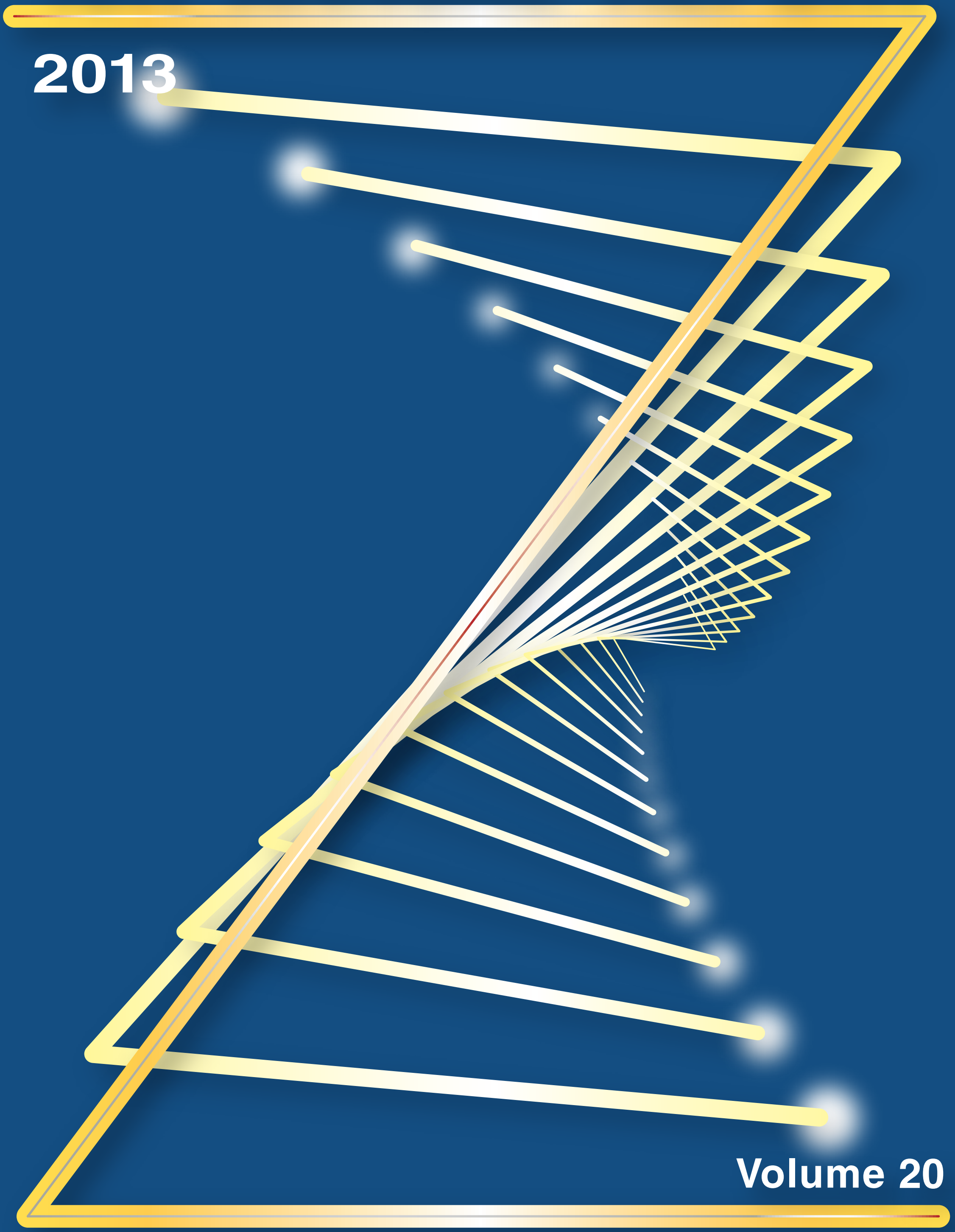
ISSN 1342-0321
IAREFM

ICR ANNUAL REPORT

2013



Volume 20

Institute for Chemical Research
Kyoto University

ICR ANNUAL REPORT 2013 (Volume 20) - ISSN 1342-0321 -
This Annual Report covers from 1 January to 31 December 2013

Editors:
Professor: SAKABE, Shuji
Professor: AOYAMA, Takashi
Professor: KURIHARA, Tatsuo
Associate Professor: IWASHITA, Yoshihisa

Editorial Staff:
Public Relations Section: HAMAOKA, Meri
INOUE, Junko
TAKEHIRA, Tokiyo
NAKANO, Yukako

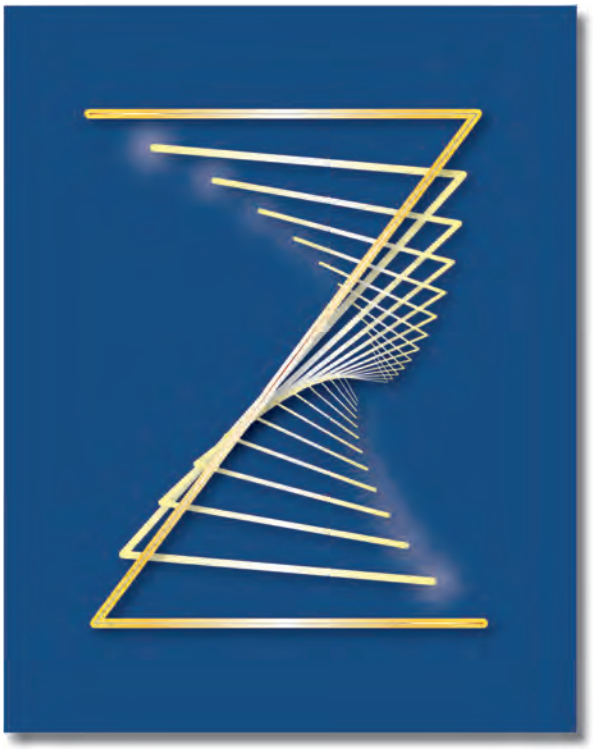
Published and Distributed by:
Institute for Chemical Research (*ICR*), Kyoto University

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

ICR ANNUAL REPORT 2013



Institute for Chemical Research
Kyoto University
Volume 20

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 100 faculty members, 200 graduate students and 50 researchers are engaged in research activities in 32 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, the first X-ray crystallographic examination of a helium atom encapsulated in fullerene, finding out diverse stoichiometry of dissolved trace metals in the Indian Ocean, and synthesis of a ball-like molecule offering a new avenue for novel three-dimensional π-conjugated molecules, 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 about 58 official international collaboration agreements) 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 last year. 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 2014

Naoki Sato

SATO, Naoki
Director

ICR News 2013

Materials Related with “Production of Synthetic Oil by the Fischer-Tropsch Process” in the Institute for Chemical Research Were Approved as Chemical Heritage

Prof MURATA, Yasujiro

Materials related with “Production of Synthetic Oil by the Fischer-Tropsch Process” in the Institute for Chemical Research (ICR) were approved as Chemical Heritage by the Chemical Society of Japan. The research works on the synthetic oil at ICR, Kyoto University and the materials for industrial process at the Takikawa Plant, the Hokkaido-jinzosekiyu, Inc. were certified. During the World War II, the Japanese government strongly pushed academia and industry to carry out research works on production of synthetic oil from coal, and the synthetic oil was produced nationwide in industrial scale. The Hokkaidojinzosekiyu, Inc., which was founded in 1938, introduced the Fisher-Tropsch process from Germany and headed for industorial production of synthetic oil from a mixture of carbon monooxide and hydrogen gases by the use of the cobalt catalysts. Professors Gen-itsu Kita and Shinjiro Kodama at the ICR, Kyoto University, succeeded in the development of the effective iron catalysts, and the research works were used in industrial process at the Takikawa Plant of the Hokkaidojinzosekiyu, Inc, located in Takikawa, Hokkaido. Although produced amounts of the synthetic oil were not much until the end of the World War II, the research works and the industrial process established the base of the petrochemical industry until today.

Chemical Heritage is one of the most important historical materials related to chemistry and chemical technology in Japan approved by the Chemical Society of Japan. The presentation ceremony of the award was held in the 93rd Spring Annual Meeting of the Chemical Society of Japan at Ritsumeikan University, Biwako Kusatsu Campus on 23 March 2013.

The certificate presentation ceremony on 23 March 2013; (left to right) Makoto Oda (Superintendent of Takikawa City Board of Education), Kohei Tamao (President of the Chemical Society of Japan), Naoki Sato (Director of ICR) at the award ceremony.

日本化学会認定化学遺産第020号

日本化学会化学遺産

認 定 証

A Chemical Heritage
authorized by
The Chemical Society of Japan

京都大学化学研究所 殿

フィッシャー・トロプシュ法による人造石油製造に関わる資料

貴下ご所有の
「フィッシャー・トロプシュ法による人造石油製造に関わる資料」を
日本の化学および化学技術にとって
歴史的に貴重な資料として
日本化学会化学遺産に認定します

平成25年3月23日

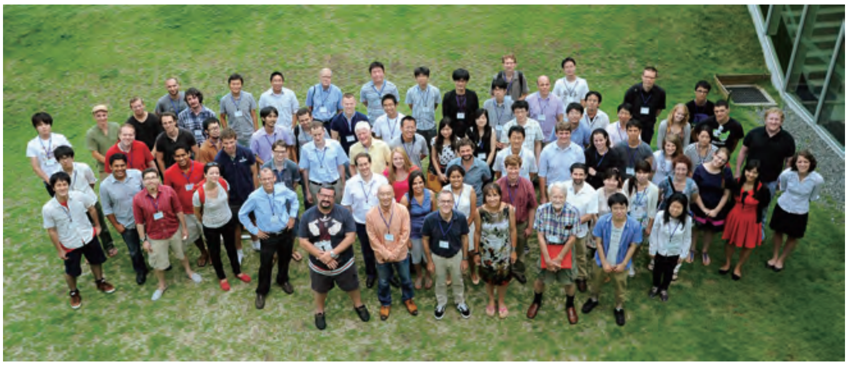
公益社団法人 日本化学会
会長 玉尾皓平

Certificate for Chemical Heritage

13th Annual International Workshop on Bioinformatics and Systems Biology (IBSB 2013)

Prof MAMITSUKA, Hiroshi

International workshop of Bioinformatics and Systems Biology (IBSB) is a student-oriented, three-day workshop, which has been annually held since 2001 by collaboration of mainly three parties; Bioinformatics Center of Kyoto University, Japan, Bioinformatics Program of Boston University, USA and Systems Biology group of Berlin, Germany. This workshop has provided graduate students, postdocs and junior faculties with good opportunities to present and discuss their research objectives, approaches and results in the emerging field of genomics, systems biology and bioinformatics. This year, IBSB 2013 was held in Kyoto, being supported by JSPS International Training Program (ITP) “International Research Training Program on Bioinformatics and Systems Biology”. The contents of IBSB 2013 were seven invited talks and more than 60 presentations, including long and short talks and poster presentations. The total number of participants reached around 90, including faculties, postdocs and graduate students of the involved institutes. These numbers are comparable with or larger than those of the past IBSB conferences, indicating significant success of IBSB 2013.



Kyoto University Joins edX Consortium

Prof UESUGI, Motonari

Kyoto University has started its attempt at providing Massive Open Online Courses (MOOCs) on a U.S-based nonprofit online learning platform, edX. As the very first KyotoUx-series course, I will be teaching “Chemistry of Life” in April 2014, trying to create a new educational path for millions of learners worldwide.

Chemistry and biology are traditionally taught as separate subjects at the high school level, where students memorize fundamental scientific principles that are universally accepted. However, at the university level and in industry, we learn that science is not as simple as we once thought. We are constantly confronted by questions about the unknown and required to use creative, integrated approaches to solve these problems. By bringing together knowledge from multidisciplinary fields, we are empowered with the ability to generate new ideas. The goal of this course is to develop skills for generating new ideas at the interface between chemistry and biology by analyzing pioneering studies.

Top performing students will have an opportunity to obtain MEXT Scholarships for postgraduate studies at Kyoto University. In addition, Kyoto University plans to offer travel awards to five students with the highest interim scores, who are interested in visiting Kyoto University for a week during summer.

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)	Senior Lecturer (part-time)
Specially Appointed Prof	Specially Appointed Professor
Program-Specific Assoc Prof	Program-Specific Associate Professor
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 (JSPS)	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
  - Supramolecular Biology
  - 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 (JSPS)
MIYAKE, Hideaki
(D Sc)

PD
SUGAMATA, Koh
(D Sc)

Guest Research Associate

VILLALBA FRANCO, José Manuel

* Also serves as Assist Prof of Pioneering Research Unit for Next Generation

Students

MIYAMOTO, Hisashi (D3)
EGAWA, Yasunobu (D2)
WASANO, Tatsuya (D2)
NAGATA, Koichi (D1)
AWANE, Hiroyuki (M2)
IKEDA, Shin (M2)
KANESATO, Shuhei (M2)
SUZUKI, Yuko (M1)

Visiting Researcher

Prof LACÔTE, Emmanuel CPE Lyon, University of Lyon, France, 11 January

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

Agou, T.; Nagata, K.; Tokitoh, N., Synthesis of a Dialumene-Benzene Adduct and Its Reactivity as a Synthetic Equivalent of a Dialumene, *Angew. Chem. Int. Ed.*, **52,** 10818-10821 (2013).

Agou, T.; Wasano, T.; Jin, P.; Nagase, S.; Tokitoh, N., Syntheses and Structures of an "Alumole" and Its Dianion, *Angew. Chem. Int. Ed.*, **52,** 10031-10034 (2013).

Sakagami, M.; Sasamori, T.; Sakai, H.; Furukawa, Y.; Tokitoh, N., 1,2-Bis(ferrocenyl)-Substituted Distibene and Dibismuthene: Sb=Sb and Bi=Bi Units as π Spacers between Two Ferrocenyl Units, *Chem. Asian J.*, **8,** 690-693 (2013).

Sasamori, T.; Tokitoh, N., A New Family of Multiple-Bond Compounds between Heavier Group 14 Elements, *Bull. Chem. Soc., Jpn.*, **86,** 1005-1021 (2013).

Synthetic Equivalent of a Dialumene

Multiply bonded species involving heavier main-group elements have been extensively investigated, whereas the chemistry of analogous species involving group 13 elements is still in its infancy. Examples for isolable neutral heavier group 13 dimetallenes with the formula of R–M=M–R (M: Al, Ga, In, Tl) remain scarce for the homologues of gallium, indium, and thallium, and have been unknown for aluminum so far.

The dialumene-benzene adduct **1** was obtained by the reduction of the 1,2-dibromodialumane in benzene. The C_6H_6 moiety of **1** was readily exchanged with C_6D_6, naphthalene, anthracene, and bis(trimethylsilyl)acetylene at room temperature, thus affording the corresponding trapping products of dialumene **2**. It was demonstrated that **1** shows unique reactivity as a synthetic equivalent of **2** for applications in the development of new organoaluminum species.

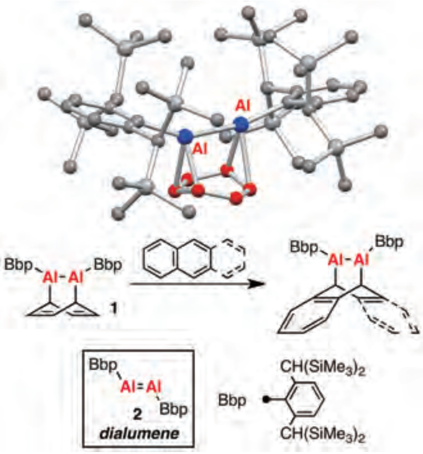


Figure 1. Structure and reactivity of dialumene-benzene adduct **1**.

Alumole and Its Dianion

Heteroles of electron-deficient group 13 elements are expected to have low-lying LUMOs owing to the orbital interactions between the empty π orbital of group 13 elements and the π* orbitals. To date, only a few examples of alumole (aluminacyclopentadienes)–Lewis base complexes have been structurally characterized. The coordination of Lewis bases to the aluminum center may substantially affect the electronic structures, therefore the synthesis of Lewis base-free alumoles has been desired to provide a basis for the elucidation of the intrinsic nature of alumoles.

We have succeeded in the synthesis of a Lewis base free alumole **3** by the introduction of bulky substituent, Mes* group. The AlC_4 ring of **3** exhibits the C–C bond alternation. Reduction of **3** with lithium afforded the lithium salt of the alumole dianion **4**. DFT calculations revealed that the 3p(Al)-π* conjugation effectively lowers the LUMO energy level of the alumole and that coordination of two lithium cations to the alumole dianion is a key factor to keep the planar AlC_4 ring structure.

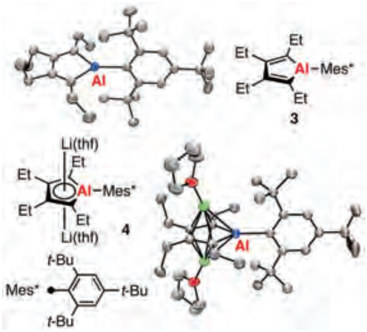


Figure 2. Structures of alumole **3** and its dianion **4**.

1,2-Bis(ferrocenyl)distibene and Dibismuthene

The d–π electron conjugated systems consisting of bimetallic complexes with π-electron spacers, M–(π-conjugated system)–M (M=transition metals), are extensively investigated from the viewpoint of their interesting electronic, optical, and magnetic properties.

We have succeeded in the synthesis of the first stable 1,2-bis(ferrocenyl)distibene **5** and 1,2-bis(ferrocenyl)-dibismuthene **6** by taking advantage of a newly developed bulky ferrocenyl group. The assessment of their structural parameters and physical properties indicated their definite Sb=Sb and Bi=Bi double-bond character. The electrochemical measurements revealed that distibene **5** and dibismuthene **6** exhibit stable, four-step (one reduction, three oxidation) redox processes reflecting the unique character of Sb=Sb and Bi=Bi π bonds, and Sb=Sb and Bi=Bi π-electron units can act as effective π spacers to couple with the two ferrocenyl moieties.

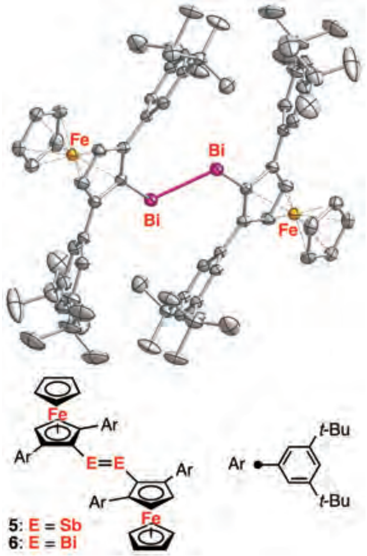


Figure 3. 1,2-Bis(ferrocenyl)distibene **5** and dibismuthene **6**.

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
YOSHIDA, Eri
(D Eng)

Assist Techn Staff

NAKAIKE, Yumi (D Eng)

Students

NISHIMURA, Hidetaka (D1)
CHAOLUMEN (D1)
FUTAGOISHI, Tsukasa (M2)
SHIMOGAWA, Hiroyuki (M2)
ZHANG, Rui (M2)
HASHIKAWA, Yoshifumi (M1)
SATO, Motoi (M1)
ENNO, Hiroki (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
Open-Cage Fullerenes
Endohedral Fullerenes
Functional Dyes
Organic Solar Cell

Selected Publications

Morinaka, Y.; Sato, S.; Wakamiya, A.; Nikawa, H.; Mizorogi, N.; Tanabe, F.; Murata, M.; Komatsu, K.; Furukawa, K.; Kato, T.; Nagase, S.; Akasaka, T.; Murata, Y., X-ray Observation of a Helium Atom and Placing a Nitrogen Atom inside He@C_{60} and He@C_{70}, *Nat. Commun.*, **4,** 1554/1-1554/5 (2013).

Morinaka, Y.; Nobori, M.; Murata, M.; Wakamiya, A.; Sagawa, T.; Yoshikawa, S.; Murata, Y., Synthesis and Photovoltaic Properties of Acceptor Materials Based on the Dimerization of Fullerene C_{60} for Efficient Polymer Solar Cells, *Chem. Commun.*, **49,** 3670-3672 (2013).

Shimogawa, H.; Mori, H.; Wakamiya, A.; Murata, Y., Impacts of Dibenzo- and Dithieno-Fused Strctures at the *b, g* Bonds in the BODIPY Skeleton, *Chem. Lett.*, **42,** 986-988 (2013).

Futagoishi, T.; Murata, M.; Wakamiya, A.; Sasamori, T.; Murata, Y., Expansion of Orifices of Open C_{60} Derivatives and Formation of an Open C_{59}S Derivative by Reaction with Sulfur, *Org. Lett.*, **15,** 2750-2753 (2013).

Zhang, R.; Murata, M.; Wakamiya, A.; Murata, Y., Synthesis and X-ray Structure of Endohedral Fullerene C_{60} Dimer Encapsulating a Water Molecule in Each C_{60} Cage, *Chem. Lett.*, **42,** 879-881 (2013).

Expansion of Orifices of Open C_{60} Derivatives and Formation of an Open $C_{59}S$ Derivative by Reaction with Sulfur

Developments of open-cage fullerenes have been attracting considerable attention from the viewpoints of host–guest chemistry as well as novel endohedral fullerenes when closing of the opening is successful with keeping the encapsulated species inside the fullerenes. We synthesized new sulfur –containing open-cage C_{60} derivatives with a huge opening by using a sulfur insertion as a key reaction. Furthermore, open-cage $C_{59}S$ derivative, in which one carbon atom was replaced by a sulfur atom, was also found to form by simply changing the reaction conditions. The structures of these derivatives were determined by the single crystal X-ray analyses, which showed the encapsulation of a water molecule inside the fullerene cages. These fullerene derivatives would be nice host compounds for other small molecules as well as potential precursors for novel endohedral fullerenes in near future.

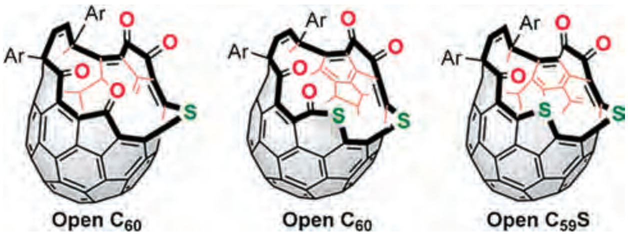


Figure 1. Novel open-cage fullerene C_{60} and $C_{59}S$ derivatives with a large opening.

Synthesis and X-ray Structure of Endohedral Fullerene C_{60} Dimer Encapsulating a Water Molecule in Each C_{60} Cage

It is well known that the chemical reactivities of endohedral metallofullerenes are very different from those of empty fullerenes due to electron transfer from the encapsulated metals to the outer fullerene cages. However, in the case of endofullerenes encapsulating electrically neutral molecule(s), very few studies have been carried out on the chemical reactivity of the outer fullerene cages. We have demonstrated that the cross dimerization of $H_2O@C_{60}$ and empty C_{60} gave three dimers of C_{60}, two of which encapsulate one or two molecules of water. Although similar reactivities toward dimerization were observed for $H_2O@C_{60}$ and empty C_{60}, the encapsulation of water molecules affected the elution order upon HPLC analysis. In addition, a small difference in the volume of the unit cell was observed in the solid state.

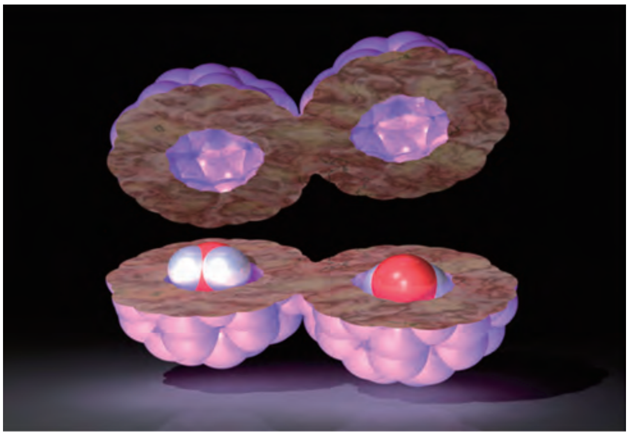


Figure 2. Space filling representation of inner space of C_{60} dimer encapsulating a water molecule in each cage.

Impacts of Dibenzo- and Dithieno-Fused Structures at the *b*, *g* Bonds in the BODIPY Skeleton

BODIPY (4,4-difluoro-4-bora-3*a*,4*a*-diaza-*s*-indacene) skeleton has unique electrochemical and optical properties, such as intense absorption profiles, high photostability, and high electron accepting ability. We recently reported that monobenzo-fusing at the *a* bond of the BODIPY skeleton effectively increases the HOMO level, whereas monobenzo-fusing at the *b* bond decreases the LUMO level. The latter is important for the molecular design toward NIR dyes or electron-transporting materials with air stability. As the fully π-expanded systems, we synthesized dibenzo[*b*,*g*]-fused and dithieno[*b*,*g*]-fused BODIPY derivatives **1** and **2**, respectively. Electrochemical and photophysical measurements demonstrated that these structural modifications effectively enhance the electron accepting ability of the BODIPY skeleton leading to the red-shifted absorption. We revealed that the impacts of the dibenzo[*b*,*g*]-fusing are more significant compared to that of the monobenzo[*b*]-fusing.

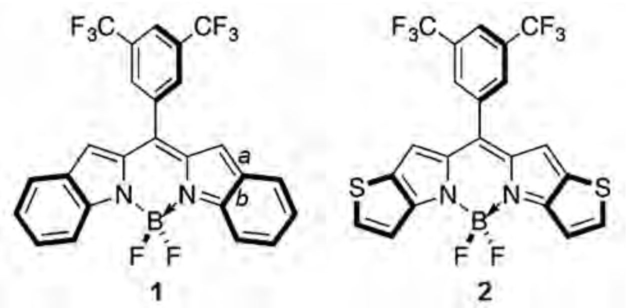


Figure 3. Ring-fused BODIPY derivatives.

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)


Techn Staff
FUJIHASHI, Akiko


Guest Res Assoc
GHOSH, Harisadhan
(Ph D)

Students

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

Visiting Researcher

Prof WILLIARD, Paul Brown University, U.S.A., 27 September

Scope of Research

KEYWORDS
Organocatalysis
Regioselective Functionalization
Dynamic Chirality
Unusual Amino Acid
Molecular Recognition

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.

Selected Publications

Kawabata, T.; Matsuda, S.; Kawakami, S.; Monguchi, D.; Moriyama, K., Stereochemical Diversity in Asymmetric Cyclization via Memory of Chirality, *J. Am. Chem. Soc.*, **128,** 15394-15395 (2006).

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).

A Properly Positioned Carboxylate in a DMAP Skeleton Accelerates Acylation Reactions

The DMAP catalyzed acylation of alcohols with acid anhydrides has been widely used for the synthesis of esters. It has been proposed that the carboxylate ion of the reactive acylpyridinium salt acts as a general base, and deprotonates the alcohols at the transition state. Therefore, the carboxylate ion plays a crucial role not only in the reactivity, but also in the regio- and stereoselectivity of the acylation reaction. We investigated the proper location of the carboxylate ion that accelerates the DMAP-catalyzed acylation of alcohols. Catalytic profiles of **1a**, **2**, **3** and **4** with an internal carboxylate and the corresponding ester **1b** and **1c** were investigated, and the relative catalytic activities were shown in Figure 1a. The transition state structure of the *N*-acetylpyridinium salts derived from the most relative catalyst **1a** with MeOH calculated by the B3LYP/6-31G* level showed that the carboxylate ion proximal to the pyridine ring in face to face geometry works as an effective general base to promote the acylation reaction (Figure 1b).

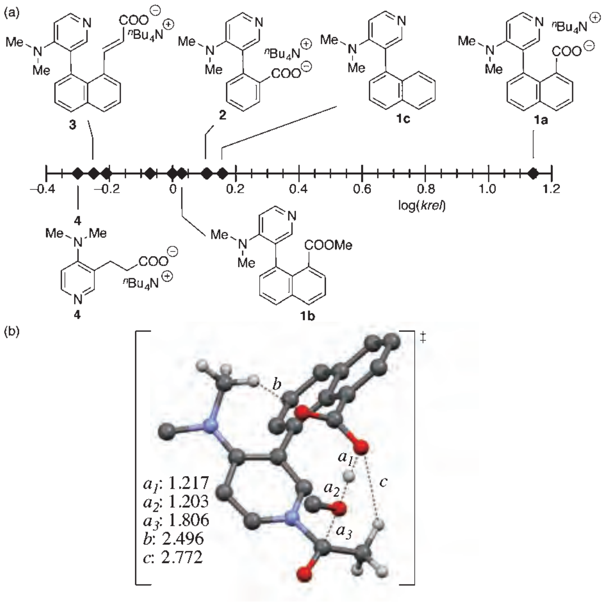


Figure 1. (a) Relative catalytic activities for acetylation of cyclohexanol. (b) Transition state structure for acetylation of *N*-acetylpyridinium ion of **1a** with MeOH.

Chemoselective Oxidation by an Electronically Tuned Nitroxyl Radical Catalyst

Nitroxyl radical **5** was disclosed to be an efficient catalyst for the oxidation of secondary alcohols. The oxoammonium generated from **5** was found to be highly reactive due to the adjacent electron-withdrawing ester groups (electronic tuning effect: Figure 2a), irrespective of the steric congestion around the active site as seen in a typical nitroxyl radical catalyst, TEMPO. Catalyst **5** promoted highly chemoselective oxidation of benzylic alcohols in the presence of aliphatic alcohols. The oxidation of the benzylic alcohols was proposed to proceed via rate-determining hydride transfer (Figure 2b).

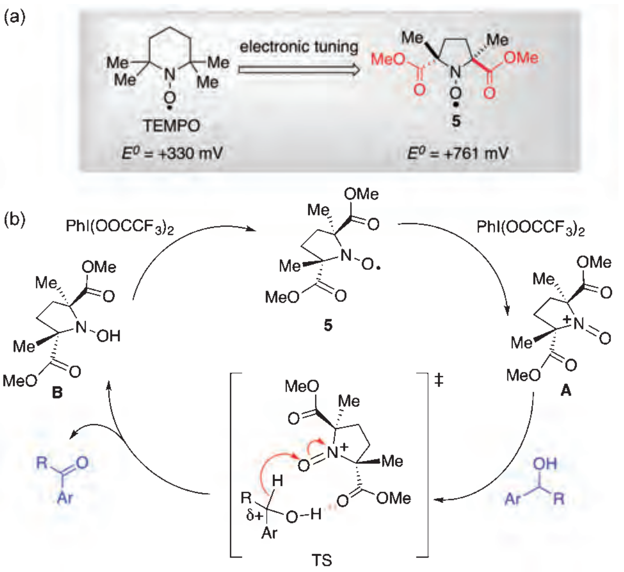
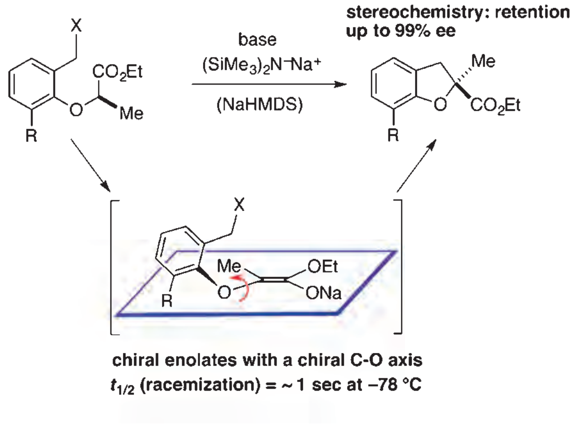


Figure 2. (a) Design of nitroxyl radical oxidation catalyst based on electronic tuning. (b) A possible reaction path via the rate-determining hydride-transfer.

The First Example of Asymmetric Synthesis via Inherently Chiral Enolates with a Chiral C-O Axis

A Novel method for asymmetric cyclization of chiral alkyl aryl ethers has been developed. The reactions were assumed to proceed via short-lived chiral enolate intermediates with a chiral C-O axis to give cyclic ethers with tetrasubstituted carbon in up to 99% ee. The half-lives of racemization of the chiral enolate intermediate was roughly estimated to be ~1 sec at −78 °C. This is the first example of asymmetric reactions that proceed via inherently chiral enolate intermediates based on the restricted rotation around a C-O bond.



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
GE, Wanyin
(D Eng)


PD
TRINH, Thang Thuy
(Ph D)


PD
YOSHIZUMI, Toshihiro
(D Eng)

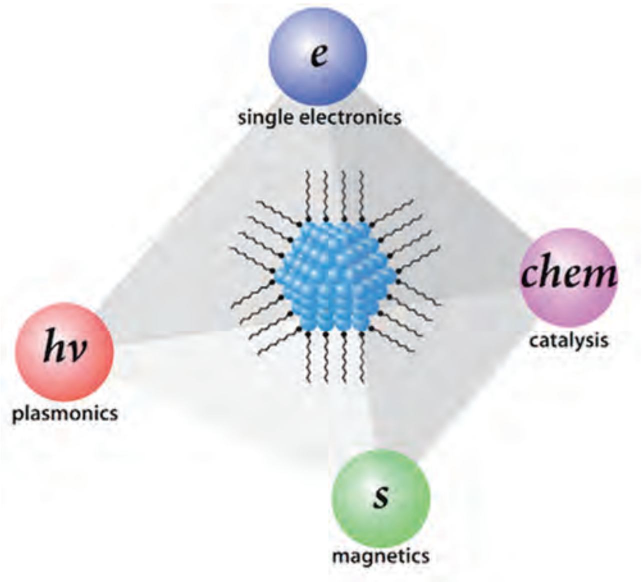
Students

TANAKA, Daisuke (D3)
YOSHINAGA, Taizo (D3)
WU, Hsin-Lun (D3)
CHEN, Lihui (D1)
KIM, Sungwon (D1)
TABUCHI, Michimasa (M1)
YAMAOKA, Satoshi (M1)
KIMURA, Masato (RS)

* Division of Synthetic Chemistry, Laboratory for Energy Quantum Manipulation

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

Teranishi, T.; Sakamoto, M., Charge Separation in Type-II Semiconductor Heterodimers, *J. Phys. Chem. Lett.*, **4,** 2867-2873 (2013).

Teranishi, T.; Inui, D.; Yoshinaga, T.; Saruyama, M.; Kanehara, M.; Sakamoto, M.; Furube, A., Crystal Structure-Selective Formation and Carrier Dynamics of Type-II $CdS\text{-}Cu_{31}S_{16}$ Heterodimers, *J. Mater. Chem. C*, **1,** 3391-3394 (2013).

Ikeda, T.; Xiong, A.; Yoshinaga, T.; Maeda, K.; Domen, K.; Teranishi,T., Polyol Synthesis of Size-controlled Rh Nanoparticles and Their Application to Photocatalytic Overall Water Splitting under Visible Light, *J. Phys. Chem. C*, **117,** 2467-2473 (2013).

Sakamoto, M. ; Tanaka, D. ; Teranishi, T., Rigid Bidentate Ligands Focus the Size of Gold Nanoparticles, *Chem. Sci.*, **4,** 824-828 (2013).

Eguchi, M.; Mitsui, D.; Wu, H.-L.; Sato, R.; Teranishi, T., Simple Reductant Concentration-Dependent Shape-Control of Polyhedral Gold Nanoparticles and Their Plasmonic Properties, *Langmuir*, **28,** 9021-9026 (2012).

Strongest π-Metal Orbital Coupling in a Porphyrin/Gold Cluster System

π-Metal coupling between the π orbital of a π-conjugated molecule and the metal orbital of a metal surface significantly modified the electronic structure of the molecule. The strength of the π-metal coupling was greatly affected by the molecular configuration on the metal surface and the distance between the molecule and the metal surface. A face-on and a close configuration of a π-conjugated molecule on the metal surface generated a strong interfacial interaction. An understanding of π-metal coupling at the interface between a π-conjugated molecule and a gold cluster is crucial for the development of various devices and materials such as single electron transistors and catalysts. SC$_0$P-coordinated gold clusters with the strongest known π-metal coupling were synthesized to investigate the interfacial interaction between the porphyrin and the gold cluster by UV-vis-NIR and transient absorption measurements. Spectroscopic investigations suggest that the strong π-metal coupling between the porphyrin and the gold cluster was in the ground state and an exciplex was formed upon photoexcitation.

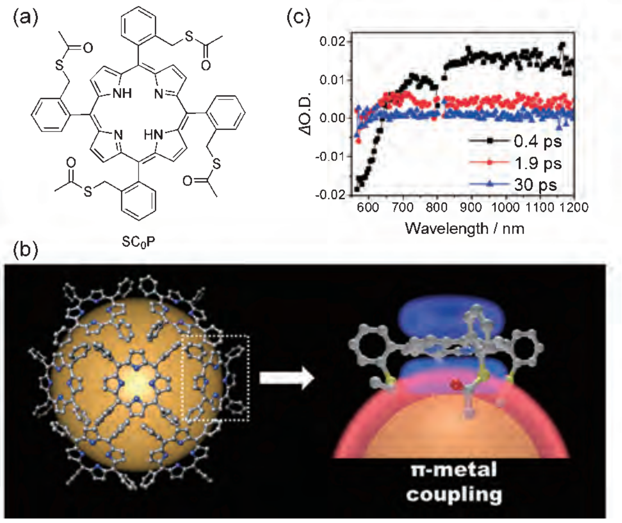


Figure 1. (a) Chemical structure of SC$_0$P. (b) Schematic illustration of SC$_0$P-coordinated gold cluster and π-metal coupling between the π orbital of a porphyrin and the metal orbital of a gold cluster. (c) Transient absorption spectra of SC$_0$P-coordinated gold clusters in DMF.

Structure Independent Photo-Induced Charge Separation in CdS/CdTe Heterostructured Nanopencils

Geometrical structure is a key to determining the properties of the semiconductor nanocrystals (NCs) because band structure and carrier dynamics of NCs are significantly affected by their size and shapes. Selective synthesis of NCs composed of two or more intrinsic chemical species tremendously expands the available geometrical structures and functions of NCs. Among them, the heterostructured NCs (HNCs) are promising nano-functional materials to the photo-electro conversion systems, sensors, and catalysts, etc. owing to the integration of independent functional units and/or efficient carrier transfer between the phases. Here, we synthesized novel anisotropically phase-segregated CdS/CdTe heterostructured nanopencils (HNPs) with preciously controlled anisotropic structure and CdS/CdTe volume, and investigated the relation between geometrical factors and the photo-induced carrier dynamics. The novel CdS/CdTe HNPs with type-II band alignment, in which the CdTe phases serve as light-absorbing layers, are successfully formed through an anion exchange of CdS nanopencils. Furthermore, the transient absorption measurement using fs-laser flash photolysis revealed that the geometry factors do not impact the charge separation rate in the present CdS/CdTe HNPs. This result provides us with an important insight necessary to design novel heterostructured nanocrystals having both efficient charge separation and integrated structure.

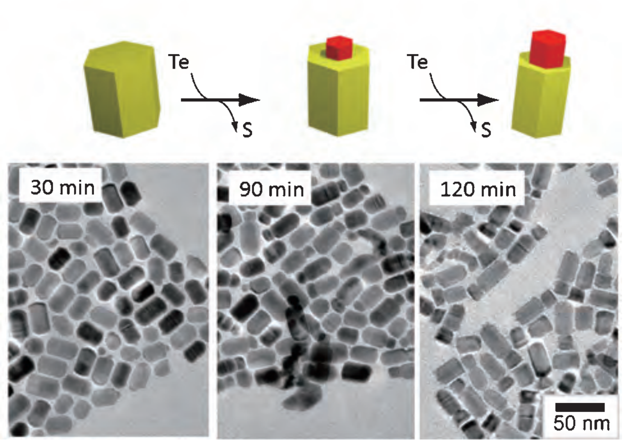


Figure 2. TEM images of the CdS/CdTe HNPs obtained by the anion exchange reaction of CdS nanopencils for 30–120 min.

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, Sungchul
(Ph D)

Researchers

HUANG, Yun
KAGATA, Hideki
(D Environmental Earth Science)
KAWANO, Yuko
KONISHI, Kyoko
MORIKI, Yoshito
NAKAMICHI, Kimiyo
SAKAUE, Motokazu
SEO, Haruna

Students

HSU, Shu-Yao (D3)
NAKANISHI, Yohei (D2)
YAHATA, Yoshikazu (D1)
AKIMOTO, Shuhei (M2)
KIDA, Katsuya (M2)
KIMURA, Keiji (M2)
KINOSE, Yuji (M1)
SHIKURI, Ryuji (M1)
TAKAHASHI, Kenichi (M1)
KIYOISHI, Ayaka (UG)
NOGAMI, Naotsugu (UG)
WADA, Ryota (UG)

Visiting Researchers

Mr. SABOURI, Hadi	University of Sydney, Australia, 24 April–7 June
Ms. ISAHAK, Natasha	University of Sydney, Australia, 24 April–7 June

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
Living Radical Polymerization
Polymer Brush
Hybrid Materials
Biointerface

Selected Publications

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

All-Solid Dye-Sensitized Solar Cell Using Self-Assembled Nanoparticles with High-Density, Concentrated Polymer Brushes

Previously, we succeeded in fabricating a solid membrane of high ionic conductivity using self-assembled nanoparticles with concentrated polymer brushes (CPBs) in an ionic liquid and in developing a novel bipolar-type of lithium-ion rechargeable batteries, where CPB represents the concentrated polymer brush (successfully and systematically synthesized by living radical polymerization techniques). This success was caused by the CPB effects (including super lubrication) originating from the highly stretched-chain conformation and high segmental density in solvent. In this work, we aimed at verifying this concept and expanding it to an iodine/iodide-redox system using poly(DEMM-TFSI) and poly(PEGMA) as a brush component on a nanoparticle. Scanning electron microscopic (SEM) observation and impedance measurement revealed that in a redox-ionic liquid, a CPB-modified nanoparticle (PSiP) was self-assembled into a solid of a high conductivity for poly (PEGMA) brush but not for poly(DEMM-TFSI) one. These results were understood by the difference in affinity between the brush component and the redox-ionic liquid. Finally, we confirmed the photovoltaic performance of the dye-sensitized solar cell (DSSC) using this new type of PSiP membrane as a novel solid-like electrolyte, in which a continuous channel was constructed in nm scale, being responsible for high ionic conductivity. This work opens up a novel route to non-flammable all-solid type of DSSC.

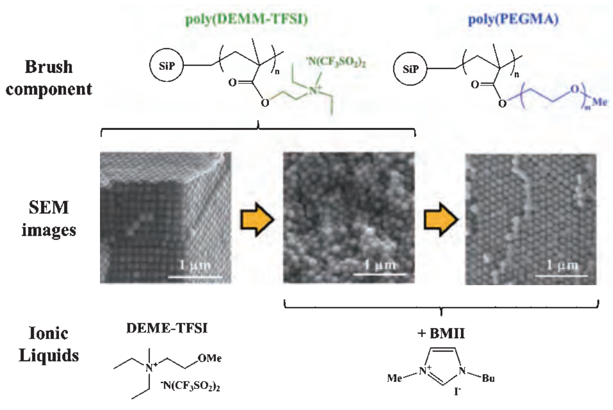


Figure 1. Cross-sectional SEM images of PSiP membranes obtained for different brush/ionic liquid components.

Fabrication of Contrast Agents for Magnetic Resonance Imaging from Polymer-Brush-Afforded Iron Oxide Magnetic Nanoparticles Prepared by Surface-Initiated Living Radical Polymerization

Iron oxide magnetite (Fe_3O_4) nanoparticles were surface-modified using initiating groups for atom transfer radical polymerization (ATRP) via a ligand-exchange reaction in the presence of a triethoxysilane derivative having an ATRP initiation site. The ATRP-initiator-functionalized Fe_3O_4 nanoparticles were used for performing the surface initiated-ATRP of methyl methacrylate. The polymerization proceeded in a living fashion so as to produce graft polymers with targeted molecular weights and narrow molecular weight distribution. The average grafting density was estimated to be as high as 0.7 chains/nm^2, which indicates the formation of so-called concentrated polymer brushes on the Fe_3O_4 nanoparticles. A similar polymerization process was conducted using a hydrophilic monomer, poly (ethylene glycol) methyl ether methacrylate (PEGMA), to prepare Fe_3O_4 nanoparticles grafted with poly(PEGMA) brushes. The blood clearance and bio-distribution of the hybrid particles were investigated by intravenously injecting particles labeled with a radio isotope, ^{125}I, into mice. It was found that some hybrid particles exhibited an excellently prolonged circulation lifetime in the blood with a half-life of about 24 h. When such hybrid particles were injected intravenously into a tumor-bearing mouse, they preferentially accumulated in the tumor tissues owing to the so-called enhanced permeability and retention effect. The tumor-targeted delivery was visualized by a T_2-enhaced magnetic resonance imaging (MRI) measurement.

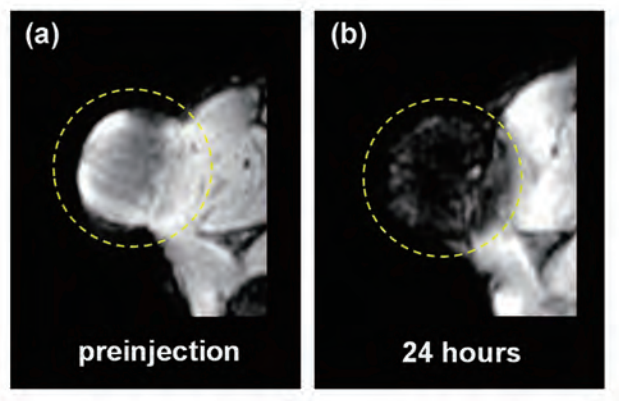


Figure 2. In vivo T_2-weighted magnetic resonance images of a tumor site taken at (a) pre-injection and (b) 24 h post-injection of suspension of PPEGMA-Fe_3O_4 nanoparticles.

Division of Materials Chemistry
– Polymer Controlled Synthesis –

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


Prof
YAMAGO, Shigeru
(D Sc)


Assoc Prof
TOSAKA, Masatoshi
(D Eng)


Assist Prof
NAKAMURA, Yasuyuki
(D Sc)


Program-Specific Assist Prof
KAYAHARA, Eiichi
(D Eng)


PD
PATEL, Kumar Vijay
(D Sc)

Students

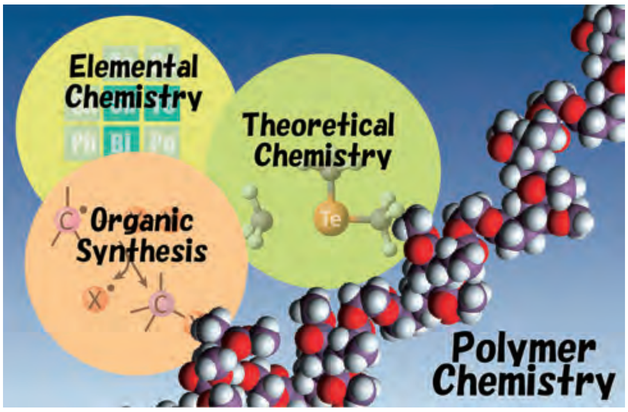
IWAMOTO, Takahiro (D3)
FUJITA, Takehiro (D2)
SAKAKIBARA, Masaya (M2)
TAKU, Setsu (M2)
FUJII, Akira (M2)
NOGUCHI, Naoki (M1)
MAEDA,Yuuki (M1)
YAMAZOE, Ryota (M1)
KOBAYASHI, Go (RS)
NAKAUCHI, Aki (RS)
FAN, Weijia (RS)
QU, Rui (RS)
OHNISHI, Hiroaki (UG)
OGIHARA, Tasuku (UG)
FUKAYAMA, Kei (UG)

Visiting Researchers

Prof VOLLHARDT, K. Peter C.	University of California, U.S.A., 20 May
Prof AMEDURI, Bruno	Centre National de la Recherché Scientifique, France, 30 October

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
Conjugated π-Molecules

Selected Publications

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, *Nat. Commun*., **4,** 2694 (2013).

Iwamoto, T.; Watanabe, Y.; Takaya, H.; Haino, T.; Yasuda, N.; Yamago, S., Size- and Orientation-Selective Encapsulation of C_{70} by Cycloparaphenylenes, *Chem. Eur. J.*, **19,** 14061-14068 (2013) (VIP article).

Yamago, S.; Yahata, Y.; Nakanishi, K.; Konishi, S.; Kayahara, E.; Nomura, A.; Goto, A.; Tsujii, Y., Synthesis of Concentrated Polymer Brushes via Surface-Initiated Organotellurium-Mediated Living Radical Polymerization (SI-TERP), *Macromolecules*, **46,** 6777-6785 (2013).

