, *Colloid Polym. Sci.*, **292,** 1143-1151 (2014).

Ohno, K.; Huang, Y.; Tsuchida, A.; Okubo, T., Colloidal Crystallization of Spindle-Shaped Hematite Particles Coated with Polymer Brush in Deionized Aqueous Suspension, *Colloid Polym. Sci.*, **292,** 723-731 (2014).

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, 6997 (2014).

Sakakibara, K.; Chithra, P.; Das, B.; Mori, T.; Akada, M.; Labuta, J.; Tsuruoka, T.; Maji, S.; Furumi, S.; Shrestha, L.; Hill, J.; Acharya, S.; Ariga, K.; Ajayaghosh, A., Aligned 1-D Nanorods of a π-Gelator Exhibit Molecular Orientation and Excitation Energy Transport Different from Entangled Fiber Networks, *J. Am. Chem. Soc.*, **136,** 8548-8551 (2014).

Sakakibara, K.; Fujisawa, T.; Hill, J.; Ariga, K., Conformational Interchange of a Carbohydrate by Mechanical Compression at the Air-Water Interface, *Phys. Chem. Chem. Phys.*, **16,** 10286-10294 (2014).

[Others]

Sakakibara, K.; Tsujii, Y., Highly Lubricating Property of Swollen Concentrated Polymer Brushes, *Kobunshi*, **63,** 281-284 (2014) (in Japanese).

Sakakibara, K.; Tsujii, Y., Polymer Dispersants for Cellulose Nanofiber Reinforced Polyolefin Composite Materials, *Kino Zairyo*, **34,** 40-45 (2014) (in Japanese).

Sakakibara, K., Cellulose Nanofiber-Based Composite Materials with Polymer Brush Components, *SEN'I GAKKAISHI*, **70,** 276-280 (2014) (in Japanese).

— Polymer Controlled Synthesis —

Yamago, S.; Kayahara, E.; Iwamoto T., Organoplatinum-Mediated Synthesis of Cyclic π-Conjugated Molecules: Towards a New Era of Three-Dimensional Aromatic Compounds, *Chem. Rec.*, **14,** 84-100 (2014).

Nakamura, Y.; Nakanishi, K.; Yamago, S.; Tsujii, Y.; Takahashi, K.; Morinaga, T.; Sato T., Controlled Polymerization of a Protic Ionic Liquid Monomer by ARGET ATRP and TERP, *Macromol. Rapid Commun.*, **35,** 642-648 (2014).

Kameda, T.; Nemoto, T.; Ogawa, T.; Tosaka, M.; Kurata, H.; Schaper, A. K., Evidence of α-helical Coiled Coils and β-sheets in Hornet Silk, *J. Struct. Biol.*, **185,** 303-308 (2014).

Kayahara, E.; Patel, V. K.; Yamago, S., Synthesis and Characterization of [5]Cycloparaphenylene, *J. Am. Chem. Soc.*, **136,** 2284-2287 (2014).

Iwamoto, T.; Kayahara, E.; Yasuda, N.; Suzuki, T.; Yamago, S., Synthesis, Characterization, and Properties of [4]Cyclo-2,7-pyrenylene: Effect of Cyclic Structure on the Electronic Properties of Pyrene Oligomers, *Angew. Chem. Int. Ed.*, **53,** 6430-6434 (2014).

Alvarez, M. P.; Burrezo, P. M.; Kertesz, M.; Iwamoto, T.; Yamago, S.; Xia, J.; Jasti, R.; Navarrete, J. T. L.; Taravillo, M.; Baonza, V. G.; Casado, J., Properties of Sizeable [n]CycloParaPhenylenes as Ultrashort Single-Wall Carbon Nanotubes by Raman Spectroscopy: Structural and Electron-Transfer Responses Under Pressure Stress, *Angew. Chem. Int. Ed.*, **53,** 7033-7037 (2014).

Fujitsuka, M.; Lu, C.; Iwamoto, T.; Kayahara, E.; Yamago, S.; Majima, T., Properties of Triplet-Excited [n]Cycloparaphenylenes ($n=8-12$): Excitation Energies Lower than Those of Linear Oligomers and Polymers, *J. Phys. Chem. A*, **118,** 4527-4532 (2014).

Fujitsuka, M.; Tojo, S.; Iwamoto, T.; Kayahara, E.; Yamago, S.; Majima, T., Radical Ions of Cycloparaphenylenes: Size-Dependence Contrary to the Neutral Molecules, *J. Phys. Chem. Lett.*, **5,** 2302-2305 (2014).

Iwamoto, T.; Slanina, Z.; Mizorogi, N.; Guo, J.; Akasaka, T.; Nagase, S.; Takaya, H.; Yasuda, N.; Kato, T.; Yamago, S., Partial Charge Transfer in Shortest Possible Metallofullerene Peapod, La@C82⊂[11] Cycloparaphenylene, *Chem. Eur. J.*, **20,** 14403-14409 (2014).

Hashimoto, S.; Nakatsuka, S.; Nakamura, M.; Hatakeyama, T., Construction of a Highly Distorted Benzene Ring in a Double Helicene, *Angew. Chem. Int. Ed.*, **53,** 14074-14076 (2014).

Hashimoto, S.; Ikuta, T.; Shiren, K.; Nakatsuka, S.; Ni, J.; Nakamura, M.; Hatakeyama, T., Triplet-Energy Control of Polycyclic Aromatic Hydrocarbons by BN Replacement: Development of Ambipolar Host Materials for Phosphorescent OLEDs, *Chem. Mater.*, **26,** 6265-6271 (2014).

Kermagoret, A.; Nakamura, Y.; Bourguignon, M.; Detrembleur, C.; Jerome, C.; Yamago, S.; Debuigne, A., Expanding the Scope of Controlled Radical Polymerization via Cobalt-tellurium Radical Exchange Reaction, *ACS Macro Lett.*, **3,** 114-118 (2014).

Nakamura, Y.; Arima, T.; Yamago, S., Modular Synthesis of Mid-Chain Functionalized Polymers by Photoinduced Diene- and Styrene-Assisted Radical Coupling Reaction of Polymer-End Radicals, *Macromolecules*, **47,** 582-588 (2014).

Hirao, T.; Tosaka, M.; Yamago, S.; Haino, T., Supramolecular Fullerene Polymers and Networks Directed by Molecular Recognition between Calix[5]arene and C_{60}, *Chem. Eur. J.*, **20,** 16138-16146 (2014).

Tosaka, M., Strain-induced Crystallization of Cross-linked Rubber, *Kobunshi Ronbunshu*, **71,** 493-500 (2014).

[Others]

Tosaka, M., Strain-Induced Crystallization of Rubber, *Polyfile*, **51,** 12-16 (2014) (in Japanese).

Yamago, S.; Kayahara, E.; Iwamoto, T., New Organic Chemistry of Three-Dimensional π-Conjugated Compounds, *Journal of Synthetic Organic Chemistry*, **72,** 992-1005 (2014) (in Japanese).

Hatakeyama, T.; Hashimoto, S.; Nakamura, M., Synthesis of Heteroatom-fused Polycyclic Aromatic Compounds via Tandem Hetero-Friedel-Crafts Reactions and Their Applications, *Journal of Synthetic Organic Chemistry*, **72,** 1391-1397 (in Japanese).

Kayahara, E.; Yamago, S., Finally Accomplished! World Smallest Carbon Nano Ring -The Development of Synthetic Methods That Enable Connection of Fibe Benzene Rings into a Circle-, *Chemistry*, **69,** 32-36 (2014) (in Japanese).

Yamago, S., Development of Novel Synthetic Method TERP, *Chemistry Today*, **521,** 50-54 (2014) (in Japanese).

— Inorganic Photonics Materials —

Minami, T.; Tokuda, Y.; Masai, H.; Ueda, Y.; Ono, Y.; Fujimura, S.; Yoko, T., Structural Analysis of Alkali Cations in Mixed Alkali Silicate Glasses by ^{23}Na and ^{133}Cs MAS NMR, *J. Asian Ceram. Soc.*, **2,** 333-338 (2014).

Tokuda, Y.; Matsuki, H.; Ueda, Y.; Masai, H.; Yoko, T., Crystal Growth of ZnO Microneedles in Water Containing Microbubbles, *New J. Glass Ceram*, **4,** 49-54 (2014).

Masai, H.; Tanimoto, T.; Okumura, S.; Teramura, K.; Matsumoto, S.; Yanagida, T.; Tokuda, Y.; Yoko T., Correlation between Preparation Conditions and the Photoluminescence Properties of Sn^{2+}Centers in $ZnO-P_2O_5$ Glasses, *J. Mater. Chem. C*, **2,** 2137-2143 (2014).

Masai, H.; Fujiwara, T.; Matsumoto, S.; Tokuda, Y.; Yoko, T.; Emission Property of Sn^{2+}-doped $ZnO-P_2O_5$ Glass, *J. Non-Cryst. Solids*, **383,** 184-187 (2014).

Yanagida, T.; Fujimoto, Y.; Masai, H., Scintillation and Dosimeter Properties of $40Li_2O-40B_2O_3-20SiO_2$ Glass with Different Sn Concentrations, *Physics and Chemistry of Glasses*, **55,** 274-279 (2014).

Masai, H.; Hino, Y.; Yanagida, T.; Fujimoto, Y.; Yoko, T., Energy Transfer from Sn^{2+} to RE^{3+} Cations in $ZnO-P_2O_5$ Glass, *Bulletin of the Chemical Society of Japan*, **87,** 556-563 (2014).

Ueda, Y.; Tokuda, Y.; Nagai, H.; Masai, H.; Yoko, T., Analysis of Electrochemical Characteristics of Organic-Inorganic Hybrid Titanophosphite Membranes, *ECS Transactions*, **58,** 45-52 (2014).

Masai, H.; Fujiwara, T.; Matsumoto, S.; Tokuda, Y.; Yoko, T., Emission Property of Sn^{2+}-Doped $ZnO-P_2O_5$ Glass, *Journal of Non-Crystalline Solids*, **383,** 184-187 (2014).

Fujimoto, Y.; Yanagida, T.; Futami, Y.; Masai, H., Fluorescence and Radiation Response Properties of Ce^{3+}-doped $CaO-Al_2O_3-B_2O_3$ Glass, *Japanese Journal of Applied Physics*, **53,** [05FK05-1]-[05FK05-3] (2014).

— Nanospintronics —

Hata, H.; Taniguchi, T.; Lee, H.-W.; Moriyama, T.; Ono, T., Spin-wave-induced Domain Wall Motion in Perpendicularly Magnetized System, *Appl. Phys. Exp.*, **7,** [33001-1]-[033001-4] (2014).

Yoshimura, Y.; Koyama, T.; Chiba, D.; Nakatani, Y.; Fukami, S.; Yamanouchi, M.; Ohno, H.; Kim, K.-J.; Moriyama, T.; Ono, T., Effect of Spin Hall Torque on Current Induced Precessional Domain Wall Motion, *Appl. Phys. Exp.*, **7,** [33005-1]-[033005-4] (2014).

Ono, S.; Hausermann, R.; Chiba, D.; Shimamura, K.; Ono, T.; Batlogg, B., High Performance Organic Field-effect Transistors with Ultra-thin HfO_2 Gate Insulator Deposited Directly onto the Organic Semiconductor, *Appl. Phys. Lett.*, **104,** [013307-1]-[013307-4] (2014).

Nagata, M.; Tanabe, K.; Moriyama, T.; Chiba, D.; Ohe, J.; Myoka, M.; Niizeki, T.; Yanagihara, H.; Kita, E.; Ono, T., Ferromagnetic Resonance in Magnetite Thin Films, *IEEE Trans. Magn.*, **50,** [1400203-1]-[1400203-3] (2014).

Fukami, S.; Yamanouchi, M.; Nakatani, Y.; Kim, K.-J.; Koyama, T.; Chiba, D.; Ikeda, S.; Kasai, N.; Ono, T.; Ohno, H., Distribution of Critical Current Density for Magnetic Domain Wall Motion, *J. of Appl. Phys.*, **115,** [17D508-1]-[17D508-3] (2014).

Ono, T., Vortices on the Move, *Nat. Nanotech.*, **9,** 96-97 (2014).

Tanigawa, H.; Suzuki, T.; Suemitsu, K.; Ohshima, N.; Kitamura, T.; Ohkochi, T.; Kotsugi, M.; Kinoshita, T.; Koyama, T.; Chiba, D.; Yoshimura, Y.; Ueda, K.; Ono, T.; Kariyada, E., Operating Principle of a Three-terminal Domain Wall Device with Perpendicularly Magnetized Ta/CoFeB/MgO Free Layer and Underlying Hard Magnets, *J. J. of Appl. Phys.*, **53,** [063002-1]-[063002-7] (2014).

Yamada, K.; Sato, T.; Nakatani, Y.; Kasai, S.; Chiba, D.; Kobayashi, K.; Thiaville, A.; Ono, T., Switching of Magnetic Vortex Core in Elliptical Disks by Nanosecond Field Pulses, *Appl. Phys. Exp.*, **7,** [063008-1]-[063008-4] (2014).

Tanaka, K.; Moriyama, T.; Nagata, M.; Seki, T.; Takanashi, K.; Takahashi, S.; Ono, T., Linewidth Broadening of Optical Precession Mode in Synthetic Antiferromagnet, *Appl. Phys. Exp.*, **7,** [063010-1]-[063010-4] (2014).

Taniguchi, T.; Kim, K.-J.; Yoshimura, Y.; Moriyama, T.; Tanigawa, H.; Suzuki, T.; Kariyada, E.; Ono, T., Different Stochastic Behaviors for Magnetic Field and Current, *Appl. Phys. Exp.*, **7,** [053005-1]-[053005-3] (2014).

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, *Appl. Phys. Exp.*, **7,** [053001-1]-[053001-4] (2014).

Ueda, K.; Kim, K.-J.; Yoshimura, Y.; Hiramatsu, R.; Moriyama, T.; Chiba, D.; Tanigawa, H.; Suzuki, T.; Kariyada, E.; Ono, T., Transition in Mechanism for Current-driven Magnetic Domain Wall Dynamics, *Appl. Phys. Exp.*, **7,** [053006-1]-[053006-4] (2014).

Chida, K.; Hata, T.; Arakawa, T.; Matsuo, S.; Nishihara, Y.; Tanaka, T.; Ono, T.; Kobayashi, K., Avalanche Electron Bunching in a Corbino Disk in the Quantum Hall Effect Breakdown Regime, *Phys. Rev. B*, **89,** [235318-1]-[235318-4] (2014).

Kim, K.-J.; Hiramatsu, R.; Moriyama, T.; Tanigawa, H.; Suzuki, T.; Kariyada, E.; Ono, T., Tradeoff between Low-power Operation and Thermal Stability in Magnetic Domain-wall-motion Devices Driven by Spin Hall Torque, *Appl. Phys. Exp.*, **7,** [053003-1]-[053003-4] (2014).

Tanaka, T.; Arakawa, T.; Maeda, M.; Kobayashi, K.; Nishihara, Y.; Ono, T.; Nozaki, T.; Fukushima, A.; Yuasa, S., Leak Current Estimated from the Shot Noise in Magnetic Tunneling Junctions, *Appl. Phys. Lett.*, **105,** [042405-1]-[042405-4] (2014).

Hiramatsu, R.; Kim, K.-J.; Nakatani, Y.; Moriyama, T.; Ono, T., Proposal for Quantifying the Dzyaloshinsky-Moriya Interaction by Domain Walls Annihilation Measurement, *J. of Appl. Phys.*, **53,** [108001-1]-[108001-3] (2014).

Gubbiotti, G.; Nguyen, T. H.; Hiramatsu, R.; Tacchi, S.; Madami, M.; Cottam, G. M.; Ono, T., Field Dependence of the Magnetic Eigenmode Frequencies in Layered Nanowires with Ferromagnetic and Antiferromagnetic Ground States: Experimental and Theoretical Study, *J. of Phys. D*, **47,** [365001-1]-[365001-10] (2014).