Nakamura, Y.; Arima, T.; Tomita, S.; Yamago, S., Photoinduced Swiching from Living Radical Polymerization to a Radical Coupling Reaction Mediated by Organotellurium Compounds, *J. Am. Chem. Soc.*, **134,** 5536-5539 (2012).

Tosaka, M.; Senoo, K.; Sato, K.; Noda, M.; Ohta, N., Detection of Fast and Slow Crystallization Processes in Instantaneously-Strained Samples of cis-1,4-Polyisoprene, *Polymer*, **53,** 864-872 (2012).

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

Curved π-conjugated molecules such as fullerenes and carbon nanotubes, which are characterized by the closed and three-dimensional (3D) structures, 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. We synthesized 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. Since 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.

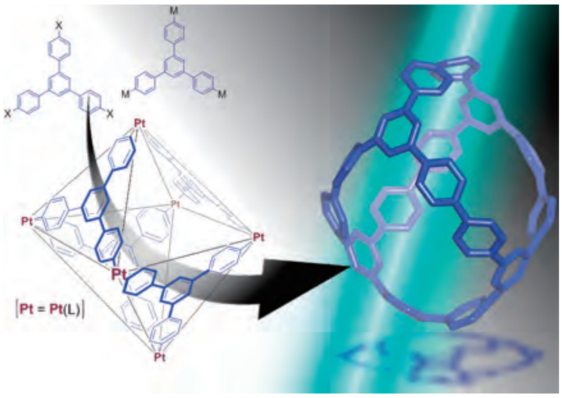


Figure 1. Synthesis of the 3D spherical π-conjugated molecule.

Synthesis of Concentrated Polymer Brushes via Surface-Initiated Organotellurium-Mediated Living Radical Polymerization

An organotellurium chain transfer agent (CTA) bearing a 2-methyltellanyl-2-methylpropionate group at one end and a triethoxysilyl group at the other was prepared and immobilized on the surface of a silicon wafer and silica nanoparticle (SiP). Surface-initiated organotellurium-mediated living radical polymerization from the immobilized CTA in the presence of nonimmobilized (free) organotellurium CTA was examined. Concentrated polymer brushes (CPBs) having surface occupancies above 0.1 were prepared by polymerization of various monomers, including styrene, methyl methacrylate, butyl acrylate, N-isopropyl acrylamide, N-vinyl pyrrolidone (NVP), and N-vinyl carbazole (NVC). All CPBs were formed in a controlled manner, with number-average molecular weights close to the theoretical values and low polydispersity indices (<1.41). Structurally well-controlled CPBs comprising unconjugated monomers, NVP and NVC, were prepared for the first time. Atomic force microscopy and transmission electron microscopy analyses of the CPBs revealed the highly stretched and anisotropic structure of the grafted polymer chain in a good solvent.

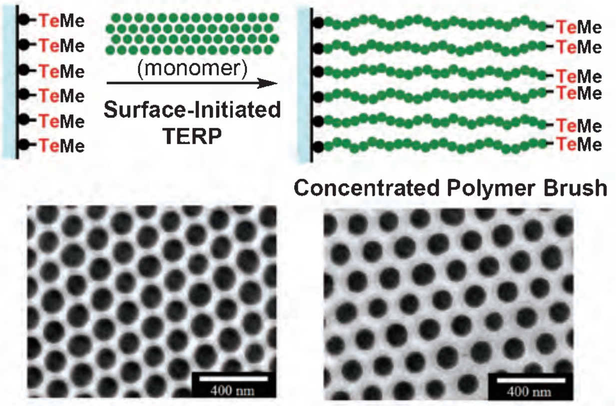


Figure 2. Surface-initiated TERP to obtain concentrated polymer brushes and TEM images of monolayers of the polystyrene-grafted silica particles.

Division of Materials Chemistry
– Inorganic Photonics Materials –

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

Prof
YOKO, Toshinobu
(D Eng)

Assoc Prof
TOKUDA, Yomei
(D Eng)

Assist Prof
MASAI, Hirokazu
(D Eng)

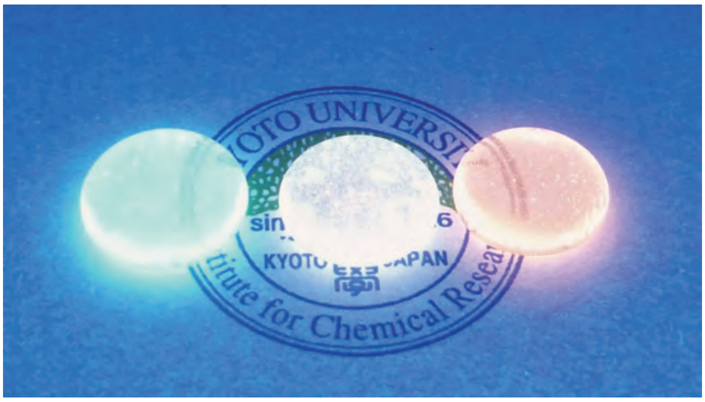
Students

HINO, Yusuke (M2)
UTSUMI, Nihiro (M2)
MINAMI, Tomohiro (M2)
MIYATA, Hiroki (M2)
OKUMURA, Shun (M1)
MATSUKI, Hiroaki (M1)
TOKUNAGA, Yuta (M1)
TAKAHASHI, Yuya (UG)
UEDA, Yuki (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
Amorphous Oxide Phosphor
Glass Structure
Organic-Inorganic Hybrids
Optical Biosensor
Environmental Remediation



Selected Publications

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.; Tanimoto, T.; Fujiwara, T.; Matsumoto, S.; Tokuda, Y.; Yoko, T., Correlation between Emission Property and Concentration of Sn^{2+} Center in the SnO-ZnO-P_2O_5 Glass, *Optics Express*, **20,** 27319-27326 (2012).

Ueda, Y.; Tokuda, Y.; Fujimura, S.; Nihei, N.; Oka, T., Removal of Radioactive Cs from Gravel Conglomerate Using Water Containing Air Bubbles, *Water Sci. Tech.*, **67,** 996-999 (2013).

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).

Topics

Fabrication of Rare Earth-free Amorphous Oxide Phosphor

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.

On the other hand, light emitting devices and various kinds of phosphors containing rare earth (RE) are being actively developed nowadays. However, the host materials for these phosphors still remain limited with respect to a high-power or short-wavelength excitation light source. If glass material without the RE cation shows light emission comparable to the crystalline phosphor, it will be considered a novel emitting material capable of much broader emission and good formability.

Recently, we have reported the highest quantum efficiency (QE) for amorphous SnO-ZnO-P_2O_5 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 RE cation ever reported. Our group has also demonstrated white light emission of RE-free Mn-doped SnO-ZnO-P_2O_5 glass. The transparent glass showed blue ~ white ~ red emission, which depended on the amount of MnO (Figure.1). 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.

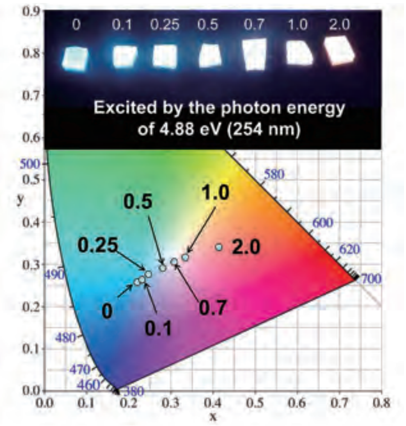


Figure 1. Chromaticity coordinates of the xMnO-2.5SnO-57.5ZnO-40P_2O_5 glasses. Inset shows a photograph of these glasses under exposure to the photon energy of 4.88 eV (254 nm).

Environmental Remediation

The Fukushima Daiichi Nuclear Power Station suffered a meltdown as a result of the Tohoku earthquake of March 11, 2011, in Japan. The accident released several kinds of radioactive elements over eastern Japan. It is well known that I-131, Cs-134, and Cs-137 are the main radioactive elements that pose a risk of human exposure (IAEA report 2006). Among these, Cs-134 and Cs-137 are the most important in terms of their effects on the environment because the half-life of I-131 is relatively short and other kinds of radioactive elements such as Pu-239 cannot spread far from the nuclear reactor (Eisenbud 1973). Therefore, removal of Cs-134 and Cs-137 from the environment is very important for protecting human health. Here, we report the effectiveness of water containing air bubbles with a diameter around 100 nm (nanobubbled water, NB water) for the removal of radioactive Cs. Laboratory experiments confirmed that NB water is more effective than purified water and as effective as water with neutral detergent in the removal of Cs-137 from gravel. Moreover, NB water retains its effectiveness even after storage for 7 days. Additionally, NB water produced from tap water was found to be effective for removal of radioactive Cs from gravel conglomerate in Fukushima, Japan.

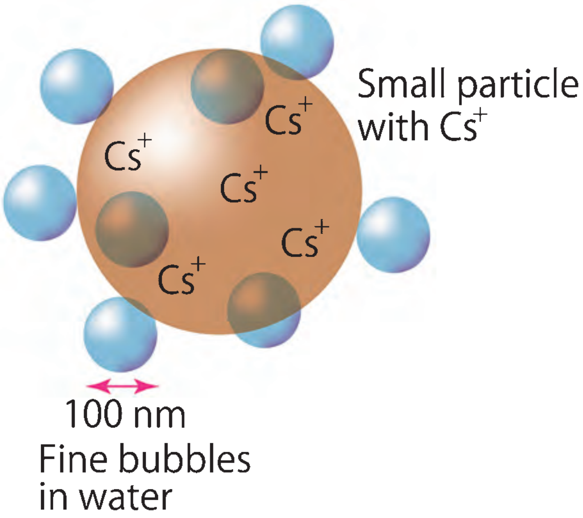


Figure 2. Schematic model of fine bubbles in water attached to clays. The fine bubbles were introduced into water by using centrifugal rotation method. The average diameter of the bubbles was determined as around 100 nm using a particle tracking analysis (NANOSIGHT LM-10, Quantum Design inc.). The mechanism for the removal of radioactive Cs is still unclear; several possibilities include surface adsorption, surface charge, and bubble nucleation. However, we consider that Cs was removed with clays.

Division of Materials Chemistry
– Nanospintronics –

http://www.scl.kyoto-u.ac.jp/~ono/onolab/public_html/english/index_e.html

Prof
ONO, Teruo
(D Sc)

Assist Prof
MORIYAMA,Takahiro
(Ph D)

Assist Prof
KIM, Kab-Jin
(Ph D)

Techn Staff
KUSUDA, Toshiyuki

PD
SHIMAMURA, Kazutoshi
(D Sc)

Students

UEDA, Kohei (D3)
MATSUO, Sadashige (D3)
NISHIHARA, Yoshitaka (D2)
HIRAMATSU, Ryo (D2)
NAGATA, Masaki (D2)
HATA, Hiroshi (D2)
KAWAGUCHI, Masashi (D1)
YOSHIMURA, Yoko (D1)
KAKIZAKAI, Haruka (M2)
YAMADA, Kihiro (M2)
TANAKA, Kensho (M1)
TANIGUCHI, Takuya (M1)
KAMIYA, Michinari (M1)

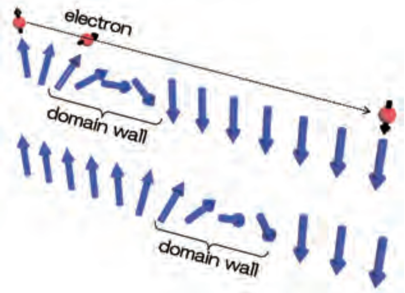
Visiting Researcher

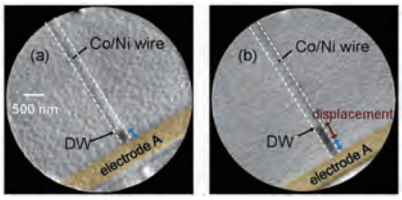
Mr. STEIN, Falk-Ulrich	University of Hamburg, Germany, 23 August – 22 November

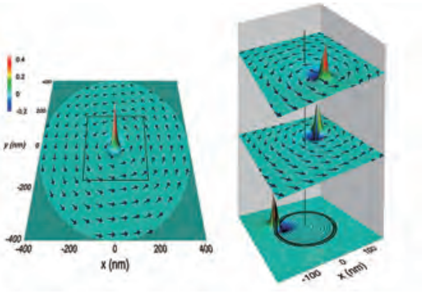
Scope of Research

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

Delmo, M. P.; Yamamoto, S.; Kasai, S.; Ono, T.; Kobayashi, K., Large Positive Magnetoresistive Effect in Silicon Induced by the Space-Charge Effect, *Nature*, **457,** 1112-1115 (2009).

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).

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.

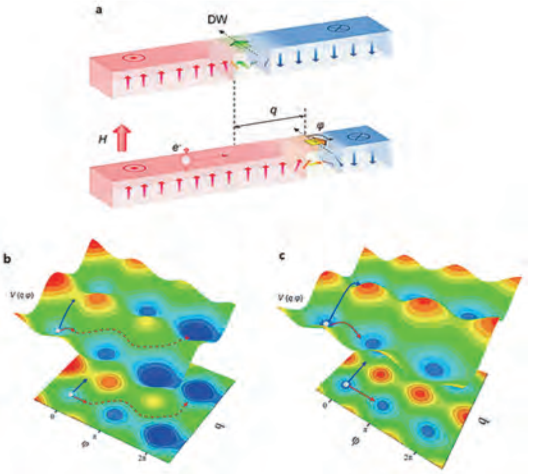


Figure 1. Schematic illustration of DW motion and energy landscape. (a) A magnetic DW in a nanowire and its collective coordinates, the position q and the tilting angle φ. (b,c) Energy landscape for the DW motion in the presence (b) and absence (c) of d.c. current.

Spin-motive Force Due to a Gyrating Magnetic Vortex

A change of magnetic flux through a circuit induces an electromotive force. By analogy, a recently predicted force that results from the motion of non-uniform spin structures has been termed the spin-motive force. Although recent experiments seem to confirm its presence, a direct signature of the spin-motive force has remained elusive. We report the observation of a real-time spin-motive force produced by the gyration of a magnetic vortex core (Figure 2). We find a good agreement between the experimental results, theory and micromagnetic simulations, which taken as a whole provide strong evidence in favour of a spin-motive force.

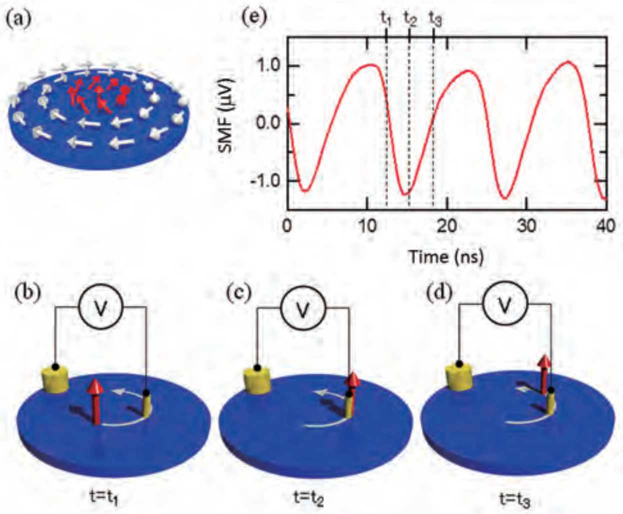


Figure 2. (a) A vortex state in a micron-size magnetic disk. (b)-(d) Illustrations of the time domain measurements in a gyrating vortex core at a time t. The vortex core is indicated by the red arrow. (e) Experimentally observed spin motive force (SMF) as a function of time.

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 (D1)
OKU, Akihiko (D1)
MURAYAMA, Tomo (M2)
TSUJI, Shogo (M2)
KOMATSU, Shohei (M1)
NAKAHASHI, Takahiro (M1)
AKISHIBA, Misao (UG)
SASAKI, Yuichiro (UG)
SHINODA, Kouki (UG)

Visiting Researchers

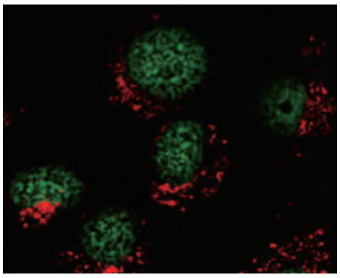
Dr. MADANI, Fatemeh	Stockholm University, Sweden, 1 December 2012–31 March 2013
Prof YU, Jaehoon	Seoul National University, Korea, R., 28 October–25 November

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

Pujals, S.; Miyamae, H.; Afonin, S.; Murayama, T.; Hirose, H.; Nakase, I.; Taniuchi, K.; Umeda, M.; Sakamoto, K.; Ulrich, A. S.; Futaki, S., Curvature Engineering: Positive Membrane Curvature Induced by Epsin N-Terminal Peptide Boosts Internalization of Octaarginine, *ACS Chem. Biol.*, **8,** 1894-1899 (2013).

Kawaguchi, Y.; Tanaka, G.; Nakase, I.; Imanishi, M.; Chiba, J.; Hatanaka, Y.; Futaki, S., Identification of Cellular Proteins Interacting with Octaarginine (R8) Cell-Penetrating Peptide by Photo-Crosslinking, *Bioorg. Med. Chem. Lett.*, **23,** 3738-3740 (2013).

Tsuji, S.; Futaki, S.; Imanishi, M., Creating a TALE Protein with Unbiased 5’-T Binding, *Biochem. Biophys. Res. Commun.*, **441,** 262-265 (2013).

Katayama, S.; Nakase, I.; Yano, Y.; Murayama, T.; Nakata, Y.; Matsuzaki, K.; Futaki, S., Effects of Pyrenebutyrate on the Translocation of Arginine-Rich Cell-Penetrating Peptides through Artificial Membranes: Recruiting Peptides to the Membranes, Dissipating Liquid-Ordered Phases, and Inducing Curvature, *Biochim. Biophys. Acta*, **1828,** 2134-2142 (2013).

Noshiro, D.; Sonomura, K.; Yu, H. H.; Imanishi, M.; Asami, K.; Futaki, S., Construction of a Ca^{2+}-Gated Artificial Channel by Fusing Alamethicin with a Calmodulin-Derived Extramembrane Segment, *Bioconjug. Chem.*, **24,** 188-195 (2013).

Curvature Engineering: Positive Membrane Curvature Induced by Epsin N-Terminal Peptide Boosts Internalization of Octaarginine

Epsin-1 is a representative protein for inducing the positive curvature necessary for the formation of clathrin-coated pits. We demonstrated that the N-terminus 18-residue peptide of epsin-1 (EpN18) has this ability *per se*, as proved by differential scanning calorimetry and solid-state NMR. Moreover, it was shown how this positive curvature promotion can be exploited for promoting the direct penetration of a representative cell-penetrating peptide (CPP), octaarginine (R_8), through artificial and plasma membranes (Figure 1). This synergistic effect has been used for the efficient delivery of a proapoptotic domain peptide (PAD), which induced high level of apoptosis only when coadministered with R_8 and EpN18, thus emphasizing the importance of positive curvature induction for achieving the desired ultimate cargo bioavailability.

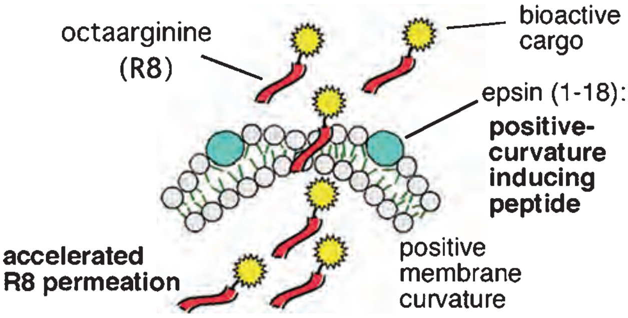


Figure 1. The synergistic effect of positive curvature induction by the epsin-1 N terminal peptide and permeation of R8 peptides.

Effects of Pyrenebutyrate on the Translocation of Arginine-Rich Cell-Penetrating Peptides (CPPs)

Arginine-rich CPPs have the ability to translocate through cell membranes. Hydrophobic counteranions such as pyrenebutyrate (PyB) have been reported to markedly promote the membrane translocation of these peptides. Using model membranes having liquid-ordered (Lo) and liquid-disordered (Ld) phases, we explored the effects of PyB on the promotion of R_8 translocation. Confocal microscopic observations of giant unilamellar vesicles (GUVs) (Figure 2) showed that PyB significantly accelerated the accumulation of R_8 on membranes containing negatively charged lipids, leading to the internalization of R_8 without collapse of the GUV structures. PyB displayed an alternative activity, increasing the fluidity of the negatively charged membranes, which diminished the distinct Lo/Ld phase separation on GUVs. Additionally, PyB induced membrane curvature, which has been suggested as a possible mechanism of membrane translocation for R8. Our results indicate that PyB may have multiple effects that promote R_8 translocation through cell membranes.

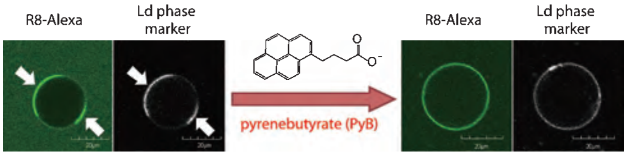


Figure 2. Confocal microscopic observations of giant unilamellar vesicles.

Construction of a Ca^{2+}-Gated Artificial Channel by Fusing Alamethicin with a Calmodulin-Derived Extramembrane Segment

Using native chemical ligation, we constructed a Ca^{2+}-gated fusion channel protein consisting of alamethicin and the C-terminal domain of calmodulin (Figure 3). At pH 5.4 and in the absence of Ca^{2+}, this fusion protein yielded a burst-like channel current with no discrete channel conductance levels. However, Ca^{2+} significantly lengthened the specific channel open state and increased the mean channel current, while Mg^{2+} produced no significant changes in the channel current. On the basis of 8-anilinonaphthalene-1-sulfonic acid (ANS) fluorescent measurement, Ca^{2+}-stimulated gating may be related to an increased surface hydrophobicity of the extramembrane segment of the fusion protein.

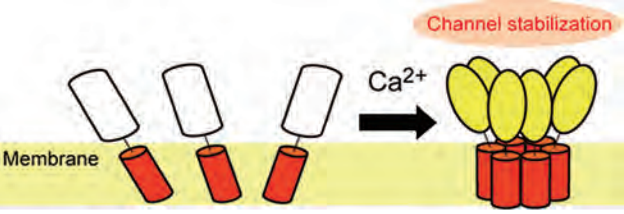


Figure 3. Construction of a Ca^{2+}-gated artificial channel protein.

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)

Assist Prof
KOEDUKA, Takao
(D Agr)

Students

KAWANISHI, Daisuke (M2)
LI, Chunjie (M2)
JING, Dongyu (M2)
OZAKI, Ayane (M1)
YIN, Ziwei (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

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 Mmode of a Classical and Electrophilic Active-site Directed Glutamate Analogue, *Acta Crystallogr. Section D*, **70,** 607-614 (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. (Stuttg.)*, doi: 10.1111/plb.12054 (2013).

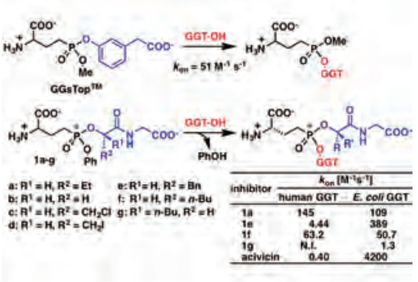
Hiratake, J.; Suzuki, H.; Fukuyama, K.; Wada, K.; Kumagai, H., γ-Glutamyltranspeptidase and Its Precursor, *Handbook of Proteolytic Enzymes, 3rd Ed.*, **820,** 3712-3719 (2013).

Ikeuchi, H.; Ahn, Y. M.; Otokawa, T.; Watanabe, B.; Hegazy, L.; Hiratake, J.; Richards, N. G. J., A Sulfoximine-Based Inhibitor of Human Asparagine Synthetase Kills L-Aspraginase-Resistant Leukemia Cells, *Bioorg. Med. Chem.*, **20,** 5915-5927 (2012).

Joyce-Brady, M.; Hiratake, J., Inhibiting Glutathione Metabolism in Lung Lining Fluid as a Strategy to Augment Antioxidant Defense, *Curr. Enz. Inhibit.*, **7,** 71-78 (2011).

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.

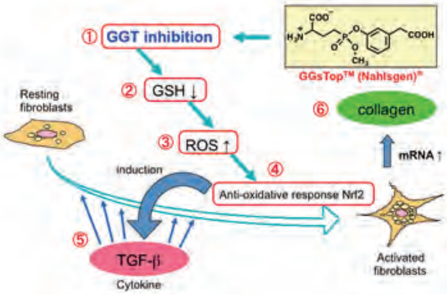


Figure 2. Mechanism for activation of human fibroblasts by GGT inhibitor, GGsTop^{TM}.

Inhibitors Targeting Human Asparagine Synthetase for Cancer Chemotherapy

A standard current clinical protocol for acute lymphoblastic leukemia (ALL) is the use of the enzyme L-asparagine amidohydrolase (ASNase) that catalyzes the hydrolysis of L-Asn to deplete circulating L-Asn in blood. The efficacy of ASNase chemotherapy, however, is hampered by the emergence of ASNase-resistant leukemic blasts; 10–12% of patients who initially go into remission undergo subsequent relapse. One widely-accepted hypothesis for ASNase resistance is the up-regulation of glutamine- and ATP-dependent asparagine synthetase (ASNS) that enables the leukemia cells to synthesize L-Asn necessary for their growth. Hence the inhibition of human ASNS is highly important in cancer chemotherapy, and we have synthesized a specific inhibitor of human ASNS. According to the proposed reaction mechanism of ASNS in which the β-carboxy group of L-Asp is activated by adenylation followed by nucleophilic substitution by ammonia to yield L-Asn, AMP and PPi, an *N*-adenylated sulfoximine **1** was synthesized as a transition-state analogue inhibitor of ASNS (Figure 3).

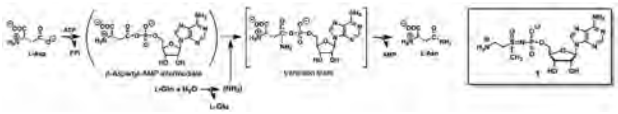


Figure 3. Reaction mechanism of asparagine synthetase and its transition-state analogue 1.

Compound **1** was found to be an extremely potent inhibitor of human ASNS; it inhibited the enzyme in a time-dependent manner with an overall K_i* of 8 nM. Furthermore, the inhibitor **1** suppressed cell proliferation of ASNase-resistant MOLT-4R leukemia cells (Figure 4) with an IC$_{50}$ of ca. 0.1 mM. Surprisingly, compound **1** induced cell death as well as suppression of cell proliferation at higher concentrations. ASNase-sensitive leukemia cells with low ASNS activity were much less sensitive toward compound **1**, suggesting that ASNS in itself was an essential enzyme for leukemia cells and was an important drug target for cancer chemotherapy.

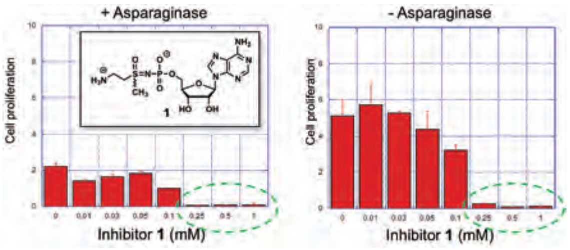


Figure 4. The effect of ASNS inhibitor **1** on the proliferation of ASNase-resistant MOLT-4 leukemia cells in the presence and absence of 1U asparaginase. (Left) MOLT-4 cells with ASNase; (right) MOLT-4R cells without ASNase. Cell proliferation is defined as the number of viable cells after 48 h incubation.

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)


Techn Staff
YASUDA, Keiko


Res
FUJIWARA-KATO, Mariko
(D Agr)

Students

NAKAI, Hideto (D3)
GOTO, Kakeru (M2)
SAITO, Ryo (M1)
SHIMAMURA, Ryota (M1)
ZHANG, Xiao-Juan (RS)

Visiting Researchers

Ms. LI, Jieru	College of Life Science, Peking University, China, P.R., 14 December 2011–13 January 2013
Ms. ZHANG, Jun	College of Life Science, Peking University, China, P.R., 27 September 2012–26 September 2013
Ms. LIN, Qing	College of Life Science, Peking University, China, P.R., 7 December 2012–6 June 2013
Prof QU, Li-Jia	College of Life Science, Peking University, China, P.R., 9–13 January

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

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 *GLABRA2*: 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).

Kusano, H.; Testerink, C.; Vermeer, J. E. M.; Tsuge, T.; Shimada, H.; Oka, A.; Munnik, T.; Aoyama, T., The *Arabidopsis* Phosphatidylinositol Phosphate 5-kinase PIP5K3 Is a Key Regulator of Root Hair Tip Growth, *Plant Cell*, **20,** 367-380 (2008).

Menon, S.; Tsuge, T.; Dohmae, N.; Takio, K.; Wei, N., Association of SAP130/SF3b-3 with Cullin-RING Ubiquitin Ligase Complexes and Its Regulation by the COP9 Signalosome, *BMC Biochem.*, **9,** 1 (2008).

Putative MATE Transporter Involved in Plant Architecture *via* Regulating Auxin Biosynthesis

Plant architecture is largely determined by genetic programs and, to some extent, by environmental cues, such as light, humidity, temperature, nutrition, and plant density. To understand how these factors are integrated into plant development, detailed studies have been focused on genetic factors that are crucial for maintenance of shoot apical meristem (SAM), initiation and outgrowth of axillary meristem (AM), proper growth rate for lateral organ development, and correct timing for reproduction and senescence. As a result, a number of gene-mutations, of which cause altered plant architecture, have been revealed to encode factors involved in biosynthesis and/or signaling of plant hormones, including auxin. Auxin is a critical factor controlling a wide variety of developmental processes, including embryogenesis, maintenance of apical dominance, and formation of lateral organs. Active auxin, mainly indole-3-acetic acid (IAA), is reported to be synthesized *de novo* by tryptophan (Trp)-dependent and/or independent pathways in the shoot apex, young leaves, and root apex. After synthesis, auxin is transported by the polar transport machinery, so that an appropriate distribution of auxin is established to maintain normal plant architecture.

We identified a dominant Arabidopsis mutant with an abnormal architecture, which we named *adp1*-D (*altered development program 1*- Dominant). The architecture of *adp1*-D was greatly altered at maturity, with increased number of axillary branches, flowers, and lateral roots (Figure 1). The growth rate of the mutant was accelerated throughout its life cycle. We found that the mutant phenotypes were caused by over-expression of *ADP1* gene, and that the gene encodes an endosome-localizing protein with sequence similarity to the multidrug and toxic compound extrusion (MATE) transporter family (Figure 2). MATE transporters are reported to be involved in a variety of important biological processes, including the exclusion of toxic organic cation and disease resistance and exhibit multi-substrate specificity in prokaryotes and eukaryotes.

Figure 1. Six-week-old wild-type (WT), and *adp1*-D heterozygous (+/-) and homozygous (-/-) plants grown under long-day conditions. The mutation of *adp1*-D caused a bushy phenotype dominantly. Bar = 1 cm.

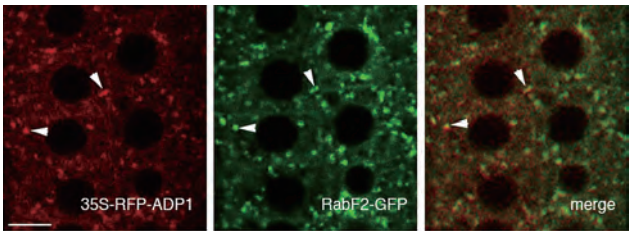


Figure 2. Co-localization of RFP-ADP1 with the endosome marker RabF2a-GFP. Arrowheads indicate Endosomes to which RFP-ADP1 and RabF2a-GFP co-localize. Bar = 15 μm.

Our molecular and genetic evidence demonstrated that the phenotypes of plants over-expressing *ADP1* were caused by reduction of local auxin levels in the meristematic regions. We further discovered that this reduction was probably due to decreased levels of auxin biosynthesis in the local meristematic regions based on the measured reduction in IAA levels and the gene expression data. Overexpression of the gene encoding the auxin-synthesizing enzyme YUCCA1 partly complemented the phenotype of *adp1*-D (Figure 3). Our results indicated that *ADP1*-mediated regulation of the local auxin level in meristematic regions is an essential determinant for plant architecture maintenance by restraining the outgrowth of lateral organs.

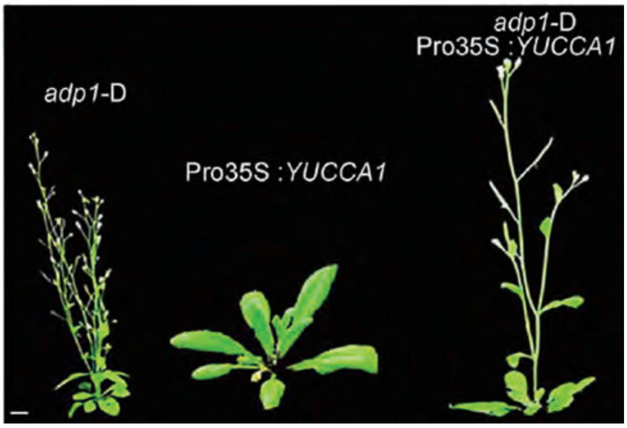


Figure 3. Thirty-five-day-old plants of *adp1*-D, Pro35S:*YUCCA1* and double mutants of *adp1*-D Pro35S:*YUCCA1*. Overexpression of *YUCCA1* partly complemented the phenotype of *adp1*-D. Bar = 1 cm.

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 Chem)


Assist Prof
SHIMOGAWA, Hiroki
(D Sc)


Proj Res*
SATO, Shinichi
(D Eng)


Proj Res**
HIRATA, Nao
(D Eng)


Proj Res**
WATANABE, Mizuki
(D Pharm Sc)


Proj Res**
JIN, Guihua
(D Med Sc)


Proj Res***
KUO, Ting-Fang
(D Sc)


Proj Res***
KATSUDA, Yousuke
(D Sc)


Proj Res**
TAKENOYA, Mihoko
(D Eng)


Proj Res***
PERRON, Amelie
(Ph D)


Guest Res Assoc
PARVATKAR, Prakash Tukaram
(Ph D)

Researcher

WATANABE, Haruhi

Assist Res Staff

NAKASHIMA, Mitsue****

Students

FRISCO, Heidie Laya (D3)
MAO, Di (D2)
TAKAYA, Junichiro (D2)
WANG, Chenyu (M2)
MBENZA, Mbambi Naasson**** (RS)

* Program-Specific Research Center Assist Prof of iCeMS
** Res (WPI) of iCeMS
*** PD (NEXT Program) of iCeMS
**** iCeMS

Visiting Researcher

Assoc Prof HOW, Siew Eng Universiti Malaysia Sabah, Malaysia, 1 May-31 October

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

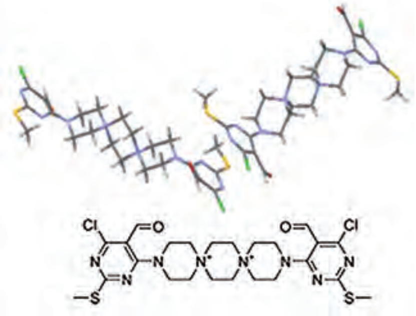
Sakano, D.; Shiraki, N.; Kikawa, K.; Yamazoe, T.; Kataoka, M.; Umeda, K.; Araki, K.; Mao, D.; Matsumoto, S.; Nakagata, N.; Andersson, O.; Stainier, D.; Endo, F.; Kume, K.; Uesugi, M.; Kume, S., VMAT2 Identified as a Regulator of Late-stage Beta Cell Differentiation, *Nat. Chem. Biol.*, **10,** 141-148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

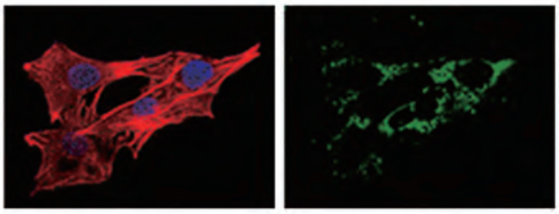
Takemoto, N.; Suehara, T.; Frisco, H.; Sato, S.; Sezaki, T.; Kusamori, K.; Kawazoe, Y.; Park, S.; Yamazoe, S.; Mizuhata, Y.; Inoue, R.; Miller, G.; Hansen, S.; Jayson, G.; Gardiner, J.; Kanaya, T.; Tokitoh, N.; Ueda, K.; Takakura, Y.; Kioka, N.; Nishikawa, M.; Uesugi, M., Small Molecule-induced Clustering of Heparan Sulfate Promotes Cell Adhesion, *J. Am. Chem. Soc.*, **135 (30),** 11032-11039 (2013).

Minami, I.; Yamada, K.; Otsuji, T. G.; Yamamoto, T.; Shen, Y.; Otsuka, S.; Kadota, S.; Morone, N.; Barve, M.; Asai, Y.; Tenkova-Heuser, T.; Heuser, J. E.; Uesugi, M.; Aiba, K.; Nakatsuji, N., A Small Molecule That Promotes Cardiac Differentiation of Human Pluripotent Stem Cells under Defined Cytokine- and Xeno-free Conditions, *Cell Reports*, **2(5),** 1448-1460 (2012).

Small Molecule-induced Clustering of Heparan Sulfate Promotes Cell Adhesion

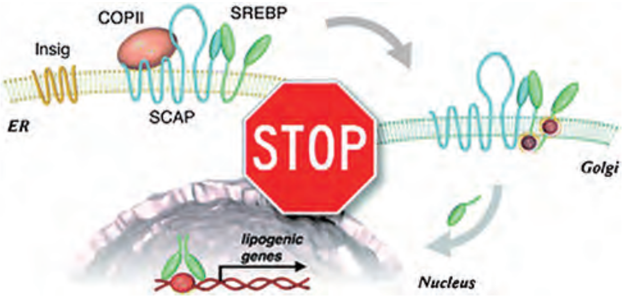
Adhesamine is an organic small molecule that promotes adhesion and growth of cultured human cells by binding selectively to heparan sulfate on the cell surface. The Uesugi research group combined chemical, physicochemical, and cell biological experiments, using adhesamine and its analogues, to examine the mechanism by which this dumbbell-shaped, non-peptidic molecule induces physiologically relevant cell adhesion. The results suggest that multiple adhesamine molecules cooperatively bind to heparan sulfate and induce its assembly, promoting clustering of heparan sulfate-bound syndecan-4 on the cell surface. A pilot study showed that adhesamine improved the viability and attachment of transplanted cells in mice. Further studies of adhesamine and other small molecules could lead to the design of assembly-inducing molecules for use in cell biology and cell therapy.

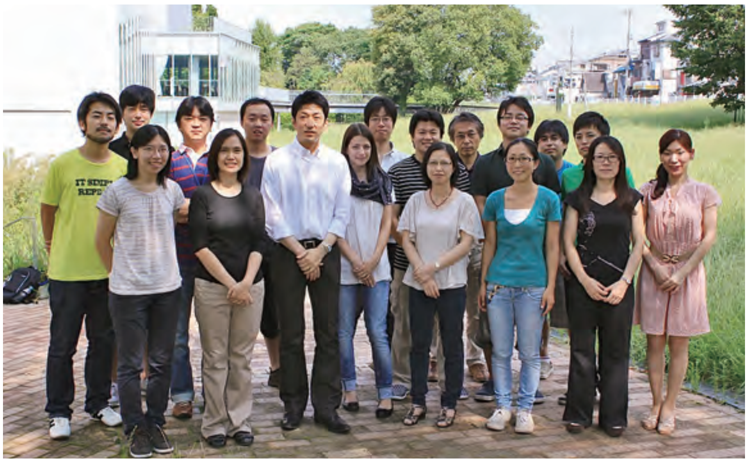




Small-molecule Inhibitors of SREBP Activation–potential for New Treatment of Metabolic Disorders

Sterol regulatory element-binding proteins (SREBPs) are transcriptional factors that control lipid and cholesterol metabolism. Activation of SREBPs in response to a decrease in cellular sterols results in acceleration of the synthesis of fatty acids, triglycerides, and cholesterol. Aberrant SREBP activity has been linked to metabolic disease states, such as obesity, fatty liver, insulin resistance, hyperlipidemia, and atherosclerosis. Thus, inhibition of SREBP activation is a potential therapeutic approach to treating metabolic disorders. Our laboratory recently discovered a number of inhibitors of SREBP activation, including fatostatin and FGH10019. Our analysis indicates that these two synthetic molecules exert their biological activities by directly interacting with SCAP (SREBP cleavage-activating protein).





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
OHTSUKI, Akimichi
(D Sc)


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


PD
LEI, Lin
(D Eng)

Lect (pt)

NISHIYAMA, Yusuke (D Sc)   JEOL Resonance

Students

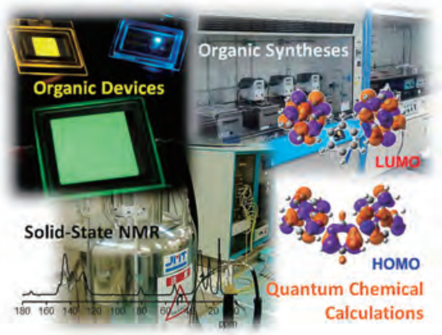
SUZUKI, Furitsu（D3）
SUZUKI, Hajime（M2）
DETANI, Masahiro（M2）
ITO, Kyohei（M1）
KURODA, Risako（M1）
TANAKA, Fumiya（M1）
ISHIBASHI, Hirotaka（UG）
HIROKAWA, Akira（UG）

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.; Fukushima, T.; Fukuchi, M.; Kaji H., Refined Structure Determination of Blue-Emitting Tris(8-hydroxyquinoline) Aluminum(III) (Alq_3) by the Combined Use of Cross-Polarization/Magic-Angle Spinning ^{13}C Solid-State NMR and First-Principles Calculation, *Journal of Physical Chemistry C*, **117,** 18809-18817 (2013).

Hayase, G.; Kanamori, K.; Fukuchi, M.; Kaji, H.; Nakanishi, K., Facile Synthesis of Marshmallow-like Macroporous Gels Usable under Harsh Conditions for the Separation of Oil and Water, *Angewandte Chemie International Edition*, **52,** 1986-1989 (2013).

Nishiyama, Y.; Fukushima, T.; Fukuchi, M.; Fujimura, S.; Kaji, H., Sensitivity Boosting in Solid-state NMR of Thin Organic Semiconductors by a Paramagnetic Dopant of Copper Phthalocyanine, *Chemical Physics Letters*, **556,** 195-199 (2013).

Hirata, S.; Totani, K.; Kaji, H.; Vacha, M.; Watanabe, T.; Adachi, C., Reversible Thermal Recording Media Using Time-Dependent Persistent Room Temperature Phosphorescence, *Advanced Optical Materials*, **1,** 438-442 (2013).

Ohtsuki, A.; Goto, A.; Kaji, H., Visible-Light-Induced Reversible Complexation Mediated Living Radical Polymerization of Methacrylates with Organic Catalysts, *Macromolecules*, **46,** 96-102 (2013).

Refined Structure Determination of Blue-Emitting Tris(8-hydroxyquinoline) Aluminum(III) (Alq_3) by the Combined Use of Cross-Polarization/Magic-Angle Spinning ^{13}C Solid-State NMR and First-Principles Calculation

The combined use of cross polarization/magic-angle spinning (CP/MAS) ^{13}C NMR experiments and gauge-including projector-augmented wave (GIPAW) isotropic chemical shift calculations is an easy and useful method for the structural refinement of organic aggregates. In this study, the method is applied to an important material for organic light-emitting diodes, tris(8-hydroxyquinoline) aluminum(III) (Alq_3). CP/MAS ^{13}C NMR spectra include precise structural information of not only the conformation of the molecules, but also the intermolecular packing. First, the structural refinements were performed for the Alq_3 in the γ- and δ-crystalline forms employing the combined method. Second, by comparing GIPAW calculations for crystals under periodic boundary conditions and those for isolated molecules extracted from the crystals, information on intramolecular structures and intermolecular structures was distinguished. It was found from the analysis that the γ-Alq_3 and δ-Alq_3 crystals have similar intramolecular structures both in the *facial* isomeric state, whereas their intermolecular packing is significantly different. Both the γ-Alq_3 and δ-Alq_3 crystals exhibit unusual blue emission, which is different from conventional green emission, and the origin of the difference has been debated. The above investigation shows that the origin of the blue-shifted emission is the isomeric states of Alq_3, not the intermolecular packing.

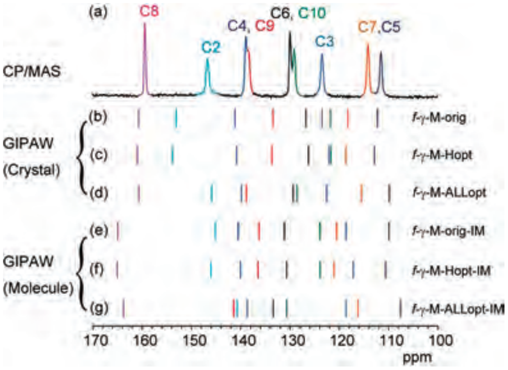


Figure 1. (a) Experimental CP/MAS ^{13}C NMR spectrum of γ-Alq_3. (b)–(g) Isotropic resonance lines of γ-Alq_3 calculated using the GIPAW method. The calculations were carried out for the crystal structures (b) proposed by Muccini et al. without further structural optimization (f-γ-M-orig), (c) after the optimization of the atomic coordinates for protons alone (f-γ-M-Hopt), and (d) after the optimization of the atomic coordinates for all atoms (f-γ-M-ALLopt). Calculations of (e)–(g) were carried out for single molecules extracted from the crystal structures used for the calculations of (b)–(d), respectively.

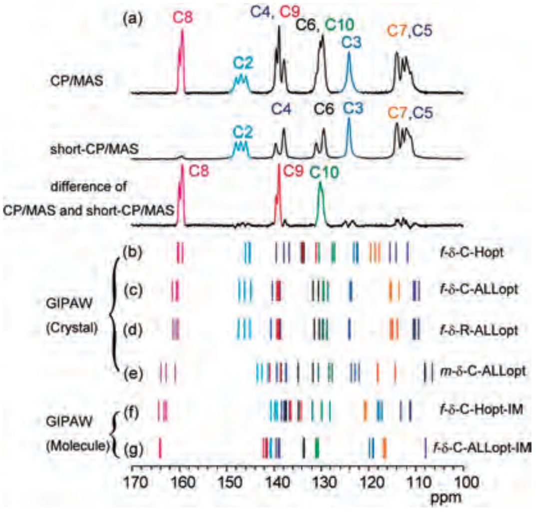


Figure 2. (a) Experimental CP/MAS, short-CP/MAS, and the difference spectra of δ-Alq_3. (b)–(g) Isotropic resonance lines of δ-Alq_3 calculated using the GIPAW method. The calculations were carried out for the crystal structures (b) proposed by Cölle et al. after the optimization of the atomic coordinates only for protons (f-δ-C-Hopt), (c) after the optimization of the atomic coordinates for all atoms (f-δ-C-ALLopt), (d) proposed by Rajeswaran et al. after the optimization of the atomic coordinates for all atoms (f-δ-R-ALLopt), and (e) proposed by Cölle et al. after the optimization of the atomic coordinates for all atoms (m-δ-C-ALLopt). All Alq_3 molecules are in facial form in (b)–(d) and in meridional form in (e). Calculations of (f) and (g) were carried out for single molecules extracted from the crystal structures used for the calculations of (b) and (c), respectively.

Visible-Light-Induced Living Radical Polymerization with Organic Catalysts

A photo-induced living radical polymerization (photo-LRP) using organic catalysts was developed. It is among the most simple and robust photo-LRPs, as it uses iodine as a capping agent and the catalysts are such common compounds as tributylamine. Under visible-light-irradiation at 350-600 nm, the polymer molecular weight and its distribution (M_w/M_n = 1.1–1.4) were well controlled for methyl methacrylate and some functional methacrylates up to fairly high conversions in many cases. Perfectly no polymerization took place without photo-irradiation, meaning that the system is an ideal polymerization switched “on” and “off” by external photo-stimulus. The polymerization rate was also finely tunable by the external irradiation power. The uses of inexpensive compounds and visible light, good polydispersity control, good tolerance to functional groups, and fine response to external photo-irradiation may be useful features of this system.

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 (D2)
KAWAHARA, Shimpei (M2)
KONAGAYA, Wataru (M2)
ZHENG, Linjie (M1)

Scope of Research

(i) Biogeochemistry of trace elements in the hydrosphere: Novel analytical methods are developed for trace metals and its isotopes. Distribution of trace elements in the hydrosphere and its 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

Analytical Chemistry
Marine Chemistry
Trace Elements
Stable Isotopes
Metal Ion Recognition

Selected Publications

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).

Tanimizu, M.; Sohrin, Y.; Hirata, T., Heavy Element Stable Isotope Ratios: Analytical Approaches and Applications, *Anal. Bioanal. Chem.*, **405,** 2771-2783 (2013).

Vu, H. T. D.; Sohrin, Y., Diverse Stoichiometry of Dissolved Trace Metals in the Indian Ocean, *Scientific Reports*, **3,** DOI: 10.1038/srep01745 (2013).

Determination of Isotopic Composition of Copper in Seawater

Copper is an essential trace metal that shows a vertical recycled-scavenged profile in the ocean. To help elucidate the biogeochemical cycling of Cu in the present and past oceans, it is important to determine the distribution of Cu isotopes in seawater. However, precise isotopic analysis of Cu has been impaired by the low concentrations of Cu as well as co-existing elements that interfere with measurements by multicollector inductively coupled plasma mass spectrometry (MC-ICP-MS). The objective of this study is to develop a simple Cu pre-concentration method using Nobias-chelate PA1 resin (Hitachi High Technologies). This extraction followed by anion exchange, allows precise analysis of the Cu isotopic composition in seawater. Using this method, Cu was quantitatively concentrated from seawater and >99.9999% of the alkali and alkaline earth metals were removed. The technique has a low procedural blank of 0.70 ng for Cu for a 2 L sample and the precision of the Cu isotopic analysis was ±0.07‰ (±2SD, $n = 6$). We applied this method to seawater reference materials (i.e., CASS-5 and NASS-6) and seawater samples obtained from the northwestern Pacific Ocean. The range of dissolved δ^{65}Cu was 0.40–0.68‰.

Figure 1. Mr. Shotaro Takano working on the R/V Hakuho Maru, who is the primary researcher of this study.

Diverse Stoichiometry of Dissolved Trace Metals in the Indian Ocean

Trace metals in seawater are essential to organisms and important as tracers of various processes in the ocean. However, we do not have a good understanding of the global distribution and cycling of trace metals, especially in the Indian Ocean. We report the first simultaneous, full-depth, and basin-scale section-distribution of dissolved (D) Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in the Indian Ocean. The samples were collected during the GEOTRACES JAPAN KH-09-5 cruise of R/V Hakuho Maru in the Indian Ocean from November 2009 to January 2010 in the northeast monsoon season. Our data reveal widespread co-limitation for phytoplankton production by DFe and occurrence of redox-related processes. The stoichiometry of the DM/phosphorus ratio agrees within a factor of 5 between deep waters in the Indian and Pacific, whereas it shows variability up to a factor of 300 among water masses within the Indian Ocean. This indicates that a consistent mechanism controls the stoichiometry in the deep waters, which are significantly depleted in Mn, Fe, and Co compared to requirements for phytoplankton.

Figure 2. Group photograph of the captain and on-board researchers and students of KH-09-5 cruise at Cape Town harbor.

Division of Environmental Chemistry
– Solution and Interface Chemistry –

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


Prof
HASEGAWA, Takeshi
(Ph D)


Assoc Prof
MATUBAYASI, Nobuyuki
(Ph D)


Assist Prof
WAKAI, Chihiro
(D Sc)


Assist Prof
SHIMOAKA, Takafumi
(D Sc)


PD
MIZUGUCHI, Tomoko
(D Sc)


PD*
ISHIZUKA, Ryosuke
(Ph D)

Students

TU, Kai-Min (D3)
NORIMOTO, Shingo (M2)
MORIMINE, Seiya (M2)
SHIOYA, Nobutaka (M1)
TANAKA, Yuki (M1)

* PD of ESICB
(Elements Strategy Initiative for Catalysts and Batteries)

Scope of Research

We investigate chemical phenomena in condensed phases. (1) 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. (2) The structure, dynamics, and reaction of solutions with nano-scale inhomogeneity and/or with fine tunability are investigated by computer simulation, and statistical-mechanical theory of solutions, and NMR spectroscopy.

KEYWORDS

Infrared and Raman Spectroscopy
Surface and Interface Chemistry
Nano Particle and Fibril Analysis
Free Energy
Solvation
Solution Theory

Selected Publications

Shimoaka, T.; Rikiyama, K.; Katsumoto, Y.; Hasegawa, T., Infrared Spectroscopic Study of Stereo-controlled Poly(*N*-isopropylacrylamide) with an Extended Chain Conformation Induced by Adsorption on a Gold Surface, *Anal. Bioanal. Chem.*, **405,** 9411-9418 (2013).

Norimoto, S.; Morimine, S.; Shimoaka, T.; Hasegawa, T., Analysis of Surface Coverage of a Self-Assembled Monolayer of Octadecyl Silane on a Si(100) Surface by Infrared External-Reflection Spectroscopy, *Anal. Sci.*, **29,** 979-984 (2013).

Wakai, C.; Shimoaka, T.; Hasegawa, T., Analysis of Hydration Process and Rotational Dynamics of Water in a Nafion Membrane Studied by ^{1}H NMR Spectroscopy, *Anal. Chem.*, **85,** 7581-7587 (2013).

Takemura, K.; Burri, R. R.; Ishikawa, T.; Ishikura, T.; Sakuraba, S.; Matubayasi, N.; Kuwata, K.; Kitao, A., Free-energy Analysis of Lysozyme–triNAG Binding Modes with All-atom Molecular Dynamics Simulation Combined with the Solution Theory in the Energy Representation, *Chem. Phys. Lett.*, **559,** 94-98 (2013).

Karino, Y.; Matubayasi, N., Interaction-component Analysis of the Urea Effect on Amino Acid Analogs, *Phys. Chem. Chem. Phys.*, **15,** 4377-4391 (2013).

Mogami, G.; Miyazaki, T.; Wazawa, T.; Matubayasi, N.; Suzuki, M., Anion-Dependence of Fast Relaxation Component in Na−, K−Halide Solutions at Low Concentrations Measured by High-Resolution Microwave Dielectric Spectroscopy, *J. Phys. Chem. A*, **117,** 4851-4862 (2013).

Analysis of Hydration Process and Rotational Dynamics of Water in a Nafion Membrane Studied by ^{1}H NMR Spectroscopy

^{1}H NMR spectroscopy is employed to reveal the hydration process of a Nafion membrane by measuring both the chemical shift and the spin-lattice relaxation time. In a former study, the hydration process was suggested to comprise two steps: the molecular adsorption of water on the sulfonic acid groups, and wetting with liquid water. The present study has revealed the first step can further be divided into two steps. By introducing a new experimental technique, the quantitatively reliable NMR measurements of protons (^{1}H) of water involved in the polymer membrane are realized. In addition, a new analytical procedure is developed using a reciprocal concentration on a saturation-adsorption model, and the hydration is clearly revealed to have three individual steps. Both the chemical shift and the relaxation time plots against the reciprocal concentration exhibit three linear parts with apparently different slopes. Of great interest is that the initial hydration is divided into two stages: the first hydration is a very strong adsorption of water probably on the hydroxyl group of the sulfonic acid group, and the second one is a relatively weak adsorption on another site of the sulfonic acid group. The third hydration is readily assigned to excess bulk (liquid-like) water as expected. These adsorption processes are readily correlated with the rotational motion of water by converting the spin-lattice relaxation time to the rotational correlation time.

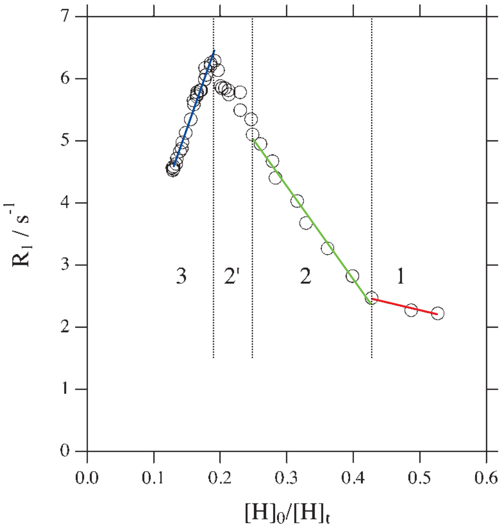


Figure 1. The spin-lattice relaxation rate (R_1) plotted against the reciprocal concentration of proton.

Free-Energy Analysis of Water Affinity in Polymer

Affinity of small molecule to polymer is an essential property for designing polymer materials with tuned permeability. In the present work, we develop a computational approach to the free energy ΔG of binding a small solute molecule into polymer using the atomistic molecular dynamics (MD) simulation combined with the method of energy representation. The binding free energy ΔG is obtained by viewing a single polymer as a collection of segments and employing an approximate functional constructed from distribution functions of the interaction energy between solute and the segment obtained from MD simulation. The binding of water is then examined against 9 typical polymers. The relationship is addressed between the segment size and the calculated ΔG, and a useful segment size is identified to compromise the performance of the free-energy functional and the sampling efficiency. It is found with the appropriate segment size that the ΔG convergence at a statistical error of ~0.2 kcal/mol is reached at ~4 ns of replica-exchange MD of the water-polymer system and that the mean absolute deviation of the computational ΔG from the experimental is 0.5 kcal/mol. The connection is further discussed between the polymer structure and the thermodynamic ΔG.

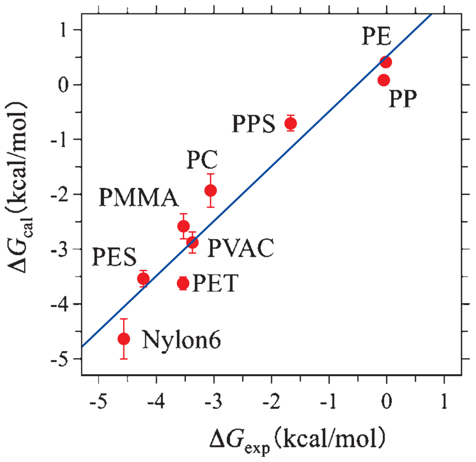


Figure 2. Comparison between the calculated free energies ΔG_{cal} and the ex- perimental ones ΔG_{exp}. The solid line represents the least-square fit expressed as $\Delta G_{cal} = 1.0\ \Delta G_{exp} + 0.5$. The error bar is expressed at 95% confidence limit (twice the standard error), and is smaller than the size of data symbol when it is not seen.

Division of Environmental Chemistry
– Molecular Microbial Science –

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

Prof
KURIHARA, Tatsuo
(D Eng)

Assist Prof
KAWAMOTO, Jun
(D Agr)

Assist Res Staff
MARUOKA, Yumi

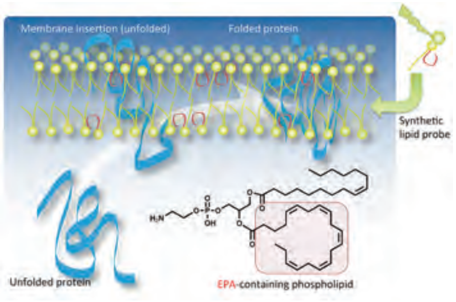
Assist Techn Staffs
UTSUNOMIYA, Machiko
KITAYAMA, Kaori

Researchers
GONG, Chunjie
CHO, Hyun-Num

Students
HIGA, Mariko (D1)
SUGIURA, Miwa (D1)
KAWAI, Soichiro (M2)
MORIMOTO, Ryohei (M2)
YAMAURA, Takayuki (M2)
ASAI, Azusa (M1)
IWANO, Yuriko (M1)
OHASHI, Sayaka (M1)
OGURA, Ryutaro (M1)
SUMIDA, Yukie (M1)
TOKUNAGA, Tomohisa (M1)
MARUYAMA, Saori (M1)

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
Molecular Microbial Science
Biochemistry
Bioengineering
Psychrotroph
Polyunsaturated Fatty Acids

Selected Publications

Dai, X.-Z.; Kawamoto, J.; Sato, S. B.; Esaki, N.; Kurihara, T., Eicosapentaenoic Acid Facilitates the Folding of an Outer Membrane Protein of the Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10, *Biochem. Biophys. Res. Commun.*, **425,** 363-367 (2012).

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

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.*, (in press) (2013).

Sato, S. B.; Park, J.; Kawamoto, J.; Sato, S.; Kurihara, T., Inhibition of Constitutive Akt (PKB) Phosphorylation by Docosahexaenoic Acid in the Human Breast Cancer Cell Line MDA-MB-453, *Biochim. Biophys. Acta.*, **1831,** 306-313 (2013).

Siwek, A.; Omi, R.; Hirotsu, K.; Jitsumori, K.; Esaki, N.; Kurihara, T.; Paneth, P., Binding Modes of DL-2-Haloacid Dehalogenase Revealed by Crystallography, Modeling and Isotope Effects Studies, *Arch. Biochem. Biophys.*, **540,** 26-32 (2013).

Yoshimune, K.; Kawamoto, J.; Kurihara, T., Proteins Involved in Cold Adaptation Cold-Adapted Microorganisms, *Cold-Adapted Microorganisms*, 97-110 (2013).

Elucidation of Metal-reducing System of a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10

A cold-adapted microorganism, *Shewanella livingstonensis* Ac10, isolated from Antarctic seawater has more than 40 kinds of cytochrome-related genes possibly involved in respiratory-linked metal reduction. In the presence of trivalent iron, ferric citrate, as a final electron acceptor for bacterial iron respiration, *S. livingstonensis* Ac10 inducibly produces eight proteins including a homolog of a phosphate-selective porin, PhoE, of *Escherichia coil*. PhoE has positively charged residues at its membrane-spanning region and acts as a channel protein to facilitate the phosphate uptake. However, the role of PhoE in the bacterial iron respiration is still unknown. In this study, we focused on a physiological role of PhoE in the iron-respiration mechanism of *S. livingstonensis* Ac10 and generated the gene-deletion mutant, Δ*phoE*, by two-step single crossover homologous recombination. When fumarate was used as a final electron receptor, Δ*phoE* grew normally. On the other hand, in the presence of ferric citrate, Δ*phoE* showed the growth retardation, and the generation of divalent iron was significantly reduced (Figure 1). Introduction of a *phoE*-expression vector suppressed the growth retardation, indicating that PhoE is required for the iron respiration of this strain. We also examined the growth of Δ*phoE* in the presence of insoluble iron oxide (III), and demonstrated that the growth of Δ*phoE* and the parent strain was almost similar. These results suggest that *S. livignstoneneis* Ac10 inducibly produces PhoE to facilitate iron uptake through membrane in the presence of soluble trivalent ferric ion.

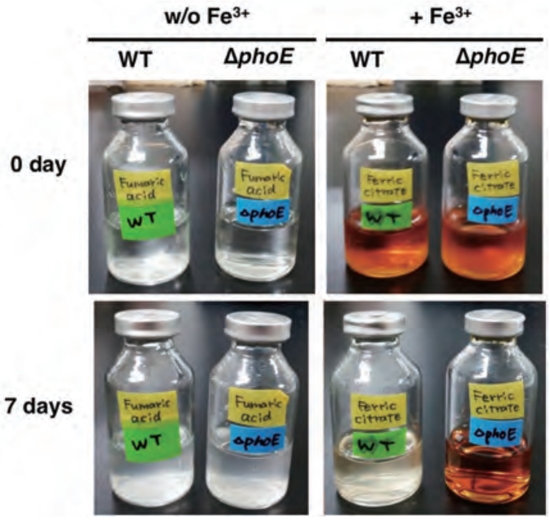


Figure 1. Respiratory iron reduction of *Shewanella livingstonensis* Ac10 and *phoE*-disrupted mutant.

Subcellular-localized 1-Acylglycerol-phosphate Acyltransferase Regulates the Cell Division of a Psychrotrophic Bacterium, *Shewanella livingstonesis* Ac10

Shewanella livingstonensis Ac10 isolated from Antarctic seawater produces a kind of polyunsaturated fatty acids, eicosapentaenoic acid (EPA), as the membrane phospholipids, which alters the physicochemical properties of cell membrane and facilitates the function of cell-division proteins and the folding of membrane proteins at low temperatures. EPA is exclusively restricted to the *sn*-2 position of phospholipids. 1-Acyl-*sn*-glycerol-3-phosphate acyltransferase (PlsC) catalyzes the acylation at the *sn*-2 position of 1-acyl-*sn*-glycerol-3-phosphate (LPA) to form phosphatidic acid (PA), suggesting that the PlsC is involved in the synthesis of EPA-containing phospholipids. *S. livingstonensis* Ac10 has five putative candidate genes coding for PlsC, PlsC1 to PlsC5. The gene-disrupted mutant of PlsC1 (Δ*plsC1*) showed the growth retardation and filamentous cells at low temperatures, and the amount of EPA-containing phospholipids was significantly decreased, indicating that PlsC1 is a key enzyme in the biogenesis of EPA-containing phospholipids. When His-tagged PlsC1 was expressed in Δ*plsC1*, the growth retardation and filamentous cell formation were suppressed, and His-tagged PlsC1 was localized at mid-cell region of *S. livingstonensis* Ac10. On the other hand, *E. coli* PlsC also catalyzes the acylation of LPA from EPA-coenzyme A similar to PlsC1 *in vitro*. Immunofluorescence microscopy was also demonstrated that His-tagged PlsC expressed in Δ*plsc1* was widely distributed in cell. These results suggest that the biogenesis of EPA-containing phospholipids synthesized by the activity of PlsC1 at mid-cell region is required for the appropriate cell division of this strain.

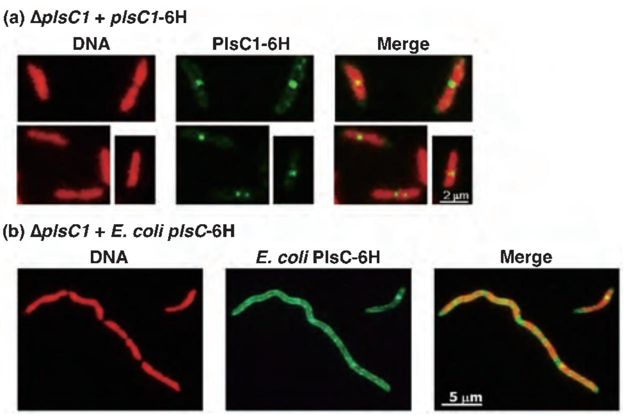


Figure 2. Subcellular localization of PlsC1 (a) and *E. coli* PlsC (b) in the *plsC1*-disrupted strain of *Shewanella livingstonensis* Ac10.

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
INOUE, Rintaro
(D Eng)

Program-Specific Res
TAKAHASHI, Nobuaki
(D Eng)

Students

MASHITA, Ryo (D1)
NABATA, Takeshi (M2)
HIRANO, Tatsumasa (M2)
MATSUURA, Tomohiko (M2)
SHIRAISHI, Yasuhiro (M1)
TAKEDA, Kazuki (M1)
MAEDE, Tadahiko (M1)
KISHIMOTO, Mizuki (UG)
FUJISHIMA, Yudai (UG)
MURAKAMI, Momoko (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

Selected Publications

Xia, T.; Ogawa, H.; Inoue, R.; Nishida, K.; Yamada, N. L.; Li, G.; Kanaya, T., Dewetting Process of Deuterated Polystyrene and Poly(vinyl methyl ether) Blend Thin Films via Phase Separation, *Macromolecules*, **46,** 4540-4547 (2013).

Kanaya, T., Polec, A. I.; Fujiwara, T.; Inoue, R.; Nishida, K.; Ogawa, H.; Ohta, N., Precursor of Shihi-Kebab above the Melting Temperature by Micro-beam X-ray Scattering, *Macromolecules*, **46,** 3031-3036 (2013).

Mashita, R.; Kishimoto, H.; Inoue, R.; Kanaya, T., Small-angle X-ray and Neutron Scattering Analyses of Highly Crosslinked Rubber with Unsaturated Carboxylic Acid, *Polym. J.*, **45,** 57-63 (2013).

Asakawa, H.; Nishida, K.; Kanaya, T.; Tosaka, M., Giant Single Crystal of Isotactic Polypropylene Showing near-equilibrium Melting Temperature, *Polym. J.*, **45,** 287-292 (2013).

Inoue, R.; Kanaya, T., Heterogeneous Dynamics of Polymer Thin Films as Studied by Neutron Scattering, *Adv. Polym. Sci.*, **252,** 107-140 (2013).

Specific Kinetic Pathway from Mesophase to Large Single Crystal of Polymer

Single crystals of polymer, especially large sized ones, have attracted the interest of researchers for many years. We have found a specific kinetic pathway to form giant single crystals of isotactic polypropylene (iPP) *via* the mesophase, whereas the crystal aggregate, the so-called spherulite, is usually obtained during the conventional crystallization of iPP from the molten state. In order to find such a kinetic pathway, multiple probes, such as wide-angle X-ray diffraction (WAXD), de-polarized light transmission (DPLT) and differential scanning calorimetry (DSC), were used in complementary.

The pre-quenched iPP mesophase was heated to 166°C at a rate of 75°C/min and maintained at this temperature for 24 h. The obtained crystallites exhibited a very high melting temperature, T_m, of 183.7°C, which is ca. 19°C higher than the iPP's nominal T_m (~165°C); namely, the observed T_m is immediately close to the literature value of iPP's equilibrium melting temperature, T_m^0 (186.2°C). The crystallites have bamboo leaf-like or needle-like morphology and are ~35 μm in length and ~3.5 μm in width. The thickness of the crystallites was estimated to be 88 nm according to the melting temperature. The number density of the crystallites in a unit volume could be controlled by adjusting the heating rate. As the result, well-isolated single crystals of iPP with the above-mentioned morphology and dimension were obtained.

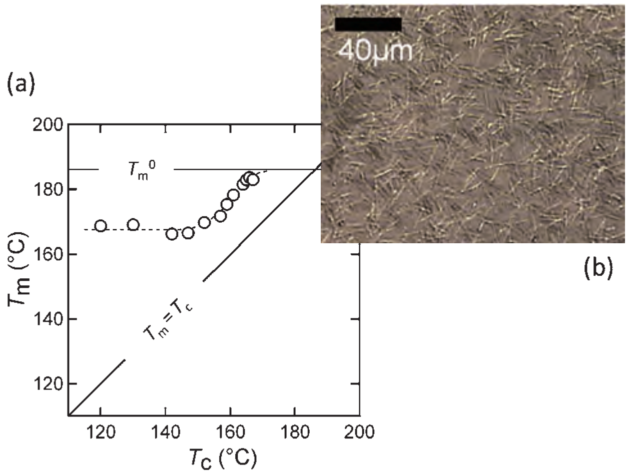


Figure 1. (a) Melting temperature, T_m, as a function of the annealing temperature, T_c. (b) Optical microscopic image of large single crystal of iPP.

Small-angle X-ray and Neutron Scattering Analyses of Crosslinked Rubber with Metal Diacrylate

Many industries, including the automobile industry, require lightweight materials with high tensile strengths and high abrasion resistances to improve the manufacturing of commercial products. Therefore, controlling the morphology and structure of functional polymeric materials is indispensable to the development of next-generation materials.

The structure of rubber crosslinked with metal diacrylate has been extensively studied because such rubber exhibits so-called "reinforcement effect" without the addition of reinforcing materials such as carbon black, silica or clay. On the other hand the structure of the matrix rubber in itself, which is a main component in these rubber materials, has not been well studied because of its structural complexity. It is considered that elucidating the structure of the matrix rubber could provide a promising approach to improve the mechanical properties of these rubber materials, we then determined to study the structure of butadiene rubber (BR) crosslinked with metal diacrylate through the complementary use of small-angle X-ray scattering (SAXS) and small angle neutron scattering (SANS). In addition to the hierarchical structure of metal aggregates we first succeeded to reveal the existence of high crosslink density segment (HC-BR) in the matrix BR. Furthermore it was also found that HC-BR was related to mechanical strength of the present studied butadiene rubber by comparing the results of the tensile measurements with the structural information from both SAXS and SANS measurements.

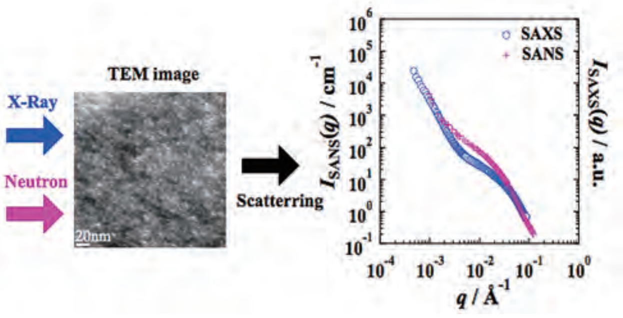


Figure 2. TEM images, SAXS and SANS profiles obtained from butadiene rubber crosslinked with metal diacrylate.

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

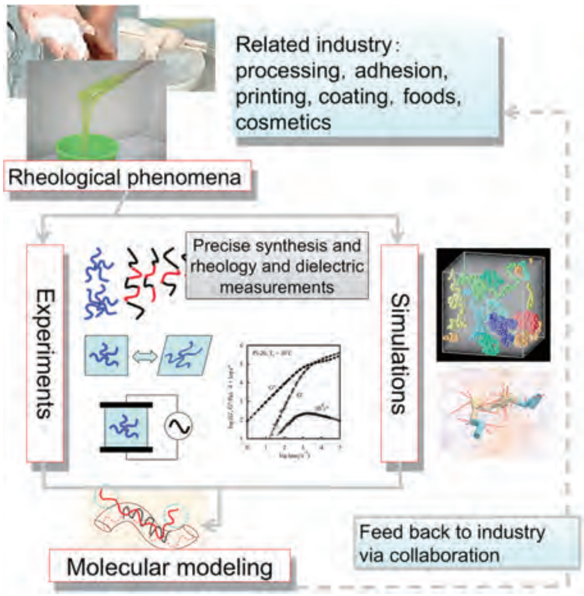
TAKADA, Jun (D3)
KAWASAKI, Yohji (D2)
NAGAO, Masahiro (M2)
EGAMI, Ryoma (M1)
KUMAZAWA, Kazuki (M1)
FURUKAWA, Yoichi (UG)
TAKAGI, Kohei (UG)

Visiting Researchers

Prof COLBY, Ralph	Pennsylvania State University, U.S.A., 13–17 May
Prof VLASSOPOULOS, Dimitris	IESL-FORTH and University of Crete, Greece, 13–17 May
Prof KWON, Youngdon	Sungkyunkwan University, Korea, R., 18–22 July
Assoc Prof KOGA, Tadanori	Stony Brook University, U.S.A., 25 July

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

Watanabe, H.; Matsumiya, Y.; van Ruymbeke, E., Component Relaxation Times in Entangled Binary Blends of Linear Chains: Reptation/CLF along Partially or Fully Dilated Tube, *Macromolecules*, **46,** 9296-9312 (2013).
Huang, Q.; Alvarez, N. J.; Matsumiya, Y.; Rasmussen, H. K.; Watanabe, H.; Hassager, O., Extensional Rheology of Entangled Polystyrene Solutions Suggests Importance of Nematic Interactions, *ACS Macro Letters*, **2,** 741-744 (2013).
Matsumiya, Y.; Kumazawa, K.; Nagao, M.; Urakawa, O.; Watanabe, H., Dielectric Relaxation of Monodisperse Linear Polyisoprene: Contribution of Constraint Release, *Macromolecules*, **46,** 6067-6080 (2013).
Masubuchi, Y.; Yaoita, T.; Matsumiya, Y.; Watanabe, H.; Ianniruberto, G.; Marrucci, G., Stretch/orientation Induced Acceleration in Stress Relaxation in Coarse-grained Molecular Dynamics Simulations, *Nihon Reoroji Gakkaishi (J. Soc. Rheol. Jpn.),* **41,** 35-37 (2013).
Langeloth, M.; Masubuchi, Y.; Böhm, M. C.; Müller-Plathe, F., Recovering the Reptation Dynamics of Polymer Melts in Dissipative Particle Dynamics Simulations via Slip-springs, *J. Chem. Phys.*, **138,** [104907] (2013).

Uniaxial Extensional Behavior of $(SIS)_p$-Type Multiblock Copolymer Systems: Structural Origin of High Extensibility

Rheological and structural behavior was examined for a series of symmetric styrene (S)− isoprene (I)− styrene (S) multiblock copolymers of $(SIS)_p$-type ($p = 1$, 2, 3, and 5 corresponding to tri-, penta-, hepta-, and undecablock) in *n*-tetradecane (C14), a selective solvent that dissolves the I block and precipitates (but swells) the S block. The molecular weights of respective blocks were almost identical for these copolymers ($M_I \cong 40$K for I block; $M_S \cong 20$K and 10K for inner and outer S blocks, respectively). At 20°C, the $(SIS)_p$/C14 systems with the copolymer concentration $C = 30$ wt % formed a bcc lattice of spherical S domains (with $T_{g,PS} \cong 38$°C) embedded in the I/C14 matrix. Under small shear and elongation in the linear regime, the systems exhibited gel-like elasticity sustained by the I blocks connecting the S domains. This linear elastic behavior, being associated with affine displacement of the S domains as revealed from small-angle X-ray scattering (SAXS) under small elongation, was very similar for all $(SIS)_p$/C14 systems having the same C. In contrast, a remarkable difference was found for those systems under large (but slow) elongation: The maximum stretch ratio at rupture, λ_{max}, significantly increased with the repeating number p of the SIS units, $\lambda_{max} \cong 1.7$, 2.2, 6.6, and ≥ 90 for $p = 1$, 2, 3, and 5, respectively. In particular, $\lambda_{max} \geq 90$ for $p = 5$ was much larger compared to the full-stretch ratio of the trapped entanglement strand ($\lambda_{full\text{-}ent} \cong 14$) and even to the full-stretch ratio of the $(SIS)_5$ copolymer chain as a whole ($\lambda_{full\text{-}copolymer} \cong 40$). For investigation of the structural origin of such remarkably high extensibility of the undecablock system ($p = 5$), SAXS and rheological tests were made under elongation followed by reversal. The tests revealed affine stretching of the lattice (affine displacements of the S domains) and negligible stress−strain hysteresis on reversal of elongation from $\lambda_{rev} < 3$ (Figure 1). In contrast, on reversal from larger λ_{rev} up to 60, nonaffine stretching of the lattice and the significant stress−strain hysteresis were observed. Thus, under large elongation, some of the S blocks were pulled out from their domains and transferred to the other S domains at 20°C, the experimental temperature not significantly lower than $T_{g,PS}$ ($\cong 38$°C) of the swollen S domains, to allow the system to deform plasto-elastically. This deformation differed from unrecoverable plastic flow, as evidenced from spontaneous, full recovery of the size, shape, and SAXS profile of the $(SIS)_5$/C14 specimen being kept at rest (without load) at 20°C for a sufficiently long time after the elongation. This recovery strongly suggests that the material preserved some memory of initial connection between the $(SIS)_5$ chains through the S domains, in particular in the direction perpendicular to the elongation, and the corresponding physical network still percolated the whole material even under large elongation (Figure 2). This argument in turn provides us with a clue for understanding the difference of λ_{max} for the series of $(SIS)_p$/C14 systems. The full percolation can survive and the material can stand with the elongation if at least two PS blocks, on average, remain intact (not pulled out) in each $(SIS)_p$ copolymer backbone. The probability of having such intact S blocks obviously increases with the repeating number p of the SIS units, which possibly resulted in the observed difference of λ_{max}.

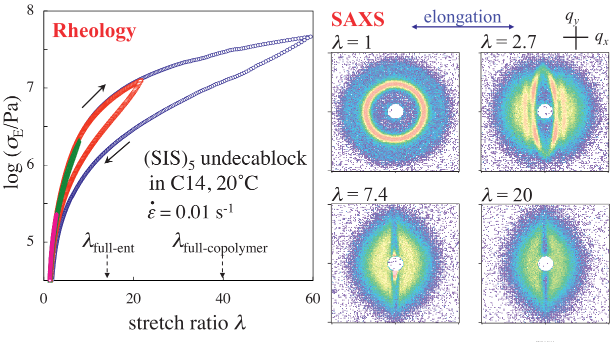


Figure 1. Left: Elongational stress σ_E of the 30 wt% $(SIS)_5$/C14 undecablock systems measured with the reverse mode at 20˚C (large unfilled symbols). The strain rate is $\dot{\varepsilon} = 0.01$ s^{-1} for both forward and reverse processes. The σ_E data are plotted against the stretch ratio λ. Right: Two-dimensional SAXS profiles $I(q_x,q_y)$ of the 30 wt% $(SIS)_5$/C14 undecablock system at stretch ratios λ as indicated. The data are shown in the range of q_x, $q_y < 0.5$ nm^{-1}.

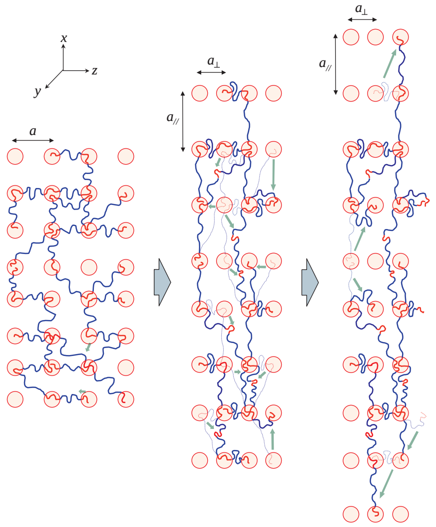


Figure 2. Schematic illustration of possible structural changes in the 30 wt% $(SIS)_5$/C14 undecablock system under large elongation. The macroscopic elongation is applied in *x* direction, and the width and thickness directions of specimen are chosen to be the *y* and *z* direction. The initial network connectivity preferentially surviving in the *y* and *z* directions provides the material with the driving force for full structural recovery after elongation.

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)

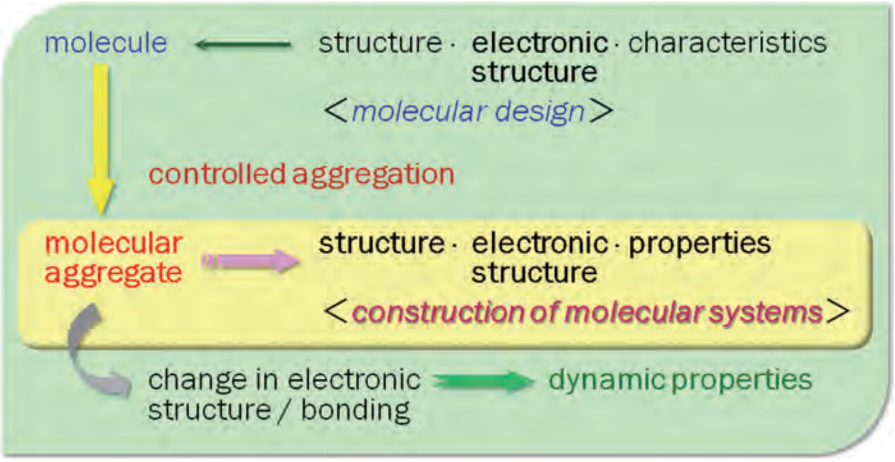
Students

HIDAKA, Yuta (M2)
SHIRAISHI, Ryo (M2)
SHINTAKU, Naoto (M1)
YAMADA, 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
α-Dispersion
Cell Suspension
Diode Behavior
Pentacene Thin Film
Voltage Stress



Selected Publications

Tsuzuki, S.; Sato, N., Origin of Attraction in Chalgogen-Nitrogen Interaction of 1,2,5-Chalcogenadiazole Dimers, *J. Phys. Chem. B*, **117,** 6849–6855 (2013).

Fabiano, S.; Yoshida, H.; Chen, Z.-H.; Facchetti, A.; Loi, M. A., Orientation-Dependent Electronic Structures and Charge Transport Mechanisms in Ultrathin Polymeric n-Channel Field-Effect Transistors, *ACS Appl. Mater. Interfaces*, **5,** 4417-4422 (2013).

Han, W.-N.; Yoshida, H.; Ueno, N.; Kera, S., Electron Affinity of Pentacene Thin Film Studied by Radiation-Damage Free Inverse Photoemission Spectroscopy, *Appl. Phys. Lett.*, **103,** [123303-1]-[123303-5] (2013).

Noshiro, D.; Sonomura, K.; Yu, H.-H.; Imanishi, M.; Asami, K.; Futaki, S., Construction of a Ca^{2+}-Gated Artificial Channel by Fusing Alamethicin with Calmodulin-Derived Extramembrane Segment, *Bioconjugate Chem.*, **24,** 188-195 (2013).

Asami, K., Dielectric Properties of Dipicrylamine-Doped Erythrocytes, Cultured Cells and Lipid Vesicles, *Bioelectrochemistry*, **92,** 14-21 (2013).

Voltage Stress Induced Reversible Diode Behavior in Pentacene Thin Films

Recently, there has been renewed interest in the current–voltage (*I*–*V*) behavior of organic materials under low electric potentials applied, where many conditions used to derive the space charge limited current model will cease to apply. Current flow is regulated there by charge injection at one or both electrodes and, as a result, interfacial effects become the dominant factor behind the measured *I*–*V* relationships. Changing the barrier energy for charge carrier injection at one or both electrodes will result in diode or diode-like behavior. This is normally achieved by using electrodes with different work functions.

In the course of *in situ* measurement of the dark conductance of pentacene films deposited under ultrahigh vacuum between two nominally identical titanium electrodes in bottom contact geometry, we consistently observed a small difference between the measured conductance for positive and negative applied voltages. A vacuum-deposited 100 nm thick pentacene film provided us with the asymmetric *I*–*V* curves and the direction and degree of the diode-like behavior vary with sample and measurement history. On further investigation it was discovered that "stressing" the sample at high voltage could reliably cause the sample to exhibit rectification in one direction or the other, depending on the polarity of the applied voltage stress. The rectification behavior, once set, was essentially permanent until reversed by a subsequent voltage stress in the opposite direction.

Analysis of the voltage and temperature dependence suggests that the current is injection limited under both forward and reverse bias. The bias stress acts to raise or lower the energy barrier for charge carrier injection, most likely through the injection of space charge into the bulk film.

Modification of the electrical properties of organic devices from sustained applied voltage bias is well known though the mechanisms are not always well understood. To our knowledge, however, bias stress induced, reversible rectification has not been reported previously for organic films.

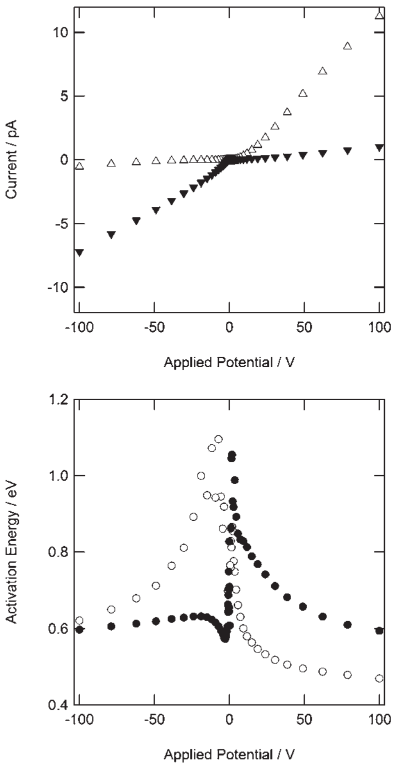


Figure 1. Variation in device current (upper) and the activation energy of electrical conductance (lower) as a function of applied potential, for the system after positive bias stress (△,○) and after negative bias (▼,●).

Electrical Properties of *E. coli* Cells Revealed by Dielectric Spectroscopy

To understand the electrical properties of the plasma membrane and the cell wall of *E. coli* cells, dielectric spectra of the cell suspensions were measured over a frequency range from 10 Hz to 10 MHz. Low-frequency dielectric dispersion, so-called the α-dispersion, was found below 10 kHz in addition to the β-dispersion, due to interfacial polarization, appeared above 100 kHz. When the cells were killed by heating at 60 ºC for 30 min, the β-dispersion disappeared completely, whereas the α-dispersion was little influenced. The disappearance of the β-dispersion suggests that the plasma (or inner) membranes in the dead cells are no longer the permeability barrier to small ions, and that the α-dispersion is not related to the membrane potential produced by diffusion of specific ions along their gradients across the plasma membrane. The intensity of the α-dispersion depended on both of the pH and ionic strength of the external medium, supporting the model that the α-dispersion results from the deformation of the ion clouds formed outside and inside the cell wall containing charged residues.

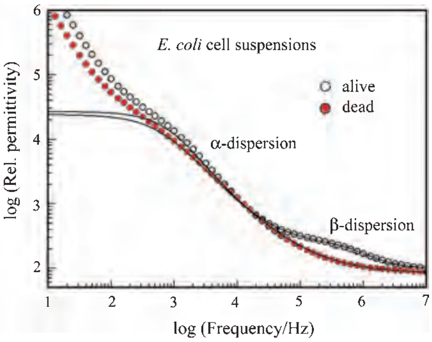


Figure 2. Dielectric spectra of *E. coli* cell suspensions.

Division of Multidisciplinary Chemistry
– Interdisciplinary Chemistry for Innovation –

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

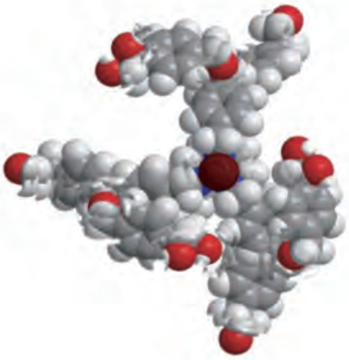
Prof
TOSHIMITSU, Akio
(D Eng)

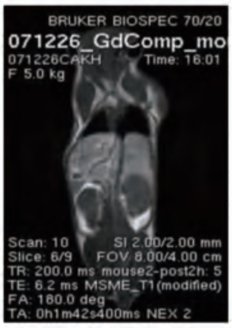
Students

SUGII, Hiroaki (M2)
IURA, Yoshihito (M1)
KAMEDA, Tetsuro (M1)
OKITSUKA, Masumi (UG)
SUZUKI, Yuki (UG)

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 metal-catalyzed reactions, and asymmetric synthesis. As for the synthetic procedure, we take note to develop atom-economic 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).

Size-controlled and Biocompatible Gd_2O_3 Nanoparticles for Dual Photoacoustic and MR Imaging

One of the most rapidly developing and exciting applications of nanotechnology in biomedical research is the development of biocompatible nanoparticles for use in multiple, powerful and highly complementary imaging modalities. Our main goal is to synthesize and isolate new size-controlled and biocompatible Gd_2O_3 nanoparticles as an unconjugated bimodal contrast agent for use in photoacoustic tomography (PAT) and magnetic resonance (MR) imaging through the fusion of inorganic nanoparticles and organic peptide coating.

Gd_2O_3 nanoparticles used in this study were obtained by applying a previously reported protocol for the alkaline hydrolysis of $Gd(NO_3)_3$ carried out in diethylene glycol (DEG) at 180°C. To isolate the DEG-coated Gd_2O_3 nanoparticles, this reaction mixture was further added to pure acetone to give dark brown precipitates. After the precipitates were dried under vacuum and dispersed in pure water, a dynamic light scattering (DLS) measurement of the isolated Gd_2O_3-DEG nanoparticles gave a sharp and reproducible peak at 100 nm during an appropriate time-window.

However, the mean size (hydrodynamic diameter) of the isolated Gd_2O_3-DEG nanoparticles increased greatly over time in pure water, which is a sign of coarse aggregation. We found that the surface modification of Gd_2O_3-DEG nanoparticles with biocompatible gelatin could be used to maintain a constant diameter even after 45 h. In addition, the size (diameter) of the new nanoparticles could be completely controlled (20–200 nm) by timing the addition of an aqueous solution of gelatin to the suspension of Gd_2O_3-DEG nanoparticles in pure water.

A transmission electron microscopy (TEM) of the new nanoparticles of a hydrodynamic diameter of 100 nm showed that the thickness of the outer layer is 10–30 nm and Gd_2O_3-DEG nanoparticles were observed as small dots (5 nm; indicated with white circles) (Figure 1). Based on the process of synthesis, it is conceivable that the outer layer of new nanoparticles consists of gelatin (indicated with black arrowheads), and the inner small dots should be unconjugated Gd_2O_3 because of its high electron density. The remaining space in the nanoparticles was filled by DEG (indicated with white arrowheads).

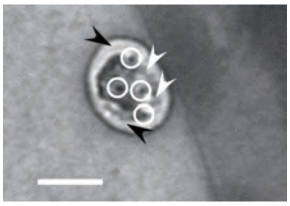


Figure 1. Transmission electron microscopy (TEM) of Gd_2O_3-DEG-gelatin nanoparticles (scale-bar; 100 nm).

Figure 2 shows a photoacoustic (PA) image of mice before and after subcutaneous injection of the new nanoparticles. After the injection, the intense signal was observed at the injected area. These signals were expected to be emitted from Gd_2O_3 nanoparticles and no PA signals for DEG or gelatin were observed.

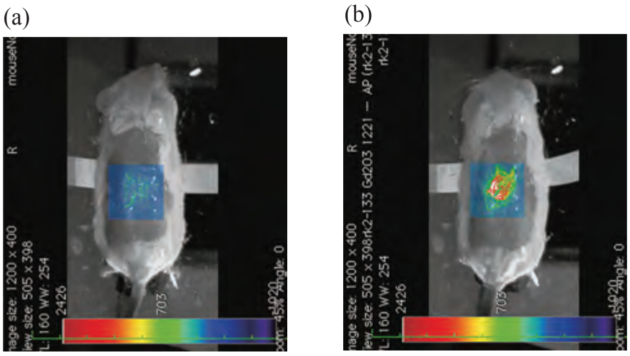


Figure 2. Photoacoustic (PA) images of mice (a) before and (b) after subcutaneous injection of Gd_2O_3-DEG-gelatin nanoparticles.

The MRI study clearly showed that the new nanoparticles are a T_1-positive MRI contrast agent, and their relaxivity r_1 is twice that of clinically available Gd-DETA. Since the relaxivity r_1 strongly depends on the rotational dynamics of molecules with a magnetic moment, the rotation of new nanoparticles could be inhibited by their gravity, which results in an increase in sensitivity as well as reduction in dose.

MR images of a whole mouse clearly showed that the new nanoparticles freely circulate in the blood vessels without undesirable accumulation in the lungs (Figure 3). We consider that these new nanoparticles could be useful as a contrast agent for angiography. In addition, signals in the liver were diminished, while signals in the colon were observed on MR imaging 24 h after injection (Figure 3b). In addition, we have confirmed that the mice 72 h after intravenous injection of the present nanoparticles were alive, and MR intensity of the liver decreased. Thus, we consider that the nanoparticles after the injection could be eliminated from the liver through the bile duct without any chemical alteration, such as generation of a free Gd^{3+} ion and the accumulation as $GdPO_4$ microcrystals in the liver.

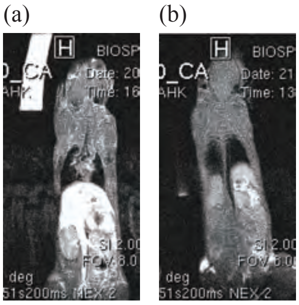


Figure 3. T1-weighted magnetic resonance (MR) images of mice (a) 5 min and (b) 24 h after intravenous injection of Gd_2O_3-DEG-gelatin nanoparticles (0.10 mmol Gd/kg).

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)

FUJISAWA, Hiroshi (Ph D)
KAZAMA, Ichiro

Lect (pt)

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

Students

IMAJO, Sohei (D3)
FUWA, Yasuhiro (D1)
KITAHARA, Ryunosuke (M2)
IKEDA, Hideki (M2)
SAGARA, Shouichiro (RS)

Visiting Researchers

Chief Scientist SWENSON, D. A.	ImpartOne Inc., U.S.A., 16 October –1 November

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).

Non-destructive Inspection for the Superconducting Cavity by XT-map System

The upper limit of the accelerating gradient of the superconducting (SC) cavity for the particle accelerator seems to be affected by the condition of the interior surface. Main causes of limiting accelerating gradient are thought to be the quench from local heat source and field emission due to defects such as scratches, dust particles in tens of µm and ruggedness of a few hundreds µm. In order to improve the performance and the production yield of the SC cavities, non-destructive inspections for finding defects on the interior surface of SC cavity have important roles.

About 15000 SC cavities with the average accelerating gradient of 32MV/m are required for the first stage plan of the International Linear collider (ILC). Because of the number of such many SC cavities to be produced, several research laboratories have made R&D of various inspection methods. As a method for survey and observation of defects on the interior surface, the high-resolution camera system, so-called Kyoto Camera, was developed. Kyoto Camera used in several research laboratories is an effective non-destructive inspection tool at the room temperature environment. On the other hand, the multi-point thermometry mapping measurements (T-map) and the multi-point X-ray radiation mapping measurements (X-map) are useful tools to survey the defect locations during the vertical test. The vertical test is the performance test of SC cavity by feeding RF power to cavities at cryogenic temperature environment (liq. He). T-map, X-map and the optical observation are complementary to each other for the purpose. Those inspections are recognized as essential processes for the local repairing of the interior surface together with the micro grinder after identified the defect locations.