Tanaka, A. M.; Maezaki, D.; Ishii, T.; Okubo, A.; Hiramatsu, R.; Ono, T.; Mibu, K., Interface Magnetism of Co_2FeGe Heusler Alloy Layers and Magnetoresistance of $Co_2FeGe/MgO/Fe$ Magnetic Tunnel Junctions, *J. of Appl. Phys.*, **116,** [163902-1]-[163902-5] (2014).

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

Nakase, I.; Osaki, K.; Tanaka, G.; Utani, A.; Futaki, S., 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, *Biochem. Biophys. Res. Commun.*, **446,** 857-862 (2014).

Azuma, Y.; Kukenshoner, 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 Modifications of *a–g* Interactions, *Chem. Commun.*, **50,** 6364-6367 (2014).

Takeuchi, T.; Popiel, H. A.; Futaki, S.; Wada, K.; Nagai, Y., Peptide-Based Therapeutic Approaches for Treatment of the Polyglutamine Diseases, *Curr. Med. Chem.*, **21,** 2575-2582 (2014).

Mitsueda, A.; Shimatani, Y.; Ito, M.; Ohgita, T.; Yamada, A.; Hama, S.; Gräslund, A.; Lindberg, S.; Langel, Ü.; Harashima, H.; Nakase, I.; Futaki, S.; Kogure K., Development of a Novel Nanoparticle by Dual Modification with the Pluripotential Cell-Penetrating Peptide PepFect6 for Cellular Uptake, Endosomal Escape and Decondensation of an siRNA Core Complex, *Biopolymers-Peptide Science*, **100,** 698-704 (2013).

Popiel, H. A.; Takeuchi, T.; Burke, J. R.; Strittmatter, W. J.; Toda, T.; Wada, K.; Nagai, Y., Inhibition of Protein Misfolding/Aggregation Using Polyglutamine Binding Peptide QBP1 as a Therapy for the Polyglutamine Diseases, *Neurotherapeutics*, **10,** 440-446 (2013).

— Chemistry of Molecular Biocatalysts —

Ida, T.; Suzuki, H.; Fukuyama, K.; Hiratake, J.; Wada, K., Crystal Structure of *Bacillus subtilis* γ-Glutamyltranspeptidase in Complex with Acivicin: Diversity of the Binding Mode of a Classical and Electrophilic Active-Site Directed Glutamate Analogue, *Acta Cryst.*, **D70,** 607-614 (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).

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).

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).

Hayashi, K.; Watanabe, B.; Nakagawa, Y.; Minami, S.; Morita, T., RPEL Proteins Are the Molecular Targets for CCG-1423, an Inhibitor of Rho Signaling., *PLoS One*, **9,** e89016 (2014).

— Molecular Biology —

Li, R.; Li, J.; Li, S.; Qin, G.; Novák, O.; Pěnčík, A.; Ljung, K.; Aoyama, T.; Liu, J.; Murphy, A.; Gu, H.; Tsuge, T.; Qu, L.-J., *ADP1* Affects Plant Architecture by Regulating Local Auxin Biosynthesis, *PLoS Genet.*, **10,** 31003954 (2014).

Zhu, D.; Wu, Z.; Cao, G.; Li, J.; Wei, J.; Tsuge, T.; Gu, H.; Aoyama, T.; Qu, L.-J., Translucent Green, an ERF Family Transcription Factor, Controls Water Balance in *Arabidopsis* by Activating the Expression of Aquaporin Genes, *Mol. Plant*, **7,** 601-615 (2014).

Tanaka, N.; Kato, M.; Tomioka, R.; Kurata, R.; Fukao, Y.; Aoyama, T.; Maeshima, M., Characteristics of a Root Hair-Less Line of *Arabidopsis thaliana* under Physiological Stresses, *J. Exp. Bot.*, **65,** 1497-1512 (2014).

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).

[Others]

Kusano, H.; Tominaga, R.; Wada, T.; Kato, M.; Aoyama, T., Phosphoinositide Signaling in Root Hair Tip Growth, *"Plant Cell Wall Patterning and Cell Shape" (ed., Fukuda, H.: Wiley-Blackwell)*, 239-268 (2014).

— Chemical Biology —

Sakano, D.; Shiraki, N.; Kikawa, K.; Yamazoe, T.; Kataoka, M.; Umeda, K.; Araki, K.; Mao, D.; Matsumoto, S.; Nakagata, N.; Andersson, O.; Stainier, D.; Endo, F.; Kume, K.; Uesugi, M.; Kume, S., VMAT2 Identified as a Regulator of Late-stage Beta Cell Differentiation., *Nat. Chem. Biol.*, **10,** 141-148 (2014).

Hirata, N.; Nakagawa, M.; Fujibayashi, Y.; Yamauchi, K.; Murata, A.; Minami, I.; Tomioka, M.; Kondo, T.; Kuo, T. F.; Endo, H.; Inoue, H.; Sato, S.; Ando, S.; Kawazoe, Y.; Aiba, K.; Nagata, K.; Kawase, E.; Chang, Y. T.; Suemori, H.; Eto, K.; Nakauchi, H.; Yamanaka, S.; Nakatsuji, N.; Ueda, K.; Uesugi, M., A Chemical Probe That Labels Human Pluripotent Stem Cells, *Cell. Rep.*, **6(6),** 1165-1174 (2014).

Araoka, T.; Mae, S.; Kurose, Y.; Uesugi, M.; Ohta, A.; Yamanaka, S.; Osafune, K., Efficient and Rapid Induction of Human iPSCs/ESCs into Nephrogenic Intermediate Mesoderm Using Small Molecule-Based Differentiation Methods, *PLoS One*, **9 (1),** e84881 (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).

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, M.; Uesugi, M., Synthetic Molecules That Protect Cells from Anoikis and Their Use in Cell Transplantation., *Angew. Chem. Int. Ed.*, **126 (42),** 11390-11395 (2014).

Ohkanda, J., Synthetic Molecules for Disrupting and Detecting Protein-protein Interactions, *Farumashia*, **50,** 1101-1106 (2014) (in Japanese).

Ohkanda, J., Peptidomimetics, *Farumashia*, **50,** 1128 (2014) (in Japanese).

Harada, K.; Aoyama, S.; Matsugami, A.; Kumar, P. K. R.; Katahira, M.; Kato, K.; Ohkanda, J., RNA-Directed Amino Acid Coupling as a Model Reaction for Primitive Coded Translation, *Chem Bio Chem.*, **15,** 794-798 (2014).

DIVISION OF ENVIRONMENTAL CHEMISTRY

— Molecular Materials Chemistry —

Lei, L.; Tanishima, M.; Goto, A.; Kaji, H.; Yamaguchi, Y.; Komatsu, H.; Jitsukawa, T.; Miyamoto, M., Systematic Study on Alkyl Iodide Initiators in Living Radical Polymerization with Organic Catalysts, *Macromolecules*, **47,** 6610-6618 (2014).

Hayase, G.; Kanamori K.; Abe K.; Yano H.; Maeno A.; Kaji, H.; Nakanishi, K., Polymethylsilsesquioxane-Cellulose Nanofiber Biocomposite Aerogels with High Thermal Insulation, Bendability and Superhydrophobicity, *ACS Appl. Mater. & Interfaces*, **6,** 9466-9471 (2014).

Suzuki, F.; Nishiyama, Y.; Kaji, H., Clarification of Isomeric Structures and the Effect of Intermolecular Interactions in Blue-emitting Aluminum Complex Alq_3 Using First-principles ^{27}Al NMR Calculations, *Chem. Phys. Lett.*, **605,** 1-4 (2014).

Wakamiya, A.; Nishimura, H.; Fukushima, T.; Saeki, A.; Seki, S.; Osaka, I.; Murata, M.; Murata, Y.; Kaji, H., On-Top π-Stacking of Quasiplanar Molecules in Hole-Transporting Materials: Inducing Anisotropic Carrier Mobility in Amorphous Films, *Angew. Chem., Int. Ed.*, **53,** 5800-5804 (2014).

Uejima, M.; Sato, T.; Detani, M.; Wakamiya, A.; Suzuki, F.; Suzuki, H.; Fukushima, T.; Tanaka, K.; Murata, Y.; Adachi, C.; Kaji, H., A Designed Fluorescent Anthracene Derivative: Theory, Calculation, Synthesis, and Characterization, *Chem. Phys. Lett.*, **602,** 80-83 (2015).

Lei, L.; Tanishima, M.; Goto, A.; Kaji, H., Living Radical Polymerization via Organic Superbase Catalysis, *Polymers*, **6,** 860-872 (2014).

Uejima, M.; Sato, T.; Tanaka, K.; Kaji, H., Enhancement of Fluorescence in Anthracene by Chlorination: Vibronic Coupling and Transition Dipole Moment Density Analysis, *Chem. Phys.*, **430,** 47-55 (2014).

Tanishima, M.; Goto, A.; Lei, L.; Ohtsuki, A.; Kaji, H.; Nomura, A.; Tsujii, Y.; Yamaguchi, Y.; Komatsu, H.; Miyamoto, M., Macromolecular Architectures Designed by Living Radical Polymerization with Organic Catalysts, *Polymers*, **6,** 311-326 (2014).

Hirata, S.; Totani, K.; Watanabe, T.; Kaji, H.; Vacha, M., Relationship between Room Temperature Phosphorescence and Deuteration Position in a Purely Aromatic Compound, *Chem. Phys. Lett.*, **591,** 119-125 (2014).

Asakura, T.; Yazawa, K.; Horiguchi, K.; Suzuki, F.; Nishiyama, Y.; Nishimura, K.; Kaji, H., Difference in the Structures of Alanine Tri- and Tetra-peptides with Antiparallel β-sheet Assessed by X-ray Diffraction, Solid-state NMR and Chemical Shift Calculations by GIPAW, *Biopolymer*, **101,** 13-20 (2014).

Tanaka, H.; Shizu, K.; Nakanotani, H.; Adachi, C., Dual Intramolecular Charge-Transfer Fluorescence Derived from a Phenothiazine-Triphenyltriazine Derivative, *J. Phys. Chem. C*, **118,** 15985-15994 (2014).

Takahashi, T.; Shizu, K.; Yasuda, T.; Togashi, K.; Adachi, C., Donor-Acceptor-Structured 1,4-Diazatriphenylene Derivatives Exhibiting Thermally Activated Delayed Fluorescence: Design and Synthesis, Photophysical Properties and OLED Characteristics, *Sci. Technol. Adv. Mater.*, **15,** 34202 (2014).

Ohkuma, H.; Nakagawa, T.; Shizu, K.; Yasuda, T.; Adachi, C., Thermally Activated Delayed Fluorescence from a Spiro-Diazafluorene Derivative, *Chem. Lett.*, **43,** 1017-1019 (2014).

— Hydrospheric Environment Analytical Chemistry —

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).

Liu, Y.; Imashuku, S.; Sasaki, N.; Ze, L.; Kawai, J.; Takano, S.; Sohrin, Y.; Seki, H.; Miyauchi, H., Portable Total Reflection X-ray Fluorescence Analysis in the Identification of Unknown Laboratory Hazards, *J. Vac. Sci. Technol. A*, **32,** [031401-1]-[031401-6] (2014).

Takano, S.; Tanimizu, M.; Hirata, T.; Sohrin, Y., Isotopic Constraints on Biogeochemical Cycling of Copper in the Ocean, *Nat. Commun.*, **5,** [5563-1]-[5663-7] (2014).

[Others]

Sohrin, Y., Ocean and Environment, *Environmental Studies -Liveral Arts in the 21st Century-*, 52-53 (2014) (in Japanese).

Sohrin, Y., Lake and Environment, *Environmental Studies -Liveral Arts in the 21st Century-*, 54-55 (2014) (in Japanese).

Sohrin, Y., Trace Metals and Their Isotopes, *Marine Geochemistry*, 78-95 (2014) (in Japanese).

Takano, S.; Sohrin, Y.; Tanimizu, M.; Hirata, T., Biogeochemical Cycling of Copper Isotopes in the Ocean Using Precise Measurement of Copper Isotopic Ratio, *Kaiyo Monthly*, **55,** 13-20 (2014) (in Japanese).

Zheng, L.; Konagaya, W.; Minami, T.; Sohrin, Y., The Determination of Bioactive Trace Metals in Seawater Using an Automated Preconcentration Device, *Kaiyo Monthly*, **55,** 21-27 (2014) (in Japanese).

Langmuir, C. H.; Broecker, W. (Translation by Sohrin, Y.), *How to Build a Habitable PLANET -The Story of Earth from the Big Bang to Humankind-*, (2014) (in Japanese).

— Solution and Interface Chemistry —

Hasegawa, T.; Shimoaka, T.; Shioya, N.; Morita, K.; Sonoyama, M.; Takagi, T.; Kanamori, T., Stratified Dipole-Arrays Model Accounting for Bulk Properties Specific to Perfluoroalkyl Compounds, *ChemPlusChem*, **79,** 1421-1425 (2014).

Shioya, N.; Shimoaka, T.; Hasegawa, T., Analysis of Molecular Orientation and Conformation of Poly (3-hexylthiophene) Thin Films on Silicon by Infrared p-Polarized Multiple-Angle Incidence Resolution Spectrometry, *Chem. Lett.*, **43,** 1198-1200 (2014).

Morimine, S.; Norimoto, S.; Shimoaka, T.; Hasegawa, T., Surface Selection Rule of Infrared Diffuse Reflection Spectrometry for Analysis of Molecular Adsorbates on a Rough Surface of a NonAbsorbing Medium, *Anal. Chem.*, **86,** 4202-4208 (2014).

Nakata, S.; Ueda, T.; Miyaji, T.; Matsuda, Y.; Katsumoto, Y.; Kitahata, H.; Shimoaka, T., Hasegawa, T., Transient Reciprocating Motion of a Self-Propelled Object Controlled by a Molecular Layer of a *N*-Stearoyl-*p*-nitroaniline: Dependence on the Temperature of an Aqueous Phase, *J. Phys. Chem. C*, **118,** 14888-14893 (2014).

Tu, K.-M.; Ishizuka, R.; Matubayasi, N., Spatial-Decomposition Analysis of Electrical Conductivity in Concentrated Electrolyte Solution, *J. Chem. Phys.*, **141,** [044126-1]-[044126-9] (2014).

Tu, K.-M.; Ishizuka, R.; Matubayasi N., Spatial-decomposition Analysis of Electrical Conductivity in Ionic Liquid, *J. Chem. Phys.*, **141,** 244507-211518 (2014).

Hasegawa, T., Basic Knowledge of Mathematical Theories of Analytical Chemistry-Simultaneous Understanding of Linear Algebra and Chemometrics, *Bunseki*, **477,** 460-467 (2014) (in Japanese)

Hasegawa, T., Characterization of Molecular Adsorbates on a Flat Surface Using Infrared and Raman Spectroscopy, *Bunseki Kagaku*, **63,** 485-495 (2014) (in Japanese)

— Molecular Microbial Science —

Fukuyama, S.; Mihara, H.; Miyake, R.; Ueda, M.; Esaki, N.; Kurihara, T., Characterization of a Thermostable 2,4-Diaminopentanoate Dehydrogenase from *Fervidobacterium nodosum* Rt17-B1, *J. Biosci. Bioeng.*, **117,** 551-556 (2014).

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,** e85045 (2014).

Hidese, R.; Mihara, H.; Kurihara, T.; Esaki, N., Global Identification of Genes Affecting Iron-Sulfur Cluster Biogenesis and Iron Homeostasis, *J. Bacteriol.*, **196,** 1238-1249 (2014).

Imai, T.; Kurihara, T.; Esaki, N.; Mihara, H., Glutathione Contributes to the Efflux of Selenium from Hepatoma Cells, *Biosci. Biotechnol. Biochem.*, **78,** 1376-1380 (2014).

[Others]

Mihara, H.; Kurihara, T.; Esaki, N., Selenocysteine Lyase: Delivering Selenium in Biosynthetic Pathway, *Selenium in the Environment and Human Health*, 181-182 (2014).

Kawamoto, J.; Kurihara, T., Proteins and Lipids of Cold-Adapted Microorganisms, *CSJ Current Review 17*, 55-61（2014）(in Japanese）.

Kurihara, T.; Kawamoto, J., Physiological Functions of a Polyunsaturated Fatty Acid, Eicosapentaenoic Acid, *Journal of Clinical and Experimental Medicine (Igaku no Ayumi)*, 1221-1227 (2014)（in Japanese）.

Kurihara, T.; Kawamoto, J., Chemical Approach to Analyze the Physiological Function of Phospholipids with Polyunsaturated Fatty Acyl Chain, *Yakugaku Zasshi*, **134,** 507-513（2014）(in Japanese）.

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

— Polymer Materials Science —

Takahara, A.; Takeda, T.; Kanaya, T.; Kido, N.; Sakurai, K.; Masunaga, H.; Ogawa, H.; Takata, M., Advanced Soft Material Beamline Consortium at SPring-8 (FSBL), *Synchrotron Radiation News*, **27,** 19-23 (2014).

Kanaya, T.; Inoue, R.; Saito, M.; Seto, M.; Yoda, Y., Relaxation Transition in Glass-forming Polybutadiene as Revealed by Nuclear Resonance X-ray Scattering, *J. Chem. Phys.*, **140,** [144906-1]-[044906-5] (2014).

Okada, K.; Tokudome, Y.; Makiura, R.; Konstas, K.; Malfatti, L.; Innocenzi, P.; Ogawa, H.; Kanaya, T.; Falcaro, P.; Takahashi, M., Micropattern Formation by Molecular Migration via UV-induced Dehydration of Block Copolymers, *Adv. Funct. Mater.*, **24,** 2801-2809 (2014).

Hemmi, K.; Matsuba, G.; Tsuji, H.; Kawai, T.; Kanaya, T.; Toyohara, K.; Oda, A.; Endou, K., Precursors in Stereo-complex Crystals of Poly (L-lacticacid)/poly (D-lactic acid) Blends under Shear Flow, *J. Appl. Cryst.*, **47,** 14-21 (2014).

Tanaka, K.; Nishida, K.; Gabrys, B. J.; Lawrence, M. J.; Kanaya, T., Critical Dissolution Ionic Strength of Aqueous Solution of Chitosan Hydrochloride Salt, *Sen'i Gakkaishi (J. Soc. Fiber Sci. Technol., Jpn)*, **70,** 225-231 (2014).

Sadakane, K.; Endo, H.; Nishida, K.; Seto, H., Lamellar/Disorder Phase Transition in a Mixture of Water/2,6-dimethylpyridine/Antagonistic Salt, *J. Solution Chem*, **43,** 1722-1731 (2014).

Hara, A.; Inoue, R.; Takahashi, N.; Nishida, K.; Kanaya, T., Trajectory of Critical Point in Polymerization-Induced Phase Separation of Epoxy/Oligoethylene Glycol Solutions, *Macromolecules*, **47,** 4453-4459 (2014).

Koido, S.; Kawai, T.; Kuroda, S.; Nishida, K.; Kanaya, T.; Kato, M.; Kurose, T.; Nakajima, K., Mesomorphic Phase Formation of Plasticized Poly (L-lactic acid), *J. Appl. Polym. Sci.*, **131, [**39762-1]-[39762-8] (2014).

Inoue, R.; Kanaya, T.; Hu, Y.; Masuda, T.; Nishida, K.; Yamamuro, O., Relationship between the Local Dynamics and Gas Permeability of Polyacetylenes Containing Polymethylated Indan/tetrahydronaphtalene Moieties, *Polymer*, **55,** 182-186 (2014).

Yamamoto, T.; Okuda, H.; Takeshita, K.; Usami, N.; Kitajima, Y.; Ogawa, H., Grazing-incidence Small-angle X-ray Scattering from Ge Nanodots Self-organized on Si(001) Examined with Soft X-rays, *Jounal of Syncrotron Radiation*, **21,** 161-164 (2014).

Okuda, H.; Yamamoto, T.; Takeshita, K.; Hirai, M.; Senoo, K.; Ogawa, H.; Kitajima, Y., Normalization of Grazing-incidence Small Angle Scattering of Phospholipid Alloy Systems at the K Absorption Edge of Phosphorous: A Standard Sample Approach, *Journal of Applied Physics*, **53,** 5 (2014).

Wernecke, J.; Okuda, H.; Ogawa, H.; Siewer, F.; Krumrey, M., Depth-Dependent Structural Changes in PS-b-P2VP Thin Films Induced by Annealing, *Macromolecules*, **47,** 5719-5727 (2014).

Zhan, J.; Matsuno, H.; Masunaga, H.; Ogawa, H.; Tanaka, K., Green Solid Films with Tunable Mechanical Properties Made from Deoxyribonucleic Acid, *NPG Asia Materials*, **6,** e92 (2014).

Takahara, A.; Takeda, T.; Kanaya, T.; Kido, N.; Sakurai, K.; Masunaga, H.; Ogawa, H.; Takata, M., Advanced Soft Material Beamline Consortium at SPring-8 (FSBL), *Synchrotron Radiation News*, **27,** 19-23 (2014).

— Molecular Rheology —

Masubuchi, Y.; Watanabe, H., Origin of Stress Overshoot under Start-up Shear in Primitive Chain Network Simulation, *ACS Macro Lett.*, **3,** 1183-1186 (2014).

Matsumiya, Y.; Masubuchi, Y.; Inoue, T.; Urakawa, O.; Liu, C.-Y.; van Ruymbeke, E.; Watanabe, H., Dielectric and Viscoelastic Behavior of Star-Branched Polyisoprene: Two Coarse-Grained Length Scales in Dynamic Tube Dilation, *Macromolecules*, **47,** 7637-7652 (2014).

van Ruymbeke, E.; Shchetnikava, V.; Matsumiya, Y.; Watanabe, H., Dynamic Dilution Effect in Binary Blends of Linear Polymers with Well-Separated Molecular Weights, *Macromolecules*, **47,** 7653-7665 (2014).

Lee, A.; Watanabe, H.; Matsumiya, Y.; Choi, K.-H.; Ahn, K. H.; Lee, S. J., Dielectric Characterization of Pigment Inks for Electrohydrodynamic Jet Printing, *Ind. Eng. Chem. Res.*, **53,** 17445-17453 (2014).

Masubuchi, Y.; Matsumiya, Y.; Watanabe, H., Test of Orientation/Stretch-Induced Reduction of Friction via Primitive Chain Network Simulations for Polystyrene, Polyisoprene, and Poly (*n*-butyl acrylate), *Macromolecules*, **47,** 6768-6775 (2014).

Matsumiya, Y.; Watanabe, H., Dielectric and Viscoelastic Behavior of low-M Linear Polyisoprene Blended in Long Matrix, *J. Soc. Rheol. Japan*, **42,** 235-244 (2014).

Masubuchi, Y.; Matsumiya, Y.; Watanabe, H.; Marrucci, G.; Ianniruberto, G., Primitive Chain Network Simulations for Pom-pom Polymers in Uniaxial Elongational Flows, *Macromolecules*, **47,** 3511-3519 (2014).

Nishikawa, M.; Ogawa, K.; Umeki, Y.; Mohri, K.; Kawasaki, Y.; Watanabe, H.; Takahashi, N.; Kusuki, E.; Takahashi, R.; Takahashi, Y.; Takakura, Y., Injectable, Self-Gelling, Biodegradable, and Immunomodulatory DNA Hydrogel for Antigen Delivery, *Journal of Controlled Release*, **180,** 25-32 (2014).

Yaoita, T.; Masubuchi, Y.; Watanabe, H., Concept of Stretch/Orientation-Induced Friction Reduction Tested with a Simple Molecular Constitutive Equation, *J. Soc. Rheol. Japan*, **42,** 207-213 (2014).

Horio, K.; Uneyama, T.; Matsumiya, Y.; Masubuchi, Y.; Watanabe, H., Rheo-Dielectric Responses of Entangled *cis*-Polyisoprene under Uniform Steady Shear and LAOS, *Macromolecules*, **47,** 246-255 (2014).

Masubuchi, Y., Simulating the Flow of Entangled Polymers, *Annual Review of Chemical and Biomolecular Engineering*, **5,** 11-33 (2014).

— Molecular Aggregation Analysis —

Murdey, R.; Sato, N., Interpretation of the Thermal Activation Energy of Conduction for Molecular Semiconductor Thin Films with Blocking Contacts, *Jpn. J. Appl. Phys.*, **53,** [05FY04-1]-[05FY04-5] (2014).

Yoshida, H., Low-energy Inverse Photoemission Study on the Electron Affinities of Fullerene Derivatives for Organic Photovoltaic Cells, *J. Phys. Chem. C*, **118,** 24377-24382 (2014).

Yoshida, H., Measuring the Electron Affinity of Organic Solids: An Indispensable New Tool for Organic Electronics (Trend 2014), *Anal. Bioanal. Chem.*, **406,** 2231-2237 (2014).

Ie, Y.; Karakawa, M.; Jinnai, S.; Yoshida, H.; Saeki, A.; Seki, S.; Yamamoto, S.; Ohkita, H.; Aso, Y., Electron-Donor Function of Methanofullerenes in Donor-Acceptor Bulk Heterojunction Systems, *Chem. Commun.*, **50,** 4123-4125 (2014).

Yoshida, H., Note: Low Energy Inverse Photoemission Spectroscopy Apparatus, *Rev. Sci. Instrum.*, **85,** [016101-1]-[016101-3] (2014).

Hidaka, Y.; Asami, K., Measurement of Dipole Potential in Bilayer Lipid Membranes by Dielectric Spectroscopy, *J. Membrane Biol.*, **247,** 721-727 (2014).

Asami, K., Low-Frequency Dielectric Dispersion of Bacterial Cell Suspensions, *Colloids Surf., B*, **119,** 1-5 (2014).

— Interdisciplinary Chemistry for Innovation —

Kondo, T.; Kimura, Y.; Yamada, H.; Toshimitsu, A., Magnetic Nanoparticles for Multimodal Bio-imaging, *Magnetic Nanoparticles: Synthesis, Physicochemical Properties and Role in Biomedicine*, 69-93 (2014).

Kondo, T.; Kimura, Y.; Yamada, H.; Toshimitsu, A., Ruthenium-Based Catalysts for Aerobic Oxidation of Alcohols, *Transition Metal Catalysis in Aerobic Alcohol Oxidation*, 70-91 (2014).

Toshimitsu, A., Organic Selenocyanates, Tellurocyanates and Related Compounds, *The Chemistry of Organic Selenium and Tellurium Compounds*, **4,** 845-884 (2013).

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

— Particle Beam Science —

Fuwa, Y.; Iwashita, Y.; Tongu, H.; Kitahara, K.: Matsumoto, T.; Michizono, S.; Fukuda, S., Focusing System with Permanent Magnets for Klystrons, *IEEE Trans. on Applied Supercond*, **24,** 502005 (2014).

Fuwa, Y.; Ikeda, S.; Kumaki, M.; Sekine, M.; Cinquegrani, D.; Romanelli, M.; Kanesue, T.; Okamura, M.; Iwashita, Y., Interaction of Plasmas in Laser Ion Source with Double Laser System, *Review of Scientific Instruments, AIP Publishing*, **85,** [02B916-1]-[02B916-3] (2014).

Fuwa, Y.; Ikeda, S.; Kumaki, M.; Sekine, M.; Munemoto, N.; Cinquegrani, D.; Romanelli, M.; Kanesue, T.; Okamura, M.; Iwashita, Y., Comparison of Graphite Materials for Targets of Laser Ion Source, *Review of Scientific Instruments, AIP Publishing*, **85,** [02B924-1]-[02B924-3] (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,** 34802 (2014).

Mishima, K.; Imajo, S.; Hino, M.; Ino, T.; Iwashita, Y.; Katayama, R.; Kitaguchi, M.; Oda, T.; Shimizu, H. M.; Utsuro, M.; Yamashita, S.; Yoshioka, T., Production of Ultra Cold Neutrons by a Doppler Shifter with Pulsed Neutrons at J-PARC, *J. Phys. Conf. Ser.*, **528,** [012030-1]-[012030-8] (2014).

[Others]

Imajo, S.; Iwashita, Y.; Shimizu, H. M.; Kitaguchi, M.; Yamashita, S.; Arimoto, Y.; Yoshioka, T.; Seki, Y., The Development of a Low Energy Neutron Accelerator for Rebunching Pulsed Neutrons, *Proceedings of 5th International Particle Accelerator Conference, IPAC'14*, 751-753 (2014).

Kitahara, R.; Fuwa, Y.; Iwashita, Y., Magnetic Field Evaluation of Multipole Permanent Magnets by Harmonic Coil with Novel Calibration, *Proceedings of 5th International Particle Accelerator Conference, IPAC’14*, 1259-1261 (2014).

Imajo, S.; Iwashita, Y.; Fuwa, Y.; Kitahara, R.; Shimizu, H. M.; Kitaguchi, M.; Mishima, K.; Ino, T., Development of Slow Neutron Accelerator for Rebunching Pulsed Neutrons, *Proceedings of 27th Linear Accelerator Conference*, THPP092 (2014).

Fuwa, Y.; Kanesue, T.; Okamura, M.; Iwashita, Y.; Ikeda, S.; Kumaki, M., Beam Dynamics of Multi Charge State Ions in RFQ Linac, *Proceedings of 27th Linear Accelerator Conference*, MOPP112 (2014).

Iwashita, Y.; Otani, M.; Mibe, T.; Yoshida, M.; Saito, N., Biperiodic L-Support DAW for Medium Beta for Muon g-2/EDM at J-PARC, *Proceedings of the 11th Annual Meeting of Particle Accelerator Society of Japan*, 568-571 (2014) (in Japanese).

Imajo, S.; Iwashita, Y.; Fuwa, Y.; Kitahara, R.; Shimizu, H. M.; Kitaguchi, M.; Mishima, K.; Ino, T., Improvement of the Ultracold Neutrons Rebuncher II, *Proceedings of the 11th Annual Meeting of Particle Accelerator Society of Japan*, 947-950 (2014) (in Japanese).

Fuwa, Y.; Ikeda, S.; Kumaki, M.; Kanesue, T.; Okamura, M.; Iwashita, Y., Analysis of Laser Plasma from Graphite Single Crystal for Laser Ion Source, *Proceedings of the 11th Annual Meeting of Particle Accelerator Society of Japan*, 560-563 (2014) (in Japanese).

Kitahara, R.; Fuwa, Y.; Iwasita, Y., Magnetic Field Evaluation of Multipole Permanent Magnets by Harmonic Coil with Higher Resolution, *Proceedings of the 11th Annual Meeting of Particle Accelerator Society of Japan*, 1175-1178 (2014) (in Japanese).

Tongu, H.; Iwashita, Y.; Hayano, H.; Yamamoto, Y., Development of SC Cavity Inspection System, XT-map, *Proceedings of the 11th Annual Meeting of Particle Accelerator Society of Japan*, 1052-1054 (2014) (in Japanese).

— Laser Matter Interaction Science —

Hashida, M.; Gemini, L.; Nishii, T.; Miyasaka, Y.; Sakagami, H.; Shimizu, M.; Inoue, S.; Limpoch, J.; Mocek, T.; Sakabe, S., Periodic Grating Structures on Metal Self-organized by Double-pulse Irradiation, *J Laser Micro Nanoen*, **9,** 234-237 (2014).

Gemini, L.; Hashida, M.; Shimizu, M.; Miyasaka, Y.; Inoue, S.; Tokita, S.; Limpouch, J.; Mocek, T.; Sakabe, S., Periodic Nanostructures Self-fromed on Silicon and Silicon Carbite by Femtosecond Laser Irradiation, *Appl. Phys. A*, **117,** 49-54 (2014).

— Electron Microscopy and Crystal Chemistry —

Aso, R.; Kan, D.; Shimakawa, Y.; Kurata, H., Control of Structural Distortions in Transition-Metal Oxide Films through Oxygen Displacement at the Heterointerface, *Adv. Funct. Mater.*, **24,** 5177-5184 (2014).

Aso, R.; Kan, D.; Shimakawa, Y.; Kurata, H., Octahedral Tilt Propagation Controlled by A-Site Cation Size at Perovskite Oxide Heterointerfaces, *Cryst. Growth Des.*, **14,** 2128-2132 (2014).

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).

Saito, H.; Kurata, H., Direct Measurement of Dispersion Relation for Surface Plasmon-Polaritons on Silver Nanoantennas, *Microscopy*, **63,** 155-159 (2014).