Our XT-map system under development in collaboration between Kyoto University and KEK is a combined system of T-map and X-map. The ruthenium oxide chip resistors with good availability and a low cost are adopted as the temperature sensors of XT-map in instead of the expensive commercial cryogenic temperature sensor or the carbon resistors. Whole T-map assemblies for 9-cell cavity will contain about 9000 (X-map: 4500) sensors. The high-density sensor distribution of the XT-map gives the high resolution. Many cabling wires for this multi-point measurement would increase the heat intrusion into the cryostat. In order to reduce the number of the signal cables significantly, CMOS analogue multiplexers have been installed in the cryogenic area. And the daisy-chained FPC boards pass a token sequentially during data scan of all analog data on each board. Because the huge amount of sensor lines are multiplexed at a hi-speed scanning rate in the vicinity of the sensors, the small number of signal lines makes the installation process easy and reduces the system complexity.

A preliminary quench detection test of XT-map was performed on a SC cavity which was known to have a quench location by a previous vertical test at KEK. As shown in Figure 3, XT-map FPC boards were installed on 1/4 area of a cell, and we succeeded in the detection of a heat generation as shown in Figure 4.

Basic design of XT-map system for non-destructive inspection during the vertical test has been established. Although sensitivity of the adopted X-map and T-map sensors are less than those used in other laboratories, both sensors show sufficient performance in our XT-map system. Issues such as insufficient thermal contact of sensors with the cavity surface found in this quench detection test will be resolved in a next version.

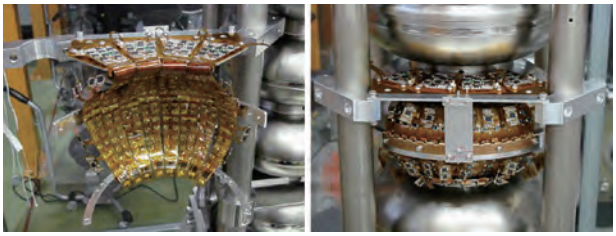


Figure 3. Installation of test of XT-map assemblies for the quench detection at KEK.

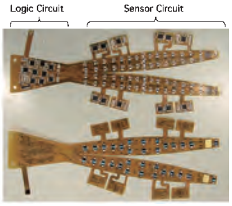


Figure 1. The double-leaf-shaped Flexible Printed Circuits films (polyimide film with several layers) for XT-map.

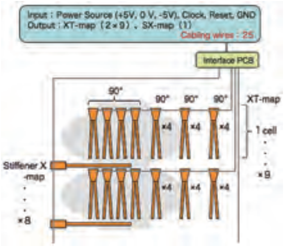


Figure 2. The schematic drawing of our inspection System (XT-map and Stiffener X-map system).

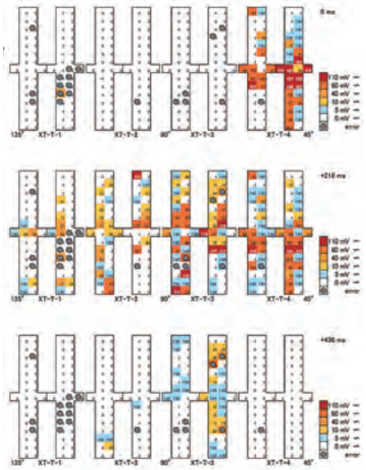


Figure 4. A typical measurement result of the quench detection test of XT-map during the vertical test. The circles are quench location previously observed by KEK T-map. The output value of 100 mV corresponds to a temperature rise from 2K to 10K.

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
HATA, Masayasu
(D Sc)

Students

MIYASAKA, Yasuhiro (D3)
IKEDA, Daiki (M2)
KAWAMOTO, Mao (M2)
MAEDA, Kazuya (M2)
MORI, Kazuaki (M2)
TERAMOTO, Kensuke (M1)
NAKASHIMA, Yuto (M1)
NISHII, Takaya (M1)

Visiting Researcher

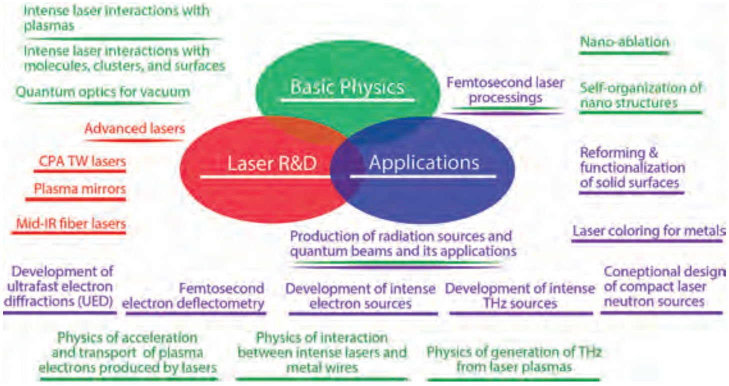
Ms. GEMINI, Laura	Czech Technical University, Czech R., 15 April–16 September

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., Metal-like Self-organization of Periodic Nanostructures on Silicon and Silicon Carbide under Femtosecond Laser Pulses, *J. Appl. Phys.*, **114,** 194903 (2013).

Shimizu, S.; Hashida, M.; Miyasaka, Y.; Tokita, S.; Sakabe S., Unidirectionally Oriented Nanocracks on Metal Surfaces Irradiated by Low-fluence Femtosecond Laser Pulses, *Appl. Phys. Lett.*, **103,** 174106 (2013).

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).

Divergence-Free Transport of Laser-Produced Fast Electrons Along a Meter-Long Wire Target

The development of ultraintense lasers has facilitated the generation of high-current charged particle beams; however, the control of such beams (collimation, transport, and focusing) remains a challenge. We report the observation that a metal wire can act as a guiding device for an electron beam. We have observed that a significant number of fast electrons can be guided over 1 m along a metal wire, without a change in beam size. The experimental results for the transverse distribution of the electron beam are well reproduced by numerical simulations of electron trajectories based on a simplified model. Numerical simulations suggest that a relatively weak steady electric field (~10^6 V/m), which does not decay for several nanoseconds, is generated around the wire and plays a key role in the long-distance guidance.

Figure 1 (a) shows the experimetnal setup for spatial distribtuion measurement of electrons. The electrons produced by irradiation of an ultraintense laser pulse on a metal wire target are detecded by stacked imaging plates (IPs). On the first layer and second of the stacked IPs, electrons with energies higher than ~40 and ~400 keV can be deteced, respectively. Figure 1 (b) shows typical single-shot images at L = 150, 400, and 1050 mm, where L is the distance from the laser irradiated spot to the end of the wire. On the first layer IP, the signal is saturated near the center to a maximum electron density of the order of 4×10^{-9} C/cm^2. The full width at half-maximum (FWHM) of the central part of the images on the second layer IP is 3 to 4 mm, at each L. The beam patterns for each wire length were highly reproducible; however, the beam size showed slight shot-to-shot fluctuation of less than ±1 mm. Assuming a typical electron energy to be 100 keV, the total charge of detected electrons was estimated to be at least 3 nC by integrating the signals below the saturation level. The total charge and diameter of the electron beam are maintained over a propagation distance of 1 m.

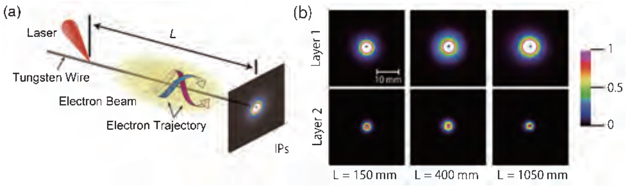


Figure 1. (a) Experimetnal setup for the observation of the spatial distributions of electrons generated from ametal wire. (b) Typical single shot images detected by IP at L = 150, 400, and 1050 mm generated from the setup in (a).

Unidirectionally Oriented Nanocracks on Metal Surfaces Irradiated by Lowfluence Femtosecond Laser Pulses

We have observed the generation of nanocracks oriented perpendicular to the incident laser polarization at fluence below ablation threshold F_{th} for W, Mo, and Cu metal targets. The number density of nanocracks increased with incident pulse number (Figure 2), but their length distributions were independent of it. From the experimental and simulation results, we proposed that an initial tiny crack on the metal surface grows to a nanocrack through local field enhancement. The enhanced field near the hole edge in longitudinal direction of the nanocrack makes the crack longer, and the low intensity field near the edge on short direction governs the space to the next crack.

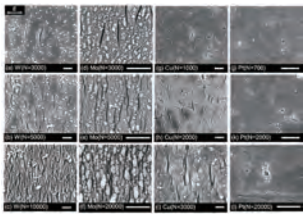


Figure 2. FESEM images of surface nanostructures on (a)-(c) W, (d)-(f) Mo, (g)-(i)Cu, and (j)-(l)Pt. The arrow in (a) shows the direction of polarization of the incident laser field, which is applied to all images. *N* is the number of incident pulses. The white bar in each image corresponds to 500 nm.

Metal-Like Self-Organization of Periodic Nanostructures on Silicon and Silicon Carbide under Femtosecond Laser Pulses

Periodic structures were generated on Si and SiC surfaces by irradiation with femtosecond laser pulses. Self-organized structures with spatial periodicity of approximately 600 nm appear on silicon and silicon carbide in the laser fluence range just above the ablation threshold and upon irradiation with a large number of pulses. As in the case of metals, the dependence of the spatial periodicity on laser fluence can be explained by the parametric decay of laser light into surface plasma waves (Figure 3). The results show that the proposed model might be universally applicable to any solid material.

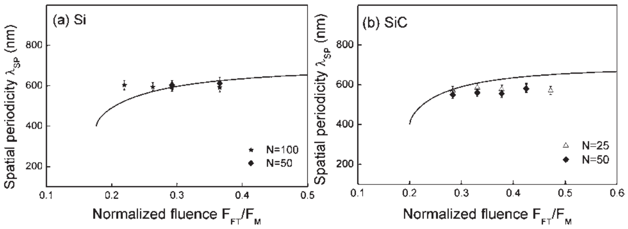


Figure 3. Evolution of spatial periodicity λ_{SP} for classical ripples with respect to normalized laser fluence for (a) Si and (b) SiC. Solid lines indicate the evolution of the spatial periodicity of ripples predicted by the parametric decay model.

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)

Assist Techn Staff

HIRAIZUMI, Yuri

Students

SAITO, Hikaru (D3)
ASO, Ryotaro (D3)
FUJIYOSHI, Yoshifumi (D2)
YAMAGUCHI, Atsushi (M2)
YAMAGUCHI, Hitomi (M2)
MITSUTA, Itaru (M1)

Visiting Researcher

Dr. SCHAPER, Andreas Karl	Philipps University Marburg, Germany, 15 March–13 May

* Nanotechnology Platform

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
STEM
ABF
Perovskite Oxide
EELS
Dispersion Curve

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 (2006).

Kiyomura, T.; Nemoto, T.; Ogawa, T.; Minari, T.; Yoshida, K.; Kurata, H.; Isoda, S., Thin-Film Phase of Pentacene Film Formed on KCl by Vacuum Deposition, *Jpn. J. Appl. Phys.*, **45,** 401-404 (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 (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 (2012).

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

Atomic Level Observation of Octahedral Distortions at the Perovskite Oxide Heterointerface

For perovskite oxides, ABO_3, slight octahedral distortions have close links to functional properties. While perovskite oxide heterostructures offer a good platform for controlling functionalities, atomistic understanding of octahedral distortion at the interface has been a challenge as it requires precise measurements of the oxygen atomic positions. Here we demonstrate an approach to clarify distortions at an atomic level using annular bright-field (ABF) imaging in aberration-corrected scanning transmission electron microscopy (STEM), which provides precise mappings of cation and oxygen atomic positions from distortion-minimized images. This technique revealed significant distortions of RuO_6 and ScO_6 octahedra at the heterointerface between a $SrRuO_3$ (SRO) film and a $GdScO_3$ (GSO) substrate. We also found that structural mismatch was relieved within only four unit cells near the interface by shifting the oxygen atomic positions to accommodate octahedral tilt angle mismatch. The present results underscore the critical role of the oxygen atom in the octahedral connectivity at the perovskite oxide heterointerface.

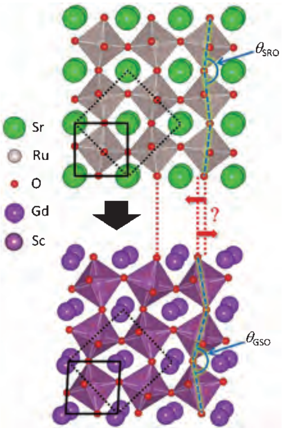


Figure 1. Crystal structures of $SrRuO_3$ (SRO) and $GdScO_3$ (GSO).

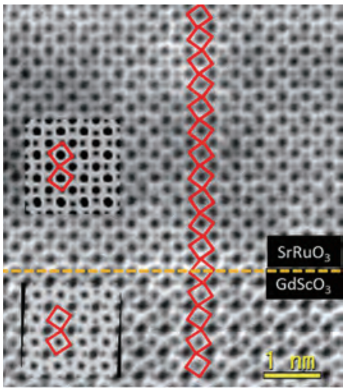


Figure 2. Atomic-scale structural characterization of SRO/GSO heterostructure by high-resolution ABF-STEM techniques. The oxygen atoms are clearly visible, revealing the projected shape of each oxygen octahedron and the connectivity of the octahedra across the heterointerface as indicated with the red open squares. Simulated images are also inserted in the image.

Optical Guided Modes Coupled with Čerenkov Radiation Excited in Si Slab Using Angular-resolved Electron Energy-loss Spectrum

Retardation effects in the valence electron energy-loss spectrum (EELS) of a Si slab are analyzed by angular-resolved EELS. The dispersion curves of the valence spectra excited in a slab are directly observed from a specimen area with several different thicknesses and are interpreted by performing a calculation of the dispersion relation using Kröger's formula. The dispersion curves observed below about 3 eV are attributed to guided modes coupled with Čerenkov radiation (ČR). The coupling between guided modes and ČR is found to be dependent on the sample thickness (*t*). For the sample with $t > 150$ nm, the intensity of the guided modes increased linearly with thickness, revealing the coupling with ČR. For $t < 150$ nm, however, the intensity of the guided modes rapidly decreased due to a diminished coupling with ČR, resulting from the thickness-dependent dispersion curves of the guided modes.

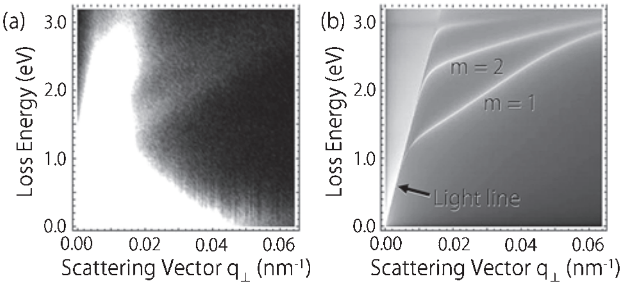


Figure 3. Experimental (a) and calculated (b) E-q maps of a Si slab of thickness t = 126 nm. Dispersion curves of 1st & 2nd order guided modes can be seen.

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)

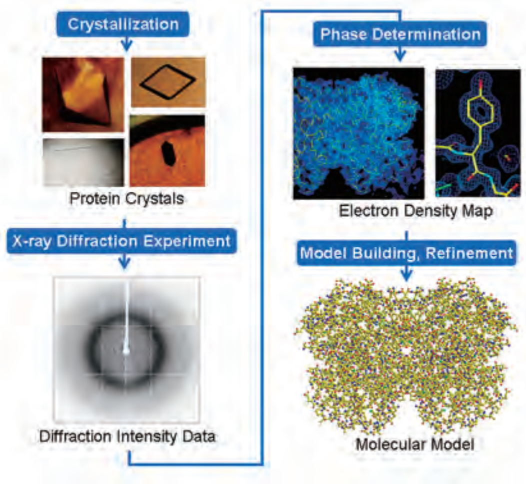
* Advanced Research Center for Beam Science, Laboratory for Structual Proteomics

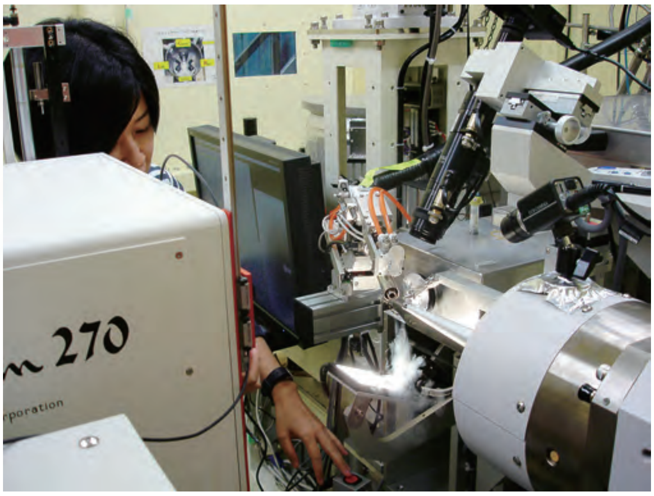
Scope of Research

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.

KEYWORDS

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





Selected Publications

Fujii, T.; Maeda, M.; Mihara, H.; Kurihara, T.; Esaki, N.; Hata, Y., Structure of a NifS 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 Oxygenase Component of a Resorcinol Hydroxylase (GraA) 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 oxygenase component (GraA) from *Rhizobium* sp. strain MTP-10005 in complex with FAD. GraA is a tetramer and its subunit consists of 409 amino acid residues with the mass of 43,305 Da.

The N-terminal His-tagged GraA was used for crystallization. The protein solution consisted of 10 mg/ml GraA, 1 mM FAD, and 50 mM Tris-HCl pH 8.0. Crystals with size of $0.1 \times 0.07 \times 0.05$ mm^3 were obtained in about 4 days by a sitting drop vapor diffusion method with a reservoir solution consisting of 20% (w/v) PEG3350 and 0.2 M KNO_3 (Figure 1). They belonged to the trigonal space group $P3_221$ with unit cell dimensions of a=b=204.4 Å, c=299.9 Å. Diffraction data were collected up to 3.2 Å resolution under cryogenic conditions at beamline BL5A, PF, Tsukuba, Japan. The structure was determined by molecular replacement and refined at 3.2 Å resolution.

In the holo-form crystal, four tetramers exist in the asymmetric unit and each subunit binds a FAD. GraA is a tetramer of four identical subunits related to one another by three molecular two-fold axes. A given pair of two subunits in the molecule form a close dimer with C-terminal α-helical domains crossed together around a molecular two-fold axis. Then, two of the close dimers form a loose dimer around another molecular two-fold axis crossing perpendicular to the former two-fold axis. Finally, the GraA tetrameric molecule adopts the structure of a dimer of dimers with three molecular two-fold axes perpendicular to one another. The subunit consists of three domains. The N-terminal domain (residues Met1–Ala121) has an α-structure mainly of antiparallel α-helices, the central domain has a β-structure of two β-sheets stacked together, and the C-terminal domain (residues Phe218–Tyr409) has a four-helix-bundle structure of long antiparallel α-helices involved in tetramer formation. The FAD is located in the space that is encompassed by these three domains (Figure 2). The FAD binds to the polypeptide chain via hydrophobic and hydrophilic interactions (Figure 3). The loop region of 13 residues (residues Gly271–Asn283), which is disordered in the apo-form, is ordered and covers FAD of another subunit (Figures 2 and 3). The turn portion of the loop occludes the entrance of the putative active site.

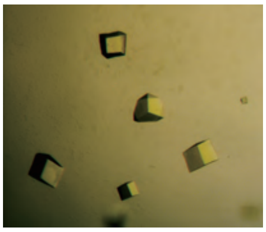


Figure 1. Crystals of the oxygenase component of a resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 in complex with FAD.

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

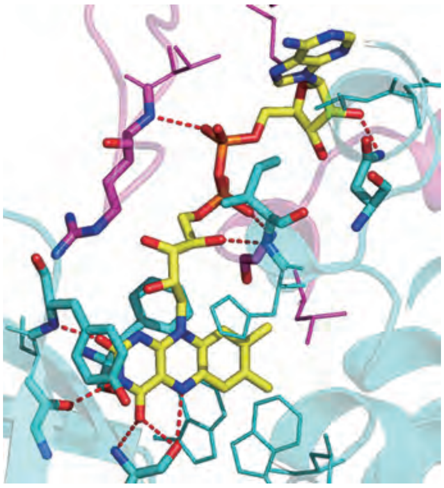


Figure 3. Structure of the FAD-binding site of the oxygenase component of a resorcinol hydroxylase (GraA) from *Rhizobium* sp. strain MTP-10005 in complex with FAD.

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)


PD(JSPS)
ADAK, Laksmikanta
(Ph D)


PD(JSPS)
GOWER, Nicholas John
(Ph D)


PD
TAKENAKA, Toshio
(D Eng)

Researchers (pt)

MINAGAWA, Toshie
WATANABE, Takeshi

Assist Res Staff (pt)

NAKAGAWA, Naohisa

Students

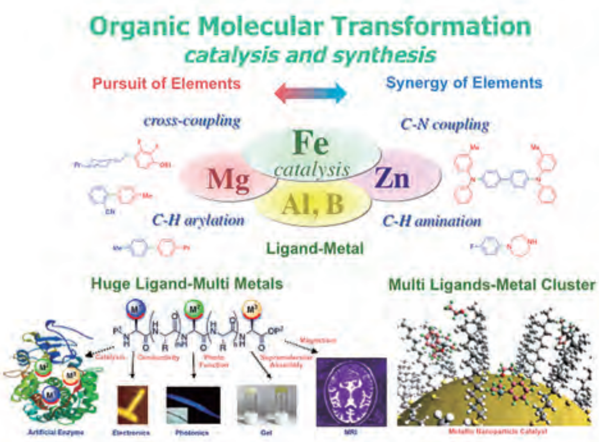
NAKAJIMA, Sho (M2)
MOCHIZUKI, Ayaka (M2)
YOSHIDA, Ryota (M2)
AGATA, Ryosuke (M1)
AOKI, Yuma (M1)
NISHIKORI, Tatsushi (M1)
ISHIBASHI, Kosuke (UG)

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

Carbon–Carbon Bond Formation
Iron Catalyst
Cross-Coupling Reaction
Metallated Peptide
Metallic Nanoparticle



Selected Publications

Kawamura, S.; Nakamura, M., Ligand-controlled Iron-catalyzed Cross Coupling of Benzylic Chlorides with Aryl Grignard Reagents, *Chem. Lett.*, **42,** 183–185 (2013).

Gabr, R. K.; Hatakeyama, T.; Takenaka, K.; Takizawa, S.; Okada, Y.; Nakamura, M.; Sasai, H., DFT Study on 5-Endo-Trig-Type Cyclization of 3-Alkenoic Acids Using Pd-SPRIX Catalyst: Importance of the Rigid Spiro Framework for Both Selectivity and Reactivity, *Chem. Eur. J.*, **19,** 9518–9525 (2013).

Jin, M.; Nakamura, M., Synthesis of Novel C_2 and C_1 Symmetrical CHIRAPHOS Derivatives and Their Application in Palladium-Catalyzed Miyaura-Michael Reaction, *Chem. Lett.*, **42,** 1035–1037 (2013).

Takaya, H.; Iwaya, T.; Ogata, K.; Isozaki, K.; Yokoi, T.; Yoshida, R.; Yasuda, N.; Seike, H.; Takenaka, T.; Nakamura, M., Synthesis, Structure, and Function of PCP Pincer Transition-Metal-Complex-Bound Norvaline Derivatives, *Synlett.*, **24,** 1910–1914 (2013).

Ogata, K.; Sasano, D.; Isozaki, K.; Yoshida, R.; Takenaka, T.; Seike, H.; Ogawa, T.; Kurata, H.; Yasuda, N.; Takaya, H.; Nakamura, M., Synthesis and Self-Assembly of NCN-Pincer Pd-Complex-Bound Norvalines., *Chem. Eur. J.*, **19,** 12356–12375 (2013).

Topics

Iron-Catalyzed Aromatic Amination for Nonsymmetrical Triarylamine Synthesis

Transition-metal-catalyzed aromatic amination is widely used for the synthesis of arylamines, which are of particular interest in the field of organic electronics and bioactive compounds. We developed a facile and environmentally benign method based on iron-catalyzed aromatic amination for synthesizing diaryl- and triarylamines. The key to the success of this protocol is the use of in situ generated magnesium amides in the presence of a lithium halide, which dramatically increases the product yield. The present method is simple and free of precious and expensive metals and ligands, thus providing a facile route to triarylamines.

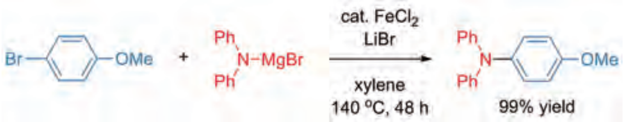


Figure 1. Iron-catalyzed aromatic amination for nonsymmetrical triarylamine synthesis.

NCN-Pincer Pd-Complex-Bound Norvalines: Synthesis and Self-Assembly

Bioorganometallic materials, which are hybrids of biogenic molecules and functional organometallic compounds, have been recently recognized as fascinating materials because of their emergent properties descending from both the metallic and biological parts. We reported the synthesis of the NCN-pincer Pd-complex-bound norvalines, their dipeptide, and self-assembly of aliphatic Pd-complex-bound norvalines. The molecular structures were determined using single-crystal X-ray structure analysis, cryogenic-temperature transmission electron microscopy (cryo-TEM), synchrotron small-angle X-ray scattering (SAXS), wide-angle X-ray scattering (WAX), and various spectroscopic analyses.

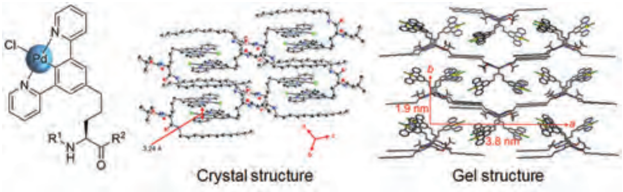


Figure 2. NCN-Pincer Pd-complex-bound norvalines: packing structure in crystal and gel state.

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 –

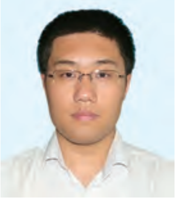
http://www.scl.kyoto-u.ac.jp/~shimakgr/indexE.html


Prof
SHIMAKAWA, Yuichi
(D Sc)


Assist Prof
KAN, Daisuke
(D Sc)


Assist Prof
SAITO, Takashi
(D Sc)


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


PD
ZHANG, Shoubao
(Ph D)

Students

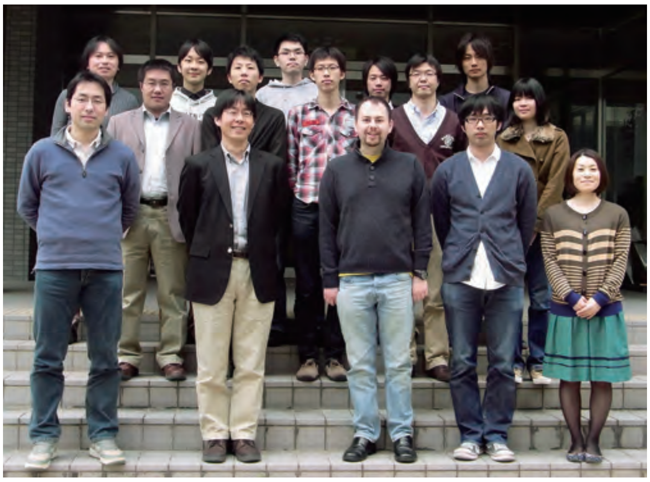
HIRAI, Kei (D2)
SEKI, Hayato (D1)
HADAME, Koji (M2)
HOSAKA, Yoshiteru (M2)
MURAKAMI, Noriaki (M2)
KUROSAKI, Ryo (M1)
SATO, Riko (M1)
MANABE, Keisuke (M1)

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.; Saito, T.; Hayashi, N.; Takano, M.; Shimakawa, Y., Ligand-hole Localization in Oxides with Unusual Valence Fe, *Sci. Rep.*, **2,** 449/1-6 (2012).

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,** 27/1-4 (2011).

Azuma, M.; Chen, W. T.; Seki, H.; Czpski, M.; Olga, S.; Oka, K.; Mizumaki, M.; Watanuki, T.; Ishimatsu, N.; Kawamura, N.; Ishiwata, S.; Tucker, M. G.; Shimakawa, Y.; Attfield, J. P., Colossal Negative Thermal Expansion in $BiNiO_3$ Induced by Intermetallic Charge Transfer, *Nat. Comm.*, **2,** 347 (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).

Kan, D.; Terashima, T.; Kanda, R.; Masuno, A.; Tanaka, K.; Chu, S.; Kan, H.; Ishizumi, A.; Kanemitsu, Y.; Shimakawa, Y.; Takano, M., Blue-light Emission at Room Temperature from Ar^+ -irradiated $SrTiO_3$, *Nat. Mater.*, **4,** 816-819 (2005).

Valence Change of A'-site Mn by A-site Doping in $La_{1-x}Na_xMn_3Ti_4O_{12}$

Recently, we have successfully synthesized a novel A-site-ordered perovskite $LaMn_3Ti_4O_{12}$. Our analysis of the X-ray diffraction, X-ray absorption spectrum, and magnetization of this compound suggested that the compound has a nominal composition of $La^{3+}Mn^{1.66+}{}_3Ti^{4+}{}_4O^{2-}{}_{12}$, with an unusually low valence Mn ion at the A'-site. Mn with a valence lower than +2 is very rare for oxides.

To precisely evaluate the cation-valence state in $AMn_3Ti_4O_{12}$, it is quite important to determine not only the overall stoichiometry but also the precise site occupancies of each ion. However, Ti/Mn mixing is not easy to explore from the structure refinements using normal (non-resonant) X-ray or neutron diffraction techniques because Ti and Mn have similar X-ray scattering factors and neutron scattering amplitudes. To overcome this, we adopted a resonant X-ray diffraction (RXRD) technique, which enables elements with close atomic numbers like Ti and Mn to be distinguished by making use of contrast between their anomalous scattering factors f' and f''.

In this study, we focus on a $La_{1-x}Na_xMn_3Ti_4O_{12}$ system, in which Na^+ substitution for La^{3+} at the A-site effectively causes the hole doping and would affect the A'-site Mn valence. $La_{1-x}Na_xMn_3Ti_4O_{12}$ ($x = 0$, 0.5, 1) were synthesized under high-pressure and high-temperature conditions, and their crystal structures and magnetic properties were investigated. Ti/Mn occupancies at the B site were also examined by using resonant X-ray diffraction, and the results confirm that they are stoichiometric with high Ti/Mn site selectivity. The Na^+ substitution changes the valence state of the A'-site Mn but not of the B-site Ti, and thus the compositions of the synthesized samples are expressed as $La_{1-x}Na_xMn^{\{(5+2x)/3\}+}{}_3Ti^{4+}{}_4O_{12}$ (Figure 1). The magnetic properties change from spin-glass-like to antiferromagnetic to spin-glass-like behavior according to the valence states of A'-site Mn.

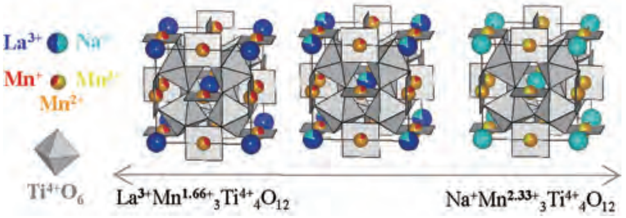


Figure 1. Crystal structure and valence Change of A'-site Mn of $La_{1-x}Na_xMn_3Ti_4O_{12}$.

Anisotropic In-Plane Lattice Strain Relaxation in Brownmilleraite $SrFeO_{2.5}$ Epitaxial Thin Films

Oxygen-deficient Fe-based perovskites exhibit various structural and physical properties depending on the amount as well as the arrangement of the oxygen vacancies. Importantly these materials with various oxygen vacancies are synthesized by either oxidation or reduction reactions of the brownmillerite $SrFeO_{2.5}$. Recently, it was also demonstrated that such reactions of the epitaxial thin films and artificial superlattices of the brownmillerite provided information about the oxygen-ion diffusion. Thus, it is important to learn the structural properties of the epitaxial thin films of the brownmillerite.

In this study we performed detailed structural characterizations and found the anisotropic in-plane lattice relaxation behavior of brownmillerite $SrFeO_{2.5}$ epitaxial thin films grown on (110) $DyScO_3$ substrates. The in-plane lattices in the films less than 50 nm thick are fixed by the substrate lattice, whereas partial in-plane lattice relaxation along the [010] direction occurs in a 50 nm thick film. When the thickness reaches 98 nm, the film eventually exhibits lattice relaxation in both the [010] and the [10–1] in-plane directions.

The high angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) observations for the partially relaxed film (Figure 2) revealed that in the bottom region, a dislocation, at which additional Fe atoms are seen, leads to formations of the stacking faults. In the surface region of the film, the complicated lattice defects propagated from the bottom result in the partial in-plane lattice relaxation associated with the disordered arrangements of the FeO_4 tetrahedra and the FeO_6 octahedra in the surface region. The preferential generation of the dislocations in the (10–1) plane can be explained by taking into account the anisotropic thermal expansion of $SrFeO_{2.5}$, which results in the increase in the lattice mismatch between the film and the substrate only along the [010] direction in the cooling process after the film deposition.

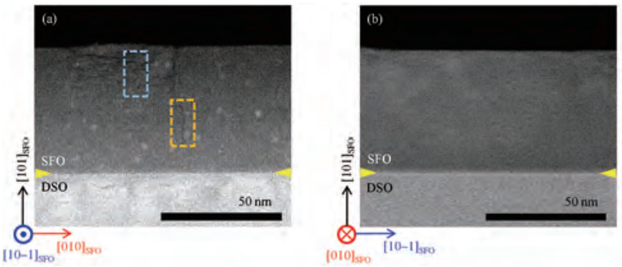


Figure 2. Anisotropic in-plane lattice strain relaxation revealed by HAADF-STEM observations. The images were taken along the (a) $[10–1]_{SFO}$ (left) and (b) $[010]_{SFO}$ (right) directions.

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
LIN, Ya-Fan
(D Sc)

Assist Res Staff

NAKAMURA-OGATA, Yuki

Researcher (pt)

ICHIHARA, Nobuko

Students

CHANG, Yung-Hung (D3)
TAKETANI, Tomoyoshi (M2)
MINAMI, Ataru (M2)
ISHIKI, Satoru (M1)
TAGUCHI Hiro-omi (M1)
IIZUKA, Eisuke (UG)
TANIGAWA, Ippei (UG)

Visiting Researcher

Prof CHEN, Jwu-Ting	National Taiwan University, Taiwan, 28 February–28 May

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

Chang, Y.-H.; Nakajima, Y.; Tanaka, H.; Yoshizawa, K.; Ozawa, F., Facile N-H Bond Cleavage of Ammonia by an Iridium Complex Bearing a Non-innocent PNP-Pincer Type Phosphaalkene Ligand, *J. Am. Chem. Soc.*, **135,** 11791-11794 (2013).

Wakioka, M.; Nakamura, Y.; Hihara, Y.; Ozawa, F.; Sakaki, S., Factors Controlling the Reactivity of Heteroarenes in Direct Arylation with Arylpalladium Acetate Complexes, *Organometallics*, **32,** 4423-4430 (2013).

Nakajima, Y.; Okamoto, Y.; Chang, Y.-H.; Ozawa, F., Synthesis, Structures, and Reactivity of Ruthenium Complexes with PNP-pincer Type Phosphaalkene Ligands, *Organometallics*, **32,** 2918-2925 (2013).

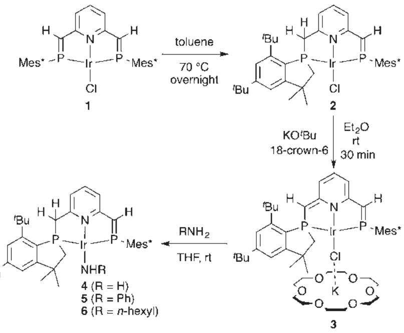
Chang, Y.-H.; Nakajima, Y.; Ozawa, F., A Bis(phosphaethenyl)pyridine Complex of Iridium(I): Synthesis and Catalytic Application to N-Alkylation of Amines with Alcohols, *Organometallics*, **32,** 2210-2215 (2013).

Wakioka, M.; Kitano, Y.; Ozawa, F., A Highly Efficient Catalytic System for Polycondensation of 2,7-Dibromo-9,9-dioctylfluorene and 1,2,4,5-Tetrafluorobenzene via Direct Arylation, *Macromolecules*, **46,** 370-374 (2013).

N–H Bond Cleavage of Ammonia by an Iridium Complex Bearing a Non-innocent PNP-Pincer Type Phosphaalkene Ligand

Late transition metal complexes with a pyridine-based PNP-pincer ligand have attracted a great deal of attention owing to their facile cleavage of non-activated bonds via non-innocent behavior of the ligand. Herein, we describe the synthesis and reactions of novel iridium complex **3** with an unsymmetrical PNP-pincer ligand composed of a dearomatized pyridine core and benzophospholanylmethyl and phosphaethenyl arms at the 2,6-positions, which was prepared in two steps from [IrCl(BPEP)] (**1**, BPEP = 2,6-bis[2-(2,4,6-tri-*tert*-butylphenyl)-2-phosphaethenyl]-pyridine) (Scheme 1).

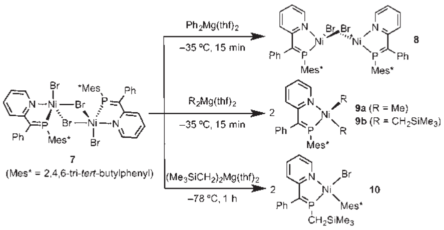
Phosphaalkenes with a P=C bond possess an extremely low-lying π^* orbital around the phosphorus atom, and thus exhibit strong π-accepting ability toward transition metals. Reflecting this particular ligand property of phosphaalkene, complex **3** undergoes extended π-conjugation over the molecule, and exhibits extremely high reactivity toward N–H bond cleavage of ammonia and amines to afford the corresponding amido complexes **4-6** in quantitative yields (Scheme 1).



Scheme 1. Synthesis of **3** and its reactivity toward ammonia and amines.

Synthesis of Phosphaethenylpyridine-Ni Complex and Its Reactivity toward Organomagnesium Reagents

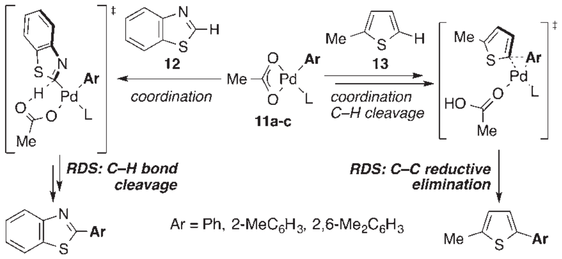
Recently, we have demonstrated that phosphaalkene ligand successfully stabilizes low oxidation state complexes like a Fe(I) aryl mesityl complex. In this study, we report the synthesis of novel phosphaalkene–Ni complex $[NiBr_2(pep)]_2$ (**7**) (PEP = 2-(1-phenyl-2-phosphaethenyl)pyridine) and its unique reactivity toward organomagnesium reagents. Complex **7** was synthesized by the reaction of PEP with $[NiBr_2(dme)]$ (dme = 1,2-dimethoxyethane) in benzene at 60°C. The reaction of **7** with $Ph_2Mg(thf)_2$ affords an one-electron reduction product, bromine-bridged Ni(I) dimer **8**. Additionally, dialkylmagnesiums ($R_2Mg(thf)_2$; R = Me, CH_2SiMe_3) also reacted with **7** at –35°C to give dialkyl Ni(II) complexes **8** and **9**. However, the reaction of dialkylmagnesiums at –78°C did not give monoalkyl complexes but gave monoaryl complexes **10** with exchange of the alkyl and Mes* groups. These results indicate that the exchange of the alkyl and Mes* groups would occur on a high-valent Ni complex intermediate.



Scheme 2. Reactivity of **7** toward organomagnesium reagents.

Factors Controlling the Reactivity of Heteroarenes in Direct Arylation with Arylpalladium Acetate Complexes

The palladium-catalyzed direct arylation of heteroarenes with aryl halides has emerged as a viable alternative to conventional cross-coupling reactions. We report a detailed mechanistic study on factors controlling the reactivity of heteroarenes in direct arylation with well-defined models of the presumed intermediate $[PdAr(O_2CMe\text{-}\kappa^2O)L]$ (**11a-c**, Ar = Ph, 2-MeC_6H_3, 2,6-$Me_2C_6H_3$). The reactivity order of heteroarenes was evaluated by competitive reactions, showing that benzothiazole (**12**, $pK_a = 27$) is significantly less reactive than 2-methylthiophene (**13**, $pK_a = 42$). The reaction of **13** obeyed simple second-order kinetics, and the deuterium-labeling experiments and DFT calculations indicated the occurrence of rate-determining reductive elimination. On the other hand, the reaction of **12** displayed saturation kinetics due to the occurrence of relatively stable coordination of **12** prior to C–H bond cleavage. This coordination stability enhances the activation barrier for C–H bond cleavage, thereby causing the modest reactivity of **12**.



Scheme 3. Reaction of **11a-c** with heteroarenes **12** and **13**.

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)

Researcher

NISHIHARA, Taishi

Students

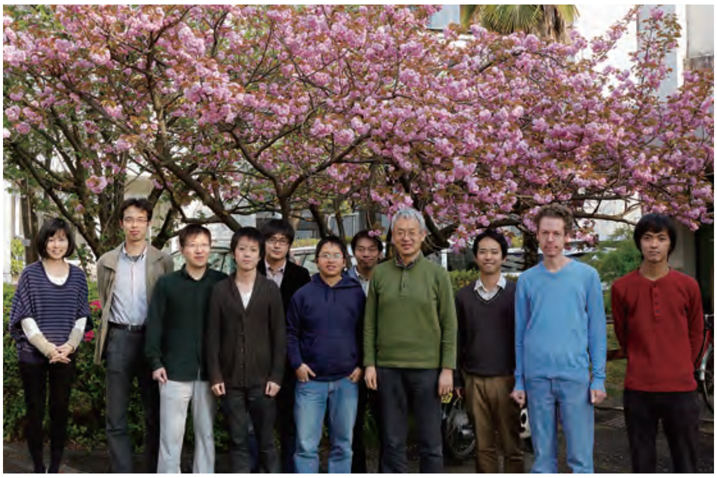
NAKAMURA, Tooru (M2)
OHNO, Kai (M1)

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 low-dimensional 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 Electron-doped $SrTiO_3$: 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).

Auger Process in Disklike InAs Quantum Structures

Fabrication and characterization of semiconductor nanostructures have been extensively studied due to interest both in the fundamental physics and potential applications in optoelectronic devices. We studied the mechanisms of upconverted photocurrent in InAs quantum structures embedded in $Al_xGa_{1-x}As$ using simultaneous measurements of photoluminescence and photocurrent spectra. Efficient upconversion was verified in samples with and without quantum dots. The dominant upconversion process from low temperatures to room temperature was found to occur through an Auger process in disklike InAs quantum structures. The results suggest the importance of shallow energy levels, which enable upconversion and efficient carrier extraction through multiparticle interactions. The disklike structure was concluded to be a suitable intermediate-band structure in terms of the energy conversion efficiency.

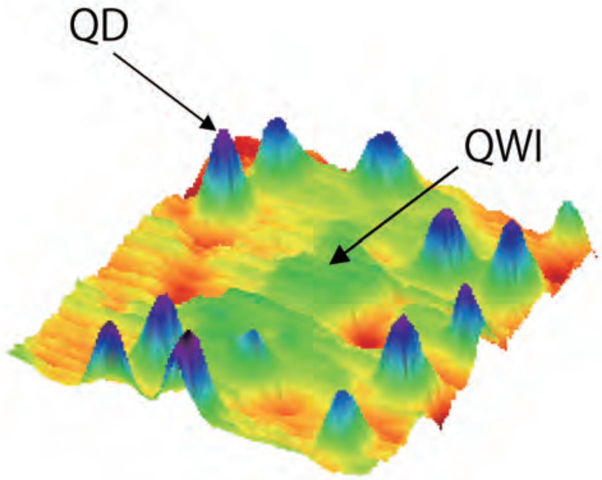


Figure 1. 3D AFM image with quantum dots (QDs) and a quantum well island (QWI) on the wetting layer of an InAs/AlGaAs layer without capping.

Charged Exciton Formation and Recombination Dynamics in Hole-doped Carbon Nanotubes

Carbon nanotubes are one of the excellent materials for studying the optical properties of excitons, because of their unique band structures and large exciton binding energies. We studied the trion (charged exciton) formation and recombination dynamics in hole-doped (7,5) single-walled carbon nanotubes (SWCNTs) by performing femtosecond transient absorption spectroscopy. The doping of SWCNTs with holes leads to a fast decay component from an exciton to a trion, and the trion decays with a lifetime of a few picoseconds. The experimental results can be explained by a quantized model accounting for the dark exciton and trion states and the hole number distribution in a SWCNT. Our findings show that the optical responses of SWCNTs can be manipulated by doping of SWCNTs with a small number of holes.

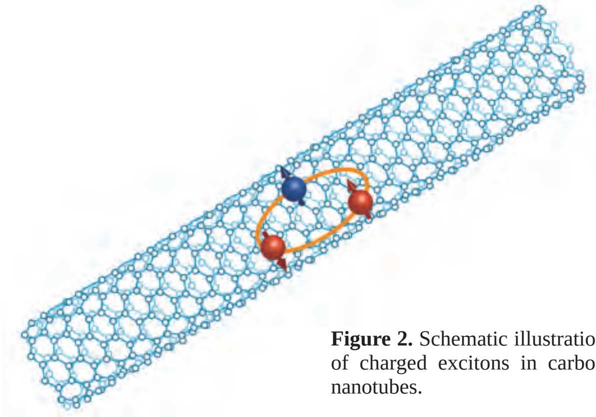


Figure 2. Schematic illustration of charged excitons in carbon nanotubes.

Current–voltage Characteristics in Ge/Si Quantum Dot Solar Cells

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. In QDs, physical processes of generation, relaxation, and recombination of carriers are determined by their nanostructures and differ from those in bulk crystals. We report studies of current–voltage characteristics in Ge/Si QD solar cells in the temperature range from 100 to 300 K. We show that even though open-circuit voltage (V_{oc}) decreases with increasing temperature, it depends on the nominal Ge thickness, indicating that V_{oc} reduction is primarily caused by a decrease in the bandgap energy of the cell. From photoluminescence decay measurements, we found that rapid carrier extraction from QDs occurred in the solar cells; this process eliminates the quasi-Fermi energy splitting between the QDs and the host semiconductor and causes V_{oc} reduction in QD solar cells.

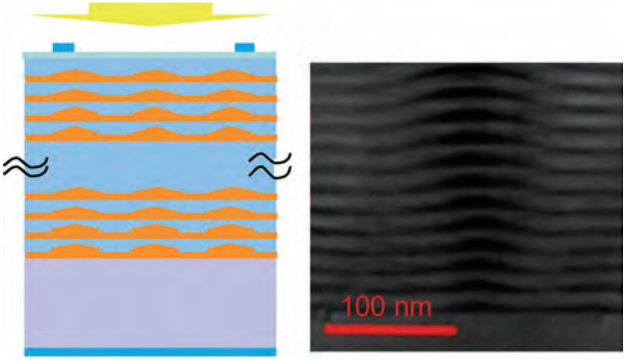


Figure 3. Schematic illustration of Ge/Si QD solar cells (left). TEM image of Ge QD array (right).

Bioinformatics Center
– Chemical Life Science –

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

Assoc Prof
GOTO, Susumu
(D Eng)

Program-Specific Assist Prof
TOKIMATSU, Toshiaki
(D Agr)

Program-Specific Assist Prof
KOTERA, Masaaki
(D Sc)

PD
JOANNIN, Nicolas
(Ph D)

Researchers

MORIYA, Yuki
NAKAGAWA, Zenichi
MUTO, Ai

Students

SHIMIZU, Yugo (D3)
MIZUTANI, Sayaka (D3)
NISHIMURA, Yosuke (D3)
FUJITA, Megumi (D3)
MIHARA, Tomoko (D3)
JIN, Zhao (D3)
SATOH, Takanori (M2)

Visiting Researcher

Assoc Prof INGALE, Arun Govindrao North Maharashtra University, India, 1 May–31 July

Scope of Research

The proteins responsible for biosynthesis, biodegradation, and transport of additional molecules, such as small metabolites, lipids and glycans, are encoded in the genome, which may indicate that all cellular functions are specified by the genomic DNA sequence. In practice, however, inferring higher-level systemic functions of the cell or the organism needs more than solely the genomic information. We are developing bioinformatics methods to integrate different types of data and knowledge on various aspects of the biological systems towards basic understanding of life as a molecular interaction/reaction system and also towards practical applications in medical and pharmaceutical sciences.

GenomeNet Database Resources

DBGET: Integrated Database Retrieval System
DBGET search
LinkDB search
KEGG: Kyoto Encyclopedia of Genes and Genomes
KEGG2 - Table of contents
KEGG PATHWAY - Systems information: pathways
KEGG BRITE - Systems information: ontologies
KEGG Organisms - Organism-specific entry points
KEGG GENES - Genomic information
KEGG LIGAND - Chemical information
KEGG MEDICUS: Health-related info resource
MEDICUS search
Reaction Ontology: Reaction classifications
varDB: Antigenic variation database
Community Databases
CYORF - Cyanobacteria annotation database
BSORF - Bacillus subtilis genome database
EXPRESSION - Gene expression profile database

KEGG pathway maps
BRITE functional hierarchies
KEGG Organisms
Metagenomes
Draft genomes

Database links

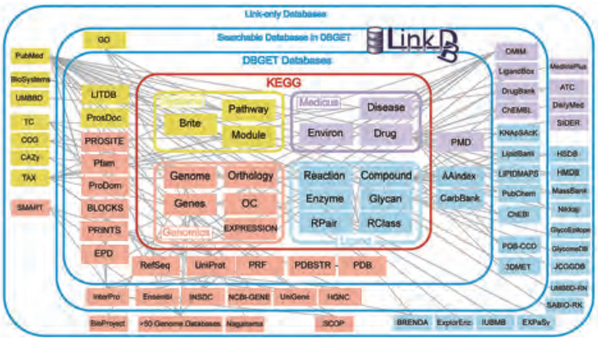
DB growth curve

GenomeNet Bioinformatics Tools

Sequence Analysis
BLAST / FASTA - Sequence similarity search
MOTIF - Sequence motif search
CLUSTALW / MAFFT / PRRN - Multiple alignment
Genome Analysis
OC Viewer - KEGG ortholog clusters
REST service is available New!
KAAS - KEGG automatic annotation server
EGassembler - EST consensus contigs
GENIES - Gene network prediction
DINIES - Drug-target network prediction
Chemical Analysis
SIMCOMP / SUBCOMP - Chemical structure search
REST service is available New!
KCaM - Glycan structure search
PathComp - Possible reaction path computation
PathSearch - Similar reaction path search
PathPred - Reaction pathway prediction
E-zyme - Enzymatic reaction prediction

Kyoto University Bioinformatics Center

GenomeNet Top page



Databases available in the DBGET/LinkDB system of the GenomeNet service. Color of each database represents the type of its contents, yellow: systems information, purple: medical information, pink: genetic information, light blue: chemical information.

KEYWORDS

GenomeNet
(Meta)genomics
Reaction Ontology
Bioinformatics
Pharmacoinformatics

Selected Publications

Kotera, M.; Tabei, Y.; Yamanishi, Y.; Tokimatsu, T.; Goto, S., Supervised *de novo* Reconstruction of Metabolic Pathways from Metabolome-scale Compound Sets, *Bioinformatics*, **29,** i135-i144 (2013).

Muto, A.; Kotera, M.; Tokimatsu, T.; Nakagawa, Z.; Goto, S.; Kanehisa, M., Modular Architecture of Metabolic Pathways Revealed by Conserved Sequences of Reactions, *J. Chem. Inf. Model*, **53,** 613-622 (2013).

Nakaya, A.; Katayama, T.; Itoh, M.; Hiranuka, K.; Kawashima, S.; Moriya, Y.; Okuda, S.; Tanaka, M.; Tokimatsu, T.; Yamanishi, Y.; Yoshizawa, A. C.; Kanehisa, M.; Goto, S., KEGG OC: A Large-scale Automatic Construction of Taxonomy-based Ortholog Clusters, *Nucleic Acids Res.*, **41,** D353-D357 (2013).

Mizutani, S.; Pauwels, E.; Stoven, V.; Goto, S.; Yamanishi, Y., Relating Drug-protein Interaction Network with Drug Side-effects, *Bioinformatics*, **28,** i522-i528 (2012).

Kotera, M.; Yamanishi, Y.; Moriya, Y.; Kanehisa, M.; Goto, S., GENIES: Gene Network Inference Engine Based on Supervised Analysis, *Nucleic Acids Res.*, **40,** W162-W167 (2012).

KEGG OC: An Automatically Constructed Comprehensive Ortholog Clusters

As the number of fully sequenced genomes is rapidly growing, it has become increasingly important to automate the identification of orthologs and the construction of ortholog clusters in order to understand functional properties and biological roles of genes in these genomes. The ortholog clusters also play a key role in functional annotation for newly sequenced genomes, because orthologs tend to have equivalent functions. KEGG OC is a novel database of ortholog clusters based on the whole genome comparison. The current version of KEGG OC contains 1,223,674 ortholog clusters, obtained by clustering 10,615,995 genes in 2,717 complete genomes. The ortholog clusters in KEGG OC were constructed by applying a novel clustering method to all possible protein coding genes in all complete genomes, based on their amino acid sequence similarities. The originality of our clustering algorithm lies in the use of a quasi-clique search (Figure 1) and a step-by-step clustering along the phylogenetic tree. In comparison with KEGG ORTHOLOGY (KO), which is not comprehensive but curated manually, almost every ortholog cluster contains a single major KO group. It suggests that the KEGG OC contains high-quality ortholog clusters. Specifically, KEGG OC has the following features. First, it consists of all fully sequenced genomes of a wide range of organisms from eukaryotes, bacteria and archaea. Second, the ortholog clusters have a hierarchical structure based on the step-by-step clustering. Third, it is computationally efficient to calculate the comprehensive ortholog clusters, which makes it possible to regularly update the contents. Forth, it is compatible with the KEGG database, which provides an easy way to link the ortholog clusters with KEGG PATHWAY, BRITE functional hierarchies, and many more.

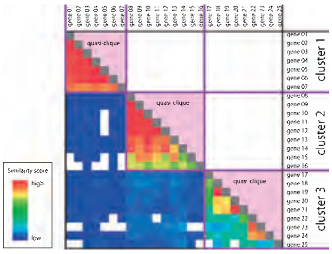


Figure 1. Overview of quasi-clique search on the adjacency matrix.

Modular Architecture of Metabolic Pathways Revealed by Conserved Sequences of Reactions

With increasing complexity of metabolic networks stored in databases, the need to describe the functional modules of metabolic networks is growing. Modular descriptions of network help us to understand complex network by split them into functionally related sub-networks. Towards better understanding of the evolution of the metabolic network, we developed a method to extract conserved sequences of reactions called ‘reaction modules’ from the analysis of all known metabolic pathways stored in the KEGG PATHWAY database. Our method is based on the similarity of chemical structure transformation patterns along the metabolic pathways. This is a purely chemical similarity measure without incorporating any protein sequence information or the EC number information. It enables us to analyze reactions with no EC numbers assigned or even with no enzymes identified. The reaction modules, which are conserved sequences of similar reactions, are systematically searched in the KEGG metabolic pathways using the similarity scoring scheme between reactions. The extracted reaction modules are repeatedly used as if they are building blocks of the metabolic network and contain chemical logic of organic reactions. We identified well-conserved, possibly ancient, reaction modules involving 2-oxocarboxylic acids (Figure 2). The chain extension module that appears as the tricarboxylic acid reaction sequence in the TCA cycle is now shown to be used in other pathways together with different types of modification modules. We also identified reaction modules and their connection patterns for aromatic ring cleavages in microbial biodegradation pathways, which are most characteristic in terms of both distinct reaction sequences and distinct gene clusters. The modular architecture of biodegradation modules will have a potential for predicting degradation pathways of xenobiotic compounds. The collection of these and many other reaction modules is made available as part of the KEGG database.

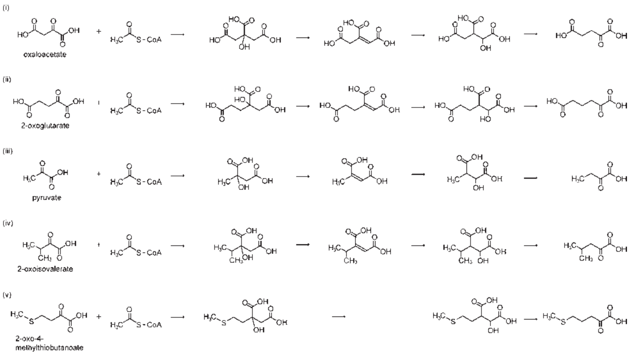


Figure 2. 2-oxocarboxylic acid chain extension module. Examples of reaction module RM001, which performs chain extension by consuming one acetyl-CoA. (i) Extension from oxaloacetate to 2-oxoglutarate in citrate cycle. (ii) 2-oxoglutarate to 2-oxoadipate in lysine biosynthesis. (iii) pyruvate (2-oxopropanoate) to 2-oxobutanoate and (iv) 2-oxoisovalerate to 2-oxoisocaproate in valine, leucine and isoleucine biosynthesis. (v) 2-oxo-4-methylthiobutanoate to 2-oxo-5-methylthiopentanoic acid, the first reaction module of a six tandem repeat of RM001 toward 2-oxo-10-methylthiodecanoate in the biosynthesis pathway of glucosinolates.

Bioinformatics Center
– Mathematical Bioinformatics –

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


Prof
AKUTSU, Tatsuya
(D Eng)


Assist Prof
HAYASHIDA, Morihiro
(D Inf)


Assist Prof
TAMURA, Takeyuki
(D Inf)

Students

NAKAJIMA, Natsu (D3)
ZHAO, Yang (D3)
LU, Wei (D3)
HASEGAWA, Takanori (D2)
MORI, Tomoya (D2)
RUAN, Peiying (D2)
UECHI, Risa (D2)
JIRA, Jindalertudomdee (D1)
CONG, Xiao (M2)
HWANG, Jaewook (M2)
BAO, Yu (RS)
CAO, Yue (RS)

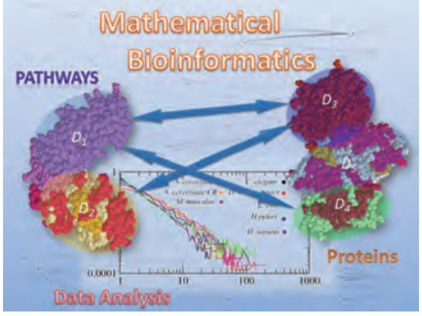
Visiting Researchers

Ms. QIU, Yushan	The University of Hong Kong, China, P.R., 20 May–15 August
Ms. TASSINARI, Anna	Boston University, U.S.A. 27 June–23 September
Mr. CHANG, Chia-Jung	National Taiwan University, Taiwan, 10 July–3 September
Assoc Prof CAI, Hongmin	South China University of Technology, China, P.R., 30 May–23August
Senior Researcher VERT, Jean-Philippe	Curie Institute, France, 27 June–25 August
Assoc Prof Em MELKMAN, Avraham Aharon	Ben Gurion University of the Negev, Israel, 20 February–24 April

Scope of Research

KEYWORDS
Scale-free Networks
Boolean Networks
Grammar-based Compression
RNA Secondary Structures
Chemical Graphs

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, scale-free networks, protein structure prediction, inference of biological networks, chemo-informatics, discrete and stochastic methods for bioinformatics.



Selected Publications

Akutsu, T.; Fukagawa, D.; Halldorsson, M. M.; Takasu, A.; Tanaka, K., Approximation and Parameterized Algorithms for Common Subtrees and Edit Distance between Unordered Trees, *Theoretical Computer Science*, **470,** 10-22 (2013).

Akutsu, T.; Tamura, T., A Polynomial-time Algorithm for Computing the Maximum Common Connected Edge Subgraph of Outerplanar Graphs of Bounded Degree, *Algorithms*, **6,** 119-135 (2013).

Nacher, J. C.; Akutsu, T., Structural Controllability of Unidirectional Bipartite Networks, *Scientific Reports*, **3,** 1647 (2013).

Zhao, Y.; Tamura, T.; Akutsu, T.; Vert, J.-P., Flux Balance Impact Degree: A New Definition of Impact Degree to Properly Treat Reversible Reactions in Metabolic Networks, *Bioinformatics*, **29,** 2178-2185 (2013).

Ruan, P.; Hayashida, M.; Maruyama, O.; Akutsu, T., Prediction of Heterodimeric Protein Complexes from Weighted Protein-Protein Interaction Networks Using Novel Features and Kernel Functions, *PLoS ONE*, **8,** e65265 (2013).

Prediction of Heterodimeric Protein Complexes from Weighted Protein-Protein Interaction Networks Using Novel Features and Kernel Functions

Identification of protein complexes is very important because many proteins express their functional activity by interacting with other proteins and forming protein complexes. Hence, many prediction methods for protein complexes from protein-protein interactions have been developed such as MCL, MCODE, RNSC, PCP, RRW, and NWE. These methods have dealt with only complexes with size of more than three because the methods often were developed based on some density of subgraphs. Heterodimeric protein complexes that consist of two distinct proteins, however, occupy a large part of whole protein complexes according to several comprehensive databases of known complexes. In this study, we proposed seven feature space mappings (F1),...,(F7) from protein-protein interaction data, in which each interaction is weighted based on reliability. Furthermore, we made use of prior knowledge on protein domains, and proposed domain composition kernel $K_c(C_i,C_j)$ for sets C_i, C_j of two distinct proteins and its combination kernel $<\varphi(C_i), \varphi(C_j)>+\alpha K_c(C_i,C_j)$ with our proposed features φ. Here, $K_c(C_i,C_j)=1$ if the domain composition of C_i is equivalent to that of C_j, otherwise 0. We performed ten-fold cross-validation computational experiments for WI-PHI protein-protein interaction data and CYC2008 protein complex catalog, and calculated the F-measures. These results suggest that our proposed kernel considerably outperforms the naive Bayes-based method, which is the best existing method for predicting heterodimeric protein complexes.

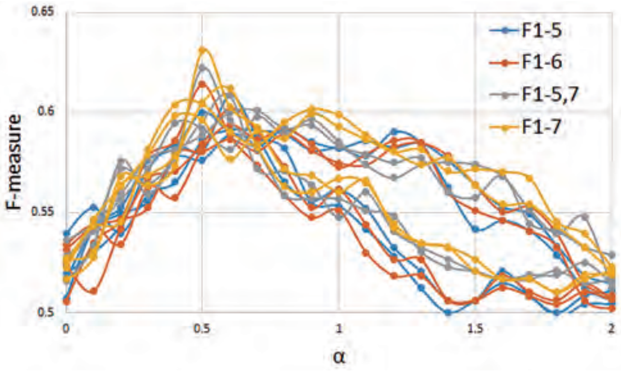


Figure 1. Result on the average F-measure using four sets (F1-5), (F1-6), (F1-5,7), (F1-7) of features and the domain composition kernel with combination parameter α=0, ..., 2.

Maximum Common Connected Edge Subgraph Problem for Chemical Compounds

Calculating similarity of two given chemical compounds is important and fundamental task in chemical informatics. The maximum common connected edge subgraph problem (MCCES) is to find a connected graph with the maximum number of edges that is isomorphic to a subgraph of each of the two input graphs. Though MCCES is useful for measuring similarity of chemical compounds, MCCES is NP-hard even for labeled partial k-trees of bounded degree, and it is reported that most chemical compounds have treewidth at most 3. On the other hand, it is also reported that 94.4% of chemical compounds have outerplanar graph structures, and the maximum degree of almost all chemical compounds is bounded by a constant(e.g., 8). In this study, we developed a polynomial time algorithm for MCCES when the two input graphs are outerplanar graphs of a bounded vertex degree, where it is known that the problem is NP-hard, even for outerplanar graphs of an unbounded degree.

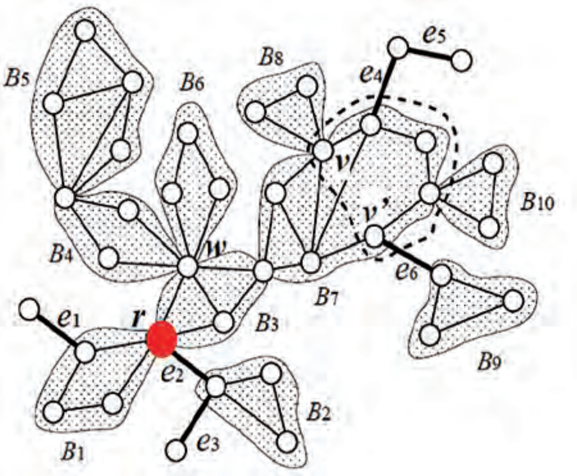


Figure 2. A graph is outerplanar if it can be drawn on a plane such that all vertices lie on the outer face without crossing of edges. Our developed algorithm treats outerplanar graphs as trees, and then dynamic programming-based methods are applied.

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

TAKAHASHI, Keiichiro (D3)
MOHAMED, Ahmed (D2)
YOTSUKURA, Sohiya (D1)
YAMAGUCHI, Shigeru (D1)
CHEN, Zhuoxin (M2)

Visiting Researchers

Lecturer HIBISHY, Hanaa	Tanta University, Egypt, 17 February–15 August
Dr. KUSTRAZE, Ia	Ilia State University, Georgia, 8 April–5 July
Mr. JOHNSTON, Ian	Boston University, U.S.A., 30 May–19 August
Mr. YU-DE Chen	National Cheng Kung University, Taiwan, 17 September–17 March

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

MLAB
Sapporo
2013

2013 International Workshop on
Machine Learning and Applications to Biology

August 5 - 6, 2013
Creative Research Institution, Hokkaido University

Register NOW. It's open to all for no charge.
All researchers and students who are interested in the talks below are welcome.

http://www.cris.hokudai.ac.jp/takigawa/mlab2013/

— 16 inspiring talks —

Samuel Kaski
(Aalto University, Finland)
Learning from Multi-Model Data Integration, Fusion, and Data Translation

Masashi Sugiyama
(Tokyo Institute of Technology, Japan)
Change Detection in Multi-Dimensional Time Series: From Distributional Change to Structural Change

Motoki Shiga
(Toyohashi University of Technology, Japan)
Non-negative Matrix Factorization with Auxiliary Information

Canh Hao Nguyen
(Kyoto University, Japan)
Discriminative Graph Embedding for Label Propagation

Koji Tsuda
(AIST, Japan)
Mining Combinatorial Regulations

Ian Johnston
(Boston University, USA)
Spatially Weighting Genes in Variable Selection for GWAS

David duVerle
(AIST, Japan)
A Regularization Path-Following Approach for Discovering Interactions in High-Dimensional Survival Data

Ichigaku Takigawa
(Hokkaido University, Japan)
Identifying Paired Substructures Significantly Shared among Interacting Structure Pairs

Ziv Bar-Joseph
(Carnegie Mellon University, USA)
Algorithm in Nature

Jean-Philippe Vert
(Mines ParisTech, France)
Fast Lasso-based Isoform Prediction from RNA-Seq Data as a Flow Problem

Martin Frith
(AIST, Japan)
Adapting Classic Alignment Techniques to Modern High-Throughput DNA

Yayoi Natsume
(JST PRESTO, Japan)
Detection of Time-Differences in Histone Modification

Shin-ichi Minato
(Hokkaido University/JST ERATO, Japan)
Recent Research Activities on BDD/ZDD-Based Discrete Structure Manipulation

Satoshi Morinaga
(NEC, Japan)
Factorized Asymptotic Bayesian Inference for Sequential/Hierarchical Latent Variable Models

Toby Dylan Hocking
(Tokyo Institute of Technology, Japan)
Learning to Compare Graph Layouts

Masayuki Karasuyama
(Kyoto University, Japan)
Latent Factor based Subnetwork Feature Selection

CRIS
北海道大学 創成研究機構
京都大学 化学研究所

Organizers: Ichigaku Takigawa (Hokkaido University)
Hiroshi Mamitsuka (Kyoto University)

Selected Publications

Zheng, X.; Ding, H.; Mamitsuka, H.; Zhu, S., Collaborative Matrix Factorization with Multiple Similarities for Predicting Drug-Target Interactions, *Proceedings of the Nineteenth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD 2013)*, 1025-1033 (2013).

Nakamura, A.; Saito, T.; Takigawa, I.; Kudo, M.; Mamitsuka, H., Fast Algorithms for Finding a Minimum Repetition Representation of Strings and Trees, *Discrete Applied Mathematics*, **161 (10-11),** 1556-1575 (2013).

Takigawa, I.; Mamitsuka, H., Graph Mining: Procedure, Application to Drug Discovery and Recent Advance, *Drug Discovery Today*, **18 (1-2),** 50-57 (2013).

Mamitsuka, H.; DeLisi, C.; Kanehisa, M., Data Mining for Systems Biology: Methods and Protocols *Methods in Molecular Biology*, **939,** (2013).

Hancock, T.; Takigawa, I.; Mamitsuka, H., Identifying Pathways of Co-ordinated Gene Expression Data Mining for Systems Biology: Methods and Protocols, *Methods in Molecular Biology*, **939,** 7, 69-85 (2013).

Global Graph Comparison for Biological Networks

We investigate the new problem of global graph comparison from statistical viewpoint, with the application in studying evolutions and preservations of biological networks of different species. Previous works on comparing graphs mainly focused on comparing graphs locally, considering graphs as a collection of subgraphs (as in the case of large chemical structures consisting of many independently functioning substructures). This does not satisfy the requirement of our application in comparing species through their corresponding metabolic, signaling or protein-protein interactions networks. Instead, in our application, the global structures of networks, such as connectivity and robustness of the networks determine the species' biological functionalities. This can contribute to building phylogenetic trees.

We formulate this problem as a graph comparison problem for labeled graphs. Considering orthologous genes from different species as the same node in different graphs, the problem boils down to comparing different graph structures on the same node set. Taking into account biological interpretation of network connectivity and robustness, we require that graph pairs are similar if they differ in the well-connected parts, and similar in sparse parts. For example, in Figure 1, graph G1 should be close to G2, and far from G3, even though both pairs have one edge difference. Therefore, we use eigenvectors and eigenvalues of graph Laplacians to derive similarities and distances (*ged*) for graphs globally [1,2].

Our formulation for this problem is shown to have many properties. It is shown to have the ability to weight edges in graphs according to their roles in network structures, potentially showing the important steps in biological processes. It is a generalization of comparing embeddings of graphs with graph Laplacians, paving way for more extensions with desirable statistical properties [2]. It has unexpected applications beyond our initial intention. We can also use it to select graph-cut clustering solutions, making it a general tool for graph data analysis. As shown in Figure 2, *ged* can differentiate bad clustering solutions with disconnected clusters from good ones [2]. This cannot be seen from usual clustering algorithms. The next step would be applying the method to comparing biological networks of different species to studies their evolutions and preservations in terms of these biological networks.

References

[1] Wicker, N.; Nguyen, C. H.; Mamitsuka, H., A New Dissimilarity Measure for Comparing Labeled Graphs, *Linear Algebra and its Applications*, **438-5,** 2331–2338 (2013).

[2] Nguyen, C. H.; Wicker, N.; Mamitsuka, H., Selecting Graph Cut Solutions via Global Graph Similarity, *IEEE Transactions on Neural Networks and Learning Systems* (in press).

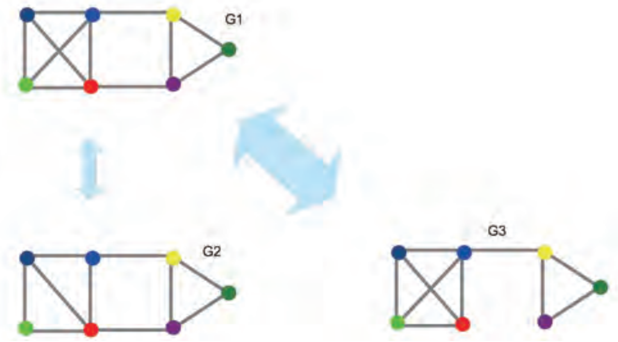


Figure 1. G1 is closer to G2 then to G3 as G3 is not robust, can be disconnected by removing one edge.

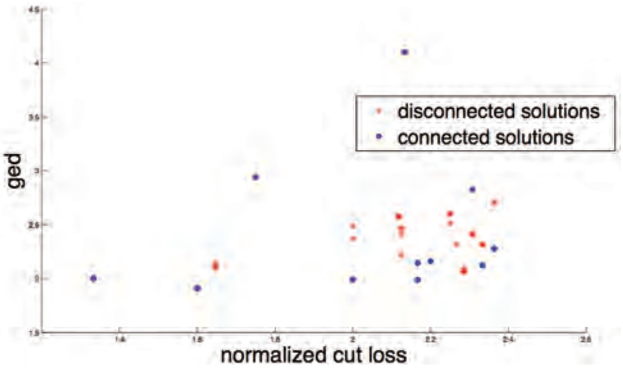


Figure 2. Small *ged* distances usually mean good clustering solutions (connected clusters).

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)

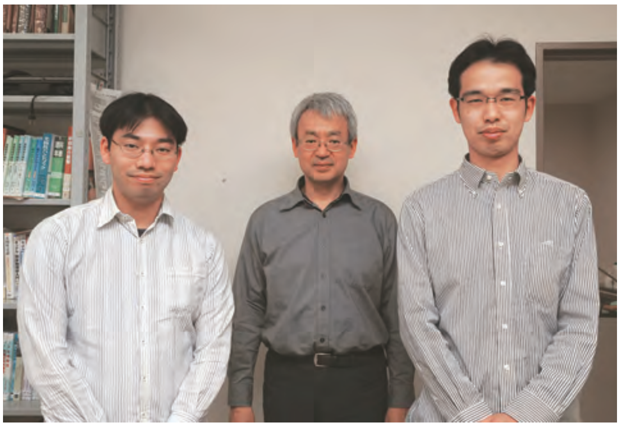
Program-Specific Assist Prof
OKANO, Makoto
(D Sc)

Prof (Supporting Faculty 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 space-resolved 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
Nanocarbon Materials
Laser Spectroscopy
Solar Energy Conversion



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, *Physical Review Letters*, **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).
Okano, M.; Kanemitsu, Y.; Chen, S.; Mochizuki, T.; Yoshita, M.; Akiyama, H.; Pfeiffer, L. N.; West, K. W., Observation of High Rydberg States of One-dimensional Excitons in GaAs Quantum Wires by Magneto-photoluminescence Excitation Spectroscopy, *Phys. Rev. B*, **86,** [085312-1]-[085312-5] (2012).
Yamada, Y.; Kanemitsu, Y., Band-edge Luminescence from $SrTiO_3$: No Polaron Effect, *Thin Solid Films*, **520,** 3843-3846 (2012).
Okano, M.; Matsunaga, R.; Matsuda, K.; Masubuchi, S.; Machida, T.; Kanemitsu, Y., Raman Study on the Interlayer Interactions and the Band Structure of Bilayer Graphene Synthesized by Alcohol Chemical Vapor Deposition, *Appl. Phys. Lett.*, **99,** [151916-1]-[151916-3] (2011).

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.

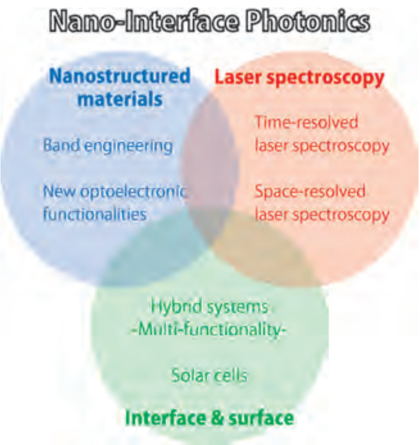


Figure 1.

Observation of Band-gap Renormalization in Hole-doped Carbon Nanotubes Using Photoluminescence Excitation Spectroscopy

Band-gap renormalization, where the band-gap energy is modified by high-density excitons or carriers, is one of the most interesting phenomena due to many-body effects in semiconductors. However, in one-dimensional semiconducting materials, it is difficult to directly determine the band-gap energy owing to extremely weak optical absorption. Therefore, we estimated the band-gap energy for hole-doped single-walled carbon nanotubes (SWCNTs) using a relationship of the exciton energy levels, which are measured by one- and two-photon photoluminescence excitation spectroscopy. As the hole-dopant concentration increases, a redshift of the first excited state (2g) and a blueshift of the ground state (1u) of the E_{11} exciton are observed. From the redshift of higher Rydberg states, we found that a reduction of the band-gap energy occurs in hole-doped SWCNTs. These findings show that a small number of holes can modulate the exciton and electronic band structures in the SWCNT one-dimensional structures.

Extremely Slow Electron Relaxation in $LaAlO_3/SrTiO_3$ Heterostructures Studied by Femtosecond Transient Absorption Spectroscopy

The interface between two insulating transition metal recently attracts much attention since the discovery of the quasi-two-dimensional electron-gas at the $LaAlO_3/SrTi_{O3}$ heterointerface. We studied the photocarrier relaxation dynamics of an n-type $LaAlO_3/SrTiO_3$ heterointerface using femtosecond transient absorption (TA) spectroscopy at low temperatures. A Drude-like free carrier absorption is observed in TA spectrum just after the photo excitation in both $LaAlO_3/SrTiO_3$ heterostructures and electron-doped $SrTiO_3$ bulk crystals. In addition, a broad absorption band gradually appears in visible spectral region within 40 ps, which corresponds to the energy relaxation of photoexcited free electrons into self-trapped polaron states. This indicates that the polaron formation time is largely enhanced at the $LaAlO_3/SrTiO_3$ heterointerface as compared to the bulk crystals, which is attributable to the splitting of the t_{2g} subbands due to the interface potential.

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

A "consensus tree" is a single phylogenetic tree that summarizes the branching structure in a given set of conflicting phylogenetic trees. We developed new deterministic algorithms for constructing several popular types of consensus trees that are faster than all the previously known ones. Given k phylogenetic trees with n leaves each and with identical leaf label sets, our algorithms run in $O(n k)$ time [majority rule consensus tree], $O(n k)$ time [loose consensus tree], $O(n^2 k)$ time [greedy consensus tree], and $\min\{O(k n^2), O(k n (k + \log^{2} n))\}$ time [frequency difference consensus tree]. We also implemented our algorithms to make sure that they are practical and applied them to various simulated data sets. These experiments suggested that the running times of our deterministic algorithms are already comparable to (and in many cases, better than) those of the randomized methods found in widely used software packages such as PHYLIP.

ACTIVITIES OF JOINT USAGE/RESEARCH CENTER

JURC Cooperative Research Subjects 2013

(1 April 2013 ~ 31 March 2014)

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

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

Development of Negative Thermal Expansion Material Based on a Perovskite $BiNiO_3$
AZUMA, Masaki, Materials and Structures Laboratory, Tokyo Institute of Technology
Host in JURC SHIMAKAWA, Yuichi

Development of Iron 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

Optical Functionalities of Silicon Photonic Crystals
TAKAHASHI, Yasushi, Research Organization for the 21st Century, Osaka Prefecture University
Host in JURC KANEMITSU, Yoshihiko

Synthesis of Sugar-Acetylenes by Iron-Catalyzed Cross-Coupling and Study on Their Stimulus-Response Luminescence
ORITA, Akihiro, Department of Applied Chemistry, Okayama University
Host in JURC NAKAMURA, Masaharu

Mechanistic Studies on the Iron Catalyzed Carbon-carbon Bond Forming Reactions Based on the Solution-phase X-ray Absorption Spectroscopy
NAGASHIMA, Hideo, Institute for Materials Chemistry and Engineering, Kyushu University
Host in JURC NAKAMURA, Masaharu

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

Co-clustering of Biological Datasets for Personalized Medicine
SHIGA, Motoki, Informatics Course, Department of Electrical, Electronic and Computer Engineering, Faculty of Engineering, Gifu University
Host in JURC MAMITSUKA, Hiroshi

Finding Frequent Similar Regions from Genome Sequences
NAKAMURA, Atsuyoshi, Graduate School of Information Science and Technology, Hokkaido University
Host in JURC MAMITSUKA, Hiroshi

Analysis and Control of Complex Bipartite Networks
JOSE, C. Nacher, 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

Interaction of Concentrated Polymer Brush Grafted Fibers with Cells
YOSHIKAWA, Chiaki, World Premier International (WPI) Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS)
Host in JURC TSUJII, Yoshinobu

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

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

Development of Novel Endosomal Escaping Peptides
KOGURE, Kentaro, Department of Biophysical Chemistry, Kyoto Pharmaceutical University
Host in JURC FUTAKI, Shiroh

Role of Water in Motor Function of F1 Protein
IKEGUCHI, Mitsunori, Graduate School in Nanobioscience, Yokohama City University
Host in JURC MATUBAYASI, Nobuyuki

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

Analysis of Molecular Adsorption of Water and Protein on a Stereo-Controlled Acrylamide Polymers
KATSUMOTO, Yukiteru, Graduate School of Science, Hiroshima 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

Investigation of Extraction Behaviors of Metal Ions in Liquid-liquid Extraction Systems Using a Novel Multidentate Ligand
MUKAI, Hiroshi, Faculty of Education, Kyoto University of Education
Host in JURC SOHRIN, Yoshiki

Study on Intermolecular Contacts of Halogen and/or 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

Elucidation of Crystallization Process of Polyurea
MATSUBA, Go, Department of Polymer Science and Engineering, Faculty of Science and Engineering, Yamagata University
Host in JURC KANAYA, Toshiji

Studies on Crystallization Process of Poly(lactic acid)/Nanofiber Composites
KAWAI, Takahiko, Department of Production Science and Technology, Graduate School of Engineering, Gunma University
Host in JURC KANAYA, Toshiji

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

X-Ray Structure Analysis of Reaction Mechanism of Catabolic Enzymes
OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University
Host in JURC HATA, Yasuo

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

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

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

Development of Methods for Discrimination and Syntheses of Chiral Molecules with Phosphoroselenoic Acid Derivatives Bearing a Binaphthyl Group
MURAI, Toshiaki, Faculty of Engineering, Gifu University
Host in JURC TOSHIMITSU, Akio

Synthesis of Novel Heterocyclic Compounds Based on High Dienophilicity of Chalcogen Multiple Bonds
SEGI, Masahito, School of Chemistry, College of Science and Engineering, Kanazawa University
Host in JURC TOSHIMITSU, Akio

Bulk Hetero Junction Photovoltaic Devices Composed of Novel Donar Polymer and Novel Fullerene Derivatives
IE, Yutaka, The Institute of Scientific and Industrial Research, Department of Soft Nanomaterials, Nanoscience and Nanotechnology Center, Osaka University
Host in JURC MURATA, Yasujiro

Reactivity of an Ethynyl Cation on the Tetrairon Core as a Lewis Acid
OKAZAKI, Masaaki, Graduate School of Science and Technology, Hirosaki University
Host in JURC OZAWA, Fumiyuki

Construction of Fullerene Organization via Molecular Recognition
HAINO, Takeharu, Graduate School of Science, Hiroshima University
Host in JURC YAMAGO, Shigeru

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

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

Development and Application of Functional Evaluation System in Genome and Metagenome
TAKAMI, Hideto, Institute of Biogeoscience, Japan Agency for Marine-Earth Science and Technology
Host in JURC GOTO, Susumu

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

Development of Novel 3-Dimensional π-Extended Molecules Directed toward Electronic Materials
SUGA, Seiji, Graduate School of Natural Science and Technology, Okayama University
Host in JURC MURATA, Yasujiro

The Mechanism of Action of Aplyronine A
KIGOSHI, Hideo, Faculty of Pure and Applied Sciences, University of Tsukuba
Host in JURC UESUGI, Motonari

Development of Self-cleavable Peptide Linkers
HAYASHI, Yoshio, Department of Medicinal Chemistry, Tokyo University of Pharmacy and Life Sciences
Host in JURC FUTAKI, Shiroh

Contribution of Constraint Release Mechanism to Dielectric and Viscoelastic Relaxation of Entangled Type-A Polymers
URAKAWA, Osamu, Graduate School of Science, Osaka University
Host in JURC MATSUMIYA, Yumi

Making of the Vertical Cross Section of Particulate Bioactive Trace Metals in the Japan Sea
NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kinki University
Host in JURC SOHRIN, Yoshiki

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

Synthesis and Functions of Multi-Bridged Naphthalene Oligomers
KURAMOCHI, Koji, Graduate School of Life and Environmental Sciences, Kyoto Prefectural University
Host in JURC KAWABATA, Takeo

Study on the Regulatory Mechanism of Plant Epidermal Cell Differentiation
TOMINAGA, Rumi, Interdisciplinary Research Organization, University of Miyazaki
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

Promotion of Wound Healing by a Synthetic Cell-adhesion Molecule
NISHIKAWA, Makiya, Graduate School of Pharmaceutical Sciences, Kyoto University
Host in JURC UESUGI, Motonari

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

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

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

Identification and Functional Analysis of Bacterial Proteins Involved in Metal Metabolism
KURATA, Atsushi, Department of Applied Biological Chemistry, Faculty of Agriculture, Kinki University
Host in JURC KURIHARA, Tatsuo

Prepararion of Oxide Glass Scintillator
YANAGIDA, Takayuki, Kyushu Institute of Technology
Host in JURC MASAI, Hirokazu

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Development of Novel Inducers of Cellular Anti-oxidative Stress Response by Inhibition of Cystine/Glutamate Antiporter xCT and γ-Glutamyltranspeptidase (GGT)
SATO, Hideyo, Department of Food and Applited Life Sciences, Faculty of Agriculture, Yamagata University
Host in JURC HIRATAKE, Jun

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

Entanglement Relaxation of Novel Tadpole-shaped Polymers
TAKANO, Atsushi, Graduate School of Engineering, Nagoya University
Host in JURC WATANABE, Hiroshi

Development of Organic Optoelectronics Based on Material Design Guided by Microwave Conductivity Technique
SAEKI, Akinori, Graduate School of Engineering, Osaka University
Host in JURC WAKAMIYA, Atsushi

Search for Biologically Active Compounds from a Synthetic Library of Nitogen Heterocycles with Chiral Tetrasubstituted Carbon
ISHIBASHI, Masami, Graduate School of Pharmaceutical Sciences, Chiba University
Host in JURC KAWABATA, Takeo

Efficient Synthesis of π-Conjugated Polymers via Direct Arylation
KANBARA, Takaki, Graduate School of Pure and Applied Sciences, Tsukuba Research Center for Interdisciplinary Materials Science, University of Tsukuba
Host in JURC OZAWA, Fumiyuki

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

New Optoelectronic Properties Arising from Nanoparticle Arrays Fabricated on 1 nm Periodic Uneven Structure
ONOE, Jun, Research Laboratory for Nuclear Reactors, Tokyo Institute of Technology
Host in JURC TERANISHI,Toshiharu

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

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

Development of Artificial Receptor-ligand Systems to Regulate Cellular Uptake of Therapeutic Molecules
NAKASE, Ikuhiko, Nanoscience and Nanotechnology Research Center, Osaka Prefecture University
Host in JURC FUTAKI, Shiroh

Adsorption Behavior of Cesium Ion on Soil Using Solid State NMR
ONO, Yuji, Fukushima Agricultural Technology Centre
Host in JURC TOKUDA, Yomei

R&Ds for Precision Measurement of Muon g-2 / EDM
MIBE, Tsutomu, Institute of Particle and Nuclear Studies, High Energy Accelerator Research Organization
Host in JURC IWASHITA, Yoshihisa

SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

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

Synthesis and Structure of Color-tunable Organotelluronium Salts
MINOURA, Mao, School of Science, Kitasato University
Host in JURC TOKITOH, Norihiro

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

Syntheses and Properties of Novel Aromatic Compounds Containing Phosphorus Atoms
NAGAHORA, Noriyoshi, Department of Chemistry, Faculty of Science, Fukuoka University
Host in JURC SASAMORI, Takahiro

Physicochemical Properties of Novel Aromatic Compounds with Heteroatoms
SAITO, Masaichi, Department of Chemistry, Graduate School of Science and Engineering, Saitama University
Host in JURC TOKITOH, Norihiro

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

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

AFM Observation of the Heterobimetallic Supramolecular Polymers Placed on the Graphite Substrate via a Pulse Valve
TAKAJO, Daisuke, Graduate School of Science, Osaka University
Host in JURC KURATA, Hiroki

Nano-electron Spectroscopic Study of Helium Bubbles in Si
MIYAMOTO, Mitsutaka, Interdisciplinary Faculty of Science and Engineering, Shimane 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

SUBJECTS ENCOURAGING JOINT PROGRAM

Electronic States and Local Structures in Transition Metal Oxides Using Synchrotron Radiated X-rays
MIZUMAKI, Masaichiro, Japan Synchrotron Radiation Research Institute, SPring-8
Host in JURC SHIMAKAWA, Yuichi

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

JURC Publications

(until 31 May 2013)

Understanding the Substrate Specificity of Conventional Calpains
Sorimachi, H.; Mamitsuka, H.; Ono, Y., *Biological Chemistry*, **393,** 853-871 (2012).

Abstract

Calpains are intracellular Ca(2+)-dependent Cys proteases that play important roles in a wide range of biological phenomena via the limited proteolysis of their substrates. Genetic defects in calpain genes cause lethality and/or functional deficits in many organisms, including humans. Despite their biological importance, the mechanisms underlying the action of calpains, particularly of their substrate specificities, remain largely unknown. Studies show that certain sequence preferences influence calpain substrate recognition, and some properties of amino acids have been related successfully to substrate specificity and to the calpains' 3D structure. The full spectrum of this substrate specificity, however, has not been clarified using standard sequence analysis algorithms, e.g., the position-specific scoringmatrix method. More advanced bioinformatics techniques were used recently to identify the substrate specificities of calpains and to develop a predictor for calpain cleavage sites, demonstrating the potential of combining empirical data acquisition and machine learning.

This review discusses the calpains' substrate specificities, introducing the benefits of bioinformatics applications. In conclusion, machine learning has led to the development of useful predictors for calpain cleavage sites, although the accuracy of the predictions still needs improvement. Machine learning has also elucidated information about the properties of calpains' substrate specificities, including a preference for sequences over secondary structures and the existence of a substrate specificity difference between two similar conventional calpains, which has never been indicated biochemically.

Characterization of Thiol-functionalized Oligo(phenylene-ethynylene)-Protected Au Nanoparticles by Scanning Tunneling Microscopy and Spectroscopy
Koo, H.; Kano, S.; Tanaka, D.; Sakamoto, M.; Teranishi, T.; Cho, G.; Majima, Y., *Appl. Phys. Lett.*, **101,** 083115 (2012).

Abstract

The electrical properties of Aunanoparticles protected by thiol-functionalized oligo(phenylene-ethynylene) (OPE), 1,4-bis-(3-mercapto-phenylethynyl)benzene have been investigated by scanning tunneling microscopy(STM) and scanning tunneling spectroscopy (STS). The STM and scanning electron microscopy images of chemisorbed OPE-protected Aunanoparticles on Au(111) surface were similar, and the densities were almost identical. OPE-protected Aunanoparticles exhibited stochastic conductance switching behaviors, and current-voltage (I–V) and log I–Vcharacteristics by STS at 100 K showed Coulomb blockade behaviors. The charging energy of Aunanoparticles was as high as 0.57 eV when the core diameter was 2.1 nm. Our results are significant for single-electron transistor memory applications.

Selective Synthesis and Crystal Structure of [10]Cycloparaphenylene
Kayahara, E.; Sakamoto, Y.; Suzuki, T.; Yamago, S., *Org. Lett.*, **14,** 3284-3287 (2012).

Abstract

[10]Cycloparaphenylene ([10]CPP) was selectively synthesized in four steps in 13% overall yield from commercially available 4,40-diiodobiphenyl by using mono-I–Sn exchange, Sn–Pt transmetalation, I–Pd exchange, and subsequent oxidative coupling reactions. The single-crystal X-ray structure of [10]CPP is described.

Current-Induced Magnetic Domain Wall Motion in a Co/Ni Nanowire with Structural Inversion Asymmetry
Koyama, T.; Hata, H.; Kim, K.-J.; Moriyama, T.; Tanigawa, H.; Suzuki, T.; Nakatani, Y.; Chiba, D.; Ono, T., *Applied Physics Express,* **6,** [033001-1]-[033001-3] (2013).

Abstract

The authors have investigated the current-induced magnetic domain wall (DW) motion in perpendicularly magnetized Co/Ni nanowire with structural inversion asymmetry (SIA). In this system, DW motion to the direction of electric current flow, not electron flow, and high DW velocity up to 110 m/s were confirmed, which have never been observed in Co/Ni systems without SIA. In addition, we found that the DW velocity showed a strong dependence on the perpendicular magnetic field in the range of ±100 Oe. These results suggest that DW in the Co/Ni nanowire with SIA moves in the steady mode, not in the precessional mode.

X-Ray Observation of a Helium Atom and Placing a Nitrogen Atom inside He@C_{60} and He@C_{70}
Morinaka, Y.; Sato, S.; Wakamiya, A.; Nikawa, H.; Mizorogi, N.; Tanabe, F.; Murata, M.; Komatsu, K.; Furukawa, K.; Kato, T.; Nagase, S.; Akasaka, T.; Murata, Y., *Nat. Commun.*, **4,** [1554-1]-[1554-5] (2013).

Abstract

X-ray diffraction study of He@C_{60} is demonstrated as the clear observation of a single helium atom inside C_{60}. In addition, the close packing of a helium atom and a nitrogen atom inside fullerenes was realized by the use of two stepwise insertion techniques, i.e. ‘‘molecular surgery’’ to synthesize the fullerenes encapsulating a helium atom followed by ‘‘nitrogen radio-frequency plasma’’ methods to generate the fullerenes encapsulating both helium and nitrogen atoms. The ESR analysis revealed that the encapsulated helium atom gives a small but detectable influence on the electronic properties of the highly reactive nitrogen atom coexisting inside the fullerenes, indicating the new usage of helium for controlling electronic properties of reactive species.