Kan, D.; Shimizu, T.; Yamada, Y.; Aso, R.; Kurata, H.; Kanemitsu, Y.; Shimakawa, Y., Band-to-Band Photoluminescence as a Probe of Electron Carriers in Nb-Doped SrTiO$_3$ Epitaxial Thin Films, *Appl. Phys. Exp.*, **7,** [015503-1]-[015503-4] (2014).

Kikkawa, J.; Terada, S.; Gunji, A.; Haruta, M.; Nagai, T.; Kurashima, K.; Kimoto, K., Understanding Li-K Edge Structure and Interband Transitions in Li$_x$CoO$_2$ by Electron Energy-Loss Spectroscopy, *Appl. Phys. Lett.*, **104,** [114105-1]-[114105-4] (2014).

Nagai, T.; Haruta, M.; Kikuchi, M.; Zhang, W.; Takeguchi, M.; Kimoto, K., Direct Observation of Atomic Columns in a Bi-2223 Polycrystal by Aberration-Corrected STEM Using a Low Accelerating Voltage, *Physica C*, **500,** 33-39 (2014).

Tanaka, D.; Inuta, Y.; Sakamoto, M.; Furube, A.; Haruta, M.; So, Y. -G.; Kimoto, K.; Hamada, I.; Teranishi, T., Strongest π-Metal Orbital Coupling in a Porphyrin/Gold Cluster System, *Chem. Sci.*, **5,** 2007-2010 (2014).

Kameda, T.; Nemoto, T.; Ogawa, T.; Tosaka, M.; Kurata, H.; Schaper, A. K., Evidence of α-Helical Coiled Coil and β-Sheets in Hornet Silk, *J. Struct. Biol.*, **185,** 303-308 (2014).

Hasegawa, G.; Kanamori, K.; Kiyomura, T.; Kurata, H.; Nakanishi K.; Abe, T., Hierarchically Porius $Li_4Ti_5O_{12}$ Anode Materials for Li- and Na-Ion Batteries: Effects of Nanoarchitectural Design and Temperature Dependence of the Rate Capability, *Adv. Energy Mater.*, [1400730-1]-[1400730-8] (2014).

[Others]

Kurata, H., Chemical Bonding State Analysis by Electron Energy-Loss Spectroscopy, *Light Metals*, **63,** 466-473 (2013) (in Japanese).

Yoshimura, T.; Ogawa, T., Observation of Nano-Structure of Surfactant Micelle by Cryogenic Electron Microscopy, *Kenbikyo*, **49,** 22-25 (2014) (in Japanese).

Haruta, M., High Resolution Electronic State Analysis Using STEM-EELS, *kenbikyo*, **49,** 132-137 (2014) (in Japanese).

Yoshida, K.; Toyoura, K.; Matsunaga, K.; Kurata, H.; Nakahira, A.; Ikuhara, H.; Sasaki, Y., Atomic-Scale Analysis of Cs^+within Zeolitic Framework by AC-(S) TEM and First Principle Calculation, *Kenbikyo*, **49,** 138-141 (2014) (in Japanese).

— Structural Molecular Biology —

Hata, Y.; Fujii, T.; Yamauchi, T.; Gogami, Y.; Oikawa, T., Structural Features and Low-Temperature Adaptation of Aspartate Racemase, *Acta Cryst.*, **A70,** C1055 (2014).

Fujii, T.; Kobayashi, K.; Yamauchi, T.; Yoshida, M.; Oikawa, T.; Hata, Y., Crystal Structure Analyses of Oxygenase Component of Resorcinol Hydroxylase, *Acta Cryst.*, **A70,** C448 (2014).

Yamauchi, T.; Fujii, T.; Yoshida, M.; Oikawa, T.; Hata, Y., Crystal Structures of Bacterial Flavin Reductase GraD and Its Complex with NADH, *Acta Cryst.*, **A70,** C448 (2014).

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Organic Main Group Chemistry —

Takaya, H.; Isozaki, K.; Nakamura, M., Metal Array Fabrication Based on the Self-Assembly of Metalated Amino Acids and Peptides, *Polymers*, **63,** 231-232 (2014) (in Japanease).

Pincella, F.; Song, Y.; Ochiai, T.; Isozaki, K.; Sakamoto, K.; Miki, K., Square-Centimeter-Scale 2D Arrays of Au@Ag Core-Shell Nanoparticles towards Practical SERS Substrates with Enhancement Factor of 107, *Chem. Phys. Lett.*, **605-606,** 115-120 (2014).

Ochiai, T.; Isozaki, K.; Nishiyama, S.; Miki, K., Enhancement of Self-Assembly of Large-Sized (> 10 nm) Gold Nanoparticles Locally on an ITO Substrate, *Appl. Phys. Express*, **7,** 65001 (2014).

Takaya, H.; Isozaki, K.; Haga, Y.; Ogata, K.; Naota, T., Synthesis and Self-Assembling Properties of Pt-Complex-Bound Oligo (glutamic acid) s, *Chem. Lett.*, **43,** 1167-1169 (2014).

Azuma, S.; Ota, M.; Ishida, A.; Isozaki, K.; Takaya, H.; Nakamura, M.; Sasamori, T.; Tokitoh, N.; Kuramochi, K.; Tsubaki, K., Dimerization Reactions of 2-Bromo-3,5,6-Trimethyl-1,4-Benzoquinone, *Chem. Lett.*, **43,** 1531-1533 (2014).

Pincella, F.; Isozaki, K.; Miki, K., A Visible Light-Driven Plasmonic Photocatalyst, *Light Sci. Appl.*, **3,** e133 (2014).

Nakamura, E.; Hatakeyama, T.; Ito, S.; Ishizuka, K.; Ilies, L.; Nakamura, M., Iron-Catalyzed Cross-Coupling Reactions, *Org. React.*, **83,** 1-209 (2014).

Hashimoto, S.; Ikuta, T.; Shiren, K.; Nakatsuka, S.; Ni, J.; Nakamura, M.; Hatakeyama, T., Triplet-Energy Control of Polycyclic Aromatic Hydrocarbons by BN Replacement: Development of Ambipolar Host Materials for Phosphorescent OLEDs., *Chem. Mater.*, **26,** 6265-6271 (2014).

Hashimoto, S.; Nakatsuka, S.; Nakamura, M.; Hatakeyama, T., Construction of a Highly Distorted Benzene Ring in a Double Helicene., *Angew. Chem. Int. Ed.*, **53,** 14074-14076 (2014).

Aoki, Y.; Imayoshi, R.; Hatakeyama, T.; Takaya, H.; Nakamura, M., Synthesis of 2,7-Disubstituted 5,10-Diaryl-5,10-Dihydrophenazines via Iron-Catalyzed Intramolecular Ring-Closing C-H Amination, *Heterocycles (Kuwajima Special Issue)*, **90,** 893-900 (2014).

[Others]

Isozaki, K.; Miki, K., Visible Light-Driven Photocatalyst with Gold Nanoparticle Arrays, *C&I Commun.*, **39,** 36-38 (2014).

— Advanced Solid State Chemistry —

Shimakawa, Y.; Mizumaki, M., Multiple Magnetic Interactions in A-Site-ordered Perovskite-structure Oxides, *J. Phys. Cond. Matter*, **26,** [473203-1]-[473203-14] (2014).

Aso, R.; Kan, D.; Shimakawa, Y.; Kurata, H., Control of Structural Distortions in Transition-metal Oxide Films through Oxygen Displacement at the Heterointerface, *Adv. Funct. Mater.*, **24,** 5177-5184 (2014).

Senn, M. S.; Chen, W. T.; Saito, T.; Garcia-Martin, S.; Attfield, J. P.; Shimakawa, Y., B-Cation Order Control of Magnetism in the 1322 Perovskite $CaCu_3Fe_2Nb_2O_{12}$, *Chem. Mater*., **26,** 4832-4837 (2014).

Murakami, N.; Kan, D.; Ichikawa, N.; Shimakawa, Y., Low-temperature Reduction of Brownmillerite $CaFeO_{2.5}$ in $LaAlO_3$/$CaFeO_{2.5}$ Heterostructures Made on $SrTiO_3$, *Dalton Trans.*, **43,** 14596-14599 (2014).

Chen, W. T.; Mizumaki, M.; Seki, H.; Senn, M. S.; 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, *Nature Comm.*, **5,** [3909-1]-[3909-7] (2014).

Zhang, S.; Saito, T.; Mizumaki, M.; Shimakawa, Y., Temperature-induced Intersite Charge Transfer Involving Cr Ions in A-Site-ordered Perovskites $ACu_3Cr_4O_{12}$ (A=La and Y), *Chem. Eur. J.*, **20,** 9510-9513 (2014).

Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Unit-cell Thick $BaTiO_3$ Blocks Octahedral Tilt Propagation Across Oxide Heterointerface, *J. Appl. Phys.*, **115,** [184304-1]-[184304-6] (2014).

Aso, R.; Kan, D.; Shimakawa, Y.; Kurata, H., Octahedral Tilt Propagation Controlled by A-Site Cation Size at Perovskite Oxide Heterointerfaces, *Cryst. Growth & Des.*, **14,** 2128-2132 (2014).

Seki, H.; Yamada, R.; Saito, T.; Kennedy, B. J.; Shimakawa, Y., High-concentration Na Doping of $SrRuO_3$ and $CaRuO_3$ *Inorg. Chem.*, **53,** 4579-4584 (2014).

Nishimura, K.; Yamada, I.; Oka, K.; Shimakawa, Y.; Azuma, M., High-pressure Synthesis of $BaVO_3$: A New Cubic Perovskite, *J. Phys. Chem. Solids*, **75,** 710-712 (2014).

Saito, T.; Yamada, R.; Ritter, C.; Senn, M.; Attfield, J. P.; Shimakawa, Y., Control of L-Type Ferrimagnetism by the Ce/vacancy Ordering in the A-Site-ordered Perovskite $Ce_{1/2}Cu_3Ti_4O_{12}$, *Inorg. Chem.*, **53,** 1578-1584 (2014).

Shimakawa, Y.; Zhang, S.; Saito, T.; Lufaso, M. W.; Woodward, P. M., Order-disorder Transition Involving the A-Site Cations in Ln^{3+} $Mn_3V_4O_{12}$ Perovskites, *Inorg. Chem.*, **53,** 594-599 (2014).

Kan, D.; Shimizu, T.; Yamada, Y.; Aso, R.; Kurata, H.; Kanemitsu, Y.; Shimakawa, Y., Band-to-band Photoluminescence as a Probe of Electron Carriers in Nb-Doped $SrTiO_3$ Epitaxial Thin Films, *Appl. Phys. Exp.*, **7,** [015503-1]-[015503-4] (2014).

Sosnowska, I.; Azuma, M.; Przeniosto, R.; Wardecki, D.; Chen, W. T.; Oka, K.; Shimakawa, Y., Crystal and Magnetic Structure in Co-substituted $BiFeO_3$, *Inorg. Chem.*, **52,** 13269-13277 (2013).

— Organotransition Metal Chemistry —

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

Chang, Y. H.; Nakajima, Y.; Tanaka, H.; Yoshizawa, K.; Ozawa, F., Mechanism of N-H Bond Cleavage of Aniline by a Dearomatized PNP-Pincer Type Phosphaalkene Complex of Iridium (I), *Organometallics*, **33,** 715-721 (2014).

Lin, Y. F.; Nakajima, Y.; Ozawa, F., Reduction of an Fe (I) Mesityl Complex Induced by π-Acid Ligands, *Dalton Trans.*, **43,** 9032-9037 (2014).

Takeuchi, K.; Minami, A.; Nakajima, Y.; Ozawa, F., Synthesis and Structures of Nickel Complexes with a PN-Chelate Phosphaalkene Ligand, *Organometallics*, **33,** 5365-5370 (2014).

Wakioka, M.; Nakamura, Y.; Hihara, Y.; Ozawa, F., Effects of PAr_3 Ligands on Direct Arylation of Heteroarenes with Isolated $[Pd(2,6\text{-}Me_2C_6H_3)(\mu\text{-}O_2CMe)(PAr_3)]_4$ Complexes, *Organometallics*, **33,** 6247-6252 (2014).

Lin, Y. F.; Ichihara, N.; Nakajima, Y.; Ozawa, F., Disproportionation of Bis (phosphaethenyl) pyridine Iron (I) Bromide Induced by tBuNC, *Organometallics*, **33,** 6700-6703 (2014).

— Photonic Elements Science —

Kan, D.; Shimizu, T.; Yamada, Y.; Aso, R.; Kurata, H.; Kanemitsu, Y., Shimakawa Y., Band-to-band Photoluminescence as a Probe of Electron Carriers in Nb-doped $SrTiO_3$ Epitaxial Thin Films, *Appl. Phys. Express*, **7,** [015503-1]-[015503-4] (2014).

Yamada, Y.; Nakamura, T.; Yasui, S.; Funakubo, H.; Kanemitsu, Y., Measurement of Transient Photoabsorption and Photocurrent of $BiFeO_3$ Thin Films: Evidence for Long-lived Trapped Photocarriers, *Phys. Rev. B*, **89,** [035133-1]-[035133-5] (2014).

Nishihara, T.; Yamada, Y.; Okano, M.; Kanemitsu, Y., Quantized Exciton-exciton Recombination in Undoped and Hole-doped Single-walled Carbon Nanotubes, *Jpn. J. Appl. Phys.*, **53,** [02BD10-1]-[02BD10-5] (2014).

Yamada, Y.; Nakamura, T.; Endo, M.; Wakamiya, A.; Kanemitsu, Y., Near-band-edge Optical Responses of Solution-Processed Organic-inorganic Hybrid Perovskite $CH_3NH_3PbI_3$ on Mesoporous TiO_2 Electrodes, *Appl. Phys. Express*, **7,** [032302-1]-[032302-4] (2014).

Le, P. Q.; Okano, M.; Yamada, Y.; Nagaoka, A.; Yoshino, K.; Kanemitsu, Y., Temperature-dependent Photocarrier Recombination Dynamics in Cu_2ZnSnS_4 Single Crystals, *Appl. Phys. Lett.*, **104,** [081907-1]-[081907-4] (2014).

Okano, M.; Nishihara, T.; Yamada, Y.; Kanemitsu, Y., Chemical Doping-induced Changes in Optical Properties of Single-walled Carbon Nanotubes, *Jpn. J. Appl. Phys.*, **53,** [05FD02-1]-[05FD02-4] (2014).

Yamada, Y.; Sato, H. K.; Hikita, Y.; Hwang, H. Y.; Kanemitsu, Y., Photocarruer Recombination and Localization Dynamics of $LaAlO_3$/$SrTiO_3$ Heterostructures, *Proc. SPIE*, **8987,** [898710-1]-[898710-7] (2014).

Yamada, Y.; Sato, H. K.; Hikita, Y.; Hwang, H. Y.; Kanemitsu, Y., Spatial Density Profile of Electrons near the $LaAlO_3/SrTiO_3$ Heterointerface Revealed by Time-resolved Photoluminescence Spectroscopy, *Appl. Phys. Lett.*, **104,** [151907-1]-[151907-4] (2014).

Okano, M.; Takabayashi, Y.; Sakurai, T.; Akimoto, K.; Shibata, H.; Niki, S.; Kanemitsu, Y., Slow Intraband Relaxation and Localization of Photogenerated Carriers in $CuIn_{1-x}Ga_xSe_2$ Thin Films: Evidence for the Existence of Long-lived High-energy Carriers, *Phys. Rev. B*, **89,** [195203-1]-[195203-6] (2014).

Sakamoto, M.; Inoue, K.; Saruyama, M.; So, Y. G.; Kimoto, K.; Okano, M.; Kanemitsu, Y.; Teranishi, T., Investigation on Photo-Induced Charge Separation in CdS/CdTe Nanopencils, *Chem. Sci.*, **5,** 3831-3835 (2014).

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).

Okano, M.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Assessment of Hot-Carrier Effects on Charge Separation in Type-II CdS/CdTe Heterostructured Nanorods, *J. Phys. Chem. Lett.*, **5,** 2951-2956 (2014).

Ihara, T.; Kanemitsu, Y., Spectral Diffusion of Neutral and Charged Exciton Transitions in Single CdSe/ZnS Nanocrystals Due to Quantum-confined Stark Effect, *Phys. Rev. B*, **90,** [195302-1]-[195302-5] (2014).

Ihara, T.; Sato. R.; Teranishi, T.; Kanemitsu, Y., Delocalized and Localized Charged Excitons in Single CdSe/CdS Dot-in-rods Revealed by Polarized Photoluminescence Blinking, *Phys. Rev. B*, **90,** [035309-1]-[035309-5] (2014).

Ono, M.; Nishihara, T.; Ihara, T.; Kikuchi, M.; Tanaka, A; Suzuki, M; Kanemitsu, Y., Impact of Surface Ligands on the Photocurrent Enhancement Due to Multiple Exciton Generation in Close-packed Nanocrystal Thin Films, *Chem. Sci.*, **5,** 2696-2701 (2014).

Tex, D. M.; Ihara, T.; Kamiya, I.; Kanemitsu, Y., Temperature and Light-intensity Dependence of Upconverted Photocurrent Generation in Shallow InAs Quantum Structures, *Jpn. J. Appl. Phys.*, **53,** [05FV01-1]-[05FV01-4] (2014).

Nishihara, T.; Segawa, Y.; Itami, K.; Kanemitsu, Y., Exciton Recombination Dynamics in Nanoring Cycloparaphenylenes, *Chem. Sci.*, **5,** 2293-2296 (2014).

Tex, D. M.; Ihara, T.; Kamiya, I.; Kanemitsu, Y., Microscopic Photoluminescence and Photocurrent Imaging Spectroscopy of InAs Nanostructures: Identification of Photocarrier Generation Sites for Intermediate-band Solar Cells, *Phys. Rev. B*, **89,** [125301-1]-[125301-8] (2014).

Tex, D. M.; Kamiya, I.; Kanemitsu, Y., Control of Hot-carrier Relaxation for Realizing Ideal Quantum-dot Intermediate-band Solar Cells, *Sci. Rep.*, **4,** [4125-1]-[4125-6] (2014).

Zhu, L.; Kim, C.; Yoshita, M.; Chen, S.; Sato, S.; Mochizuki, T.; Akiyama, H.; Kanemitsu, Y., Impact of Sub-cell Internal Luminescence Yields on Energy Conversion Efficiencies of Tandem Solar Cells: A Design Principle, *Appl. Phys. Lett.*, **104,** [031118-1]-[031118-5] (2014).

Hoshi, Y.; Tayagaki, T.; Kiguchi, T.; Usami, N., Control of Geometry in Si-based Photonic Nanostructure Formed by Maskless Wet Etching Process and Its Impact on Optical Properties, *Thin Solid Films*, **557,** 338-341 (2014).

Tayagaki, T.; Hoshi, Y.; Ooi, K.; Kiguchi, T.; Usami, N., Carrier Extraction Dynamics from Ge/Si Quantum Wells in Si Solar Cells, *Thin Solid Films*, **557,** 368-371 (2014).

Tayagaki, T.; Hoshi, Y.; Kishimoto, Y.; Usami, N., Enhanced Photocarrier Generation in Large-scale Photonic Nanostructures Fabricated from Vertically Aligned Quantum Dots, *Opt. Express*, **22,** A225-A232 (2014).

Tayagaki, T.; Kishimoto, Y.; Hoshi, Y.; Usami, N., Simulation Study of Ge/Si Heterostructure Solar Cells Yielding Improved Open-circuit Voltage and Quantum Efficiency, *Jpn. J. Appl. Phys.*, **53,** [110312-1]-[110312-4] (2014).

Tayagaki, T.; Kishimoto, Y.; Hoshi, Y.; Usami, N., Light Tapping by Direction-dependent Light Transmission at Front-surface Photonic Nanostructures, *Appl. Phys. Express*, **7,** [122301-1]-[122301-4] (2014).

Yamada, Y.; Kanemitsu, Y., Band-to-band Photoluminescence and Photocarrier Dynamics in $SrTiO_3$, *Kotai Butsuri*, **49,** 25-33 (2014) (in Japanese).

Yamada, Y.; Wakamiya, A.; Kanemitsu, Y., Perovskite Semiconductor Solar Cells, *Kotai Butsuri*, **49,** 545-553 (2014) (in Japanese).

Kanemitsu, Y., Multiple Carrier Interactions in Semiconductor Nanostructures for High-efficiency Solar Cell Applications, *Oyo Butsuri*, **83,** 986 (2014) (in Japanese).

BIOINFORMATICS CENTER
— Chemical Life Science —

Katayama, T.; Wilkinson, M. D.; Aoki-Kinoshita, K. F.; Kawashima, S.; Yamamoto, Y.; Yamaguchi, A.; Okamoto, S.; Kawano, S.; Kim, J.; Wang, Y.; Wu, H.; Kano, Y.; Ono, H.; Bono, H.; Kocbek, S.; Aerts, J.; Akune, Y.; Antezana, E.; Arakawa, K.; Aranda, B.; Baran, J.; Bolleman, J.; Bonnal, R. J. P.; Buttigieg, P. L.; Campbell, M. P.; Chen, Y.; Chiba, H.; Cock, P. J. A.; Cohen, K. B.; Constantin, A.; Duck, G.; Dumontier, M.; Fujisawa, T.; Fujiwara, T.; Goto, N.; Hoehndorf, R.; Igarashi, Y.; Itaya, H.; Ito, M.; Iwasaki, W.; Kalas, M.; Katoda, T.; Kim, T.; Kokubu, A.; Komiyama, Y.; Kotera, M.; Laibe, C.; Lapp, H.; Lütteke, T.; Marshall, M. S.; Mori, T.; Mori, H.; Morita, M.; Murakami, K.; Nakao, M.; Narimatsu, H.; Nishide, H.; Nishimura, Y.; Nystrom-Persson, J.; Ogishima, S.; Okamura, Y.; Okuda, S.; Oshita, K.; Packer, N. H.; Prins, P.; Ranzinger, R.; Rocca-Serra, P.; Sansone, S.; Sawaki, H.; Shin, S.; Splendiani, A.; Strozzi, F.; Tadaka, S.; Toukach, P.; Uchiyama, U.; Umezaki, M.; Vos, R.; Whetzel, P. L.; Yamada, I.; Yamasaki, C.; Yamashita, R.; York, W. S.; Zmasek, C. M.; Kawamoto, S.; Takagi, T., BioHackathon Series in 2011 and 2012: Penetration of Ontology and Linked Data in Life Science Domains, *J. Biomed. Semantics*, **5,** 5 (2014).

Kanehisa, M.; Goto, S.; Sato, Y.; Kawashima, M.; Furumichi, M.; Tanabe, M., Data, Information, Knowledge and Principle: Back to Metabolism in KEGG, *Nucleic Acids Res.*, **42,** D199-D205 (2014).

Ingale, A. G.; Goto, S., Prediction of CTL Epitope, in silico Modeling and Functional Analysis of Cytolethal Distending Toxin (CDT) Protein of Campylobacter jejuni, *BMC Res. Notes*, **7,** 92 (2014).

Kotera, M.; Goto, S.; Kanehisa, M., Predictive Genomic and Metabolic Analysis for the Standardization of Enzyme Data, *Perspectives in Science*, **1,** 24-32 (2014).

Mizutani, S.; Noro, Y.; Kotera, M.; Goto, S., Pharmacoepidemiological Characterization of Drug-induced Adverse Reaction Clusters towards Understanding of Their Mechanisms, *Comput. Biol. Chem.*, **50,** 50-59 (2014).

Yamanishi, Y.; Kotera, M.; Moriya, Y.; Sawada, R.; Kanehisa, M.; Goto, S., DINIES: Drug-target Interaction Network Inference Engine Based on Supervised Analysis, *Nucleic Acids Res.*, **42,** W39-W45 (2014).

Kotera, M.; Tabei, Y.; Yamanishi, Y.; Muto, A.; Moriya, Y.; Tokimatsu, T.; Goto, S., Metabolome-scale Prediction of Intermediate Compounds in Multistep Metabolic Pathways with a Recursive Supervised Approach, *Bioinformatics*, **30,** i165-i174 (2014).

Jin, Z.; Kotera, M.; Goto, S., Virus Proteins Similar to Human Proteins as Possible Disturbance on Human Pathways, *Syst. Synth. Biol.*, **8,** 283-295 (2014).

Wilson, W. H.; Gilg, I. C.; Duarte, A.; Ogata, H., Development of DNA Mismatch Repair Gene, MutS, as a Diagnostic Marker for Detection and Phylogenetic Analysis of Algal Megaviruses, *Virology*, **466-467,** 123-128 (2014).

Kotera, M.; Nishimura, Y.; Nakagawa, Z.; Muto, A.; Moriya, Y.; Okamoto, S.; Kawashima, S.; Katayama, T.; Tokimatsu, T.; Kanehisa, M.; Goto, S., PIERO Ontology for Analysis of Biochemical Transformations: Effective Implementation of Reaction Information in the IUBMB Enzyme List, *J. Bioinform. Comput. Biol.*, doi:10.1142/S0219720014420013. (2014).

[Others]

Ogata, H.; Takemura, M., Pandora's Box Brought by Giant Viruses, *Seibutsu-no-Kagaku Iden*, **68,** 194-199 (2014) (in Japanese).

Goto, S., KEGG Database for Functional Genomics, *Journal of the Society of Instrument and Control Engineers*, **53,** 432-437 (2014) (in Japanese).

— Mathematical Bioinformatics —

Hayashida, M.; Akutsu, T., Domain-Based Approaches to Prediction and Analysis of Protein-Protein Interactions, *Int. J. Knowledge Discovery in Bioinformatics*, **4,** 24-41 (2014).

Wang, M.; Zhao, X. M.; Tan, H.; Akutsu, T.; Whisstock, J. C.; Song, J., Cascleave 2.0, a New Approach for Predicting Caspase and Granzyme Cleavage Targets, *Bioinformatics*, **30,** 71-80 (2014).

Qiu, Y.; Tamura, T.; Ching, W. K.; Akutsu, T., On Control of Singleton Attractors in Multiple Boolean Networks: Integer Programming-Based Method, *BMC Systems Biology*, **8(Suppl)1,** [S7-1]-[S7-10] (2014).

Ruan, P.; Hayashida, M.; Maruyama, O.; Akutsu, T., Prediction of Heterotrimeric Protein Complexes by Two-Phase Learning Using Neighboring Kernels, *BMC Bioinformatics*, **15(Suppl)2,** S6 (2014).

Nakajima, N.; Akutsu, T., Exact and Heuristic Methods for Network Completion for Time-Varying Genetic Networks, *Biomed Research International*, **2014,** [684014-1]-[684014-13] (2014).

Lu, W.; Tamura, T.; Song, J.; Akutsu, T., Integer Programming-Based Method for Designing Synthetic Metabolic Networks by Minimum Reaction Insertion in a Boolean Model, *PLoS One*, **9,** [e92637-1]-[e92637-14] (2014).

Cai, H.; Ruan, P.; Ng, M.; Akutsu, T., Feature Weight Estimation for Gene Selection: a Local Hyperlinear Learning Approach, *BMC Bioinformatics*, **15,** [70-1]-[70-13] (2014).

Nakajima, N.; Akutsu, T., Network Completion for Static Gene Expression Data, *Adv. Bioinformatics*, **2014,** [382452-1]-[382452-9] (2014).

Akutsu, T.; Tamura, T.; Fukagawa, D.; Takasu, A., Efficient Exponential-Time Algorithms for Edit Distance between Unordered Trees, *J. Disc. Algorithms*, **25,** 79-93 (2014).

Suzuki, M.; Nagamochi, H.; Akutsu, T., Efficient Enumeration of Monocyclic Chemical Graphs with Given Path Frequencies, *J. Cheminformatics*, **6,** [31-1]-[31-18] (2014).

Hayashida, M.; Ruan, P.; Akutsu, T., Proteome Compression via Protein Domain Compositions, *Methods*, **67,** 380-385 (2014).

Kamada, M.; Sakuma, Y.; Hayashida, M.; Akutsu, T., Prediction of Protein-Protein Interaction Strength Using Domain Features with Supervised Regression, *The Scientific World Journal*, **2014,** [240673-1]-[240673-7] (2014).

Koyano, H.; Tsubouchi, T.; Kishino, H.; Akutsu, T., Archaeal β Diversity Patterns under the Seafloor along Geochemical Gradients, *J. Geophys. Res. - Biogeosciences*, **119,** 1770-1788 (2014).

Hasegawa, T.; Mori, T.; Yamaguchi, R.; Imoto, S.; Miyano, S.; Akutsu, T., An Efficient Data Assimilation Schema for Restoration and Extension of Gene Regulatory Networks Using Time-Course Observation Data, *J. Comp. Biol.*, **21,** 785-798 (2014).

Nacher, J. C.; Akutsu, T., Analysis of Critical and Redundant Nodes in Controlling Directed and Undirected, *J. Complex Networks*, **2,** 394-412 (2014).

Takeuchi, R.; Tamura, T.; Nakayashiki, T.; Tanaka, Y.; Muto, A.; Wanner, B. L.; Mori, H., Colony-Live —A High-Throughput Method for Measuring Microbial Colony Growth Kinetics — Reveals Diverse Growth Effects of Gene Knockouts in *Escherichia coli*, *BMC Microbiology*, **14,** 171 (2014).

Hayashida, M.; Koyano, H.; Akutsu, T., Measuring the Similarity of Protein Structures Using Image Local Feature Descriptors SIFT and SURF, *Proc. 8th Int. Conf. Systems Biology*, 167-171 (2014).

Akutsu, T.; Jansson, J.; Takasu, A.; Tamura, T., On the Parameterized Complexity of Associative and Commutative Unification, *Lecture Notes in Computer Science*, **8894,** 15-27 (2014).

— Bio-knowledge Engineering —

Mohamed, A.; Hancock, T.; Nguyen, C. H.; Mamitsuka, H., NetPathMiner: R/Bioconductor Package for Network Path Mining through Gene Expression, *Bioinformatics*, **30(21),** 3139-3141 (2014).

Kayano, M.; Shiga, M.; Mamitsuka, H., Detecting Differentially Coexpressed Genes from Labeled Expression Data: A Brief Review, *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, **11(1),** 154-167 (2014).

Nguyen, C. H.; Wicker, N.; Mamitsuka, H., Selecting Graph Cut Solutions via Global Graph Similarity, *IEEE Transactions on Neural Networks and Learning Systems*, **25(7),** 1407-1412 (2014).

Ding, H.; Takigawa, I.; Mamitsuka, H.; Zhu, S., Similarity-based Machine Learning Methods for Predicting Drug-target Interactions: A Brief Review, *Briefings in Bioinformatics*, **15(5),** 737-747 (2014).

Takahashi, K.; Takigawa, I.; Mamitsuka, H., SiBIC: A Web Server for Generating Gene Set Networks Based on Biclusters Obtained by Maximal Frequent Itemset Mining, *PLoS One*, **8(12),** e82890 (2013).

Karasuyama, M.; Mamitsuka, H., Multiple Graph Label Propagation by Sparse Integration, *IEEE Transactions on Neural Networks and Learning Systems*, **24(12),** 1999-2012 (2013).

ENDOWED RESEARCH SECTION

— Nano-Interface Photonics (SEI Group CSR Foundation) —

Kan, D.; Shimizu, T.; Yamada, Y.; Aso, R.; Kurata, H.; Kanemitsu, Y.; Shimakawa Y., Band-to-Band Photoluminescence as a Probe of Electron Carriers in Nb-Doped $SrTiO_3$ Epitaxial Thin Films, *Appl. Phys. Express*, **7,** [015503-1]-[015503-4] (2014).

Yamada, Y.; Nakamura, T.; Yasui, S.; Funakubo, H.; Kanemitsu, Y., Measurement of Transient Photoabsorption and Photocurrent of $BiFeO_3$ Thin Films: Evidence for Long-Lived Trapped Photocarriers, *Phys. Rev. B*, **89,** [035133-1]-[035133-5] (2014).

Nishihara, T.; Yamada, Y.; Okano, M.; Kanemitsu, Y., Quantized Exciton-Exciton Recombination in Undoped and Hole-Doped Single-Walled Carbon Nanotubes, *Jpn. J. Appl. Phys.*, **53,** [02BD10-1]-[02BD10-5] (2014).