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
FUKUZUMI, Shunichi
(D Eng)

Professor, Department of Material and Life Science, Graduate School of Engineering, Osaka University
(2-1 Yamada-oka, Suita, Osaka 565-0871)

Lectures at *ICR*

Development and Future of Artificial Photosynthesis

Vis Prof
HASHIMOTO, Shun-ichi
(D Pharm Sc)

Professor, Laboratory of Synthetic and Industrial Chemistry, Faculty of Pharmaceutical Sciences, Hokkaido University
(Kita-12 Nishi-6, Kita-ku, Sapporo 060-0812)

Vis Prof
NAGASHIMA, Hideo
(D Eng)

Professor, Institute for Materials Chemistry and Engineering, Kyusyu University
(6-1 Kasuga Kohen, Kasuga-shi, Fukuoka 816-0811)

Lectures at *ICR*

Living Radical Polymerization and Hyper-branched Polymer; Homogeneous Catalytic System inspired by Industry-Academia Partnership

Iron Carbonyl Complexes which Easily Generate Active Species; Utilization in Catalytic Reactions

Vis Prof
IMANISHI, Nobuyuki
(D Eng)

Professor, Department of Chemistry for Materials, Faculty of Engineering and Graduate School of Engineering, Mie University
(1577 Kurimamachiya-cho, Tsu 514-8507)

Lectures at *ICR*

Fundamental Basics in Electrochemistry

Advanced Electrochemistry and Next-generation Fuel Cells

Vis Prof
CHEN, Jwu-Ting
(Ph D)

Professor, Department of Chemistry, National Taiwan University
(No. 1, Sec. 4, Roosevelt Road, Taipei, 10617)

Lectures at *ICR*

Alternating Ethylene/norbornene Copolymerization Catalyzed by Organopalladium Complexes Bearing Aminopyridines–An Unusual Example of Ligand Design Leading to the Control of Geometric Isomerism-reactivity Relationship

Vis Assoc Prof
YUSA, Shin-ichi
(D Sc)

Associate Professor, Division of Synthetic Chemistry and Biochemistry, Graduate School of Engineering, University of Hyogo
(2167 Shosya Himeji, Hyogo 671-2280)

Lectures at *ICR*

Control of Self-Assembled Structure by Chemical Structure of Polymers

Development of Functional Fine Particles Using the Interface

Vis Assoc Prof
NISHIOKA, Jun
(Ph D)

Associate Professor, Pan-Okhotsk Research Center, Institute of Low Temperature Science, Hokkaido University
(Kita-19, Nishi-8, Kita-ku, Sapporo 060-0819)

Lectures at *ICR*

The Role of the Subpolar Region in the Material Cycle and Biological Productivity in the North Pacific Ocean

Vis Assoc Prof
YATSUI, Takashi
(D Eng)

Associate Professor, Graduate School of Engineering, The University of Tokyo
(Yayoi, Bunkyo-ku, Tokyo 113-8656)

Lectures at *ICR*

Advances of Nanofabrication Using Dressed Photons

Advancement of Photochemical Reaction Using Dressed Photons

Vis Assoc Prof
SHIBUYA, Tetsuo
(D Sc)

Associate Professor, Laboratory of Sequence Analysis, The Institute of Medical Science, Human Genome Center, The University of Tokyo
(4-6-1, Shirokanedai, Minato-ku, Tokyo 108-8639)

Lectures at *ICR*

Indexing Protein 3-D Structures for Faster Structural Similarity Queries

Prof Em KANEHISA, Minoru (D Sc)

Appointed as Res (pt) at ICR,
1 April 2012–31 March 2014

PERSONAL

Awards

TOKITOH, Norihiro

Alexander von Humboldt Research Award (Re-invitation)

"New Perspectives in the Chemistry of Phosphinidenoids and Their Heavier Homologues"

Alexander von Humboldt Foundation

8 October, 2013

WASANO, Tatsuya

ICR Award for Graduate Students

"Syntheses and Structures of an "Alumole" and Its Dianion"

Institute for Chemical Research, Kyoto University

13 December 2013

WAKAMIYA, Atsushi

Incentive Award of Japan Association for Chemical Innovation

"Creation of Low Band Gap Materials with High Charge Transporting Properties"

Japan Association for Chemical Innovation

30 May 2013

NISHIMURA, Hidetaka

Mazume Research Encouragement Prize Award

Graduate School of Engineering, Kyoto University

12 June 2013

YOSHIMURA, Tomoyuki

ICR Award for Young Scientists

"Asymmetric Induction via Short-lived Chiral Enolates with a Chiral C-O Axis"

Institute for Chemical Research

13 December 2013

KINOSHITA, Tomohiko

Best Presentation Award

The 133rd Annual Meeting of the Pharmaceutical Society of Japan

"Synthesis of Gamma-lactams with Tetra-substituted Carbon via Asymmetric N-C acyl Migration Based on Memory of Chirality"

The Pharmaceutical Society of Japan

30 March 2013

TERANISHI, Toshiharu

Materials and Structures Laboratory Director Award 2013

“Development of Single Electron Devices Using Gold Clusters as Single Electron Islands”

Materials and Structures Laboratory, Tokyo Institute of Technology

17 July 2013

YAMAGO, Shigeru

Technology Award

51st Annual Conference of the Adhesion Society of Japan

“Industrialization and Development of Adhesive Using Living Radical Polymerization”

The Adhesion Society of Japan

21 June 2013

ONO, Teruo

German Innovation Award—Gottfried Wagener Prize (2nd Prize)

“Development of Non-Volatile Memory Using Spin Dynamics”

German Research and Innovation Forum Tokyo, German Chamber of Commerce and Industry in Japan

18 June 2013

KIM, Kab-Jin

ICR Award for Young Scientists (Foreign Researchers’ Category)

“Two-barrier Stability that Allows Low-power Operation in Current-induced Domain-wall Motion”

Institute for Chemical Research, Kyoto University

13 December 2013

IMANISHI, Miki

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

“Study of Designing DNA Binding Proteins to Control Cellular Functions”

Minister of Education, Culture, Sports, Science and Technology

16 April 2013

SOHRIN, Yoshiki

The Steel Foundation for Environmental Protection Technology President Award

“Three-dimensional Analysis of the Oceanic Environment Using Trace Metals”

Steel Foundation for Environmental Protection Technology

6 September 2013

TAKANO, Shotaro

ICR Award for Graduate Students

“Determination of Isotopic Composition of Dissolved Copper in Seawater by Multi-collector Inductively Coupled Plasma Mass Spectrometry after Pre-concentration Using an Ethylene-diaminetriacetic Acid Chelating Resin”

Institute for Chemical Research, Kyoto University

13 December 2013

HASEGAWA, Takeshi

Advanced Analysis Technology Award - JAIMA Instrument Development Award 2013

The 62nd Annual Meeting of Japan Society for Analytical Chemistry

“Development of the Principle and the Equipment of Multiple-angle Incidence Resolution Spectrometry”

Japan Society of Analytical Chemistry (JSAC)

11 September 2013

SHIOYA, Nobutaka

The Best Oral Presentation Award

The 30th Kyushu Colloid Colloquium

"Molecular Orientation Analysis of a Spin-Coated Film of Poly (3-hexylthiophene-2,5-diyl) on Calcium Fluoride Analyzed by Infrared Multiple-Angle Incidence Resolution Spectrometry"

The Chemical society of Japan, Division of Colloid and Surface Chemistry (Kyushu Branch)

9 August 2013

INOUE, Rintaro

Promotive Award of the Society of Fiber Science and Technology, Japan, Kansai

The 35th Meeting of the Society of Fiber Science and Technology, Japan, Kansai

"Distribution of Glass Transition Temperature in Polymer Thin Film as Studied by Neutron Reflectivity"

The Society of Fiber Science and Technology, Japan

22 November 2013

ASO, Ryotaro

JSAP Young Scientist Oral Presentation Award

The 34th JSAP Autumn Meeting

"Local Structure and Strain Analysis of Epitaxially Grown $SrRuO_3$Thin Film by STEM"

The Japan Society of Applied Physics

16 September 2013

HATAKEYAMA, Takuji

The CSJ Award for Young Chemist 2012

"Development of Iron-catalyzed Cross-coupling Reactions Based on Mechanistic Studies"

The Chemical Society of Japan

23 March 2013

MURAKAMI, Noriaki

JSPM Award for Best Presentation by Student

The 111th Spring Meeting of Japan Society of Powder and Powder Metallurgy

"Oxygen Diffusion during Low-temperature CaH_2 Reduction Reaction in $LaAlO_3/CaFeO_{2.5}/SrTiO_3$ Heterostructure"

Japan Society of Powder and Powder Metallurgy

29 May 2013

TAKEUCHI, Katsuhiko

Reaxys PhD Prize 2013 Finalists

"Access to a Stable Si_2N_2 4-Membered Ring with Non-Kekulé Singlet Biradical Character from a Disilyne"

Reaxys

22 September 2013

MORI, Tomoya

IPSJ Yamashita SIG Research Award

"An Improved Clique-Based Method for Computing Edit Distance between Rooted Unordered Trees"

Information Processing Society of Japan

6 March 2013

Paper Awards

SAKAGAMI, Michiyasu; SASAMORI, Takahiro; SAKAI, Heisuke[1]; FURUKAWA, Yukiko[1]; TOKITOH, Norihiro

BCSJ Award

"1,2-Bis(ferrocenyl)dipnictenes: Bimetallic Systems with a Pn=Pn Heavy π-Spacer (Pn: P, Sb, and Bi)"

15 October 2013

[1] Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University

SOHRIN, Yoshiki, et. al.

Geochemical Journal Award 2013

Goldschmidt Conference 2013

"The Molybdenum Isotopic Composition of the Modern Ocean"

NAKAGAWA, Yusuke; TAKANO, Shotaro; FIRDAUS, Mochamad Lutfi; NORISUYE, Kazuhiro; SOHRIN, Yoshiki

Geochemical Society of Japan

27 August 2013

SHIMIZU, Masahiro

The Distinguished Paper Award

The Papers of Technical Meeting on "Fundamentals and Materials", IEE Japan

"Self-formation of Nanostructures on Metal Surface under Femtosecond Laser Irradiation"

The Institute of Electrical Engineering of Japan

25 April 2013

Poster Awards

HIRANO, Toshiko

The Best Poster Presentation Award

The 30th Joint Symposium (The 80th Meeting of the Association of Organic Micro-Analysts in the Japan Society for Analytical Chemistry/The 92th Meeting of the Technical Committee on Measurement of Mechanical Quantities in the Society of Instrument and Control Engineers)

"Examination of Interfering Factor in the Determination of Bromine in Organic Compound with the Automatic Analyzer"

Organizing Committee of the 30th Joint Symposium

30 May 2013

WASANO, Tatsuya

The Best Poster Award

The 3rd CSJ Chemistry Festa 2013

"Synthesis and Properties of "Alumole" and Its Dianion"

The Chemical Society of Japan

11 November 2013

MORINAKA, Yuta

CSJ Student Presentation Award 2013

The 93rd Annual Meeting, Chemical Society of Japan

“Organic Synthesis of Helium-Containing Fullerenes and Generation of Novel Endofullerenes Encapsulating Two Different Atoms”

The Chemical Society of Japan

18 April 2013

FUTAGOISHI, Tsukasa

Young Scientist Poster Award

The 44th Fullerenes-Nanotubes-Graphene General Symposium

“Synthesis of C_{60} Derivatives Having a Sulfur-containing Opening and X-ray Structure of N_2 Encapsulated Molecule”

The Fullerenes, Nanotubes and Graphene Research Society

6 August 2013

SHIMOGAWA, Hiroyuki

Poster Award

24th Symposium on Physical Organic Chemistry

“Development of Green Dyes Containing an Intramolecular B–N Coordination Bond for Dye-Sensitized Solar Cells”

The Society of Physical Organic Chemistry

7 September 2013

KURIBAYASHI, Toshifumi

Best Poster Award

Symposium on Molecular Chirality 2013

“Synthesis of Amide Functionalized Helicene via Intramolecular Amidation”

Molecular Chirality Research Organization (MCRO)

11 May 2013

YANAGI, Masanori

Best Poster Prize

1st International Conference and 6th Symposium on Organocatalysis

“Regioselective Deoxygenation of Glucose Derivatives”

Organizing Committee of 1st International Conference and 6th Symposium on Organocatalysis

28 May 2013

OTSUKI, Haruka

Best Poster Award

The 33rd Seminar on the Society of Synthetic Organic Chemistry, Japan, Kinki Branch

“Mechanistic Investigation of Asymmetric Aldol Reaction via Axially Chiral Enolates”

The Society of Synthetic Organic Chemistry, Japan, Kinki Branch

2 August 2013

TSUDA, Ayumi

Chemistry Letters Award

The 43rd Congress of Heterocyclic Chemistry

“Kinetic Resolution of Topologically Chiral Racemic Rotaxanes by Organocatalysis”

Organizing Committee of 43rd Congress of Heterocyclic Chemistry

19 October 2013

TAKEUCHI, Hironori

Best Poster Award

“Total Synthesis of Natural Saccharides by Organocatalytic Regioselective Functionalization of Unprotected D-Glucose”

39th Symposium on Progress in Organic Reactions and Synthesis -Application in the Life Science-

Organizing Committee of 39th Symposium on Progress in Organic Reactions and Synthesis -Application in the Life Science-

6 November 2013

SAKAMOTO, Masanori

Poster Award

The 11th Annual Meeting of Society of Nano Science and Technology

"Controlling the Shape and Anisotropy of Nanoparticles by Rigid Multidentate Ligands"

Society of Nano Science and Technology

8 June 2013

SATO, Ryota

Poster Award

The 64th Divisional Meeting on Colloid and Interface Chemistry

"Exchange Coupling Interaction in $L1_0$-FePd/α-Fe Nanocomposite Magnets with Optimum Nanostructure"

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

19 September 2013

NAKANISHI, Yohei

The Best Poster Award

The 15th Symposium of Research Group on Polymer Surface and Interface

"Development of Dye-sensitized Solar Cell Using Membrane of Self-assembled Nanoparticles with Polymer Brushes: Effects of Polymer Brushes"

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

1 February 2013

KINOSE, Yuji

The Best Poster Award

The 2013 Autumn Meeting of the Society of Fiber Science and Technology

"Synthesis of Novel Hairy-Rod Type Cellulosic Derivatives via ATRP"

The Society of Fiber Science and Technology, Japan

6 September 2013

KAYAHARA, Eiichi

Wiley Presentation Award on Gordon Research Conference

2013 Gordon Research Conference on Physical Organic Chemistry

"Synthesis of a Ball-Like Three Dimensional π-Conjugated Compound and Its Physical Properties"

GRC, Willy

29 June 2013

NAGATA, Masaki

Best Poster Award

" Ferromagnetic Resonance in Magnetite Thin Films"

ISAMMA 2013

22 July 2013

NAKASE, Ikuhiko

Journal of Controlled Release Poster Award

2nd International Conference on Biomaterials Science

"Tumor Accumulation of Arginine-rich Cell-penetrating Peptides and Delivery of Anticancer Drug in vivo"

21 March 2013

OKU, Akihiko

Best Poster Prize

The 45th Peptide Summer School for Young Scientists

"Development of Deubiquitinating Enzyme-Resistant Ubiquitin Dimer"

The Japanese Peptide Society

30 July 2013

NORIMOTO, Shingo

Spectroscopy & Innovation Consortium Award

The 7th International Conference on Advanced Vibrational Spectroscopy (ICAVS7)

"Analysis of the Preparation Process of a Self-assembled Monolayer on Silicon by FT-IR Spectroscopy"

Spectroscopy & Innovation Consortium

30 August 2013

MARUYAMA, Saori

Poster Presentation Award

The 14th Annual Meeting of Japanese Society of Extremophiles

"Study of Metal-Reducing Mechanism of a Psychrotrophic Bacterium, *Shewanella livingstonensis* Ac10"

Japanese Society of Extremophiles

26 October 2013

MATSUURA, Tomohiko

The Poster Presentation Award

International Discussion Meeting on Polymer Crystallization 2013

"Precursor in Shear-induced Crystallization of Isotactic Polystyrene above Melting Temperature by Micro-beam SAXS and WAXS"

International Discussion Meeting on Polymer Crystallization 2013

3 July 2013

MIZUTANI, Sayaka

NORO, Yosuke

KOTERA, Masaaki

GOTO, Susumu

Excellent Poster Award

2013 Annual Convention of Japanese Society for Bioinformatics (JSBi 2013)

"A Biclustering Approach to Associating Adverse Drug Events with the Patients' Physiological Backgrounds"

Japanese Society for Bioinformatics

31 October 2013

PUBLICATIONS
INTERNATIONAL RESEARCH COLLABORATIONS
SELECTED GRANTS
THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Sakagami, M.; Sasamori, T.; Sakai, H.; Furukawa, Y.; Tokitoh, N., 1,2-Bis(ferrocenyl)-Substituted Distibene and Dibismuthene: Sb=Sb and Bi=Bi Units as π Spacers between Two Ferrocenyl Units, *Chem. Asian J.*, **8,** 690-693 (2013).

Maruo, S.; Nishio, K.; Sasamori, T.; Tokitoh, N.; Kuramochi, K.; Tsubaki, K.**,** Biomimetic Synthesis of Zeylanone and Zeylanone Epoxide by Dimerization of 2-Methyl-1,4-naphthoquinone, *Org. Lett.*, **15,** 1556-1559 (2013).

Nishino, R.; Furuta, T.; Kan, K.; Sato, M.; Yamanaka, M.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Investigation of the Carboxylate Position during the Acylation Reaction Catalyzed by Biaryl DMAP Derivatives with an Internal Carboxylate, *Angew. Chem. Int. Ed.*, **52,** 6445-6449 (2013).

Takemoto, N.; Suehara, T.; Frisco, H. L.; Sato, S.; Sezaki, T.; Kusamori, K.; Kawazoe, Y.; Park, S. M.; Yamazoe, S.; Mizuhata, Y.; Inoue, R.; Miller, G. J.; Hansen, S. U.; Jayson, G. C.; Gardiner, J. M.; Kanaya, T.; Tokitoh, N.; Ueda, K.; Takakura, Y.; Kioka, N.; Nishikawa, M.; Uesugi, M., Small-Molecule-Induced Clustering of Heparan Sulfate Promotes Cell Adhesion, *J. Am. Chem. Soc.*, **135,** 11032-11039 (2013).

Agou, T.; Wasano, T.; Jin, P.; Nagase, S.; Tokitoh, N., Syntheses and Structures of an “Alumole” and Its Dianion, *Angew. Chem. Int. Ed.*, **52,** 10031-10034 (2013).

Agou, T.; Nagata, K.; Tokitoh, N., Synthesis of a Dialumene-Benzene Adduct and Its Reactivity as a Synthetic Equivalent of a Dialumene, *Angew. Chem. Int. Ed.*, **52,** 10818-10821 (2013).

Sasamori, T.; Tokitoh, N., A New Family of Multiple-Bond Compounds between Heavier Group 14 Elements, *Bull. Chem. Soc. Jpn.*, **86,** 1005-1021 (2013).

Sakagami, M.; Sasamori, T.; Sakai, H.; Furukawa, Y.; Tokitoh, N., 1,2-Bis(ferrocenyl)dipnictenes: Bimetallic Systems with a Pn=Pn Heavy π-Spacer (Pn: P, Sb, and Bi), *Bull. Chem. Soc. Jpn.*, **86,** 1132-1143 (2013).

Sasamori, T.; Sakagami, M.; Tokitoh, N., Step-wise Sulfurization of Stable 1,2-bis(ferrocenyl)diphosphene, *J. Sulf. Chem.*, **34,** 677-683 (2013).

— Structural Organic Chemistry —

Morinaka, Y.; Sato, S.; Wakamiya, A.; Nikawa, H.; Mizorogi, N.; Tanabe, F.; Murata, M.; Komatsu, K.; Furukawa, K.; Kato, T.; Nagase, S.; Akasaka, T.; Murata, Y., X-Ray Observation of a Helium Atom and Placing a Nitrogen Atom inside He@C_{60} and He@C_{70}, *Nat. Commun.*, **4,** [1554-1]-[1554-5] (2013).

Morinaka, Y.; Nobori, M.; Murata, M.; Wakamiya, A.; Sagawa, T.; Yoshikawa, S.; Murata, Y., Synthesis and Photovoltaic Properties of Bulky Acceptor Materials Based on the Dimerization of Fullerene C_{60} for Efficient Polymer Solar Cells, *Chem. Commun.*, **49,** 3670-3672 (2013).

Mitsudo, K.; Harada, J.; Tanaka, Y.; Mandai, H.; Nishioka, C.; Tanaka, H.; Wakamiya, A.; Murata, Y.; Suga, S., Synthesis of Hexa(furan-2-yl)benzenes and Their π-Extended Derivatives, *J. Org. Chem.*, **78,** 2763-2768 (2013).

Futagoishi, T.; Murata, M.; Wakamiya, A.; Sasamori, T.; Murata, Y., Expansion of Orifices of Open C_{60} Derivatives and Formation of an Open C_{59}S Derivative by Reaction with Sulfur, *Org. Lett.*, **15,** 2750-2753 (2013).

Zhang, R.; Murata, M.; Wakamiya, A.; Murata, Y., Synthesis and X-Ray Structure of Endohedral Fullerene C_{60} Dimer Encapsulating a Water Molecule in Each C_{60} Cage, *Chem. Lett.*, **42,** 879-881 (2013).

Hitosugi, S.; Iizuka, R.; Yamasaki, T.; Zhang, R.; Murata, Y.; Isobe, H.**,** Assessment of Fullerene Derivatives as Rolling Journals in a Finite Carbon Nanotube Bearing, *Org. Lett.*, **15,** 3199-3201 (2013).

Chen, J. Y.-C.; Li, Y.; Frunzi, M.; Lei, X.; Murata, Y.; Lawler, R. G.; Turro, N. J., Nuclear Spin Isomers of Guest Molecules in H_2@C_{60}, H_2O@C_{60} and Other Endofullerenes, *Phil. Trans. R. Soc. A*, **371,** [20120429-1]-[20120429-16] (2013).

Murata, Y.; Chuang, S.-C.; Tanabe, F.; Murata, M.; Komatsu, K., Recognition of Hydrogen Isotopomers by an Open-Cage Fullerene, *Phil. Trans. R. Soc. A*, **371,** [20110629-1]-[20110629-6] (2013).

Room, T.; Peedu, L.; Ge, M.; Huvonen, U.; Nagel, U.; Ye, S.; Xu, M.; Bacic, Z.; Mamone, S.; Levitt, M. H.; Carravetta, M.; Chen, J. Y.-C.; Lei, X.; Turro, N. J.; Murata, Y.; Komatsu, K., Infrared Spectroscopy of Small-Molecule Endofullerenes, *Phil. Trans. R. Soc. A*, **371,** [20110631-1]-[20110631-25] (2013).

Horsewill, A. J.; Goh, K.; Rols, S.; Ollivier, J.; Johnson, M. R.; Levitt, M. H.; Carravetta, M.; Mamone, S.; Murata, Y.; Chen, J. Y.-C.; Johnson, J. A.; Lei, X.; Turro, N. J., Quantum Rotation and Translation of Hydrogen Molecules Encapsulated inside C_{60}: Temperature Dependence of INS Spectra, *Phil. Trans. R. Soc. A*, **371,** [20110627-1]-[20110627-15] (2013).

Filidou, V.; Mamone, S.; Simmons, S.; Karlen, S. D.; Anderson, H. L.; Kay, C. W. M.; Bango, A.; Rastrelli, F.; Murata, Y.; Komatsu, K.; Lei, X.; Li, Y.; Turro, N. J.; Levitt, M. H.; Morton, J. J. L., Probing the C_{60} Triplet State Coupling to Nuclear Spins Inside and Out, *Phil. Trans. R. Soc. A*, **371,** [20120475-1]-[20120475-17] (2013).

Shimogawa, H.; Mori, H.; Wakamiya, A.; Murata, Y., Impacts of Dibenzo- and Dithieno-Fused Strctures at the b, g Bonds in the BODIPY Skeleton, *Chem. Lett.*, **42,** 986-988 (2013).

Mamone, S.; Concistre, M.; Heinmaa, I.; Carravetta, M.; Kuprov, I.; Wall, G.; Denning, M.; Lei, X.; Chen, J. Y.-C.; Li, Y.; Murata, Y.; Turro, N. J.; Levitt, M. H., Nuclear Magnetic Resonance of Hydrogen Molecules Trapped inside C_{70} Fullerene Cages, *ChemPhysChem*, **14,** 3121-3130 (2013).

Li, Y.; Lei, X.; Chen, J. Y.-C.; Murata, Y.; Turro, N. J.; Lawler, R. G., Paramagnet Enhanced Nuclear Spin Relaxation in H_2O@Open-C_{60} and H_2@Open-C_{60}, *Org. Lett.*, **15,** 4746-4749 (2013).

Wakamiya, A.; Murakami, T.; Yamaguchi, S., Benzene-fused BODIPY and Fully-fused BODIPY Dimer: Impacts of the Ring-fusing at the b Bond in the BODIPY Skeleton, *Chem. Sci.*, **4,** 1002-1007 (2013).

[Others]

Murata, Y., Creation of Spherical π-Space Encapsulating Active Molecules and Control of Its Function, *Emergence of Highly Elaborated π-Space and Its Function, CMC Publishing*, 64-67, (2013) (in Japanese).

Murata, Y., π-Electron Science of Endofullerenes Encapsulating Molecules, *Science of π-Electron Systems, Kagakudojin*, 70-76 (2013) (in Japanese).

Kaji, H.; Suzuki, F.; Wakamiya, A.; Murata, Y.; Sato, T.; Tanaka, K., Quantum Chemical Analysis of Electron Transporting Materials for OLED, *Monthly Display*, **19,** 49-52 (2013) (in Japanese).

Murata, M.; Murata, Y.; Komatsu, K., Organic Synthesis of Endohedral Fullerenes Encapsulating Helium, Dihydrogen, and Water, *Organic Nanomaterials*, 225-240 (2013).

— Synthetic Organic Chemistry —

Yoshimura, T.; Kinoshita, T.; Yoshioka, H.; Kawabata, T., Asymmetric Intermolecular Conjugate Addition of Amino Acid Derivatives via Memory of Chirality: Total Synthesis of Manzacidin A, *Org. Lett.*, **15,** 864-867 (2013).

Furuta, T.; Nikaido, M.; Yamamoto, J.; Kuribayashi, T.; Kawabata T., Synthesis of Axially Chiral Amino Acid Derivatives via the Selective Monoesterification of 1,1’-Biaryl-2,2’-dicarboxylic Acids, *Synthesis*, **45,** 1312-1318(2013).

Nishino, R.; Furuta, T.; Kan, K.; Sato, M.; Yamanaka, M.; Sasamori, T.; Tokitoh, N.; Kawabata, T., Investigation of the Carboxylate Position during the Acylation Reaction Catalyzed by Biaryl DMAP Derivatives with an Internal Carboxylate, *Angew. Chem. Int. Ed.*, **52,** 6445-6449 (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).

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 fo Ester Enolates via Momory of Chirality, *J. Am. Chem. Soc.*, **135,** 13294-13297 (2013).

Mishiro, K.; Furuta, T.; Sasamori, T.; Hayashi, K.; Tokitoh, N.; Futaki, S.; Kawabata, T., A Cyclochiral Conformational Motif Constructed Using a Robust Hydrogen Bonding Network, *J. Am. Chem. Soc.*, **135,** 13644-13647 (2013).

— Advanced Inorganic Synthesis —

Teranishi, T.; Sakamoto, M., Charge Separation in Type-II Semiconductor Heterodimers, *J. Phys. Chem. Lett.*, **4,** 2867-2873 (2013).

Teranishi, T.; Inui, D.; Yoshinaga, T.; Saruyama, M.; Kanehara, M.; Sakamoto, M.; Furube, A., Crystal Structure-Selective Formation and Carrier Dynamics of Type-II CdS-$Cu_{31}S_{16}$ Heterodimers, *J. Mater. Chem. C*, 3391-3394 (2013).

Hackenberger, G.; Azuma, Y.; Kano, S.; Tanaka, D.; Sakamoto, M.; Teranishi, T.; Ohno, Y.; Maehashi, K.; Matsumoto, K.; Majima, Y., Silicon-Nitride-Passivated Bottom-Up Single-Electron Transistors, *Jpn. J. Appl. Phys.*, **52,** [110101-1]-[110101-5] (2013).

Li, C.; Sun, L.; Sun, Y.; Teranishi, T., One-Pot Controllable Synthesis of Au@Ag Heterogeneous Nanorods with Highly Tunable Plasmonic Absorption, *Chem. Mater.*, **25,** 2580-2590 (2013).

Ikeda, T.; Xiong, A.; Yoshinaga, T.; Maeda, K.; Domen, K.; Teranishi, T., Polyol Synthesis of Size-controlled Rh Nanoparticles and Their Application to Photocatalytic Overall Water Splitting under Visible Light, *J. Phys. Chem. C*, **117,** 2467-2473 (2013).

Sagarzazu, G.; Inoue, K.; Saruyama, M.; Sakamoto, M.; Teranishi, T.; Masuo, S.; Tamai, N., Ultrafast Dynamics and Single Particle Spectroscopy of Au-CdSe Nanorods, *Phys. Chem. Chem. Phys.*, **15,** 2141-2152 (2013).

Sakamoto, M.; Tanaka, D.; Teranishi, T., Rigid Bidentate Ligands Focus the Size of Gold Nanoparticles, *Chem. Sci.*, **4,** 824-828 (2013).

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

Sato, O.; Kasai, T.; Sato, M.; Sakajiri, K.; Tsujii, Y.; Kang, S.; Watanabe, J.; Tokita, M., High-Density Poly(hexyl methacrylate) Brushes Offering a Surface for Near-Zero Azimuthal Anchoring of Liquid Crystals at Room Temperature, *J. Mater. Chem. C*, **1,** 7992-7995 (2013).

Yamago, S.; Yahata, Y.; Nakanishi, K.; Konishi, S.; Kayahara, E.; Nomura, A.; Goto, A.; Tsujii, Y., Synthesis of Concentrated Polymer Brushes via Surface-Initiated Organotellurium-Mediated Living Radical Polymerization, *Macromolecules*, **46,** 6777-6785 (2013).

Ohno, K.; Mori, C.; Akashi, T.; Yoshida, S.; Tago, Y.; Tsujii, Y.; Tabata, Y., Fabrication of Contrast Agents for Magnetic Resonance Imaging from Polymer-Brush-Afforded Iron Oxide Magnetic Nanoparticles Prepared by Surface-Initiated Living Radical Polymerization, *Biomacromolecules*, **14,** 3453-3462 (2013).

Ohno, K.; Tabata, H.; Tsujii. Y., Surface-Initiated Living Radical Polymerization from Silica Particles Functionalized with Poly(ethylene glycol)-Carrying Initiator, *Colloid Polym. Sci.*, **291,** 127-135 (2013).

Sakakibara, K.; Granstrom, M.; Kilpelainen, I.; Helaja, J.; Heinilehto, S.; Inoue, R.; Kanaya, T.; Hill, J. P.; Nakatsubo, F.; Tsujii, Y.; Ariga, K., Light-Harvesting Nanorods Based on Pheophorbide-Appending Cellulose, *Biomacromolecules*, **14,** 3223-3230 (2013).

Sato, O.; Kasai, T.; Nomura, A.; Tsujii, Y.; Kang, S.; Tokita, M.; Watanabe, J., Viscoelastic PS Brush Surface Offering Strong Anchoring at Low Temperature and Near-Zero Anchoring at High Temperature for LC Molecules, *Liquid Crystals*, **40,** 221-227 (2013).

Hore, M. J. A.; Ford, J.; Ohno, K.; Composto, R. J.; Hammouda, B., Direct Measurements of Polymer Brush Conformation Using Small-Angle Neutron Scattering (SANS) from Highly Grafted Iron Oxide Nanoparticles in Homopolymer Melts, *Macromolecules*, **46,** 9341-9348 (2013).

Moraes, J.; Ohno, K.; Maschmeyer, T.; Perrier, S., Synthesis of Silica-Polymer Core-Shell Nanoparticles by Reversible Addition-Fragmentation Chain Transfer Polymerization, *Chem. Commun.*, **49,** 9077-9088 (2013).

Moraes, J.; Ohno, K.; Maschmeyer, T.; Perrier, S., Monodisperse, Charge-Stabilized, Core-Shell Particles via Silica-Supported Reversible Addition-Fragmentation Chain Transfer Polymerization for Cell Imaging, *Chem. Mater.*, **25,** 3522-3527 (2013).

Moraes, J.; Ohno, K.; Gody, G.; Maschmeyer, T.; Perrier, S., The Synthesis of Well-Defined Poly(vinylbenzyl chloride)-Grafted Nanoparticles via RAFT Polymerization, *Beilstein J. Org. Chem.*, **9,** 1226-1234 (2013).

Mori, T.; Sakakibara, K.; Endo, H.; Akada, M.; Okamoto, K.; Shundo, A.; Lee, M. V.; Ji, Q.; Fujisawa, T.; Oka, K.; Matsumoto, M.; Sakai, H.; Abe, M.; Hill, J. P.; Ariga, K., Langmuir Nanoarchitectonics: One-Touch Fabrication of Regularly Sized Nanodisks at the Air-Water Interface, *Langmuir*, **29,** 7239-7248 (2013).

— Polymer Controlled Synthesis —

Yamago, S.; Nakamura, Y., Recent Progress in the Use of Photoirradiation in Living Radical Polymerization, *Polymer*, **54,** 981-994 (2013).

Tosaka, M.; Senoo, K., Gold Nanoparticle/PDMS Composite Exhibiting Anisotropic Plasmon Resonance, *J. Soc. Mater. Sci. Jpn.*, **62,** 13-17 (2013) (in Japanese).

Asakawa, H.; Nishida, K.; Kanaya, T.; Tosaka, M., Giant Single Crystal of Isotactic Polypropylene Showing Near-Equilibrium Melting Temperature, *Polymer J.*, **45,** 287-292 (2013).

Iwamoto, T.; Watanabe, Y.; Takaya, H.; Haino, T.; Yasuda, N.; Yamago, S., Size- and Orientation-Selective Encapsulation of C_{70} by Cycloparaphenylenes, *Chem. Eur. J.*, **19,** 14061-14068 (2013).

Nakamura, Y.; Yamago, S., Organotellurium-Mediated Living Radical Polymerization under Photoirradiation by a Low-Intensity Light-Emitting Diode, *Beilstein J. Org. Chem.*, **9,** 1607-1612 (2013).

Tosaka, M.; Noda, M.; Ito, K.; Senoo, K.; Aoyama, K.; Ohta, N., Strain- and Temperature-Induced Polymorphism of Poly(dimethylsiloxane), *Colloid Polym. Sci.*, **291,** 2719-2724 (2013).

Fujitsuka, M.; Iwamoto, T.; Kayahara, E.; Yamago, S.; Majima, T., Enhancement of Quinoidal Character of Smaller [n]Cycloparaphenylenes Probed by Raman Spectroscopy, *ChemPhysChem*, **14,** 1570-1572 (2013).

Kayahara, E.; Iwamoto, T.; Suzuki, T.; Yamago, S., Selective Synthesis of [6], [8], and [10]Cycloparaphenylenes, *Chem. Lett.*, **42,** 621-623 (2013).

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

Kayahara, E.; Kouyama, T.; Kato, T.; Takaya, H.; Yasuda, N.; Yamago, S., Isolation and Characterization of Cycloparaphenylene Radical Cation and Dication, *Angew. Chem. Int. Ed.*, **52,** 13722-13726 (2013).

Yamago, S.; Yahata, Y.; Nakanishi, K.; Konishi, S.; Kayahara, E.; Nomura, A.; Goto, A.; Tsujii, Y., Synthesis of Concentrated Polymer Brushes via Surface-Initiated Organotellurium-Mediated Living Radical Polymerization (SI-TERP), *Macromolecules*, **46,** 6778-6785 (2013).

[Others]

Tosaka, M., Crystallization of Highly Strained Polymer Network, *Sin'i Gakkaishi*, **69,** 81- 87 (2013) (in Japanese).

Tosaka, M., High Resolution TEM of Grain Boundaries in Polymer Crystals, *J. Adhesion Soc. Jpn.*, **49,** 381-388 (2013) (in Japanese).

Yamago, S., Development and Application of Organotellium-mediated Living Radical Polymerization, TERP, *Mirai Zairyo*, **13,** 15-21 (2013) (in Japanese).

Yamago, S., Recent Progress in Organotellium-Mediated Living Radical Polymerization, TERP, *Syokubai*, **55,** 65-70 (2013) (in Japanese).

— Inorganic Photonics Materials —

Ueda, Y.; Tokuda, Y.; Fujimura, S.; Nihei, N.; Oka, T., Cesium Transfer from Granule Conglomerate, Asphalt, and Concrete Using Water-Containing Nanosized Air Bubbles, *ECS Trans.*, **50,** 1-6 (2013).

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).

Ueda, Y.; Tokuda, Y.; Shigeto, F.; Nihei, N.; Oka, T., Removal of Radioactive Cs from Gravel Conglomerate Using Water Containing Air Bubbles, *Water Science and Technology*, **67,** 996-999 (2013).

Masai, H.; Shirai, R.; Yoshida, K.; Takahashi, Y.; Ihara, R.; Fujiwara, T.; Tokuda, Y.; Yoko, T., Fabrication of $Sr_{0.5}Ba_{0.5}Nb_2O_6$ Nanocrystallite-Precipitated Transparent Phosphate Glass-Ceramics, *Journal of American Ceramics Society*, **96,** 3576-3583 (2013).

Masai, H.; Shirai, R.; Miyazaki, T.; Yoshida, K.; Fujiwara, T.; Tokuda, Y.; Yoko, T., ^{31}PNMR and IR Study of Highly Water-stable SrO-BaO-Nb_2O_5-P_2O_5 Glass and Glass-ceramics, *Chemistry Letters*, **42,** 1305-1307 (2013).

Masai, H.; Yamada, Y.; Okumura, S.; Kanemitsu, Y.; Yoko, T., Photoluminescence of Te^{4+} Center in Zinc Borate Glass, *Optics Letters*, **38,** 3780-3783 (2013).

Masai, H.; Hino, Y.; Yanagida, T.; Fujimoto, Y.; Fukuda, K.; Yoko, T., Excitation Light Source Dependence of Emission in Sn^{2+}-Ce^{3+} Codoped ZnO-P_2O_5 Glasses, *Journal of Applied Physics*, **114,** [083502-1]-[083502-6] (2013).

Masai, H.; Miyata, H.; Tanimoto, T.; Tokuda, Y.; Yoko, T., Preparation of Sn-Doped Zinc Phosphate Amorphous Thin Film and Its Emission Properties, *Journal of American Ceramics Society*, **96,** 382-384 (2013).

Masai, H., Preparation of Rare-earth-free Oxide Glass Phosphors, *Journal of Ceramic Society of Japan*, **121,** 150-155 (2013).

Masai, H.; Tanimoto, T.; Fujiwara, T.; Matsumoto, S.; Tokuda, Y.; Yoko, T., Localized Sn^{2+} Emission Center Independent of the Optical Basicity of Zinc Phosphate Glass, *Chemistry Letters*, **42,** 132-134 (2013).

— Nanospintronics —

Nakano, K.; Tanabe, K.; Hiramatsu, R.; Chiba, D.; Ohshima, N.; Kasai, S.; Sato, T.; Nakatani, Y.; Sekiguchi, K.; Kobayashi, K.; Ono, T., Real-time Observation of Electrical Vortex Core Switching, *Appl. Phys. Lett.*, **102,** [072405-1]-[072405-3] (2013).

Koyama, T.; Hata, H.; Kim, K.-J.; Moriyama, T.; Tanigawa, H.; Suzuki, T.; Nakatani, Y.; Chiba, D.; Ono, T., Current-Induced Magnetic Domain Wall Motion in a Co/Ni Nanowire with Structural Inversion Asymmetry, *Applied Physics Express*, **6,** [033001-1]-[033001-3] (2013).

Yamada, K.; Kakizakai, H.; Shimamura, K.; Kawaguchi, M.; Fukami, S.; Ishiwata, N.; Chiba, D.; Ono, T., Electric Field Modulation of Magnetic Anisotropy in MgO/Co/Pt Structure, *Applied Physics Express*, **6,** [073004-1]-[073004-3] (2013).

Kakizakai, H.; Yamada, K.; Kawaguchi, M.; Shimamura, K.; Fukami, S.; Ishiwata, N.; Chiba, D., Direct Observation of Domain Wall Motion in Co/Pt Wire under Gate Electric Field, *Japanese Journal of Applied Physics*, **52,** [070206-1]-[070206-3] (2013).

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., Two-barrier Stability that Allows Low-power Operation in Current-induced Domain-wall Motion, *Nature Communications*, **4,** [2011-1]-[2011-6] (2013).

Hiramatsu, R.; Koyama, T.; Hata, H.; Ono, T.; Chiba, D.; Fukami, S., Domain Wall Pinning by a Stray Field from NiFe on a Co/Ni Nanowire, *Journal of the Korean Physical Society*, **63,** 608-612 (2013).

Kawaguchi, M.; Shimamura, K.; Fukami, S.; Matsukura, F.; Ohno, H.; Moriyama, T.; Chiba, D.; Ono, T., Current-Induced Effective Fields Detected by Magnetotrasport Measurements, *Applied Physics Express*, **6,** [113002-1]-[113002-4] (2013).

DIVISION OF BIOCHEMISTRY
— Biofunctional Design-Chemistry —

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*, **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).

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).

Takeuchi, T.; Matile, S., Sensing Applications of Synthetic Transport Systems, *Chem. Commun. (Camb)*, **49,** 19-29 (2013).

Tsuji, S.; Futaki, S.; Imanishi, M., Creating a TALE Protein with Unbiased 5'-T Binding, *Biochem. Biophys. Res. Commun.*, **441,** 262-265 (2013).

Kawaguchi, Y.; Tanaka, G.; Nakase, I.; Imanishi, M.; Chiba, J.; Hatanaka, Y.; Futaki, S., Identification of Cellular Proteins Interacting with Octaarginine (R8) Cell-penetrating Peptide by Photo-crosslinking, *Bioorg. Med. Chem. Lett.*, **23,** 3738-3740 (2013).

Noshiro, D.; Sonomura, K,; Yu, H. H.; Imanishi, M.; Asami, K.; Futaki, S., Construction of a Ca(2+)-gated Artificial Channel by Fusing Alamethicin with a Calmodulin-derived Extramembrane Segment, *Bioconjug. Chem.*, **24,** 188-195 (2013).

Mishiro, K.; Furuta, T.; Sasamori, T.; Hayashi, K.; Tokitoh, N.; Futaki, S.; Kawabata, T., A Cyclochiral Conformational Motif Constructed Using a Robust Hydrogen Bonding Network, *J. Am. Chem. Soc.*, **135,** 13644-13647 (2013).

Pujals, S.; Miyamae, H.; Afonin, S.; Murayama, T.; Hirose, H.; Nakase, I.; Taniuchi, K.; Umeda, M.; Sakamoto, K.; Ulrich, A.; Futaki, S., Curvature Engineering: Positive Membrane Curvature Induced by Epsin N-Terminal Peptide Boosts Internalization of Octaarginine, *ACS Chem. Biol.*, **8,** 1894-1899 (2013).

Gehin, C.; Montenegro, J.; Bang, E.-K.; Cajaraville, A.; Takayama, S.; Hirose, H.; Futaki, S.; Matile, S.; Riezman, H., Dynamic Amphiphile Libraries to Screen for the "Fragrant" Delivery of siRNA into HeLa Cells and Human Primary Fibroblasts, *J. Am. Chem. Soc.*, **135,** 9295-9298 (2013).

Katayama, S.; Nakase, I.; Yano, Y.; Murayama, T.; Nakata, Y.; Matsuzaki, K.; Futaki, S., Effects of Pyrenebutyrate on the Translocation of Arginine-rich Cell-penetrating Peptides through Artificial Membranes: Recruiting Peptides to the Membranes, Dissipating liquid-ordered Phases, and Inducing Curvature, *Biochim. Biophys. Acta*, **1828,** 2134-2142 (2013).

Yamazaki, C. M.; Nakase, I.; Endo, H.; Kishimoto, S.; Mashiyama, Y.; Masuda, R.; Futaki, S.; Koide, K., Collagen-like Cell-penetrating Peptides, *Angew. Chem. Int. Ed. Engl.*, **52,** 5497-5500 (2013).

Madani, F.; Abdo, R.; Lindberg, S.; Hirose, H.; Futaki, S.; Langel, Ü.; Gräslund, A., Modeling the Endosomal Escape of Cell-Penetrating Peptides Using a Transmembrane pH Gradient, *Biochim. Biophys. Acta*, **1828,** 1198-1204 (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).

Futaki, S.; Hirose, H.; Nakase, I., Arginine-rich Peptides: Methods of Translocation through Biological Membranes, *Curr. Pharm. Design*, **19,** 2863-2868 (2013).

— Chemistry of Molecular Biocatalysts —

Hiratake, J.; Suzuki, H.; Fukuyama, K.; Wada, K.; Kumagai, H., γ-Glutamyltranspeptidase and Its Precursor, *Handbook of Proteolytic Enzymes, 3rd Ed.*, **820,** 3712-3719 (2013).

Koeduka, T.; Suzuki, S.; Iijima, Y.; Ohnishi, T.; Suzuki, H.; Watanabe, B.; Shibata, D.; Umezawa, T.; Pichersky, E.; Hiratake, J., Enhancement of Production of Eugenol and Its Gllycosides in Transgenic Aspen Plants via Genetic Engineering, *Biochem. Biophys. Res. Commun.*, **436,** 73-78 (2013).

Tanaka, R.; Yamamoto, S.; Watanabe, B.; Hiratake, J.; Ohkita, M.; Matsumura, Y., Basis for Ttreatment of Oxidative Stress Injury -Novel Selective γ-Glutamyl Transpeptiease Inhibitors for Acute Ischemic Nephropathy-, *Kiendy and Free Radical*, **11(11),** 146-149 (2013) (in Japanese).

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 (Stuttg).*, doi: 10.1111/plb.12054. (2013).

— Molecular Biology —

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).

Takai, A.; Satoh, M.; Matsuyama, T.; Ito, A.; Nakata, R.; Aoyama, T.; Inoue, H., Secretion of Miraculin through the Function of a Signal Peptide Conserved in the Kunitz-type Soybean Trypsin Inhibitor Family, *FEBS Lett.*, **587,** 1767-1772 (2013).

Franciosini, A.; Lombardi, B.; Iafrate, S.; Pecce, V.; Mele, G.; Lupacchini, L.; Kondou, Y.; Gusmaroli, G.; Aki, S.; Tsuge, T.; Deng, X. W.; Matsui, M.; Vittorioso, P.; Costantino, P.; Serino, G., The *Arabidopsis* COP9 SIGNALOSOME INTERACTING F-BOX KELCH 1 Protein Forms an SCF Ubiquitin Ligase and Regulates Hypocotyl Elongation, *Mol. Plant*, **6,** 1616-1629 (2013).

— Chemical Biology —

Kumagai, H.; Suemori, H.; Uesugi, M.; Nakatsuji, N.; Kawase, E., Identification of Small Molecules that Promote Human Embryonic Stem Cell Self-Renewal, *Biochem. Biophys. Res. Commun.*, **434(4),** 710-716 (2013).

Suzuki, T.; Arai, M. A.; Nakashima, M.; Uesugi, M., Merging Chemistry and Biology in Emerging Countries, *Chem. Biol.*, **20(4),** 461-465 (2013).

Natsume, A.; Ito, M.; Katsushima, K.; Ohka, F.; Hatanaka, A.; Shinjo, K.; Sato, S.; Takahashi, S.; Ishikawa, Y.; Takeuchi, I.; Shimogawa, H.; Uesugi, M.; Okano, H.; Kim, S. U.; Wakabayashi, T.; Issa, J. P.; Sekido, Y.; Kondo, Y., Chromatin Regulator PRC2 Is a Key Regulator of Epigenetic Plasticity in Glioblastoma, *Cancer Res.*, **73(14),** 4559-4570 (2013).

Takemoto, N.; Suehara, T.; Frisco, H.; Sato, S.; Sezaki, T.; Kusamori, K.; Kawazoe, Y.; Park, S. M.; Yamazoe, S.; Mizuhata, Y.; Inoue, R.; Miller, G. J.; Hansen, S. U.; Jayson, G. C.; Gardiner, J.; Kanaya, T.; Tokitoh, N.; Ueda, K.; Takakura, Y.; Kioka, N.; Nishikawa, M.; Uesugi, M., Small-Molecule-Induced Clustering of Heparan Sulfate Promotes Cell Adhesion, *J. Am. Chem. Soc.*, **135(30),** 11032-11039 (2013).

Kita, M.; Hirayama, Y.; Yoneda, K.; Yamagishi, K.; Chinen, T.; Usui, T.; Sumiya, E.; Uesugi, M.; Kigoshi, H., Inhibition of Microtubule Assembly by A Complex of Actin and Antitumor Macrolide Aplyronine A, *J. Am. Chem. Soc.*, **135(48),** 18089-18095 (2013).

Molzan, M.; Kasper, S.; Röglin, L.; Skwarczynska, M.; Sassa, T.; Inoue, T.; Breitenbuecher, F.; Ohkanda, J.; Kato, N.; Schuler, M.; Ottmann, C., Stabilization of Physical RAF/14-3-3 Interaction by Cotylenin A as Treatment Strategy for Ras Mutant Cancers, *ACS Chem. Biol.*, **8,** 1869-1875 (2013).

Anders, C.; Higuchi, Y.; Koschinsky, K.; Bartel, M.; Schumacher, B.; Thiel, P.; Nitta, H.; Preisig-Müller, R.; Schlichthörl, G.; Renigunta, V.; Ohkanda, J.; Daut, J.; Kato, N.; Ottmann, C., A Semi-synthetic Fusicoccane Stabilizes a Protein-protein Interaction and Enhances the Expression of K+ Channels at the Cell Surface, *Chem. Biol.*, **20,** 583-593 (2013).

Hayashi, D.; Kato, N.; Kuzuyama, T.; Sato, Y.; Ohkanda, J., Antimicrobial *N*-(2-chlorobenzyl)-Substituted Hydroxamate Is an Inhibitor of 1-Deoxy-D-xylulose 5-Phosphate Synthase, *Chem. Commun.*, **49,** 5535-5537 (2013).

Maki, T.; Kawamura, A.; Kato, N.; Ohkanda, J., Chemical Ligation of Epoxide-containing Fusicoccins and Peptide Fragments Guided by 14-3-3 Protein, *Mol. BioSyst.*, **9,** 940-943 (2013).

Machida, S.; Tsubamoto, M.; Kato, N.; Harada, K.; Ohkanda, J., Peptidomimetic Modification Improves Cell Permeation of Bivalent Farnesyltransferase Iinhibitors, *Bioorg. Med. Chem.*, **21,** 4004-4010 (2013).