Yamada, Y.; Nakamura, T.; Endo, M.; Wakamiya, A.; Kanemitsu, Y., Near-band-edge Optical Responses of Solution-Processed Organic-Inorganic Hybrid Perovskite $CH_3NH_3PbI_3$ on Mesoporous TiO_2 Electrodes, *Appl. Phys. Express*, **7,** [032302-1]-[032302-4] (2014).

Le, P. Q.; Okano, M.; Yamada, Y.; Nagaoka, A.; Yoshino, K.; Kanemitsu, Y., Temperature-Dependent Photocarrier Recombination Dynamics in Cu_2ZnSnS_4 Single Crystals, *Appl. Phys. Lett.*, **104,** [081907-1]-[081907-4] (2014).

Okano, M.; Nishihara, T.; Yamada, Y.; Kanemitsu, Y., Chemical Doping-Induced Changes in Optical Properties of Single-Walled Carbon Nanotubes, *Jpn. J. Appl. Phys.*, **53,** [05FD02-1]-[05FD02-4] (2014).

Yamada, Y.; Sato, H. K.; Hikita, Y.; Hwang, H. Y.; Kanemitsu, Y., Photocarruer Recombination and Localization Dynamics of $LaAlO_3$/$SrTiO_3$ Heterostructures, *Proc. SPIE*, **8987,** [898710-1]-[898710-7] (2014).

Yamada, Y.; Sato, H. K.; Hikita, Y.; Hwang, H. Y.; Kanemitsu, Y., Spatial Density Profile of Electrons near the $LaAlO_3/SrTiO_3$ Heterointerface Revealed by Time-Resolved Photoluminescence Spectroscopy, *Appl. Phys. Lett.*, **104,** [151907-1]-[151907-4] (2014).

Okano, M.; Takabayashi, Y.; Sakurai, T.; Akimoto, K.; Shibata, H.; Niki, S.; Kanemitsu, Y., Slow Intraband Relaxation and Localization of Photogenerated Carriers in $CuIn_{1-x}Ga_xSe_2$ Thin Films: Evidence for the Existence of Long-Lived High-Energy Carriers, *Phys. Rev. B*, **89,** [195203-1]-[195203-6] (2014).

Sakamoto, M.; Inoue, K.; Saruyama, M.; So, Y. G.; Kimoto, K.; Okano, M.; Kanemitsu, Y.; Teranishi, T., Investigation on Photo-Induced Charge Separation in CdS/CdTe Nanopencils, *Chem. Sci.*, **5,** 3831-3835 (2014).

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).

Okano, M.; Sakamoto, M.; Teranishi, T.; Kanemitsu, Y., Assessment of Hot-Carrier Effects on Charge Separation in Type-II CdS/CdTe Heterostructured Nanorods, *J. Phys. Chem. Lett.*, **5,** 2951-2956 (2014).

Yamada, Y.; Kanemitsu, Y., Band-to-band Photoluminescence and Photocarrier Dynamics in $SrTiO_3$, *Kotai Butsuri*, **49,** 25-33 (2014) (in Japanese).

Yamada, Y.; Wakamiya, A.; Kanemitsu, Y., Perovskite Semiconductor Solar Cells, *Kotai Butsuri*, **49,** 545-553 (2014) (in Japanese).

HAKUBI PROJECT
— Algorithmic Graph Theory with Applications to Bioinformatics —

Do, H. H.; Jansson, J.; Sadakane, K.; Sung, W.-K., Fast Relative Lempel-Ziv Self-Index for Similar Sequences, *Theoretical Computer Science*, **532,** 14-30 (2014).

Jansson, J.; Lingas, A., Computing the Rooted Triplet Distance between Galled Trees by Counting Triangles, *Journal of Discrete Algorithms*, **25,** 66-78 (2014).

Asahiro, Y.; Jansson, J.; Miyano, E.; Ono H., Degree-Constrained Graph Orientation: Maximum Satisfaction and Minimum, Violation, Proc. 11th International Workshop on Approximation and Online, Algorithms (WAOA 2013), *Lecture Notes in Computer Science*, **8447,** 24-36 (2014).

Floderus, P.; Jansson, J.; Levcopoulos, C.; Lingas, A.; Sledneu, D., 3D Rectangulations and Geometric Matrix Multiplication, Proc. 25th International Symposium on Algorithms and Computation, (ISAAC 2014), *Lecture Notes in Computer Science*, **8889,** 65-78 (2014).

Jansson, J.; Sung, W.-K.; Vu, H.; Yiu, S.-M., Faster Algorithms for Computing the R* Consensus Tree, Proc. 25th International Symposium on Algorithms and Computation, (ISAAC 2014), *Lecture Notes in Computer Science*, **8889,** 414-425 (2014).

Akutsu, T.; Jansson, J.; Takasu, A.; Tamura, T., On the Parameterized Complexity of Associative and Commutative Unification, Proc. 9th International Symposium on Parameterized and Exact Computation, (IPEC 2014), *Lecture Notes in Computer Science*, **8894,** 15-27 (2014).

INTERNATIONAL RESEARCH COLLABORATIONS

[Belgium]
Université Catholique de Louvain, Institute on Condensed Matter and Nano-science

University of Liège, Department of Chemistry

[Chile]
Pontificia Universidad Católica de Chile, Facultad de Ciencias Biológicas

[China, P.R.]
Fudan University, School of Computer Sciences

Fudan University, Shanghai Key Lab of Intelligent Information Processing

Peking University, College of Life Sciences

The Chinese Academy of Sciences, Institute of Chemistry

[France]
Centre National de la Recherche Scientifique, Station Biologique de Roscoff

Universite´ de Rennes, Sciences Chimiques de Rennes

University Lille 1, UFR de Mathematics

[Germany]
GEOMAR, Helmholtz Centre for Ocean Research

Philipps University Marburg, Center for Materials Science

Philipps University of Marburg, Center for Materials Sciences, EM&Mlab

Technische Universität Darmstadt, Department of Chemistry

[India]
North Maharashtra University, School of Life Sciences

[Italy]
Universita' degli Studi di Napoli Federico II, Dipartimento di Ingegneria Chimica

University of Padova, Department of Chemistry

[Korea, R.]
Jeju National University, School of Mechatronics Engineering

Seoul National University, Institute of Chemical Process

[Singapore]
National University of Singapore, Department of Chemistry

[Spain]
Ciudad Universitaria, Facultad de Ciencias Químicas

University Complutense of Madrid, Department of Physical Chemistry, Chemistry Faculty

University of Málaga, Department of Physical Chemistry

[Switzerland]
Institute of Geochemistry and Petrology, Department of Earth Sciences

Paul Scherrer Institut, Laboratory for Muon-Spin Spectroscopy

Universität Bern, Institut für Geologie

[U.K.]
Imperial College London, Department of Earth Science and Engineering

King's College London, Department of Pharmacy

Plymouth Marine Laboratory

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

University of Nottingham, School of Physics & Astronomy

University of Oxford, Department of Materials

University of Southampton, School of Chemistry

[U.S.A.]
Arizona State University, Department of Chemistry and Biochemistry

Arizona State University, School of Earth and Space Exploration

Boston University, Department of Chemistry and Division of Materials Science & Engineering and Center for Nanoscience & Nanotechnology

Boston University, School of Medicine, The Pulmonary Center

Brown University, Department of Chemistry

Columbia University, Department of Chemistry

Emory University, School of Medicine, Department of Pediatrics

Georgetown University, Department of Chemistry and Institute of Soft Matter

Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory

Stanford University, Department of Applied Physics

University of Connecticut, Department of Chemistry

University of Maryland, Department of Plant Science and Landscape Architecture

University of Pennsylvania, Department of Materials Science and Engineering

University of Pittsburgh, Department of Medicine

*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.
Development of Pt–Silylyne Complexes and Their Application to Synergetic and Tandem Activation of Small Molecules
Grant-in-Aid for Challenging Exploratory Research
1 April 2012–31 March 2014

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 2015

Sasamori, T.
Construction of Novel d-π Conjugated Systems Containing Heavier Main Group Elements and Their Functions
Grant-in-Aid for Young Scientists (A)
1 April 2011–31 March 2014

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

— 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.
Creation of Paramagnetic Endofullerenes by Organic Synthesis
Grant-in-Aid for Challenging Exploratory Research
1 April 2012–31 March 2014

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

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

— Synthetic Organic Chemistry —

Kawabata, T.
Regioselective Molecular Transformation Based on Organocatalytic Molecular Recognition
Grant-in Aid for Scientific Research on Innovative Area
25 July 2011–31 March 2016

Kawabata, T.
Regioselective Molecular Transformation of Multifunctionalized Molecules
Grant-in Aid for Scientific Research (S)
30 May 2014–31 March 2019

Furuta, T.
Development of Regio- and Stereoselective Reactions of Polyfunctionalized Molecules by Axially Chiral Catalysts
Grant-in-Aid for Scientific Research (C)
28 April 2011–31 March 2014

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

— 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, JST
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.
Fabrication of Nanocrystal Superstructure toward Novel Artificial Photosynthesis
Precursory Research for Embryonic Science and Technology, JST
1 April 2012–31 March 2015

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

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

Tsujii, Y.
Development of Novel Nanosystem by Hierarchically Assembling Concentrated Polymer Brushes
CREST (Core Research for Evolutional Science and Technology), 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

Tsujii, Y.
High-Reliable Li-ion Battery Electrolytes Supported with Well-Designed Polymeric Monoliths
NEDO Project for New Energy Venture Business Technology Innovation Program
1 April 2013–28 February 2014

Ohno, K.
Pharmacokinetics of Well-Defined Polymer Brush-Afforded Fine Particles
Grants-in Aid for Young Scientists (A)
1 April 2011–31 March 2014

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
CREST (Core Research for Evolutional Science and Technology), JST
1 October 2010–31 March 2016

Yamago, S.
Highly Value-added Polymer Material Created by New Living Radical Polymerization Agent
NexTEP (Next Generation Technology Transfer Program), 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.
Development of Novel Spin Dynamics Devices
Grant-in-Aid for Scientific Research(S)
1 April 2011–31 March 2016

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

Futaki, S.
Library Design for Targeting HTLV-1 Related Proteins and the Selection
Grant-in-Aid for Challenging Exploratory Research
1 April 2013–31 March 2015

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 —

Hiratake, J.
Search for Pharmaceuticals Based on Asparagine Synthetase Inhibitors
Grant-in-Aid for Scientific Research (C)
1 April 2011–31 March 2014

Hiratake, J.
Molecular Mechanisms for Pyrethrin Biosynthesis
GDSL Lipase for Development of Insect-Resistant Recombinant Plants
1 April 2013–31 March 2016

Hiratake, J.
Development and Applications of Specific Inhibitors of γ-Glutamyl Transpeptidase
A Grant from the Japan Foundation for Applied Enzymology
28 April 2014–27 April 2015

Watanabe, B.
A Study on Biosynthesis and Dynamics of Archaeal Membrane Lipids Using Synthetic Lipid Molecules
Grant-in-Aid for Young Scientists (B)
1 April 2013–31 March 2015

— Molecular Biology —

Aoyama, T.
Regulatory Mechanisms for Functional Morphologies of Plants
Bilateral Program for Joint Research between JSPS and NSFC
1 April 2012–31 March 2015

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

— Chemical Biology —

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

Uesugi, M.
Chemical Biological Exploration of New Functions of Endogenous Lipid-related Molecules
CREST (Core Research for Evolutional Science and Technology), JST
1 October 2014–31 March 2020

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

Goto, A.
High Performance Color Material by Living Radical Polymerization with Organic Catalysts
A-STEP (Adaptable and Seamless Technology Transfer Program through Target-Driven R&D), JST
1 November 2011–31 March 2015

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

— 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

— Solution and Interface Chemistry —

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

Hasegawa, T.
Generation of a New Energy State by Excitation of Multipole via Light Absorption and Its Application to Surface-enhance Raman Scattering Spectrometry
Grant-in-Aid for Scientific Research (B)
1 April 2011–31 March 2014

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.
Functional Analysis and Application of Phospholipids Containing Polyunsaturated Fatty Acids in Bacterial Cell Membrane
Grant-in-Aid for Scientific Research (B)
1 April 2012–31 March 2015

Kurihara, T.
Exploration of Cold-Adapted Microorganisms to Develop the Low-temperature Bioprocessing
Grant-in-Aid for Scientific Research (B)
1 April 2013–31 March 2016

Kawamoto, J.
Exploration of Functional Metal-Nanoparticle-Producing Bacteria from Extreme Environments
Grant-in-Aid for Scientific Research (B)
1 April 2012–31 March 2015

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 2015

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

Kanaya, T.
Photon and Quantum Basic Research Coordinated Development Program, JST
1 September 2013–31 March 2018

Nishida, K.
Property Control of Water-soluble Cellulose Derivatives
Grant-in-Aid for Scientific Research (C)
1 April 2011–31 March 2014

Ogawa, H.
Development of the Micro-GISAXS System for Functional Polymer Thin Films
Grant-in-Aid for Young Scientist (B)
1 April 2013–31 March 2015

— Molecular Rheology —

Watanabe, H.
Non-linear Feedbacks between Polymer Dynamics and Phase Separation Kinetics in Polymer Blends
Grant-in-Aid for Scientific Research (A)
1 April 2012–31 March 2015

Masubuchi, Y.
Molecular Friction of Polymers under Stretch and Oriented State
Grant-in-Aid for Scientific Research (B)
1 April 2014–31 March 2017

Masubuchi, Y.
Relaxation Mechanisms of Polymers under Fast Flow
Grant-in-Aid for Scientific Research (B)
1 April 2011–31 March 2014

Matsumiya, Y.
Molecular Picture of the Correlation Length in Polymer Dynamics
Grant-in-Aid for Scientific Research (C)
1 April 2012–31 March 2015

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.
Innovative High-performance Ion Source by the RF Phase Direct Injection of the Short Pulse Laser Plasma
Grant-in-Aid for Challenging Exploratory Research
1 April 2012–31 March 2014

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 Program
1 April 2013–31 March 2017

— Laser Matter Interaction Science —

Sakabe, S.
Demonstration of Ultra-fast Electron Diffraction Using Fast Electrons Accelerated in Plasmas by an Intense Femtosecond Laser
Grant-in-Aid for Scientific Research (S)
1 April 2011–31 March 2016

Sakabe, S.
Long-distance Acceleration of Surface Plasma Electrons Along a Metal Wire by the Surface Wave Induced by Ultra-intense Laser Pulses
Grant-in-Aid for Challenging Exploratory Research
1 April 2013–31 March 2015

Sakabe, S.
Fundamental Study for Mechanism Clarification of Laser Colored Metal Surface
Amada Foundation for Metal Work Technology
15 December 2011–31 March 2014

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, MEXT
2 July 2012–31 March 2022

Haruta, M.
Atomic Resolution Polarized Spectrum Analysis
Grant-in-Aid for Research Activity Start-up
30 August 2013–31 March 2014

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 —

Isozaki, K.
Development of Novel Gold Nanoparticle Catalysts Bearing Molecular Interfacial Reaction Fields
The Science Research Promotion Fund of Research Institute for Production Development
1 November 2014–31 October 2015

Iwamoto, T.
Aromatic C-H Functionalization via Cation-π Interaction
Grant-in-Aid for Research Activity Start-up
29 August 2014–31 March 2016

— 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

Ozawa, F.
Development of Highly Efficient Catalysts for Synthesizing of π-Conjugated Polymers via Direct Arylation
ACT-C (Advanced Catalytic Transformation Program for Carbon Utilization), 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 —

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

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

Kotera, M.
Reaction Network Prediction for ab initio Reconstruction of Metabolic Pathways Biosynthesis Machinery
Grant-in-Aid for Scientific Research on Innovative Areas, MEXT
1 April 2013–31 March 31 2015

Kotera, M.
Information Technology Development for the Comparative Genomics of Various Insects
Grant-in-Aid for Young Scientists (B)
1 April 2013–31 March 2016

— 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.
Estimating Data Structures from Various Semi-Structured Data
Grants-in-Aid for Scientific Research (B)
1 April 2012–31 March 2015

Karasuyama, M.
Extracting Sub-Structures from Graph-Structured Data
Grants-in-Aid for Young Scientists (B)
1 April 2014–31 March 2017

Takeuchi, I.; Hatano, K.; Karasuyama, M.
Theory and Applications of Optimality Guaranteed Screening for Big-Data Analysis
Grants-in-Aid for Scientific Research (B)
1 April 2014–31 March 2017

Natsume, Y.
In silico Analysis of Histone Modification Dynamics that Regulate Developmental Processes
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2010–31 March 2015

THESES

ARAKAWA, Tomonori
D Sc, Kyoto University
"Dynamics and Spin Dependent Transport in Mesoscopic Junctions"
Supervisor: Prof ONO, Teruo
29 July 2014

ASO, Ryotaro
D Sc, Kyoto University
"Local Structure and Strain Analysis of Transition Metal Oxide Films by STEM"
Supervisor: Prof KURATA, Hiroki
24 March 2014

CHANG, Yung-Hung
D Eng, Kyoto University
"Studies on PNP-Pincer Type Phosphaalkene Complexes of Iridium"
Supervisor: Prof OZAWA, Fumiyuki
18 April 2014

CHO, Hyun-nam
D Agr, Kyoto University
"Studies on 1-Acyl-*sn*-Glycerol-3-Phosphate Acyltransferase of *Shewanella livingstonensis* Ac10"
Supervisor: Prof KURIHARA, Tatsuo
24 March 2014

FUKUYAMA, Sadanobu
D Agr, Kyoto University
"Catalytic and Structural Characteristics of 2,4-Diaminopentanoate Dehydrogenase from *Fervidobacterium nodosum*"
Supervisor: Prof KURIHARA, Tatsuo
24 March 2014

HUANG, Yun
D Eng, Kyoto University
"Synthesis of Novel Polymer-Brush-Afforded Hybrid Particles for Well-Organized Assemblies"
Supervisor: Prof TSUJII, Yoshinobu
23 July 2014

IWAMOTO, Takahiro
D Eng, Kyoto University
"Studies on Synthesis and Host-Guest Chemistry of Cycloparaphenylenes"
Supervisor: Prof YAMAGO, Shigeru
24 March 2014

KINOSHITA, Tomohiko
D Pharm Sc, Kyoto University
"Studies on Intermolecular Conjugate Addition and Dieckmann Condensation Based on Memory of Chirality"
Supervisor: Prof KAWABATA, Takeo
24 March 2013

MATSUO, Sadashige
D Sc, Kyoto University
"Investigation of Quantum Interferences in Bi_2Se_3 Thin Films"
Supervisor: Prof ONO, Teruo
14 January 2014

MIYASAKA, Yasuhiro
D Sc, Kyoto University
"Laser Nano Ablation Induced by the Iinteraction of Femtosecond Laser with Metal Surface"
Supervisor: Prof SAKABE Shuji
24 September 2014

SAITO, Hikaru
D Sc, Kyoto University
"Propagation Mode Analysis of Nano-Materials for Optics Using Angle-Resolved EELS"
Supervisor: Prof KURATA, Hiroki
24 March 2014

UEDA, Kohei
D Sc, Kyoto University
"Investigation of the Mechanisms in Current-Induced Domain Wall Motion"
Supervisor: Prof ONO, Teruo
14 January 2014

YAOITA, Takatoshi
D Eng, Kyoto University
"Friction of Polymer Chains under Fast Deformation"
Supervisor: Prof WATANABE, Hiroshi
25 November 2014

ZHAO, Yang
D Inf, Kyoto University
"Computational Methods for Analyzing Chemical Graphs and Biological Networks"
Supervisor: Prof AKUTSU, Tatsuya
24 March 2014

THE 114TH ICR ANNUAL SYMPOSIUM

SEMINARS

MEETINGS AND SYMPOSIA

THE 114TH ICR ANNUAL SYMPOSIUM

(12 December 2014)

ORAL PRESENTATION

OHNO, Kohji (Chemistry of Polymer Materials)
“Precision Design and Applications of Polymer-brush-afforded Hybrid Particles”

FRISCO-CABANOS, Heidie L. (Chemical Biology)
“Synthetic Molecules That Protect Cells from Anoikis and Their Use in Cell Transplantation”

OGAWA, Hiroki (Polymer Materials Science)
“Structural Analysis of the Polymer Surfaces and Interfaces with SR-GISAXS”

YOSHIDA, Hiroyuki (Molecular Aggregation Analysis)
“A New Experimental Method to Determine the Electron Affinity of Organic Semiconductors and Its Application to Organic Electronics”

— ICR Award for Young Scientists —
KAYAHARA, Eiichi (Polymer Controlled Syinthesis)
“Synthesis and Physical Properties of a Ball-like Three-dimensional π-Conjugated Molecule”

— ICR Award for Young Scientists (Foreign Researchers’ Category) —
TEX, David Michael (Photonic Elements Science)
“Control of Hot-carrier Relaxation for Realizing Ideal Quantum-dot Intermediate-band Solar Cells”

— ICR Award for Graduate Students —
NAGATA, Koichi (Organoelement Chemistry)
“Syntheses and Structures of Terminal Arylalumylene Complexes”

— ICR Award for Graduate Students —
NISHIMURA, Hidetaka (Structural Organic Chemistry)
“On-top π-stacking of Quasiplanar Molecules in Hole-transporting Materials: Inducing Anisotropic Carrier Mobility in Amorphous Films”

— ICR Award for Graduate Students (Foreign Students’ Category) —
MOHAMED, Ahmed Mohmed (Bio-knowledge Engineering)
“NetPathMiner: R/Bioconductor Package for Network Path Mining through Gene Expression”

— ICR Grants for Promoting Integrated Research —
YOSHIMURA, Tomoyuki
“Spectroscopic Detection of Chiral Molecules of Theoretical Existence”

WAKIOKA, Masayuki
“Development of the Synthetic Method for Precise Control of Primary Structures of π-Conjugated Polymers via Direct Arylation Polymerization: Combination of Experimental and Theoretical Approaches”

LE, Quang Phuong
“Investigation of Photocarrier Dynamics in Perovskite-based Solar Cells”

YAMADA, Yasuhiro
“Dielectric Screening Effects on the Optical Properties of Nanomaterials”

SATO, Ryota
“Strategic Synthesis of High-Performance Core-Shell Structured Catalytic Nanoparticles with Low Pt Loading”

TAKEUCHI, Katsuhiko
“Synthesis and Applications of Non-Innocent PNP-Pincer Type Phosphaalkene Ligands”

POSTER PRESENTATIONS

LW : Laboratory Whole Presentation
LT : Laboratory Topic
GE : General Presentation

— Organoelement Chemistry —

LW “Studies on the Synthesis and Properties of Novel Organic Compounds Containing Heavier Elements”

GE HIRANO, Koki; MIYAKE, Hideaki; SASAMORI, Takahiro; TOKITOH, Norihiro
“Synthesis, Properties, and Structures of Group 6 Metal Carbonyl Complexes Bearing a Triphospha[3]radialene Ligand”

— Structural Organic Chemistry —

LW “Research Activities in Structural Organic Chemistry Laboratory”

GE ZHANG, Rui; MURATA, Michihisa; WAKAMIYA, Atsushi; MURATA, Yasujiro
“Synthesis and X-ray Structure of Open-Cage Thiafullerene $C_{69}S$ and Oxafullerene $C_{69}O$ Derivatives”

GE CHAOLUMEN; ENNO, Hiroki; MURATA, Michihisa; WAKAMIYA, Atsushi; MURATA, Yasujiro
“Synthesis, Structure, and Properties of Dibenzo[*a*,*f*]perylene Bisimide Derivatives”

— Synthetic Organic Chemistry —

LW “Recent Advances of Research in Synthetic Chemistry Laboratory”

LT YANAGI, Masanori; TSUDA, Ayumi; UEDA, Yoshihiro; FURUTA, Takumi; KAWABATA, Takeo
“Counter-anion Induced Accelerative Acylation by Nucleophilic Catalysis”

— Advanced Inorganic Synthesis —

LW “Poster Lab Whole Presentation of Advanced Inorganic Synthesis, Division of Synthetic Chemistry”

GE YAMAOKA, Satoshi; SAKAMOTO, Masanori; TERANISHI, Toshiharu
“Synthesis of Gold Nanoparticles Protected by Novel Bulky Porphyrin Ligand”

GE KIMURA, Masato; SAKAMOTO, Masanori; FURUBE, Akihiro; TERANISHI, Toshiharu
“Synthesis and Optical Properties of Heterostructured Au/ZnS Nanoparticles”

GE MATSUMOTO, Kenshi; SATO, Ryota; TRINH, Thang Thuy; SAKUMA, Noritugu; TERANISHI, Toshiharu
“Grain Size Dependence of Magnetic Properties in $L1_0$-FePd/α-Fe Nanocomposite Magnets”

GE EGUCHI, Daichi; SAKAMOTO, Masanori; TERANISHI, Toshiharu
“Synthesis of Stable Gold Clusters Face-coordinated by Porphyrin Derivatives Containing Disulfide Groups”

— Chemistry of Polymer Materials —

LT HSU, Shu-Yao; ISHIGE, Ryohei; OHNO, Kohji; TSUJII, Yoshinobu
“Synthesis of Concentrated Polymer Brushes with Extraordinarily Large Thicknesses by Living Radical Polymerization and Characterization of Their Tribological Properties”

GE NAKANISHI, Yohei; ISHIGE, Ryohei; SAKAKIBARA, Keita; OHNO, Kohji; TSUJII, Yoshinobu; OGAWA, Hiroki; KANAYA, Toshiji; MORINAGA, Takashi; SATO, Takaya
“Structural Analysis by Ultra-small-angle X-ray Scattering Method for Membranes of Self-assembled Nanoparticles with Polymer Brushes”

— Polymer Controlled Synthesis —

LW “Research Activity of Polymer Controlled Synthesis Group”

GE MAEDA, Yuki; KAYAHARA, Eiichi; YAMAGO, Shigeru
“Synthetic Study on Cyclic-Conjugated Porphyrin Oligomers”

GE FUJII, Akira; YAMAGO, Shigeru
“Propargyl Tellurides for Living Radical Polymerization”

— Inorganic Photonics Materials —

GE OKUMURA, Shun
“Structural Analysis of Local Coordination State of Sn^{2+} Center in Oxide Glass”

GE TOKUNAGA, Yuta
“Preparation of Proton Conductive Organic-inorganic Hybrid Phosphite Membranes with Proton Conductivity”

GE MATSUKI, Hiroaki
“Protein Adsorption Characteristic of Organic-Inorganic Hybrid Material Containing Gold Nanoparticles”

— Nanospintronics —

GE YOSHIMURA, Yoko; KIM, Kab-Jin; TANIGUCHI, Takuya; UEDA, Kohei; HIRAMATSU, Ryo; MORIYAMA, Takahiro; ONO, Teruo
“Real-time Observation of Domain Wall Motion in Ferromagnetic Wires”

GE KAWAGUCHI, Masashi; MORIYAMA, Takahiro; ONO, Teruo
“Layer Thickness Dependence of the Current Induced Effective Field”

— Biofunctional Design-Chemistry —

LW “Research Activity at Biofunctional Design Chemistry”

GE MURAYAMA, Tomo; PUJALS, Silvia; FUTAKI, Shiroh
“Curvature Sensitive Membrane Perturbation by Amphypathic Peptides of Adenovirus Protein VI”

— Chemistry of Molecular Biocatalysts —

LW “Research Activities in the Laboratory of Chemistry of Molecular Biocatalysts”

GE OZAKI, Ayane; Li, Chunjie; WATANABE, Bunta; HIRATAKE, Jun
“Irreversible Inhibition and Reactivation of Human γ-Glutamyl Transpeptidase by Mechanism-Based Inhibitors”

— Molecular Biology —

LW “Research Activities in the Laboratory of Molecular Biology”

— Chemical Biology —

LW “Create New World of Bioactive Synthetic Small Molecules”

— Molecular Materials Chemistry —

LW “Research Activities in Molecular Materials Chemistry Laboratory”

GE LEI, Lin; TANISHIMA, Miho; GOTO, Atsushi; KAJI, Hironori
“Design of Initiators in Organo-catalyzed Living Radical Polymerization”

— Hydrospheric Environment Analytical Chemistry —

LW “The Determination of Bioactive Trace Metals in Seawater Using an Automated Preconcentration Device”

LT MINAMI, Tomoharu; KONAGAYA, Wataru; ZHENG, Linjie; SOHRIN, Yoshiki
“Vertical Profiles of Dissolved and Total Dissolvable Bioactive Trace Metals along 165°E in Western North Pacific”

— Solution and Interface Chemistry —

GE TANAKA, Yuki; SHIMOAKA, Takafumi; MORITA, Kohei; SONOYAMA, Masashi; TAKAGI, Toshiyuki; KANAMORI, Toshiyuki; HASEGAWA, Takeshi
“Surface Chemistry and Spectroscopic Studies on a Chemical Model Accounting for Material Characteristics of Perfluoroalkyl Compounds”

GE SHIOYA, Nobutaka; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
“Infrared Spectroscopic Study of Molecular Orientation of p-type Organic Semiconductor Thin Film”

— Molecular Microbial Science —

LW “Laboratory of Molecular Microbial Science”

LT OGURA, Ryutaro; KAWAMOTO, Jun; KURIHARA, Tatsuo
“Study on Polyunsaturated Fatty Acid-biosynthesis Enzymes Involved in the Microdomain Formation in Bacterial Membrane”

— Polymer Materials Science —

LW “Investigation of Polymer Structure for Creation of New Polymer Properties”

GE MURAKAMI, Momoko; MATSUURA, Tomohiko; TAKAHASHI, Nobuaki; NISHIDA, Koji; KANAYA, Toshiji
“Shear-induced Structure Formation Process of Isotactic Polystyrene above Nominal Melting Temperature”

GE KISHIMOTO, Mizuki; INOUE, Rintaro; OGAWA, Hiroki; NISHIDA, Koji; KANAYA, Toshiji
“Effect of Interactions between Polymer Thin Film and Substrate on the Glass Transition Temperature”

— Molecular Rheology —

LW “Research Activities in Molecular Rheology Laboratory”

— Molecular Aggregation Analysis —

LT YAMADA, Kazuto; YOSHIDA, Hiroyuki; TSUTSUMI, Jun’ya; SATO, Naoki
“Electronic States of Organic Semiconductor Thin Films: Impact of Polarization Energy, Band-dispersion and Molecular Orientation”

GE SHINTAKU, Naoto; MURDEY, Richard; YOSHIDA, Hiroyuki; SATO, Naoki
“The Energy Gap of a Radical Molecular Thin Film and the Energy Level Alignment at the Interface with Conductive Substrates”

— Interdisciplinary Chemistry for Innovation —

LW “Research Activities of Interdisciplinary Chemistry for Innovation”

— Particle Beam Science —

LW “Status of Accelerator Laboratory, Advanced Research Center for Beam Science”

LT KITAHARA, Ryunosuke; IWASHITA, Yoshihisa; NOP Group
“A Report of the Neutron Life Time Measurement at J-PARC/BL05”

— Laser Matter Interaction Science —

GE MIYASAKA, Yasuhiro; HASHIDA, Masaki; NISHII, Takaya; INOUE, Shunsuke; SAKABE, Shuji
“Physics of Nano Ablation for Metals by Femtosecond Laser Irradiation”

GE MAEDA, Kazuya; INOUE, Shunsuke; TOKITA, Shigeki; HASHIDA, Masaki; SAKABE, Shuji
“Improvement of Contrast with Plasma Mirror Installed in T^6 Laser System”

GE NISHII, Takaya; HASHIDA, Masaki; MIYASAKA, Yasuhiro; INOUE, Shunsuke; SAKABE, Shuji
“Formation of Laser Induced Periodic Surface Structures on Metal”

GE NAKASHIMA, Yuto; INOUE, Shunsuke; TERAMOTO, Kensuke; NAKAMIYA, Yoshihide; MIYASAKA, Yasuhiro; HASHIDA, Masaki; SAKABE, Shuji
“Generation and Acceleration of Proton Beams by Interaction of Thin Foils and Laser Pulses”