DIVISION OF ENVIRONMENTAL CHEMISTRY

— Molecular Materials Chemistry —

Shuto, A.; Kushida, T.; Fukushima, T.; Kaji, H.; Yamaguchi, S., π-Extended Planarized Triphenyl-boranes with Thiophene Spacers, *Org. Lett.*, **15,** 6234-6237 (2013).

Suzuki, F.; Fukushima, T.; Fukuchi, M.; Kaji, H., Refined Structure Determination of Blue-Emitting Tris(8-hydroxyquinoline) Aluminum(III) (Alq_3) by the Combined Use of Cross-Polarization/Magic-Angle Spinning ^{13}C Solid-State NMR and First-Principles Calculation, *J. Phys. Chem. C*, **117,** 18809-18817 (2013).

Asakura, T.; Suzuki, Y.; Yazawa, K.; Aoki, A.; Nishiyama, Y.; Nishimura, K.; Suzuki, F.; Kaji, H., Determination of Accurate ^{1}H Positions of (Ala-Gly)n as a Sequential Peptide Model of *Bombyx mori* Silk Fibroin before Spinning (Silk I), *Macromolecules*, **46,** 8046-8050 (2013).

Iwahara, N.; Sato, T.; Tanaka, K.; Kaji, H., Vibronic Couplings in C_{60} Derivatives for Organic Photovoltaics, *Chem. Phys. Lett.*, **590,** 169-174 (2013).

Hayase, G.; Kanamori, K.; Hasegawa, G.; Maeno, A.; Kaji, H.; Nakanishi, K., A Superamphiphobic Macroporous Silicone Monolith with Marshmallow-like Flexibility, *Angew. Chem. Int. Ed.*, **52,** 10788-10791 (2013).

Goto, A.; Ohtsuki, A.; Ohfuji, H.; Tanishima, M.; Kaji, H., Reversible Generation of a Carbon-Centered Radical from Alkyl Iodide Using Organic Salts and Their Application as Organic Catalysts in Living Radical Polymerization, *J. Am. Chem. Soc.*, **135,** 11131-11139 (2013).

Hirata, S.; Totani, K.; Kaji, H.; Vacha, M.; Watanabe, T.; Adachi, C., Reversible Thermal Recording Media Using Time-Dependent Persistent Room Temperature Phosphorescence, *Adv. Opt. Mater.*, **1,** 438-442 (2013).

Uejima, M.; Sato, T.; Tanaka, K.; Kaji, H., Vibronic Coupling Density Analysis for the Chain-length Dependence of Reorganization Energies in Oligofluorenes: A Comparative Study with Oligothiophenes, *Phys. Chem. Chem. Phys.*, **15,** 14006-14016 (2013).

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 (2013).

Hirata, S.; Totani, K.; Zhang, J.; Yamashita, T.; Kaji, H.; Marder, S. R.; Watanabe, T.; Adachi, C., Efficient Persistent Room Temperature Phosphorescence in Organic Amorphous Materials under Ambient Conditions, *Adv. Funct. Mater.*, **23,** 3386-3397 (2013).

Hayase, G.; Kanamori, K.; Fukuchi, M.; Kaji, H.; Nakanishi, K., Facile Synthesis of Marshmallow-like Macroporous Gels Usable under Harsh Conditions for the Separation of Oil and Water, *Angew. Chem. Int. Ed.*, **52,** 1986-1989 (2013).

Ohtsuki, A.; Goto, A.; Kaji, H., Visible-Light-Induced Reversible Complexation Mediated Living Radical Polymerization of Methacrylates with Organic Catalysts, *Macromolecules*, **46,** 96-102 (2013).

Nishiyama, Y.; Fukushima, T.; Fukuchi, M.; Fujimura, S.; Kaji, H., Sensitivity Boosting in Solid-state NMR of Thin Organic Semiconductors by a Paramagnetic Dopant of Copper Phthalocyanine, *Chem. Phys. Lett.*, **556,** 195-199 (2013).

— Hydrospheric Environment Analytical Chemistry —

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).

Tanimizu, M.; Sohrin, Y.; Hirata, T., Heavy Element Stable Isotope Ratios: Analytical Approaches and Applications, *Anal. Bioanal. Chem.*, **405,** 2771-2783 (2013).

Vu, H. T. D.; Sohrin, Y., Diverse Stoichiometry of Dissolved Trace Metals in the Indian Ocean, *Scientific Reports*, **3,** DOI: 10.1038/srep01745 (2013).

Sohrin, Y. (Ed. Okada, T.; Hayashita, T.), Determination of Trace Metals in Seawater, *Tokoton Yasashii Ion Koukan no Hon*, 114 (2013) (in Japanese).

Sohrin, Y. (Ed. Arikawa, Y.; Oguma, K.; Tsunoda, K.), Stoichiometric Calculation, Acid-base Reaction, Acid-base Titration, *Basic Master Series Analytical Chemistry*, 21-59 (2013) (in Japanese).

Sohrin, Y., Trace Elements, *Nippon Kaiyo Gakkai Souritsu 70 Shunen Kinen Shi*, 22 (2013) (in Japanese).

— Solution and Interface Chemistry —

Shimoaka, T.; Rikiyama, K.; Katsumoto, Y.; Hasegawa, T., Infrared Spectroscopic Study of Stereo-controlled Poly(*N*-isopropylacrylamide) with an Extended Chain Conformation Induced by Adsorption on a Gold Surface, *Anal. Bioanal. Chem.*, **405,** 9411-9418 (2013).

Norimoto, N.; Morimine, S.; Shimoaka, T.; Hasegawa, T., Analysis of Surface Coverage of a Self-Assembled Monolayer of Octadecyl Silane on a Si(100) Surface by Infrared External-Reflection Spectroscopy, *Anal. Sci.*, **29,** 979-984 (2013).

Wakai, C.; Shimoaka, T.; Hasegawa, T., Analysis of the Hydration Process and Rotational Dynamics of Water in a Nafion Membrane Studied by ^{1}H NMR Spectroscopy, *Anal. Chem.*, **85,** 7581-7587 (2013).

Tsuchiizu, A., Hasegawa, T., Katsumoto, Y., Water Sorption on a Thin Film of Stereocontrolled Poly(*N*-Ethylacrylamide) and Poly(*N*, *N*-Diethylacrylamide), *MATEC Web of Conferences*, **4,** [03001-1]-[03001-4] (2013).

Ito, Y.; Yoshidome, T.; Matubayasi, N.; Kinoshita, M.; Ikeguchi, M., Molecular Dynamics Simulations of Yeast F_1-ATPase before and after 16° Rotation of the γ Subunit, *J. Phys. Chem. B*, **117,** 3298-3307 (2013).

Mogami, G.; Miyazaki, T.; Wazawa, T.; Matubayasi, N.; Suzuki, M., Anion-Dependence of Fast Relaxation Component in Na-, K-Halide Solutions at Low Concentrations Measured by High-Resolution Microwave Dielectric Spectroscopy, *J. Phys. Chem. A*, **117,** 4851-4862 (2013).

Kimura, H.; Nakahara, M.; Matubayasi, N., Solvent Effect on Pathways and Mechanisms for D-Fructose Conversion to 5-Hydroxymethyl-2-furaldehyde: In Situ ^{13}C NMR Study, *J. Phys. Chem. A*, **117,** 2102-2113 (2013).

Yoshida, K.; Matubayasi, N.; Uosaki, Y.; Nakahara, M., Effect of Heavy Hydrogen Isotopes on the Vibrational Line Shape for Supercritical Water through Rotational Couplings, *J. Chem. Phys.*, **138,** [134508-1]-[134508-12] (2013).

Karino, Y.; Matubayasi, N., Interaction-Component Analysis of the Urea Effect on Amino Acid Analogs, *Phys. Chem. Chem. Phys.*, **15,** 4377-4391 (2013).

Ishikawa, T.; Burri, R. R.; Kamatari, Y. O.; Sakuraba, S.; Matubayasi, N.; Kitao, A.; Kuwata, K., A Theoretical Study of the Two Binding Modes between Lysozyme and tri-NAG with an Explicit Solvent Model Based on the Fragment Molecular Orbital Method, *Phys. Chem. Chem. Phys.*, **15,** 3646-3654 (2013).

Takemura, K.; Burri, R. R.; Ishikawa, T.; Ishikura, T.; Sakuraba, S.; Matubayasi, N.; Kuwata, K.; Kitao, A., Free-Energy Analysis of Lysozyme–triNAG Binding Modes with All-Atom Molecular Dynamics Simulation Combined with the Solution Theory in the Energy Representation, *Chem. Phys. Lett.*, **559,** 94-98 (2013).

Kameda, Y.; Deguchi, H.; Kubota, Y.; Furukawa, H.; Yagi, Y.; Imai, Y.; Tatsumi, M.; Yamazaki, N.; Watari, N.; Hirata, T.; Matubayasi, N., High-Energy X-ray Diffraction Study on the Intramolecular Structure of 2-Aminoethanol in the Liquid State, *Bull. Chem. Soc. Japan*, **86,** 99-103 (2013).

Ishizuka, R.; Yoshida, N., Extended Molecular Ornstein-Zernike Integral Equation for Fully Anisotropic Solute Molecules: Formulation in a Rectangular Coordinate System, *J. Chem. Phys.*, **139,** 084119-084128 (2013).

— Molecular Microbial Science —

Sato, S. B.; Park, J.; Kawamoto, J.; Sato, S.; Kurihara, T., Inhibition of Constitutive Akt (PKB) Phosphorylation by Docosahexaenoic Acid in the Human Breast Cancer Cell Line MDA-MB-453, *Biochim. Biophys. Acta*, **1831,** 306-313 (2013).

Siwek, A.; Omi, R.; Hirotsu, K.; Jitsumori, K.; Esaki, N.; Kurihara, T.; Paneth, P., Binding Modes of DL-2-Haloacid Dehalogenase Revealed by Crystallography, Modeling and Isotope Effects Studies, *Arch. Biochem. Biophys.*, **540,** 26-32 (2013).

Ohke, Y.; Sakoda, A.; Kato, C.; Sambongi, Y.; Kawamoto, J.; Kurihara, T.; Tamegai, H., Regulation of Cytochrome *c*- and Quinol Oxidases, and Piezotolerance of Their Activities in the Deep-Sea Piezophile *Shewanella violacea* DSS12 in Response to Growth Conditions, *Biosci. Biotechnol. Biochem.*, **77,** 1522-1528 (2013).

Yoshimune, K.; Kawamoto, J.; Kurihara, T., Proteins Involved in Cold Adaptation, *Cold-Adapted Microorganisms*, 97-110 (2013).

Kurihara, T.; Kawamoto, J., Novel Micromdomain at Bacterial Cell Membrane, *Kagaku to Seibutsu*, **51,** 358-360 (2013) (in Japanese).

[Others]

Kawamoto, J.; Kurihara, T., Physiological Function of Polyunsaturated Fatty Acid in Bacteria, *Oleoscience*, **13,** 221-229 (2013) (in Japanes).

Kurihara, T., Global Environment and Microorganisms, *Oceanochemistry Res.*, **26,** 28-30 (2013) (in Japanese).

DIVISION OF MULTIDISCIPLINARY CHEMISTRY
— Polymer Materials Science —

Inoue, R.; Kanaya, T., Heterogeneous Dynamics of Polymer Thin Films as Studied by Neutron Scattering, *Adv. Polym. Sci.*, **252,** 107-140 (2013).

Kanaya, T., Glass Transition, Dynamics and Heterogeniety of Polymer Thin Films, *Adv. Polym. Sci.*, **252,** (2013).

Mashita, R.; Kishimoto, H.; Inoue, R.; Kanaya, T., Small-angle X-ray and Neutron Scattering Analyses of Highly Crosslinked Rubber with Unsaturated Carboxylic Acid, *Polym. J.*, **45,** 57-63 (2013).

Mita, K.; Okumura, K.; Kimura, K.; Isaki, T.; Takenaka, M.; Kanaya, T., Simultaneous Small- and Wide-Angle X-ray Scattering Studies on the Crystallization Dynamics of Poly(4-methylpentene-1) from Melt, *Polym. J.*, **45,** 79-86 (2013).

Okada, K.; Higashioji, H.; Nakagawa, T.; Uchida, H.; Takahashi, K.; Inoue, R.; Nishida, K.; Kanaya, T., Structural Analysis of Poly(ethylene terephthalate) during Uniaxial Drawing above the Glass Transition Temperature, *Polym. J.*, **45,** 50-56 (2013).

Asakawa, H.; Nishida, K.; Kanaya, T.; Tosaka, M., Giant Single Crystal of Isotactic Polypropylene Showing Near-Equilibirum Melting Temperature, *Polym. J.*, **45,** 287-292 (2013).

Matsuba, G.; Ito, C.; Zhao, Y.; Inoue, R.; Nishida, K.; Kanaya, T., In-situ Small-Angle X-ray and Neutron Scattering Measurements on a Blend Deuterated and Hydrogenated Polyethylenes during Uniaxial Drawing, *Polym. J.*, **45,** 293-299 (2013).

Kanaya, T.; Polec, A. I.; Fujiwara, T.; Inoue, R.; Nishida, K.; Ogawa, H.; Ohta, N., Precursor of Shish-Kebab above the Melting Temperature by Microbeam X-ray Scattering, *Macromolecules*, **46,** 3031-3036 (2013).

Xia, T.; Ogawa, H.; Inoue, R.; Nishida, K.; Yamada, N. L.; Li, G.; Kanaya, T., Dewetting Process of Deuterated Polystyrene and Poly(vinyl methyl ether) Blend Thin Films via Phase Separation, *Macromolecules*, **46,** 4540-4547 (2013).

Takemoto, N.; Suehara, T.; Frisco, H. L.; Sato, S.; Sezaki, T.; Kusamori, K.; Kawazoe, Y.; Park, S. M.; Yamazoe, S.; Mizuhata, Y.; Inoue, R.; Miller, G. J.; Hansen, S. U.; Jayson, G. C.; Gardiner, J. M.; Kanaya, T.; Tokitoh, N.; Ueda, K.; Takakura, Y.; Kioka, N.; Nishizawa, M.; Uesugi, M., Small-Molecule-Induced Clustering of Heparan Sulfate Promotes Cell Adhesion, *J. Am. Chem. Soc.*, **135,** 11032-11039 (2013).

Sakakibara, K.; Granström, M.; Kilpeläinen, I.; Helaja, J.; Heinilehto, S.; Inoue, R.; Kanaya, T.; Hill, J. P.; Nakatsubo, F.; Tsujii, Y.; Ariga, K., Light-Harvesting Nanorods Based on Pheophorbide-Appending Cellulose, *Biomacromolecules*, **14,** 3223-3230 (2013).

Ogawa, H.; Masunaga, H.; Sasaki, S.; Goto, S.; Tanaka, T.; Seike, T.; Takahashi, S.; Takeshita, K.; Nariyama, N.; Ohashi, H.; Ohata, T.; Furukawa, T.; Matsushita, T.; Ishizawa, Y.; Yagi, N.; Takata, M.; Kitamura, H.; Takahara, A.; Sakurai, K.; Tashiro, K.; Kanaya, T.; Amemiya, Y.; Horie, K.; Takenaka, M.; Jinnai, H.; Okuda, H.; Akiba, I.; Takahashi, I.; Yamamoto, K.; Hikosaka, M.; Sakurai, S.; Shinohara, Y.; Okada, A., Experimental Station for Multiscale Surface Structural Analyses of Soft-Material Films at SPring-8 via a GISWAX/GIXD/XR-Integrated System, *Polym. J.*, **45,** 109-116 (2013).

Fujiwara, S.; Yamada, T.; Matsuo, M.; Takahashi, N.; Kamazawa, Y.; Kawakita, Y.; Shibata, K., Internal Dynamics of Protein during Amyloid Fibril Formation Observed by Neutron Scattering, *J. Phys. Soc. Jpn.*, **82,** SA019-1-SA019-5 (2013).

Arai, M.; Kajimoto, R.; Nakamura, M.; Inamura, Y.; Nakajima, K.; Shibata, K.; Takahashi, N.; Suzuki, J.; Takata, S.; Yamada, T.; Itoh, S., Recent Developments of Instruments in a Spallation Neutron Source at J-PARC and Those Prospects in the Future, *J. Phys. Soc. Jpn.*, **82,** [SA024-1]-[SA024-14] (2013).

Inoue, R.; Nakamura, M.; Matsui, K.; Kanaya, T.; Nishida, K.; Hino, M., Distribution of Glass Transition Temperature in Multilayered Poly(methyl methacrylate) Thin Film Supported on a Si Substrate as Studied by Neutron Reflectivity, *Phys. Rev. E*, **88,** [032601-1]-[032601-6] (2013).

[Others]

Kanaya, T., Crystalline and Amorphous Structure of Polymer, *Structure and Physical Properties of Polymer*, 219-288 (2013) (in Japanese).

— Molecular Rheology —

Langeloth, M.; Masubuchi, Y.; Böhm, M. C.; Müller-Plathe, F., Recovering the Reptation Dynamics of Polymer Melts in Dissipative Particle Dynamics Simulations via Slip-Springs, *J. Chem. Phys.*, **138,** [104907-1]-[104907-8] (2013).

Masubuchi, Y.; Sukumaran, S. K., Cross-Correlation Contributions to Orientational Relaxations in Primitive Chain Network Simulations, *J. Soc. Rheol. Jpn.*, **41,** 1-7 (2013).

Furuichi, K.; Nonomura, C.; Masubuchi, Y.; Watanabe, H., Nonlinear Stress Relaxation of Scarcely Entangled Chains in Primitive Chain Network Simulations, *J. Soc. Rheol. Jpn.*, **41,** 13-19 (2013).

Masubuchi, Y.; Yaoita, T.; Matsumiya, Y.; Watanabe, H.; Ianniruberto, G.; Marrucci, G., Stretch/Orientation Induced Acceleration in Stress Relaxation in Coarse-Grained Molecular Dynamics Simulations, *J. Soc. Rheol. Jpn.*, **41,** 35-37 (2013).

Matsumiya, Y.; Watanabe, H.; Takano, A.; Takahashi, Y., Uniaxial Extensional Behavior of $(SIS)_p$-Type Multiblock Copolymer Systems: Structural Origin of High Extensibility, *Macromolecules*, **46,** 2681-2695 (2013).

Suzuki, S.; Uneyama, T.; Watanabe, H., Concentration Dependence of Nonlinear Rheological Properties of Hydrophobically Modified Ethoxylated Uretane Aqueous Solutions, *Macromolecules*, **46,** 3497-3504 (2013).

Matsumiya, Y.; Kumazawa, K.; Nagao, M.; Urakawa, O.; Watanabe, H., Dielectric Relaxation of Monodisperse Linear Polyisoprene: Contribution of Constraint Release, *Macromolecules*, **46,** 6067-6080 (2013).

Huang, Q.; Alvarez, N. J.; Matsumiya, Y.; Rasmussen, H. K.; Watanabe, H.; Hassager, O., Extensional Rheology of Entangled Polystyrene Solutions Suggests Importance of Nematic Interactions, *ACS Macro Letters*, **2,** 741-744 (2013).

Watanabe, H.; Matsumiya, Y.; van Ruymbeke, E., Component Relaxation Times in Entangled Binary Blends of Linear Chains: Reptation/CLF along Partially or Fully Dilated Tube, *Macromolecules*, **46,** 9296-9312 (2013).

[Others]

Masubuchi, Y., Molecular Simulations for Rheology of Polymeric Materials, *Nippon Gomu Kyokaishi*, **86,** 113-118 (2013) (in Japanese).

— Molecular Aggregation Analysis —

Tsuzuki, S.; Sato, N., Origin of Attraction in Chalgogen-Nitrogen Interaction of 1,2,5-Chalcogenadiazole Dimers, *J. Phys. Chem. B*, **117,** 6849-6855 (2013).

Yoshida, H., Low-Energy Inverse Photoemission Spectroscopy Using a High-Resolution Grating Spectrometer in the Near Ultraviolet Range, *Rev. Sci. Instrum.*, **84,** [103901-1]-[103901-5] (2013).

Fabiano, S.; Yoshida, H.; Chen, Z.-H.; Facchetti, A.; Loi, M. A., Orientation-Dependent Electronic Structures and Charge Transport Mechanisms in Ultrathin Polymeric n-Channel Field-Effect Transistors, *ACS Appl. Mater. Interfaces*, **5,** 4417-4422 (2013).

Han, W. N.; Yoshida, H.; Ueno, N.; Kera, S., Electron Affinity of Pentacene Thin Film Studied by Radiation-Damage Free Inverse Photoemission Spectroscopy, *Appl. Phys. Lett.*, **103,** [123303-1]-[123303-5] (2013).

Han, W. N.; Yonezawa, K.; Makino, R.; Kato, K.; Hinderhofer, A.; Murdey, R.; Shiraishi, R.; Yoshida, H.; Sato, N.; Ueno, N.; Kera, S., Quantitatively Identical Orientation-Dependent Ionization Energy and Electron Affinity of Diindenoperylene, *Appl. Phys. Lett.*, **103,** [253301-1]-[253301-4] (2013).

Noshiro, D.; Sonomura, K.; Yu, H.-H.; Imanishi, M.; Asami, K.; Futaki, S., Construction of a Ca^{2+}-Gated Artificial Channel by Fusing Alamethicin with Calmodulin-Derived Extramembrane Segment, *Bioconjugate Chem.*, **24,** 188-195 (2013).

Asami, K., Dielectric Properties of Dipicrylamine-Doped Erythrocytes, Cultured Cells and Lipid Vesicles, *Bioelectrochemistry*, **92,** 14-21 (2013).

— Interdisciplinary Chemistry for Innovation —

Kondo, T.; Kanda, T.; Takagi, D.; Wada, K.; Kimura, Y.; Toshimitsu, A., Dehydrogenative *N*-Heterocyclization of 2-(2-Aminoaryl) ethyl Alcohols to Indole Derivatives Catalyzed by (μ-Oxo)tetraruthenium Cluster / 1,2-Bis(diphenylphosphino)benzene, *Heterocycles*, **85,** 1015-1022 (2012).

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

— Particle Beam Science —

[Others]

Kubo, T.; Iwashita, Y.; Saeki, T., RF Electromagnetic Field and Vortex Penetration in Multilayered Superconductors, *Proc. of International Conference on RF Superconductivity, SRF2013*, TUP007 (2013).

Iwashita, Y.; Tongu, H.; Hayano, H., Update on Study of Welding Porosity in b EBW, *Proc. of International Conference on RF Superconductivity, SRF2013*, TUP061 (2013).

Tongu, H.; Iwashita, Y.; Hayano, H.; Yamamoto, Y., XT-map System for Locatiig SC Cavity Quench Position, *Proc. of International Conference on RF Superconductivity, SRF2013,* TUP114 (2013).

Iwashita, T.; Fuwa, Y.; Hashida, M.; Sakabe, S.; Tokita, S.; Tongu, H.; Otani, K.; Hayano, H.; Watanabe, K.; Yamamoto, Y., Update on Detection and Study of Welding Porosity in Niobium EBW, *Proc. of European Linear Collider Workshop, ECFA LC2013* (2013).

Iwashita, T.; Fuwa, Y.; Hashida, M.; Sakabe, S.; Tokita, S.; Tongu, H.; Otani, K., Efforts on Nondestructive Inspections for SC Cavities, *Proc. of International Particle Accelerator Conference, IPAC'13*, 2352-2354 (2013).

Fuwa, Y.; Iwashita, T.; Okamura, M., Multi-strip Current Monitor for Pulsed Laser Plasma Diagnostics, *Proc. of International Particle Accelerator Conference, IPAC'13*, 538-540 (2013).

Fuwa, Y.; Ikeda, H.; Iwashita, T.; Kitahara, R.; Nasu, Y.; Tongu, H.; Fukuda, S.; Matsumoto, T.; Okamura, M., Anisotropic Ferrite Magnet Focusing System for Klystrons, *Proc. of International Particle Accelerator Conference, IPAC'13*, 2756-2758 (2013).

Kubo, T.; Saeki, T.; Iwashita, Y., RF Field-Attenuation Formulae for the Multilayer Coating Model, *Proc. of International Particle Accelerator Conference, IPAC'13*, 2343-2345 (2013).

Imajo, S.; Iwashita, Y.; Gertenbort, P.; Arimoto, Y.; Shimizu, H. M.; Kitaguchi, M.; Yoshioka, T.; Seki, Y., Rebunching Ultracold Neutrons by Magnetic Deceleration for the Neutron EDM Experiment at J-PARC, *Proc. of International Particle Accelerator Conference, IPAC'13*, 1187-1189 (2013).

Kitahara, R.; Nasu, Y.; Fuwa, Y.; Iwasita, Y., Development of Harmonic Field Measurement System with Higher Resolution ADC, *Proc. of International Particle Accelerator Conference, IPAC'13*, 3330-3332 (2013).

Imajo, S.; Iwashita, Y.; Kitaguchi, M.; Shimizu, H. M.; Arimoto, Y.; Yoshioka, T.; Seki, Y., The Improvement of the Ultracold Neutrons Rebuncher, *Proceedings of the 10th Annual Meeting of Particle Accelerator Society of Japan*, SAP019 (2013) (in Japanese).

Kitahara, R.; Nasu, Y.; Fuwa, Y.; Iwasita, Y., Rotating Coil System for ILC Final Focus Magnet Multipole part 2, *Proceedings of the 10th Annual Meeting of Particle Accelerator Society of Japan*, SUP064 (2013) (in Japanese).

Fuwa, Y.; Ikeda, S.; Kumaki, M.; Sekine, M.; Okamura, M.; Iwashita, Y., Laser Ion Source with a Multi Pulse Laser, *Proceedings of the 10th Annual Meeting of Particle Accelerator Society of Japan*, SAP047 (2013) (in Japanese).

Tongu, H.; Iwashita, Y.; Kusuda, T.; Hayano, H.; Yamamoto, Y., Device Construction for the Development of CS Cavity Inspection System, *Proceedings of the 10th Annual Meeting of Particle Accelerator Society of Japan*, SAP116 (2013) (in Japanese).

— Laser Matter Interaction Science —

Gemini, L.; Hashida, M.; Shimizu, M.: Miyasaka, Y.; Inoue, S.; Tokita, S.; Limpouch, J.; Mocek, T.; Sakabe, S., Metal-like Self-Organization of Periodic Nanostructures on Silicon and Silicon Carbide under Femtosecond Laser Pulses, *J. Appl. Phys.*, **114,** [194903-1]-[194903-5] (2013).

Shimizu, S.; Hashida, M.; Miyasaka, Y.; Tokita, S.; Sakabe, S., Unidirectionally Oriented Nanocracks on Metal Surfaces Irradiated by Low-Fluence Femtosecond Laser Pulses, *Appl. Phys. Lett.*, **103,** [174106-1]-[174106-4] (2013).

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,** [155001-1]-[155001-4] (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,** [174106-1]-[174106-4] (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,** [191106-1]-[191106-4] (2013).

— Electron Microscopy and Crystal Chemistry —

Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Thickness-Dependent Structure-Property Relationships in Strained (110) $SrRuO_3$ Thin Films, *Adv. Funct. Mater.*, **23,** 1129-1136 (2013).

Kohara, K.; Yamamoto, S.; Seinberg, L.; Murakami, T.; Tsujimoto, M.; Ogawa, T.; Kurata, H.; Kageyama, H.; Takano, M., Carboxylated SiO_2-Coated α-Fe Nanoparticles: Towards a Versatile Platform for Biomedical Applications, *Chem. Commun.*, **49,** 2563-2565 (2013).

Wiengmoon, A.; Pearce, J. T. H.; Chairuangsri, T.; Isoda, S.; Saito, H.; Kurata, H., HRTEM and HAADF-STEM Study of the Precipitate at Peak Aging of Cast A319 Aluminum Alloy, *Micron*, **45,** 32-36 (2013).

Saito, H.; Chen, C. H.; Kurata, H., Optical Guided Modes Coupled with Čerenkov Radiation Excited in Si Slab Using Angular-Resolved Electron Energy-Loss Spectrum, *J. Appl. Phys.*, **113,** [113509-1]-[113509-7] (2013).

Yoshida, K.; Sasaki, Y.; Kurata, H., High-Resolution Imaging of Zeolite with Aberration-Corrected Transmission Electron Microscopy, *AIP Adv.*, **3,** [042113-1]-[042113-9] (2013).

Morita, C.; Imura, Y.; Ogawa, T.; Kurata, H.; Kawai, T., Thermal-Sensitive Viscosity Transition of Elongated Micelles Induced by Breaking Intermolecular Hydrogen Bonding of Amide Groups, *Langmuir*, **29,** 5450-5456 (2013).

Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Epitaxial Strain Effect in Tetragonal $SrRuO_3$ Thin Films, *J. Appl. Phys.*, **113,** [173912-1]-[173912-7] (2013).

Bindi, L.; Schaper, A. K.; Kurata, H.; Menchetti, S., The Composite Modulated Structure of Cupropearceite and Cupropolybasite and Its Behavior toward Low Temperature, *Am. Min.*, **98,** 1279-1284 (2013).

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).

Hirai, K.; Kan, D.; Aso, R.; Ichikawa, N.; Kurata, H.; Shimakawa, Y., Anisotropic In-Plane Lattice Strain Relaxation in Brownmillerite $SrFeO_{2.5}$ Epitaxial Thin Films, *J. Appl. Phys.*, **114,** [053514-1]-[053514-6] (2013).

Yoshida, K.; Toyoura, K.; Matsunaga, K.; Nakahira, A.; Kurata, H.; Ikuhara, Y. H.; Sasaki, Y., Atomic Sites and Stability of Cs^+ Captured within Zeolitic Nanocavities, *Sci. Rep.*, **3,** [2457-1]-[2457-5] (2013).

Haruta, M.; Nagai, T.; Lugg, N. R.; Neish, M. J.; Nagao, M.; Kurashima, K.; Allen, L. J.; Mizoguchi, T.; Kimoto, K., Atomic Resolution Chemical Bond Analysis of Oxygen in La_2CuO_4, *J. Appl. Phys.*, **114,** [083712-1]-[083712-8] (2013).

Neish, M. J.; Lugg, N. R.; Findlay, S. D.; Haruta, M.; Kimoto, K.; Allen, L. J., Detecting the Direction of Oxygen Bonding in $SrTiO_3$, *Phys. Rev. B*, **88,** [115120-1]-[115120-14] (2013).

Aso, R.; Kurata, H.; Namikoshi, T.; Hashimoto, T.; Kuo, S. W.; Chang, F. C.; Hasegawa, H.; Tsujimoto, M.; Takano, M.; Isoda, S., Quantitative Imaging of Tg in Block Copolymers by Low-Angle Annular Dark-Field Scanning Transmission Electron Microscopy, *Macromolecules*, **46,** 8589-8595 (2013).

Okajima, M. K.; Nguyen, Q. T.; Nakamura, M.; Ogawa, T.; Kurata, H.; Kaneko, T., Double-Metal Complexation of Heterogels Containing Cyanobacterial Polysaccharides, *J. Appl. Polym. Sci*., **128,** 676-683 (2013).

Ogata, K.; Sasano, D.; Yokoi, T.; Isozaki, K.; Yoshida, R.; Takenaka, T.; Seike, H.; Ogawa, T.; Kurata, H.; Yasuda, N.; Takaya, H.; Nakamura, M., Synthesis and Self-Assembly of NCN-Pincer Pd-Complex-Bound Norvalines, *Chem. -A Eur. J*., **19,** 12356-12375 (2013).

Okajima, M. K.; Kumar, A.; Fujiwara, A.; Mitsumata, T.; Kaneko, D.; Ogawa, T.; Kurata, H.; Isoda, S.; Kaneko, T., Anionic Complexes of MWCNT with Supergiant Cyanobacterial Polyanions, *Biopolymers*, **99,** 1-9 (2013).

— Structural Molecular Biology —

[Others]

Hata, Y.; Yamauchi, T.; Fujii, T.; Yoshida, M.; Oikawa, T., Crystal Structure of Flavin Reductase from *Rhizobium* sp. strain MTP-10005, *Abstract of AsCA'13*, P-020 (2013).

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Organic Main Group Chemistry —

Hatakeyama, T.; Imayoshi, R.; Yoshimoto, Y.; Ghorai, S. K.; Jin, M.; Takaya, H.; Norisue, K.; Sohrin, Y.; Nakamura, M., Iron-Catalyzed Aromatic Amination for Nonsymmetrical Triarylamine Synthesis, *J. Am. Chem. Soc.*, **134,** 20262-20265 (2012).

Kawamura, S.; Nakamura, M., Ligand-controlled Iron-catalyzed Cross-coupling of Benzylic Chlorides with Aryl Grignard Reagents, *Chem. Lett.*, **42,** 183-185 (2013).

Gabr, R. K.; Hatakeyama, T.; Takenaka, K.; Takizawa, S.; Okada, Y.; Nakamura, M.; Sasai, H., DFT Study on 5-Endo-Trig-Cyclization of 3-Alkenoic Acids Using Pd-SPRIX Catalyst: Importance of the Rigid Spiro Framework for Both Selectivity and Reactivity, *Chem. Eur. J.*, **19,** 9518-9525 (2013).

Jin, M.; Nakamura, M., Synthesis of Novel C_2 and C_1 Symmetrical CHIRAPHOS Derivatives and Their Application in Palladium-Catalyzed Miyaura-Michael Reaction, *Chem. Lett.*, **42,** 1035-1037 (2013).

Takaya, H.; Iwaya, T.; Ogata, K.; Isozaki, K.; Yokoi, T.; Yoshida, R.; Yasuda, N.; Seike, H.; Takenaka, T.; Nakamura, M., Synthesis, Structure, and Function of PCP Pincer Transition-Metal-Complex-Bound Norvaline Derivatives, *Synlett*, **24,** 1910-1914 (2013).

Isozaki, K.; Haga, Y.; Ogata, K.; Naota, T.; Takaya, H., Metal Array Fabrication Based on Ultrasound-induced Self-assembly of Metalated Dipeprides, *Dalton Trans.*, **42,** 15953-15966 (2013).

Ogata, K.; Sasano, D.; Isozaki, K.; Yoshida, R.; Takenaka, T.; Seike, H.; Ogawa, T.; Kurata, H.; Yasuda, N.; Takaya, H.; Nakamura, M., Synthesis and Self-Assembly of NCN-Pincer Pd-Complex-Bound Norvalines, *Chem. Eur. J.*, **19,** 12356-12375 (2013).

Ochiai, T.; Isozaki, K.; Pincella, F.; Taguchi, T.; Nittoh, K.; Miki, K., Plasmon-Resonant Optics on an Indium-Tin-Oxide Film for Exciting a Two-Photon Photochromic Reaction, *Appl. Phys. Express*, **6,** 102001 (2013).

Mouri, S.; Hijikata, D.; Isozaki, K.; Yonezawa, N.; Okamoto, A., [2,7-Diethoxy-8-(4-Fluorobenzoyl)Naphthalene-1-yl](4-Fluorophenyl)Methanone, *Acta Cryst. E*, **E69,** o637 (2013).

Sakamoto, R.; Hijikata, D.; Isozaki, K.; Yonezawa, N.; Okamoto, A., Bis (1-Benzoyl-7-Methoxynaphthalen-2-yl) Terephthalate, *Acta Cryst. E*, **E69,** o557 (2013).

Hijikata, D.; Sakamoto, R.; Isozaki, K.; Yonezawa, N.; Okamoto, A., 1,8-Bis (4-Fluorobenzoyl) Naphthalen-2,7-Diyl Dimethanesulfonate, *Acta Cryst. E*, **E69,** o544 (2013).

Terashima, Y.; Takayama, M.; Isozaki, K.; Maeda, H., Ion-based Materials of Boron-modified Dipyrrolyldiketones as Anion Receptors, *Chem. Commun.*, **49,** 2506-2508 (2013).

Mouri, S.; Yoshiwaka, S.; Isozaki, K.; Yonezawa, N.; Okamoto, A., Head-to-tail Square-shaped Cyclic Hydrogen Bonds Leading Centrosymmetric Dimeric Aggregates: 1,8-Dibenzoyl-2,7-Dihydroxynaphthalene and a Comparison with Its Aanalogous Benzoylnaphthalene, *Acta Cryst. C*, **C69,** 1541-1544 (2013).

Iwamoto, T.; Watanabe, Y.; Takaya, H.; Haino, T.; Yasuda, N.; Yamago, S., Size- and Orientation-Selective Encapsulation of C_{70} by Cycloparaphenylenes, *Chem. Eur. J.*, **19,** 14061-14068 (2013).

Kayahara, E.; Kouyama, T.; Kato, T.; Takaya, H.; Yasuda, N.; Yamago, S., Isolation and Characterization of the Cycloparaphenylene Radical Cation and Dication, *Angew. Chem. Int. Ed.*, **52,** 1-6 (2013).

Kitayama, T.; Nakahira, M.; Yamasaki, K.; Inoue, H.; Imada, C.; Yonekura, Y.; Awata, M.; Takaya, H.; Kawai, Y.; Ohnishi, K.; Murakami, A., Novel Synthesis of Zerumbone-Pendant Derivatives and Their Biological Activity, *Tetrahedron*, **69,** 10152-10160 (2013).

[Others]

Takaya, H., Metal Array Fabrication Based on Self-Assembly of Metalated Amino Acids and Peptides, *In Briefs in Molecular Science Series Vol. 26, Metal-Molecular Assembly for Functional Materials*, **26,** Chapter 6, 49-60 (2013).

Takaya, H.; Isozaki, K.; Nakamura, M., Metal Array Fabrication Based on Self-Assembly of Metalated Amino Acdis and Peptides toward Artificial Enzymes, *FBC Lett.*, **42,** 10-18 (2013) (in Japanese).

— Advanced Solid State Chemistry —

Senn, M.; Arevalo-Lopez, A.; Saito, T.; Shimakawa, Y.; Attfield, J. P., Nonmagnetic Spin-singlet Dimer Formation and Coupling to the Lattice in the 6H Perovskite Ba$_3$CaRu$_2$O$_9$, *J. Phy.: Cond. Matter*, **25,** [496008-1]-[496008-6] (2013).

Kan, D.; Shimakawa, Y., Transient Behavior in Pt/Nb-doped SrTiO$_3$ Schottky Junctions, *Appl. Phys. Lett.*, **103,** [142910-1]-[142910-5] (2013).

Kobayashi, Y.; Li, Z.; Hirai, K.; Tassel, C.; Loyer, F.; Ichikawa, N.; Abe, N.; Yamamoto, T.; Shimakawa, Y.; Yoshimura, K.; Takano, M.; Kageyama, H., Gas Phase Contributions to Topochemical Hydride Reduction Reactions, *J. Solid State Chem.*, **207,** 190-193 (2013).

Zhang, S.; Saito, T.; Chen, W. T.; Mizumaki, M.; Shimakawa, Y., Solid Solutions of Pauli-paramagnetic CaCu$_3$V$_4$O$_{12}$ and Antiferromagnetic CaMn$_3$V$_4$O$_{12}$, *Inorg. Chem.*, **52,** 10610-10614 (2013).

Singh, V. R.; Verma, V. K.; Ishigami, K.; Shibata, G.; Yamazaki, Y.; Fujimori, A.; Takeda, Y.; Okane, T.; Saitoh, Y.; Yamagami, H.; Nakamura, Y.; Azuma, M.; Shimakawa, Y., Enhanced Ferromagnetic Moment in Co-doped BiFeO$_3$Thin Films Studied by Soft X-ray Circular Dichroism, *J. Appl. Phys.*, **114,** [103905-1]-[103905-6] (2013).

Mizumaki, M.; Yoshii, K.; Hayashi, N.; Saito, T.; Shimakawa, Y.; Takano, M., Magnetocaloric Effect of Ferromagnetic Perovskite BaFeO$_3$, *J. Appl. Phys.*, **114,** [073901-1]-[073901-6] (2013).

Hirai, K.; Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Anisotropic In-plane Lattice Strain Relaxation in Brownmillerite SrFeO$_{2.5}$ Epitaxial Thin Films, *J. Appl. Phys.*, **114,** [053514-1]-[053514-6] (2013).

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).

Oka, K.; Nabetani, K.; Sakaguchi, C.; Seki, H.; Czapski, M.; Shimakawa, Y.; Azuma, M., Tuning Negative Thermal Expansion in Bi$_{1-x}$Ln$_x$NiO$_3$ (Ln=La, Nd, Eu, Dy), *Appl. Phys. Lett.*, **114,** [073901-1]-[073901-6] (2013).

Mizumaki, M.; Saito, T.; Uozumi, T.; Shimakawa, Y., Electronic Structure of Cu in Ferromagnetic CaCu$_3$Sn$_4$O$_{12}$, *J. Phys.: Conference Series*, **103,** [061909-1]-[061909-3] (2013).

Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Epitaxial Strain Effect in Tetragonal SrRuO$_3$ Thin Films, *J. Appl. Phys.*, **113,** [173912-1]-[173912-7] (2013).

Chen, W. T.; Mizumaki, M.; Saito, T.; Shimakawa, Y., Frustration Relieved Ferrimagnetism in Novel A- and B-site-ordered Quadruple Perovskite, *Dalton Transactions*, **42,** 10116-10120 (2013).

Matsumoto, K.; Kan, D.; Ichikawa, N.; Hosokawa, S.; Kageyama, H.; Shimakawa, Y., Oxygen Incorporation into Infinite-Layer Structure AFeO$_2$ (A = Sr, Ca), *Chem. Lett.*, **42,** 732-734 (2013).

Wadati, H.; Kato, K.; Wakisaka, Y.; Sudayama, T.; Hawthorn, D. G.; Regier, T. Z.; Onishi, N.; Azuma, M.; Shimakawa, Y.; Mizokawa, T.; Tanaka, A.; Sawatzky, G. A., Impact of Mn-O-O-Mn Superexchange Pathways in a Honeycomb Lattice Mn Oxide with Small Charge-transfer Energy, *Solid State Comm.*, **162,** 18-22 (2013).

Kan, D.; Aso, R.; Kurata, H.; Shimakawa, Y., Thickness-dependent Structure-property Relationships in Strained (110) SrRuO$_3$ Thin Films, *Adv. Func. Mater.*, **23,** 1129-1136 (2013).

Tohyama, T.; Senn, M. S.; Saito, T.; Chen, W. T.; Tang, C. C.; Attfield, J. P.; Shimakawa, Y., Valence Change of A'-site Mn by A-site Doping in La$_{1-x}$Na$_x$Mn$_3$Ti$_4$O$_{12}$, *Chem. Mater.*, **25,** 178-183 (2013).

Zhang, S.; Saito, T.; Mizumaki, M.; Chen, W. T.; Tohyama, T.; Shimakawa, Y., Site-Selective Doping Effect in AMn$_3$V$_4$O$_{12}$ (A = Na$^+$, Ca^{2+}, and La^{3+}), *J. Am. Chem. Soc.*, **135,** 6056-6060 (2013).

Shimakawa, Y., Reduction and Oxidation of Transition-Metal Oxide Thin Films: Solid State Chemistry with Epitaxially Grown Thin Films, *Bull. Chem. Soc. Jpn.*, **86,** 299-311 (2013).

Shimakawa, Y.; Chen, W. T.; Saito, T., New A-site Ordered Perovskite-structure Oxides with Intriguing Functional Properties, *Proceeding of the 2012 Powder Metallurgy World Congress*, 16F-T14-14/1-6 (2012).

Tohyama, T.; Saito, T.; Shimakawa, Y., Material Design, Synthesis and Magnetic Properties of Novel A-Site-Ordered Perovskites Amn$_3$Al$_4$O$_{12}$, *Proceeding of the 2012 Powder Metallurgy World Congress*, 16F-T14-15/1-6 (2012).

Hirai, K.; Kan, D.; Ichikawa, N.; Shimakawa, Y., Epitaxial Growth of Brownmillerite-structure Sr$_{1-x}$La$_x$FeO$_{2.5}$ Thin Films, *Proceeding of the 2012 Powder Metallurgy World Congress*, 16F-T14-18/1-6 (2012).

— Organotransition Metal Chemistry —

Chang, Y. H.; Nakajima, Y.; Tanaka, H.; Yoshizawa, K.; Ozawa, F., Facile N-H Bond Cleavage of Ammonia by an Iridium Complex Bearing a Non-innocent PNP-Pincer Type Phosphaalkene Ligand, *J. Am. Chem. Soc.*, **135,** 11791-11794 (2013).

Wakioka, M.; Nakamura, Y.; Hihara, Y.; Ozawa, F.; Sakaki, S., Factors Controlling the Reactivity of Heteroarenes in Direct Arylation with Arylpalladium Acetate Complexes, *Organometallics*, **32,** 4423-4430 (2013).

Nakajima, Y.; Okamoto, Y.; Chang, Y. H.; Ozawa, F., Synthesis, Structures, and Reactivity of Ruthenium Complexes with PNP-pincer Type Phosphaalkene Ligands, *Organometallics*, **32,** 2918-2925 (2013).

Chang, Y. H.; Nakajima, Y.; Ozawa, F., A Bis (phosphaethenyl) pyridine Complex of Iridium(I): Synthesis and Catalytic Application to *N*-Alkylation of Amines with Alcohols, *Organometallics*, **32,** 2210-2215 (2013).

Okazaki, M.; Taniwaki, W.; Miyagi, K.; Takano, M.; Kaneko, S.; Ozawa, F., Lewis Acid Chemistry of a Cationic [CCH] Subunit in a Bisdisphenoidal Eight-Atom Tetrairon-Tetracarbon Cluster, *Organometallics*, **32,** 1951-1957 (2013).

Wakioka, M.; Kitano, Y.; Ozawa, F., A Highly Efficient Catalytic System for Polycondensation of 2, 7-Dibromo-9, 9-dioctylfluorene and 1, 2, 4, 5-Tetrafluorobenzene via Direct Arylation, *Macromolecules*, **46,** 370-374 (2013).

Takeuchi, K.; Hounjet, L. J.; Stephan, D. W., Frustrated Lewis Pair Route to Hydrodesilylation of Silylphosphines, *Organometallics*, **32,** 4469-4472 (2013).

— Photonic Elements Science —

Le, P. Q.; Okano, M.; Yamada, Y.; Nagaoka, A.; Yoshino, K.; Kanemitsu, Y., Photocarrier Localization and Recombination Dynamics in Cu_2ZnSnS_4 Single Crystals, *Appl. Phys. Lett.*, **103,** [191902/1-191902/4] (2013).

Yoshikawa, N.; Hirori, H.; Watanabe, H.; Aoki, T.; Ihara, T.; Kusuda, R.; Wolpert, C.; Fujiwara, T. K.; Kusumi, A.; Kanemitsu, Y.; Tanaka, K., Biexciton State Causes Photoluminescence Fluctuations in CdSe/ZnS Core/Shell Quantum Dots at High Photoexcitation Densities, *Phys. Rev. B*, **88,** [155440/1-155440/5] (2013).

Masai, H.; Yamada, Y.; Okumura, S.; Kanemitsu, Y.; Yoko, T., Photoluminescence of Te^{4+} Center in Zinc Borate Glass, *Opt. Lett.*, **38,** 3780-3783 (2013).

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).

Nishihara, T.; Yamada, Y.; Okano, M.; Kanemitsu, Y., Trion Formation and Recombination Dynamics in Hole-Doped Single-Walled Carbon Nanotubes, *Appl. Phys. Lett.*, **103,** [023101/1-023101/4] (2013).

Tex, D. M.; Kamiya, I.; Kanemitsu, Y., Efficient Upconverted Photocurrent through Auger Process in Disk-like InAs Quantum Structures for Intermediate-Band Solar Cells, *Phys. Rev. B*, **87,** [245305/1-245305/7] (2013).

Kimoto, Y.; Okano, M.; Kanemitsu, Y., Observation of Eexcited-State Excitons and Band-Gap Renormalization in Hole-Doped Carbon Nanotubes Using Photoluminescence Excitation Spectroscopy, *Phys. Rev. B*, **87,** [195416/1-195416/5] (2013).

Hirano, D.; Kimoto, T.; Kanemitsu, Y., Determination of Phase Diagram of Electron-Hole Systems in 4H-SiC, *J. Phys. Soc. Jpn.*, **82,** [063703/1-063703/4] (2013).

Okano, M.; Nishihara, T.; Yamada, Y.; Kanemitsu, Y., Dynamics of Excitons and Trions in Semiconducting Carbon Nanotubes, *Proc. SPIE*, **8623,** 86231F (2013).

Kanemitsu, Y., Multiple Exciton Generation and Recombination in Carbon Nanotubes and Nanocrystals, *Acc. Chem. Res.*, **46,** 1358-1366 (2013).

Yamada, Y.; Kanemitsu, Y., Photoluminescence Spectra of Perovskite Oxide Semiconductors, *J. Lumin.*, **133,** 30-34 (2013).