GE TERAMOTO, Kensuke; INOUE, Shunsuke; NAKASHIMA, Yuto; WATANABE, Kota; NAKAMIYA, Yoshihide; TOKITA, Shigeki; HASHIDA, Masaki; SAKABE, Shuji
“Generation, Acceleration and Guidance of Electrons by Intense Laser Irradiation”

GE MORI, Kazuaki; HASHIDA, Masaki; NAGASHIMA, Takeshi; INOUE, Shunsuke; HANGYO, Masanori; SAKABE, Shuji
“THz Wave Generation from Cluster Plasma Produced by Intense Laser”

— Electron Microscopy and Crystal Chemistry —

LW “Research Activities in Division of Electron Microscopy and Crystal Chemistry”

GE FUJIYOSHI, Yoshifumi; NEMOTO, Takashi; KURATA, Hiroki
“EELS Mapping of Localized Surface Plasmon and Its Analysis”

— Structural Molecular Biology —

LW “Introduction of Structural Molecular Biology Laboratory”

— Organic Main Group Chemistry —

LW “Research of Organic Main Group Chemistry”

GE NISHIKORI, Tatsushi; NAKAGAWA, Naohisa; IWAMOTO, Takahiro; HATAKEYAMA, Takuji; TAKAYA, Hikaru; NAKAMURA, Masaharu
“*Anti*-Selective Iron-Catalyzed Carbosilylation of Alkynes”

GE ISHIBASHI, Kosuke; ISOZAKI, Katsuhiro; TAGUCHI, Tomoya; TAKAYA, Hikaru; NAKAMURA, Masaharu; MIKI, Kazushi
“Reaction Rate-Acceleration of Hydrosilane Alcoholysis with Self-Assembled Monolayer-Capped Gold Nanoparticles”

— Advanced Solid State Chemistry —

LW “Introduction of Advanced Solid State Chemistry Laboratory”

GE SEKI, Hayato; SAITO, Takashi; SHIMAKAWA, Yuichi
“Crystal Structure and Physical Properties of Novel Perovskites $SrFe_{1-x}Ni_xO_3$”

— Organotransition Metal Chemistry —

LW “Activity Report: Organotransition Metal Chemistry Laboratory”

GE IIZUKA, Eisuke; WAKIOKA, Masayuki; OZAWA, Fumiyuki
“Synthesis of D-A Type π-Conjugated Polymer with Dithienosilole Units via Direct Arylation Polymerization”

GE CHANG, Yung-Hung; TAKEUCHI, Katsuhiko; OZAWA, Fumiyuki
“Hydrosilylation of CO_2 Catalyzed by PNP-Pincer Type Phosphaalkene Complexes of Iridium and Its Applications”

— Photonic Elements Science —

LW “Recent Research Topics of Photonic Elements Science Group”

— Chemical Life Science —

LW “Research Topics in Laboratory of Chemical Life Science”

LT MIHARA, Tomoko; GOTO, Susumu; OGATA, Hiroyuki
“A Study of Amino Acid Biosynthetic Enzymes Encoded in Viral Genomes”

— Mathematical Bioinformatics —

LW “Enumeration of Tree-like Chemical Compounds with Benzene Rings and EnuMol Server”

— Bio-knowledge Engineering —

GE KARASUYAMA, Masayuki; MAMITSUKA, Hiroshi
“Sparse Multiple Graph Integration for Label Propagation”

— Nano-Interface Photonics —

LW “Research Topics in Nano-interface Photonics Group”

— Research Center for Low Temperature and Materials Sciences —

LT TERASHIMA, Takahito
“Artificial Superlattices of Heavy Fermion Antiferromagnets”

SEMINARS

Prof ANDO, Shinji
Department of Chemistry and Materials Science, Tokyo Institute of Technology, Tokyo, Japan
"Control in Electrical State and Conformation of Polyimides and Design of Their Nanohybridization"
27 August 2014

Prof BACK, Christian
Universitat Regensburg, Germany
"Imaging the Current Induced Spin Wave Doppler Shift"
26 June 2014

Prof BAUMGATTNER, Thomas
University of Calgary, Canada
"Organophosphorus Avenues toward Powerful Electron Acceptors and Self-Assembled Nanomaterials"
14 November 2014

Prof BETTINGER, Holger
Institut für Organische Chemie, Universität Tübingen, Tübingen, Germany
"From Reactive Intermediates to Polycyclic Aromatic Hydrocarbons"
8 April 2014

Dr. BLANC-MATHIEU, Romain
Institut Sophia Agrobiotech, INRA, Sophia Agrobiotech, France
"Population Genomics of *Ostreococcus tauri*: Diversity and Evolution of the Smallest Photosynthetic Eukaryote"
24 September 2014

Prof BODWELL, Graham, J.
Memorial University of Newfoundland, Canada
"Large Scale Synthesis and Chemistry of 1,1,n,n Tetramethyl[n](2,11) teropyrenophanes"
22 October 2014

Prof BRADDOCK, Chris
Imperial College London, U.K.
"Studies on Halogenated Marine Natural Products as Inspired by Their Probable Biogenesis"
22 October 2014

Dr. CARDARELLI, Maura
Department of Biology and Biotechnology, Sapienza University of Rome, Italy
"The Role of ARF8 and ARF6 in Late Stamen Development in *Arabidopsis*"
14 October 2014

Prof CHIDA, Noritaka
Faculty of Science and Technology, Department of Applied Chemistry, Keio University, Kanagawa, Japan
"Synthetic Study of Bioactive Natural Products: Approach from Chiral Pool Method"
26 February 2014

Prof CHIU, Ya-Ping
Department of Physics, National Sun Yat-sen University, Taiwan
"Atomic-Scale Interface Electronic Structures Across Hetero-Epitaxial Structure by Cross-Sectional STM"
22 July 2014

Prof CHOW, Tahsin J.
Academia Sinica Institute of Chemistry, Taiwan
"The Synthesis of Acenes and Their Semiconducting Properties"
6 October 2014

Prof CHUANG, John Shih-Ching
National Chiao Tung University, Taiwan
"Fullerenes Functionalization through Metal-Catalyzed C-H Bond Activation and Phosphine-Catalysis: From Methodology to Application"
12 July 2014

Prof COZZI, Giorgio
University of Milan, Milan, Itary
"Electrophilicity and Nucleophilicity Scales in a Rational Approach towards SN1-type Stereoselective Organocatalytic Reactions"
14 November 2014

Prof DE LA HIGUERA, Colin
University of Nantes, Nantes, France
"Learning Probabilistic Context-Free Grammars"
16 September 2014

Prof DESAULNIERS, Jean-Paul
Faculty of Science, University of Ontario Institute of Technology, Ontario, Canada
"Training the RISC Complex Some New Tricks"
19 November 2014

Mr. FLODERUS, Peter
Lund University, Lund, Sweden
"A Polynomial to Count Induced Subgraphs Quickly"
2 September 2014

Assoc Prof GHOSH, Suhrit
Indian Association for the Cultivation of Science, India
"Stimuli-responsive Amphiphilic Polymers"
9 December 2014

Prof HARA, Kenji
Catalysis Research Center, Hokkaido Univerisy, Hokkaido, Japan
"Catalyst Preparation on Mesoporous Materials"
31 October 2014

Prof HE, Junpo
Fudan University, China, P.R.
"Precise Control of Polymer Chain Structure Using Living Anion Polymerization"
1 August 2014

Prof JIA, Yngxing
Peking University, China, P.R.
"Total Synthesis of Polycyclic Indole Alkaloids and Development of Synthetic Methodology"
8 December 2014

Prof JUNG, Hyun Suk
Sungkyunkwan University, Korea, R.
"Nanostructured Charge Collecting Materialsfor Next Generation Perovskite Solar Cells"
26 November 2014

Dr. KAMATANI, Asayuki
Phizer Japan Inc., Tokyo, Japan
“Stories behind Crizotinib”
9 September 2014

Prof KANN, Maricel G.
University of Maryland, Baltimore County, U.S.A.
“A Protein-Domain Approach for the Analysis of Disease Mutations”
3 April 2014

Mr. KOBAYASHI, Toshio
Japan Drilling Co., Ltd., Tokyo, Japan
“Debris Mitigation for Nuclear Power Plant by Using the CO2 Laser”
21 November 2014

Prof KOYAMA, Kazuyoshi
High Energy Accelerator Research Organization, Ibaraki, Japan
“Laser-driven Particle Acceleration”
24 September 2014

Director KROL, Alain
CNRS-University of Strasbourg, France
“Recoding UGA as Selenocysteine during Selenoprotein Synthesis”
16 April 2014

Dr. KUWATA, Akira
Tohoku National Fisheries Research Institute, Fisheries Research Agency, Miyagi, Japan
“Diatoms and Parmales: Evolution, Ecology and Natural History”
22 August 2014

Dr. LUGG, Nathan
School of Engineering, The University of Tokyo, Tokyo, Japan
“Removing the Effects of Channelling from Spectrum Images in STEM”
14 October 2014

Prof MARROWS, Christopher
University of Leeds, U.K.
“Giant Topological Hall Effect in Strained $Fe_{0.7}Co_{0.3}Si$ Epilayers”
15 May 2014

Prof MELEDANDRI, Carla
The University of Otago, New Zealand
“Development of Silver Nanoparticle Materials for Use in Clinical Dentistry”
10 February 2014

Prof MICHL, Josef
University of Colorado, U.S.A.
“The Catalytic Properties of $LiCB_{11}Me_{12}$”
31 October 2014

Prof MURAI, Shinji
Nara Institute of Science, Nara, Japan
“Encouraging Creativity Reaching to Amazing Discovery”
12 May 2014

Dr. MUROOKA, Yoshie
École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland
“Magnetic Dynamics Studied by Time-resolved Electron Microscopy”
23 July 2014

Prof NG, Michael
Department of Mathematics, Hong Kong Baptist University, Hong Kong, China. P.R.
“Spectral Clustering for Tensor Data”
29 May 2014

Dr. NOMURA, Akihiro
National Institute for Materials Science (NIMS), Ibaraki, Japan
“Polymeric Amine Incorporated Porous Silicas as Adsorbents for Trapping of Formaldehyde Indoor Air Pollutants”
2 April 2014

Dr. OKUBO, Ayako
Integrated Support Center for Nuclear Nonproliferation and Nuclear Security, Japan Atomic Energy Agency, Ibaraki, Japan
“Research and Development for the Nuclear Forensics and Safeguard in JAEA”
8 September 2014

Prof PARK, Jongwook
The Catholic University of Korea, Bucheon, Korea, R.
“Synthesis and Electroluminescence Properties of Highly Efficient Blue Fluorescence Emitters Using Dual Core Chromophores”
15 January 2014

Prof PIERS, Warren
Department of Chemistry, University of Calgary, Calgary, Canada
“Perfluoroarylborane Catalyzed Frustrated Lewis Pair Hydrosilations: Mechanism, Applications and Scope”
22 October 2014

Prof PRATT, Derek
University of Ottawa, Canada
“Chemistry of Phenolic, Anionic and Organosulfur Radical-trapping Antioxidants”
20 March 2014

Prof ROHMER, Michel
CNRS-University of Strasbourg, France
“Biosynthesis of Isoprene Units via the MEP Pathway in Bacteria and Plants: Electron and Proton Transfers in the Formation of Isopentenyl Diphosphate and Dimethylallyl Diphosphate”
10 October 2014

Dr. SERINO, Giovanna
Department of Biology and Biotechnology, Sapienza University of Rome, Italy
“CULLIN Neddylation is Globally Regulated during Seedling Development in *Arabidopsis thaliana*”
14 October 2014

Assoc Prof SHIBUYA, Tetsuo
Human Genome Center, Institute of Medical Science, The University of Tokyo, Tokyo, Japan
“de Bruijn Graph Problems”
19 March 2014

Dr. SHIMIZU, M. Hirohiko
Laboratory for Particle Properties, Department of Physics, Nagoya University, Nagoya, Japan
“Monochromating Optics of Epithermal Neutron and Its Applications”
4 July 2014
31 October 2014

Prof SUNAZUKA, Toshiaki
Kitasato Institute for Life Sciences & Graduate School of Infection Control Sciences, Kitasato University, Tokyo, Japan
“Total Synthesis of Novel Polycyclic Indole Alkaloides”
6 August 2014

Dr. TAKAHASHI, Hiroki
Department of Physics, ETH Zurich, Switzerland
“Ultrasensitive Solid-State NMR by High-Field Dynamic Nuclear Polarization and Nano-scale MRI Using Magnetic Resonance Force Microscopy”
6 November 2014

Assoc Prof TAKEMURA, Masaharu
Tokyo University of Science, Tokyo, Japan
"The Origin of the Nucleus: Giant Viruses Unveil the Enigmatic Root of Eukaryotes"
24 June 2014

Assoc Prof TAKEUCHI, Ichiro
Nagoya Institute of Technology, Japan
"An Algorithmic Framework for Computing Validation Performance Bounds by Using Suboptimal Models"
19 March 2014

Prof WEIGAND, Jan J.
Department of Chemistry and Food Chemistry, Technische Universität Dresden, Dresden, Germany
"Highly-Reactive Phosphorus Building Blocks — New Concepts in Synthesis"
19 July 2014

Dr. YAMADA, Takeshi
Kitasato Institute for Life Sciences & Graduate School of Infection Control Sciences, Kitasato University, Tokyo, Japan
"Chemoselective Functionalization of Bioactive Polyol Natural Products Using Organocatalyst"
4 July 2014

Prof YEH, Ming-Chang
National Taiwan Normal University, Taiwan
"Facile Synthesis of Heterocycles via Iron- and Iridium-Prompted Cyclization Reactions"
4 November 2014

MEETINGS AND SYMPOSIA

Asian Chemical Biology Initiative 2014 Manila Meeting
Organized by UESUGI, Motonari
24-27 January 2014 (Manila, Philippines)

Workshop on Novel Functional Oxides
Organized by SHIMAKAWA, Yuichi
8-9 July 2014 (Kyoto, Japan)

MEXT Project of Integrated Research on Chemical Synthesis
"The 4th International Conference on MEXT Project of Integrated Research on Chemical Synthesis (ICOMC2014 Pre-symposium in Kyoto)"
Organized by OZAWA, Fumiyuki
10-11 July 2014 (Uji, Japan)

The 7th Workshop on Next-generation Optical Materials and Their Applications
Organized by MASAI, Hirokazu
28 July 2014 (Uji, Japan)

ICR-Polymer Physics Workshop 2014
Organized by MASUBUCHI, Yuichi
18 September 2014 (Uji, Japan)

International Symposium of Fiber Science and Technology (ISF 2014)
"Special Session S3: Flow and Deformation Induced Polymer Crystallization"
Organized by Institute for Chemical Research, Kyoto University
28 September-1 October 2014 (Tokyo, Japan)

ICR Symposium on Polymer Crystals 2014 (ICRSPC2014)
Organized by Institute for Chemical Research, Kyoto University
2-3 October 2014 (Kyoto, Japan)

ICRIS-NMR '14: Technological Frontiers in Solid-State NMR: A French-Japanese Workshop
Organized by Institute for Chemical Research (ICR), Kyoto University, Co-organized by Joint Usage/Research Center (JURC), ICR, Kyoto University (TOKITOH, Norihiro as Chair, WATANABE, Hiroshi; KAJI, Hironori; NISHIYAMA, Yusuke; FUKUSHIMA, Tatsuya; SUZUKI, Katsuaki; SHIZU, Katsuyuki as Organizers)
4-5 October 2014 (Uji, Japan)

International Symposium on the Synthesis and Application of Curved Organic π-Molecules and Materials (CURO-π)
Organized by YAMAGO, Shigeru
19-21 October 2014 (Uji, Japan)

KUBIC-NII Joint Seminar on Bioinformatics 2014
Organized by Bioinformatics Center, Institute for Chemical Research, Kyoto University and National Institute of Informatics
17 November 2014 (Uji,Japan)

Short Course on Analytical Chemistry (3) -Advanced Course-
Organized by HASEGAWA, Takeshi
18 December 2014 (Uji, Japan)

INDEX

NAME INDEX

KEYWORD INDEX

Institute for
Chemical
Research

Kyoto University