Tayagaki, T.; Hoshi, Y.; Usami, N., Investigation of the Open-Circuit Voltage in Solar Cells Doped with Quantum Dots, *Sci. Rep.*, **3,** [2703/1-2703/5] (2013).

Hoshi, Y.; Pan, W.; Kiguchi, T.; Ooi, K.; Tayagaki, T.; Usami, N., Control of Dip Shape in Photonic Nanostructures by Maskless Wet-Etching Process and Its Impact on Optical Properties, *Jpn. J. Appl. Phys.*, **52,** [080202/1-080202/4] (2013).

BIOINFORMATICS CENTER

— Chemical Life Science —

Frost, K.; Johansson, E.; Shanks, R.; Goto, S.; Kirwan, G. M., Thermoplastic Starch Films: DOE and O2PLS Methodology for Optimization and Increased Understanding of Polymer Processing, *Polymer Testing*, **32,** 343-352 (2013).

Nakaya, A.; Katayama, T.; Itoh, M.; Hiranuka, K.; Kawashima, S.; Moriya, Y.; Okuda, S.; Tanaka, M.; Tokimatsu, T.; Yamanishi, Y.; Yoshizawa, A. C.; Kanehisa, M.; Goto, S., KEGG OC: A Large-scale Automatic Construction of Taxonomy-based Ortholog Clusters, *Nucleic Acids Res.*, **41,** D353-D357 (2013).

Muto, A.; Kotera, M.; Tokimatsu, T.; Nakagawa, Z.; Goto, S.; Kanehisa, M., Modular Architecture of Metabolic Pathways Revealed by Conserved Sequences of Reactions, *J. Chem. Inf. Model.*, **53,** 613-622 (2013).

Kirwan, G. M.; Hancock, T.; Hassell, K.; Niere, J. O.; Nugegoda, D.; Goto, S.; Adams, M. J., Nuclear Magnetic Resonance Metabonomic Profiling Using tO2PLS, *Anal. Chim. Acta*, **781,** 33-40 (2013).

Kotera, M.; Tabei, Y.; Yamanishi, Y.; Tokimatsu, T.; Goto, S., Supervised de novo Reconstruction of Metabolic Pathways from Metabolome-scale Compound Sets, *Bioinformatics*, **29,** i135-i144 (2013).

Iwata, H.; Mizutani, S.; Tabei, Y.; Kotera, M.; Goto, S.; Yamanishi, Y., Inferring Protein Domains Associated with Drug Side Effects Based on Drug-target Interaction Network, *BMC Syst. Biol.*, **7,** [S18/1-S18/11] (2013).

Kotera, M.; Tabei, Y.; Yamanishi, Y.; Moriya, Y.; Tokimatsu, T.; Kanehisa, M.; Goto, S., KCF-S: KEGG Chemical Function and Substructure for Improved Interpretability and Prediction in Chemical Bioinformatics, *BMC Syst. Biol.*, **7,** [S2/1-S2/17] (2013).

— Mathematical Bioinformatics —

Hayashida, N.; Kamada, M.; Song, J.; Akutsu, T., Prediction of Protein-RNA Residue-base Contacts Using Two-dimensional Conditional Random Field with the Lasso, *BMC Systems Biology*, **7(suppl 2),** S15 (2013).

Zhao, Y.; Hayashida, M.; Jindalertudomdee, J.; Nagamochi, H.; Akutsu, T., Breadth First Search Approach to Enumeration of Tree-like Chemical Compounds, *Journal of Bioinformatics and Computational Biology*, **6,** 1343007 (2013).

Melkman, A. A.; Akutsu, T., An Improved Satisfiability Algorithm for Nested Canalyzing Functions and its Application to Determining a Singleton Attractor of a Boolean Network, *Journal of Computational Biology*, **20,** 958-969 (2013).

Jiang, H.; Tamura, T.; Ching, W. K.; Akutsu, T., On the Complexity of Inference and Completion of Boolean Networks from Given Singleton Attractors, *IEICE Transactions on Fundamentals of Electronics, Communications and Computer Sciences*, **E96-A,** 2265-2274 (2013).

Zhao, Y.; Tamura, T.; Akutsu, T.; Vert, J. P., Flux Balance Impact Degree: A New Definition of Impact Degree to Properly Treat Reversible Reactions in Metabolic Networks, *Bioinformatics*, **29,** 2178-2185 (2013).

Uechi, L.; Akutsu, T., Stability and Restoration Phenomena in Competitive Systems, *Progress of Theoretical and Experimental Physics*, **2013,** [103J01:1-103J01:18] (2013).

Takemoto, K.; Tamura, T.; Akutsu, T., Theoretical Estimation of Metabolic Network Robustness against Multiple Reaction Knockouts Using Branching Process Approximation, *Physica A*, **392,** 5525-5535 (2013).

Wang, M.; Sun, Z.; Akutsu, T.; Song, J., Recent Advances in Predicting Functional Impact of Single Amino Acid Polymorphisms: A Review of Useful Features, Computational Methods and Available Tools, *Current Bioinformatics*, **8,** 161-176 (2013).

Ruan, P.; Hayashida, M.; Maruyama, O.; Akutsu, T., Prediction of Heterodimeric Protein Complexes from Weighted Protein-protein Interaction Networks Using Novel Features and Kernel Functions, *PLoS One*, **8,** e65265 (2013).

Lai, Y.; Hayashida, M.; Akutsu, T., Survival Analysis by Penalized Regression and Matrix Factorization, *The Scientific World Journal*, **2013,** 632030 (2013).

Nacher, J. C.; Akutsu, T., Structural Controllability of Unidirectional Bipartite Networks, *Scientific Reports*, **3,** 1647 (2013).

Chen, X.; Akutsu, T.; Tamura, T.; Ching, W. K., Finding Optimal Control Policy in Probabilistic Boolean Networks with Hard Constraints by Using Integer Programming and Dynamic Programming, *Int. J. Data Min. Bioinform.*, **7,** 322-343 (2013).

Akutsu, T.; Nagamochi, H., Comparison and Enumeration of Chemical Graphs, *Computational and Structural Biotechnology Journal*, **5,** [e201302004:1-e201302004:9] (2013).

Akutsu, T.; Tamura, T., A Polynomial-time Algorithm for Computing the Maximum Common Connected Edge Subgraph of Outerplanar Graphs of Bounded Degree, *Algorithms*, **6,** 119-135 (2013).

Akutsu, T.; Fukagawa, D.; Halldorsson, M. M.; Takasu, A.; Tanaka, K., Approximation and Parameterized Algorithms for Common Subtrees and Edit Distance between Unordered Trees, *Theoretical Computer Science*, **470,** 10-22 (2013).

Nacher, J. C.; Akutsu, T., Analysis on Critical Nodes in Controlling Complex Networks Using Dominating Sets, *Proc. 2013 International Conference on Signal-Image Technology & Internet-Based Systems*, 649-654 (2013).

Akutsu, T.; Tamura, T.; Melkman, A. A.; Takasu, A., On the Complexity of Finding a Largest Common Subtree of Bounded Degree, *Proc. 19th International Symposium on Fundamentals of Computation Theory*, 4-15 (2013).

Nakajima, N.; Akutsu, T., Network Completion for Time Varying Genetic Networks, *Proc. 7th International Conference on Complex, Intelligent and Software Intensive Systems*, 553-558 (2013).

Sakuma, Y.; Kamada, M.; Hayashida, M.; Akutsu, T., Inferring Strengths of Protein-protein Interactions Using Support Vector Regression, *Proc. 2013 International Conference on Parallel and Distributed Processing Techniques and Applications* (2013).

Nacher, J. C.; Akutsu, T., Analysis on Controlling Complex Networks Based on Dominating Sets, *Journal of Physics: Conference Series*, **410,** [012104:1-012104:4] (2013).

— Bio-knowledge Engineering —

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

Zheng, X.; Ding, H.; Mamitsuka, H.; Zhu, S., Collaborative Matrix Factorization with Multiple Similarities for Predicting Drug-Target Interactions, *Proceedings of the Nineteenth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD 2013)*, 1025-1033 (2013).

Shiga, M.; Mamitsuka, H., Variational Bayes Co-clustering with Auxiliary Information, *Proceedings of the 4th MultiClust Workshop on Multiple Clusterings, Multi-view Data, and Multi-source Knowledge-driven Clustering (MultiClust 2013),* Article No.5 (2013).

Nakamura, A.; Saito, T.; Takigawa, I.; Kudo, M.; Mamitsuka, H., Fast Algorithms for Finding a Minimum Repetition Representation of Strings and Trees, *Discrete Applied Mathematics*, **161(10-11),** 1556-1575 (2013).

Gu, J.; Feng, W.; Zeng, J.; Mamitsuka, H.; Zhu, S., Efficient Semi-supervised MEDLINE Document Clustering with MeSH Semantic and Global Content Constraints, *IEEE Transactions on Cybernetics*, **43(4),** 1265-1276 (2013).

Wicker, N.; Nguyen, C. H.; Mamitsuka, H., A New Dissimilarity Measure for Comparing Labeled Graphs, *Linear Algebra and its Applications*, **438(5),** 2331-2338 (2013).

Yamamoto, T.; Nakayama, K.; Hirano, H.; Tomonaga, T.; Ishihama, Y.; Yamada, T.; Kondo, T.; Kodera, Y.; Sato, Y.; Araki, N.; Mamitsuka, H.; Goshima, N., Integrated View of the Human Chromosome X-centric Proteome Project, *Journal of Proteome Research*, **12(1),** 58-61 (2013).

Takigawa, I.; Mamitsuka, H., Graph Mining: Procedure, Application to Drug Discovery and Recent Advance, *Drug Discovery Today*, **18(1-2),** 50-57 (2013).

[Others]

Takigawa, I.; Tsuda, K.; Mamitsuka, H., An in silico Model for Interpreting Polypharmacology in Drug-Target Networks, *In Silico Models for Drug Discovery*, **5,** 67-80 (2013).

Hancock, T.; Takigawa, I.; Mamitsuka, H., Identifying Pathways of Co-ordinated Gene Expression, *Data Mining for Systems Biology: Methods and Protocols*, **7,** 69-85 (2013).

Mamitsuka, H.; DeLisi, C.; Kanehisa, M., Data Mining for Systems Biology: Methods and Protocols, *Methods in Molecular Biology*, **939,** (2013).

ENDOWED RESEARCH SECTION
—Nano-Interface Photonics (SEI Group CSR Foundation) —

Yamada,Y.; Kanemitsu, Y., Photoluminescence Spectra of Perovskite Oxide Semiconductors, *Journal of Luminescence*, **133,** 30-34 (2013).

Okano, M.; Nishihara, T.; Yamada, Y.; Kanemitsu, Y., Dynamics of Excitons and Trions in Semiconducting Carbon Nanotubes, *Proc. of SPIE*, **8623,** 86231F (2013).

Kimoto, Y.; Okano, M.; Kanemitsu, Y., Observation of Excited-state Excitons and Band-gap Renormalization in Hole-doped Carbon Nanotubes Using Photoluminescence Excitation Spectroscopy, *Phys. Rev. B*, **87,** [195416-1]-[195416-5] (2013).

Nishihara, T.; Yamada, Y.; Okano, M.; Kanemitsu, Y., Trion Formation and Recombination Dynamics in Hole-Doped Single-Walled Carbon Nanotubes, *Appl. Phys. Lett.*, **103,** [023101-1]-[023101-4] (2013).

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).

Masai, H.; Yamada, Y.; Okumura, S.; Kanemitsu, Y.; Yoko, T., Photoluminescence of a Te^{4+} Center in Zinc Borate Glass, *Opt. Lett.*, **38,** 3780-3783 (2013).

Le, P. Q.; Okano, M.; Yamada, Y.; Nagaoka, A.; Yoshino, K.; Kanemitsu, Y., Photocarrier Localization and Recombination Dynamics in Cu_2ZnSnS_4 Single Crystals, *Appl. Phys. Lett.*, **103,** [191902-1]-[191902-4] (2013).

INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]
Monash University, School of Physics

The University of Melbourne, School of Physics

The University of Sydney, School of Chemistry

[Belgium]
Université Catholique de Louvain, Institute on Condensed Matter and Nano-science

[Canada]
The University of British Columbia, Division of Neurology, Department of Medicine

[China, P.R.]
Dalian University of Technology, Department of Polymer Materials, School of Chemical Engineering

Fudan University, School of Computer Science

Fudan University, Shanghai Key Lab of Intelligent Information Processing

Sichuan University, College of Polymer Science and Engineering

[Czech R.]
Academy of Sciences of the Czech Republic, Institute of Organic Chemistry and Biochemistry

ASCR, HiLASE Project, Institute of Physics

Czech Technical University in Prague, FNSPE

[Denmark]
Danmarks Tekniske Universitet, Department of Chemical and Biochemical Engineering

[Estonia]
National Institute of Chemical Physics and Biophysics

[Finland]
University of Helsinki, Department of Chemistry

University of Oulu, Center of Microscopy and Nanotechnology

[France]
Institut Laue-Langevin

Institut Pasteur, Bioinformatique Structurale

Université de Rennes, Sciences Chimiques de Rennes

Université Lille 1, UFR de Mathématiques

[Germany]
German Cancer Consortium (DKTK)

Karlsruhe Institute of Technology, Institute of Organic Chemistry and CFN

Philipps University Marburg, Center for Materials Sciences

Technische Universität Darmstadt, Eduard-Zintl-Institut für Anorganische und Physikalische Chemie and Center of Smart Interfaces

The Max-Planck-Society, Chemical Genomics Centre

University Hospital Essen, Department of Medical Oncology, West German Cancer Center

University of Marburg, Institute for Physiology and Pathophysiology

[Italy]
Università degli Studi di Firenze, Dipartimento di Scienze della Terra

Università degli Studi di Napoli “Federico II”, Dipartimento di Ingegneria Chimica

Università degli Studi di Padova, Dipartimento di Scienze Chimiche

[Korea, R.]
Chung-Ang University College of Medicine, Medical Research Institute

[Netherlands]
Eindhoven University of Technology, Department of Biomedical Engineering

Eindhoven University of Technology, Molecular Cell and Structural Biology

[Sweden]
Lund University, Department of Theoretical Chemistry

Stockholm University, Department of Biochemistry and Biophysics

[Switzerland]
University of Geneva, School of Chemistry and Biochemistry

[Taiwan]
Academia Sinica, Research Center for Applied Sciences

National Chiao Tung University, Department of Applied Chemistry

National Sun Yat-sen University, Department of Materials and Optoelectronic Science

[Thailand]
Naresuan University, Faculty of Science

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

The University of Manchester, Manchester Institute of Biotechnology, School of Chemistry, Faculty of EPS

The University of Nottingham, School of Physics and Astronomy

University College London, Department of Electronic and Electrical Engineering

University College London, Institute of Structural and Molecular Biology

University College London, London Centre for Nanotechnology

University of Oxford, Department of Chemistry

University of Oxford, Department of Materials

University of Southampton, School of Chemistry

[U.S.A.]
Brown University, Department of Chemistry

Columbia University, Department of Chemistry

National Institute of Standards and Technology, Center for Neutron Research

New York University, Department of Chemistry

Temple University, Fels Institute for Cancer Research and Molecular Biology

University of Michigan, Department of Molecular, Cellular and Developmental Biology

University of Pennsylvania, Department of Materials Science & Engineering

University of Pennsylvania, Penn Regional Nanotechnology Facility

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

Tokitoh, N.
Construction of Polycyclic Aromatic Compounds Containing Heavier Group 14 Elements and Development of Their Functions by Utilizing the Features of Main Group Elements
Grant-in-Aid for Scientific Research (B)
1 April 2010–31 March 2013

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.
Synthesis of Phthalocyanine Derivatives Bearing Phosphorus Atoms as Skeletal Elements and Their Properties
Grant-in-Aid for Scientific Research on Innovative Area "π-Space"
1 April 2011–31 March 2013

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
Grant-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 and Function of Spherical π-Space Encapsulating an Active Small Molecule
Grant-in-Aid for Scientific Research on Innovative Areas "π-Space"
1 December 2008–31 March 2013

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

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

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.
Fine Organic Synthesis Based on Catalytic Regioselective Functionalization
Grant-in Aid for Scientific Research (A)
1 April 2009–31 March 2013

Kawabata, T.
Regioselective Molecular Transformation Based on Organocatalytic Molecular Recognition
Grant-in Aid for Scientific Research on Innovative Area
1 October 2011–31 March 2015

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

Yoshimura, T.
Synthesis of Novel Amino Acids and Natural Products Derived from Amino Acids via Memory of Chirality
Grant-in-Aid for Young Scientists (B)
28 April 2011–31 March 2013

— Advanced Inorganic Synthesis —

Teranishi, T.
Development of Structure-Specific Energy-Related Functional Materials Using Heterostructured Nanoparticles
Grant-in-Aid for Scientific Research (A)
1 April 2011–31 March 2014

Teranishi, T.
Study on Correlation between Structure and Hydrogen Storing Properties of Palladium Nanoparticles
Grant-in-Aid for Challenging Exploratory Research
1 April 2012–31 March 2014

Teranishi, T.
Synthesis of Macrocyclic π-Conjugated Ligand-Protected Gold Clusters and Fabrication of Nano-Gap Single Electron Devices
CREST (Core Research for Evolutional Science and Technology), JST
1 October 2008–31 March 2014

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.
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, METI
1 October 2012–31 March 2022

Teranishi, T.
Development of Green Sustainable Chemical Process
Mirai Kaitaku Research Project, METI
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 2015

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
Industrial Technology Research Grant Program, NEDO
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.
Development of Next-Generation MRI Contrast Agent
Industrial Technology Research Grant Program, NEDO
1 July 2009–30 June 2013

Ohno, K.
Pharmacokinetics of Well-Defined Polymer Brush-Afforded Fine Particles
Grant-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
Grant-in-Aid for Young Scientist (B)
1 April 2012–31 March 2014

— 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

— Inorganic Photonics Materials —

Yoko, T.
Organic-inorganic Material for Biosensor Application
Grant-in-Aid for Challenging Exploratory Research
1 April 2011–31 March 2014

—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 Rhythmic Gene Expression Systems Based on the Cellular Clock
Grant-in-Aid for Scientific Research on Innovative Areas
1 April 2012–31 March 2014

Takeuchi, T.
Structure-activity Relationship Study of Membrane Proteins by Regulation of Their Oligomer Formation
Grant-in-Aid for Research Activity Start-up
1 October 2013–31 March 2015

— 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 2013

— 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 2015

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

— 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

— Solution and Interface Chemistry —

Hasegawa, T.
Structural Analysis and Control of an Organic Thin Film of Solar Cell Using MAIR Spectroscopy
Grant for Basic Science Research Projects, Sumitomo Foundation
1 November 2012–30 November 2013

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

Hasegawa, T.
Operando Analysis of Concentration and Diffusion of Negatively-Adsorptive Chemical Species in A Monolayer Formed at An Air/Water Interface
Grant-in-Aid for Scientific Research on Innovative Areas "Molecular Sciences of Soft Interface"
1 April 2011–31 March 2013

Matubayasi, N.
Free-Energy Analysis of ATP hydrolysis
Grant-in-Aid for Scientific Research on Innovative Areas "Hydration and ATP Energy"
1 December 2008–31 March 2013

— 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.
Development of Biocatalysts for Remediation of Environments Polluted with Persistent Organohalogen Compounds
Grant-in-Aid for Challenging Exploratory Research
1 April 2012–31 March 2014

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

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

— Polymer Materials Science —

Kanaya, T.
Non-equilibrium Intermediate States and Polymer Crystallization–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

Nishida, K.
Control of Higher-order Structures of Polymer Materials by Fast Temperature Variation
Researcher Exchange Program between JSPS and DAAD
1 September 2013–20 October 2013

— Molecular Rheology —

Watanabe, H.
Nonlinear Feedback between Phase Growth and Chain Dynamics in Polymer Blends
Grant-in-Aid for Scientific Research (A)
1 April 2012–31 March 2015

Masubuchi, Y.
Relaxation of Polymer Chain under Flow
Grant-in-Aid for Scientific Research (B)
1 April 2011–31 March 2014

Matsumiya, Y.
Molecular Interpretation of Cooperative Length of Polymer Segment
Grant-in-Aid for Scientific Research (C)
1 April 2012–31 March 2015

— Molecular Aggregation Analysis —

Yoshida, H.
Inverse-Photoemission Spectroscopy with Zero Kinetic Energy Electrons for Measuring the Unoccupied Electronic States of Organic Semiconductors
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2009–31 March 2013

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

— Particle Beam Science —

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

— 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.
Development of Single-shot Ultrafast Electron Diffraction Using Femtosecond Electron Pulses Generated by an Ultra Intense Short Pulse Laser
The Mitsubishi Foundation
1 October 2012–30 September 2013

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

Hashida, M.
Amorphous Metal Thin Film with the Surface of Periodic Nanostructures Self-formed by Femtosecond Laser Pulses
Grant-in-Aid for Scientific Research (C)
1 April 2010–31 March 2013

— Electron Microscopy and Crystal Chemistry —

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

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

— Organic Main Group Chemistry —

Nakamura, M.
Development of Selective Organic Synthesis Based on Iron Catalysis
Funding Program for Next Generation World-Leading Researchers (NEXT Program)
1 March 2011–31 March 2014

Takaya, H.
A Comprehensive Research on Iron- and Nickel-Catalyzed Organic Reactions: Development of New Catalyst, New Reactions, New Spectroscopic Methods
CREST (Core Research for Evolutional Science and Technology), JST
1 April 2011–31 March 2016

Takaya, H.
New Catalyst toward Biorefinery of Lignins Based on Metal-Conjugate Amino Acids and Peptides
CREST (Core Research for Evolutional Science and Technology), JST
1 April 2011–31 March 2016

Hatakeyama, T.
Synthesis of Helical π-Conjugated Molecules toward Next Generation Semiconductors
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2011–31 March 2015

Hatakeyama, T.
Synthesis of Heterographene Derivatives by Tandem Hetero-Friedel-Ctafts Reactions
Grant-in-Aid for Young Scientists (A)
1 April 2011–31 March 2014

— 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.
Development of Highly Efficient Direct Arylation Catalysts for the Synthesis of π-Conjugated Polymers
Grant-in-Aid for Scientific Research (B)
1 April 2011–31 March 2014

Wakioka, M.
Development of Living Polymerization Based on Direct Arylation
Grant-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, JST
1 October 2012–31 March 2018

— Photonic Elements Science —

Kanemitsu, Y.
Microscopic Spectroscopy of Highly Excited State in Semiconductor Nanostructures and Exploring Novel Optical Functionality
Grant-in-Aid for Scientific Research on Innovative Areas, ”Optical Science of Dynamically Correlated Electrons”
13 November 2008–31 March 2013

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

Tayagaki, T.
Controlling of the Many-body Interaction between Photoexcited Carriers toward Hot Carrier Solar Cells
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2009–31 March 2013

Tayagaki, T.
Integration of Nanostructures in Crystalline Silicon Solar Cells for Advanced Management of Photons and Carriers
ALCA (Advanced Low Carbon Technology Research and Development Program), JST
1 October 2011–31 March 2017

BIOINFORMATICS CENTER
— Chemical Life Science —

Goto, S.
Key Technology Development for Data Integration and Application to Emerging Fields
Life Science Database Integration Project, JST
1 April 2011–31 March 2014

Kotera, M.
Reaction Network Prediction for ab initio Reconstruction of Metabolic Pathways
Biosynthesis Machinery, Grant-in-Aid for Scientific Research on Innovative Areas
1 April 2013–31 March 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.; Kawabata, T.; Nagamochi, H.; Hayashida, M.
An Approach to Novel Structural Design by Combining Discrete Methods and Kernel Methods
Grant-in-Aid for Scientific Research (A)
1 April 2010–31 March 2015

— Bio-knowledge Engineering —

Mamitsuka, H.
Estimating Data Structures from Various Semi-Structured Data
Grant-in-Aid for Scientific Research (B)
1 April 2012–31 March 2015

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

CHIDA, Kensaku
D Sc, Kyoto University
"Electrical Noise Measurements on Non-Equilibrium Quantum Hall System"
Supervisor: Prof KOBAYASHI, Kensuke
15 January 13

FUKUSHIMA, Tatsuya
D Eng, Kyoto University
"Solid-State NMR Studies on Local and Aggregated Structures of Organic Semiconductor Materials"
Supervisor: Prof KAJI, Hironori
25 March 13

FURUICHI, Kenji
D Eng, Kyoto University
"Nonlinear Stress Relaxation of Entangled Polymer Chains in Primitive Network Simulation"
Supervisor: Prof WATANABE, Hiroshi
23 July 13

GONG, Chunjie
D Agr, Kyoto University
"Characterization of Proteins Involved in the Biosynthesis of Eicosapentaenoic Acid in *Shewanella livingstonensis* Ac10"
Supervisor: Prof KURIHARA, Tatsuo
25 March 13

HAMADA, Shohei
D Pharm Sc, Kyoto University
"Development of Electronically Tuned Nitroxyl Radical Catalysts"
Supervisor: Prof KAWABATA, Takeo
25 March 13

HASHIMOTO, Sigma
D Eng, Kyoto University
"Syntheses of Polycyclic Aromatic Compounds with Heteroatom Junctions via Tandem Hetero-Friedel-Crafts Reactions"
Supervisor: Prof NAKAMURA, Masaharu
25 March 13

HISADA, Hiromoto
D Agr, Kyoto University
"Studies on Gene Expression and Promoter Analyses for Protein Production in *Aspergillus oryzae*"
Supervisor: Prof HIRATAKE, Jun
23 May 13

IMAI, Takeshi
D Agr, Kyoto University
"Studies on Mammalian Selenite Metabolism"
Supervisor: Prof KURIHARA, Tatsuo
25 March 13

INOUE, Shunsuke
D Sc, Kyoto University
"Femtosecond Electron Deflectometry for Measuring Ultrafast Transient Fields Induced by Intense Laser Pulses"
Supervisor: Prof SAKABE, Shuji
25 March 13

KAMADA, Mayumi
D Inf, Kyoto University
"Analysis and Prediction Methods for Protein Structure and Function"
Supervisor: Prof AKUTSU, Tatsuya
25 March 13

KATAYAMA, Sayaka
D Pharm Sc, Kyoto University
"Membrane Accumulation of Arginine-Rich Cell-Penetrating Peptides Promoting Their Membrane Translocation"
Supervisor: Prof FUTAKI, Shiroh
25 March 13

KAWAMURA, Shintaro
D Eng, Kyoto University
"Development of Iron-Catalyzed Cross-Coupling Reacions with Organoaluminum, magnesium and –zinc Reagents Directed toward Controlled Organic Synthesis"
Supervisor: Prof NAKAMURA, Masaharu
25 March 13

KIMURA, Hiroshi
D Sc, Kyoto University
"In-situ NMR Study of the Mechanism and Kinetics of Hydrothermal Reactions of Monosaccharides and Oligosaccharides"
Supervisor: Assoc Prof MATUBAYASI, Nobuyuki
25 March 13

MISHIRO, Kenji
D Pharm Sc, Kyoto University
"Development of Substrate Specific Reactions and Creation of Optically Active Molecules Based on Hydrogen Bonding"
Supervisor: Prof KAWABATA, Takeo
25 March 13

MORINAKA, Yuta
D Eng, Kyoto University
"Studies on Properties of Endohedral Fullerenes and Development of Fullerene Derivatives for Organic Photovoltaic Devices"
Supervisor: Prof MURATA, Yasujiro
25 March 13

MUTO, Ai
D Sc, Kyoto University
"Modular Architecture of Metabolic Pathways Revealed by Conserved Sequences of Reactions"
Supervisor: Assoc Prof GOTO, Susumu
24 September 13

NAKAO, Masao
D Sc, Kyoto University
"Resonance Coupling Induced Enhancement of Indirect Transverse Cooling in a Laser-cooled Ion Beam"
Supervisor: Prof NODA, Akira
23 January 2013

NISHINO, Reiko
D Pharm Sc, Kyoto University
“Development of DMAP Derivatives with an Internal Carboxylate and Their Catalytic Profile”
Supervisor: Prof KAWABATA, Takeo
25 March 13

SAKAGAMI, Michiyasu
D Sc, Kyoto University
“Studies on Construction of Novel d-π Conjugated Systems Reflecting Unique Properties of Low-Coordinated Heavier Group 15 Elements”
Supervisor: Prof TOKITOH, Norihiro
26 March 13

SHIMAMURA, Kazutoshi
D Sc, Kyoto University
“Electric Field Control of Magnetic Properties Using Electrical Double-Layers”
Supervisor: Prof ONO, Teruo
15 January 13

SHINTANI, Megumi
D Sc, Kyoto University
“Interaction and Dynamics of Phospholipid Membranes Studied by Solution-state NMR and Molecular Dynamics Simulation”
Supervisor: Assoc Prof MATUBAYASI, Nobuyuki
23 May 13

SOUDA, Hikaru
D Sc, Kyoto University
“Efficiency Enhancement of Indirect Transverse Laser Cooling with Synchro-Betatron Resonant Coupling by Suppression of Beam Intensity”
Supervisor: Prof NODA, Akira
23 January 13

TANABE, Kenji
D Sc, Kyoto University
“Study on Spin Motive Force Excited in Magnetic Vortices”
Supervisor: Prof ONO, Teruo
15 January 13

UEDA, Yoshihiro
D Pharm Sc, Kyoto University
“Organocatalytic Regioselective Total Synthesis and Functionalization of Natural Glycosides”
Supervisor: Prof KAWABATA, Takeo
25 March 13

YAMADA, Masako
D Sc, Kyoto University
“ToF-lens for Focusing Pulsed White Neutron Beam Using Permanent Magnet Sextupole with Modulation Capability”
Supervisor: Assoc Prof IWASHITA, Yoshihisa
23 January 2013

THE 113TH
ICR ANNUAL
SYMPOSIUM

SEMINARS
MEETINGS AND
SYMPOSIA

THE 113TH ICR ANNUAL SYMPOSIUM

(13 December 2013)

ORAL PRESENTATION

IWASHITA, Yoshihisa (Particle Beam Science)
“Accelerator and Science”

NISHIDA, Koji (Polymer Materials Science)
“Non-equilibrium Property in Crystalline Polymer Elucidated by Rapid Temperature Variation Method and Its Application to Structural Control”

KUO, Ting-Fang (Chemical Biology)
“A Chemical Probe for Human Pluripotent Stem Cells”

HAYASHIDA, Morihiro (Mathematical Bioinformatics)
“EnuMol: Enumeration System for Chemical Compounds”

–ICR Award for Young Scientists–
YOSHIMURA, Tomoyuki (Synthetic Organic Chemistry)
“Asymmetric Induction via Short-lived Chiral Enolates with a Chiral C-O Axis”

–ICR Award for Young Scientists (Foreign Researchers’ Category)–
KIM, Kab-Jin (Nanospintronics)
“Two-barrier Stability that Allows Low-power Operation in Current-induced Domain-wall Motion”

−ICR Award for Graduate Students−
WASANO, Tatsuya (Organoelement Chemistry)
“Syntheses and Structures of an “Alumole” and its Dianion”

TAKANO, Shotaro (Hydrospheric Environment Analytical Chemistry)
“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”

–ICR Grants for Young Scientists–
AGOU, Tomohiro
“Development of Catalysts for Small Molecule Activation Based on the Characteristics of Heavier Group 14 Elements”

WAKAMIYA, Atsushi
“Development of Charge-transporting Materials Using Quasi-planar Structure as a Key Scaffold”

TEX, David
“Towards Green Optoelectronic Devices Using Quantum Disks”

MASAI, Hirokazu
“Study on Emission Mecahnism of Oxide Glass Phosphor Containing ns^2-Type Emission Center”

KAWAMOTO, Jun
“Study of Physiological Function of Long-chain Polyunsaturated Fatty Acids by *in-situ* Chemical Modification”

POSTER PRESENTATIONS

LW : Laboratory Whole Presentation
LT : Laboratory Topic
GE : General Presentation

— Organoelement Chemistry —

LW “Studies on the Synthesis and Properties of Novel Organic Compounds Containing Heavier Elements”

— Structural Organic Chemistry —

LW “Research Activities in Structural Organic Chemistry Laboratory”

GE ENDO, Masaru; SASAMORI, Takahiro; WAKAMIYA, Atsushi; TOKITOH, Norihiro; MURATA, Yasujiro
“Preparation of Efficient Organic-Inorganic Hybrid Solar Cells”

GE MURATA, Michihisa; SUGANO, Yasunori; WAKAMIYA, Atsushi; MURATA, Yasujiro
“Synthesis and Properties of π-Extended Pyracylene”

— Synthetic Organic Chemistry —

LW “Research in Laboratory of Synthetic Organic Chemistry ～ Toward the Development of Attractive Molecular Transformation ～ ”

GE YANAGI, Masanori; UEDA, Yoshihiro; FURUTA, Takumi; KAWABATA, Takeo
“Regioselective Deoxygenation of Sugars”

— Advanced Inorganic Synthesis —

LW “Research Activities in Advanced Inorganic Synthesis”

GE SATO, Ryota; TRINH, Thang Thuy; TERANISHI, Toshiharu
“Fabrication of $L1_0$-FePd/α-Fe Nanocomposite Magnets”

GE SAKAMOTO, Masanori; TANAKA, Daisuke; TERANISHI, Toshiharu
“Rigid Bidentate Ligands Focus the Size of Gold Nanoparticles”

— Chemistry of Polymer Materials —

LW “Research Activities in the Laboratory of Chemistry of Polymer Materials”

GE KINOSE, Yuji; SAKAKIBARA, Keita; OHNO, Kohji; TSUJII, Yoshinobu
“Synthesis of Cellulosic Bottle Brush with Regioselectively Substituted Side Chains”

— Polymer Controlled Synthesis —

LW “Research Activity of Polymer Controlled Synthesis Laboratory”

GE ZHAI, Xue; KAYAHARA, Eiichi; YAMAGO, Shigeru
“Synthesis of Sulfur-Containing Cycloparaphenylene Analogues from Cyclic Organoplatinum Complexes and Their Physical Properties”

GE FUJITA, Takehiro; YAMAGO Shigeru
“Stereospecific Radical Polymerization of Acrylimides Bearing Chiral Oxazolidinones in the Presence of Lewis Acid”

— Inorganic Photonics Materials —

GE HINO, Yusuke; MASAI, Hirokazu; TOKUDA, Yomei; YOKO, Toshinobu
“Correlation between Co-activator and Emission Property in SnO-ZnO-P_2O_5 Glasses”

GE MIYATA, Hiroki; MASAI, Hirokazu; TOKUDA, Yomei; YOKO, Toshinobu
“Fabrication of Light Emitting Amorphous Thin Film in the System of SnO-ZnO-P_2O_5 via Liquid Phase Synthesis”

GE MINAMI, Tomohiro; TOKUDA, Yomei; MASAI, Hirokazu; YOKO, Toshinobu
“Structure Analysis of Alkali Ion in Mixed Alkali Silicate Glasses”

GE UTSUMI, Nihiro; TOKUDA, Yomei, MASAI, Hirokazu; YOKO, Toshinobu
“Titano-borosilicate Hybrid Materials Prepared by Solventless Ethanol Condensation”

— Nanospintronics —

GE NAGATA, Masaki; MORIYAMA,Takahiro; TANABE, Kenji; CHIBA, Daichi; ONO, Teruo
“Spin Motive Force Induced in Magnetite Thin Films”

GE HATA, Hiroshi; HIRAMATSU, Ryo; TANIGUCHI, Takuya; KOYAMA, Tomohiro; CHIBA, Daichi; KIM, Kab-Jin; MORIYAMA, Takahiro; ONO, Teruo
“Quantitative Estimation of Antisymmetric Exchange Interaction by Spin Wave Resonances”

GE NISHIHARA,Yoshitaka; ONO, Teruo; ARAKAWA, Tomonori; TANAKA, Takahiro; NORIMOTO, Shota; KOBAYASHI, Kensuke
“Shot Noise at a Quantum Point Contact on a High-electron-mobility Transistor”

GE HIRAMATSU, Ryo
“Observation of Metastable Bound State between Domain Walls in an Asymmetric Co/Ni Nanowire”

— Biofunctional Design-Chemistry —

LW “Research Activities in Biofunctional Design Chemistry”

GE TSUJI, Shogo; IMANISHI, Miki; FUTAKI, Shiroh
“Directed Evolution of a TALE Protein for Unconstrained DNA Binding”

— Chemistry of Molecular Biocatalysts —

LW “Recent Activities of Laboratory of Chemistry of Molecular Biocatalysts”

GE KAWANISHI, Daisuke; KOEDUKA, Takao; SUGIMOTO, Koichi; OZAWA, Rika; TAKABAYASHI, Zyunzi; WATANABE, Bunta; HIRATAKE, Jun
“Structure and Biological Activities of Prenylated Phenylpropanoids”

GE LI, Chunjie; KOEDUKA, Takao; WATANABE, Bunta; HIRATAKE, Jun
“Development of Strong Mechanism-Based Carbamate Inhibitors of Human Gamma-Glutamyl Transpeptidase”

— Molecular Biology —

LW “Research Topics from the Molecular Biology Laboratory”

— Chemical Biology —

GE WANG, Chenyu; KUSUMOTO, Atsushi; KATO, Nobuo; UESUGI, Motonari; OHKANDA, Junko
“Design and Synthesis of Fusicoccin-J-based Chemical Probes for Elucidation of Structural Effects on 14-3-3 Labeling”

— Molecular Materials Chemistry —

LW “Research Activities in Molecular Materials Chemistry Laboratory”

GE OHTSUKI, Akimichi; GOTO, Atsushi; KAJI, Hironori
“Photo-Induced Controlled Radical Polymerization with Organic Catalysts in a Wide Range of Wavelengths”

GE SUZUKI, Hajime; FUKUSHIMA, Tatsuya; KAJI, Hironori
“Degradation Analysis of Blue Phosphorescent Organic LEDs by Solution NMR Spectroscopy”

— Hydrospheric Environment Analytical Chemistry —

GE KONAGAYA, Wataru; MINAMI, Tomoharu; SOHRIN, Yoshiki
“Ocean Sections and Stoichiometry of Dissolved Bioactive Trace Metals in the North Pacific Ocean”

GE KAWAHARA, Shimpei; UMETANI, Shigeo; SOHRIN, Yoshiki
“Solid-phase Extraction of Alkali Metal Ions with Solvent Impregnated Resins Containing Strongly Acidic β-Diketones and Neutral Ligand”

— Solution and Interface Chemistry —

GE WAKAI, Chihiro; SHIMOAKA Takafumi; HASEGAWA, Takeshi
“NMR Studies on Water Molecules Adsorbed on Nafion Film by Spin-Lattice Relaxation Time and Chemical Shift Measurements”

GE SHIMOAKA, Takafumi; RIKIYAMA, Kazuaki; KATSUMOTO, Yukiteru; WAKAI, Chihiro; HASEGAWA, Takeshi
“Effects of Molecular Water on the Secondly Structure of Poly(*N*-isopropylacrylamide) with a High Isotacticity in an Acetone Solution Studied by Infrared and NMR Spectroscopies”

— Molecular Microbial Science —

LW “Laboratory of Molecular Microbial Science”

GE CHO, Hyun-Nam; KAWAMOTO, Jun; KURIHARA, Tatsuo
“Subcellular Localization and Physiological Function of 1-Acyl-*sn*-glycerol-3-phosphate Acyltransferase of EPA-producing Bacterium, *Shewanella livingstonensis* Ac10”

— Polymer Materials Science —

LW “Reserach Progress in the Laboratory of Polymer Materials Science”

GE HIRANO, Tatsumasa; NISHIDA, Koji; ASAKAWA, Harutoshi; INOUE, Rintaro; KANAYA, Toshiji
“Crystallization Behavior of Isotactic Polypropylene from Mesophase”

GE NABATA, Takeshi; INOUE, Rintaro; NISHIDA, Koji; KANAYA, Toshiji
“Observation of Structure Formation in Isotactic Polystyrene for Glass and Cold Crystallization”

GE MATSUURA, Tomohiko; INOUE, Rintaro; NISHIDA, Koji; KANAYA, Toshiji
“Precursor in Shear-induced Polymer Crystallization”

— Molecular Rheology—

LW “Research Activities in Molecular Rheology Laboratory”

— Molecular Aggregation Analysis —

GE ASAMI, Koji
“Electrical Properties of *E. coli* Cells Revealed by Dielectric Spectroscopy”

GE YOSHIDA, Hiroyuki
“New Experimental Method to Examine Unoccupied States and Electron Affinities of Organic Semiconductors”

— Interdisciplinary Chemistry for Innovation —

LW “Research Activities of Interdisciplinary Chemistry for Innovation”

— Particle Beam Science —

LW “Present Status of Accelerator Laboratory for Beam Science”

GE KITAHARA, Ryunosuke; IWASHITA, Yoshihisa; KITAGUCHI, Masaaki; SHIMIZU, Hirohiko
“Hg co-magnetometer for Measurement of Neutron Electric Dipole Moment”

— Laser Matter Interaction Science —

LW “Recent Research at Laser Matter Interaction Science”

GE IKEDA, Daiki; INOUE, Shunsuke; HATA, Masayasu; HASHIDA, Masaki; SAKABE, Shuji
“Characteristics of Electrons Accelerated by Intense Femtosecond Laser Pulsesβα”

GE KAWAMOTO, Mao; HASHIDA, Masaki; MIYASAKA, Yasuhiro; SHIMIZU, Masahiro; HATA, Masayasu; INOUE, Shunsuke; TOKITA, Shigeki; SAKABE, Shuji
“Femtosecond Laser Coloring of Metal Surface”

GE HATA, Masayasu; INOUE, Shunsuke; IKEDA, Daiki; TERAMOTO, Kensuke; NAKASHIMA, Yuto; MORI, Kazuaki
“Computer Simulation of High-intense Femtosecond Laser Plasma Interaction”

GE MORI, Kazuaki; HASHIDA, Masaki; NAGASHIMA, Takeshi; INOUE, Shunsuke; TOKITA, Shigeki; HANGYO, Masanori; SAKABE, Shuji
“THz Generation from Plasma Produced by the Interaction of Intense Laser with Clusters”

GE MIYASAKA, Yasuhiro; HASHIDA, Masaki; NISHII, Takaya; INOUE, Shunsuke; SAKABE, Shuji
“Mechanism of Femtosecond Laser Nano Ablation for Metals ～ Dependence of Ablation Rate on Polarization for Oblique Incidence ～ ”

— Electron Microscopy and Crystal Chemistry—

LW “Researches in Laboratory of Electron Microscopy and Crystal Chemistry”

GE FUJIYOSHI, Yoshifumi; KARIYA, Ayuta; NEMOTO, Takashi; KURATA, Hiroki
“The Dielectric-substrate Effect for the Localized Surface Plasmon (LSP) Excited Around an Ag Nanoparticle”

— Structural Molecular Biology —

LW “Introduction of Structural Molecular Biology Laboratory”

— Organic Main Group Chemistry —

LW “Researches in Laboratory of Organic Main Group Chemistry”

GE YOSHIDA, Ryota; ISOZAKI, Katsuhiro; YOKOI, Tomoya; TAKENAKA, Toshio; TAKAYA, Hikaru; NAKAMURA, Masaharu
“Ruthenium Complex-Bound Norvaline-Catalyzed Oxidation of Electron-Rich Aromatic Compounds with Hydrogen Peroxide”

GE NAKAJIMA, Sho; HASHIMOTO, Toru; NAKAGAWA, Naohisa; IMAYOSHI, Ryuji; GOWER, Nicholas J.; ADAK, Laksmikanta; HONMA, Tetsuo; SUNADA, Yusuke; NAGASHIMA, Hideo; ISOZAKI, Katsuhiro; HATAKEYAMA, Takuji; TAKAYA, Hikaru; NAKAMURA, Masaharu
“The Structure and Reactivity of Aryl-Iron Intermediate in Iron-Catalyzed Cross-Coupling Reaction”

— Advanced Solid State Chemistry —

LW “Introduction of the Laboratory of Advanced Inorganic Chemistry”

GE HIRAI, Kei; KAN, Daisuke; ICHIKAWA, Noriya; MIBU, Ko; SHIMAKAWA, Yuichi
"Metal-insulator Transition in $SrFeO_{2.875}$ Epitaxial Thin Films"

— Organotransition Metal Chemistry —

LW "Activity Report: Organotransition Metal Chemistry Laboratory"

GE WAKIOKA, Masayuki; ICHIHARA, Nobuko; KITANO, Yutaro; OZAWA, Fumiyuki
"A Highly Efficient Catalyst for the Synthesis of Alternating Copolymers via Direct Arylation Polymerization"

— Photonic Elements Science —

LW "Recent Research at Photonic Elements Science"

— Chemical Life Science —

LW "Recent Development of the Life Science Database for the Data Integration and Improved Usage in the Big-data Era"

GE MUTO, Ai; OZAKI, Katsuhisa; GOTO, Susumu; KOTERA, Masaaki
"Construction of an Ortholog Database of Lepidopteran Insects"

— Mathematical Bioinformatics —

GE ZHAO, Yang
"Flux Balance Impact Degree: A New Definition of Impact Degree to Properly Treat Reversible Reactions in Metabolic Networks"

— Bio-knowledge Engineering —

GE NGUYEN, Hao Canh; MAMITSUKA, Hiroshi
"Discriminative Graph Embedding for Label Propagation"

— Nano-Interface Photonics —

LW "Recent Research Topics in Nanointerface Photonics Group"

—Research Center for Low Temperature and Materials Sciences —

GE TERASHIMA, Takahito
"Control of Inversion Symmetry Breaking in Artificially Engineered Superlattices of Heavy Fermion Superconductor"

SEMINARS

Prof AKAI, Shuji
Graduate School of Pharmaceutical Sciences, Osaka University, Osaka, Japan
“Control of Regiochemistry of Benzyne Reactions and the Mechanistic Study”
9 July 2013

Prof ALEZRA, Valerie
Universite Paris Sud, Paris, France
“Non Proteinogenic Amino Acids: Asymmetric Synthesis and Their Use as Building Blocks of Foldamers”
27 September 2013

Prof AMEDURI, Bruno
Centre National de la Recherché Scientifique, France
“Recent Advances in the Controlled Radical (Co)Polymerization of Fluoroalkenes”
30 October 2013

Prof BEGLEY, Tadhg P.
Department of Chemistry, Texas A&M University, U.S.A.
“Molecular Microbial Science Seminar”
28 May 2013

Assoc Prof CAI, Hongmin
South China University of Technology, China, P.R.
“Feature Selection via Local Hyperplane Approximation”
5 June 2013

Dr CHANMUANG, Chutimun
Faculty of Gems, Burapha University, Thailand
“Transmission Electron Microscopy and Related Phase Transformation of the Ag-Cu-Pd Jewelry Sterling”
11 November 2013

Prof CHEN, Chun-Wei
Department of Materials Science and Engineering, National Taiwan University, Taiwan
“Tunable Graphene Based Optics, Electronics and Photonics”
1 August 2013

Prof CHEN, Jwu-Ting
Department of Chemistry, National Taiwan University, Taiwan
“Alternating Ethylene/norbornene Copolymerization Catalyzed by Organopalladium Complexes Bearing Aminopyridines–An Unusual Example of Ligand Design Leading to the Control of Geometric Isomerism-reactivity Relationship”
9 April 2013

Mr. CHENG, Ran
The University of Texas at Austin, U.S.A.
“Dynamics of Antiferromagnets Driven by Spin Current”
13 June 2013

Assoc Prof CHESI, Graziano
The University of Hong Kong, China, P.R.
“Equilibria and Stability Investigation in Genetic Regulatory Networks”
24 May 2013

Prof COLBY, Ralph
Department of Materials Science and Engineering and Chemical Engineering, Pennsylvania State University, U.S.A.
“Ionomer Design, Synthesis and Characterization for Ion-Conducting Energy Materials”
14 May 2013

Assoc Prof CUTURI, Marco
Graduate School of Informatics, Kyoto University, Kyoto, Japan
“Sinkhorn Distances: Lightspeed Computation of Optimal Transport”
21 November 2013

Dr D. A. Swenson
Chief Scientist, ImpartOne Inc., U.S.A.
“Compact Neutron Source based on the RFI Linac Structure”
22 October 2013
“A Possible Design for the Mid-Beta section of the G-2 Muon Linac”
24 October 2013

Prof EGERTON, Raymond Frank
Physics Department, University of Alberta, Edmonton, Canada
“Choice of Operating Voltage for a Transmission Electron Microscope”
9 April 2013

Prof FELDHOFF, Armin
Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, Germany
“Perovskite-based Oxygen-transporting Membranes”
6 June 2013

Prof FUJITA, Tetsuro
Emeritus Professor, Kyoto University, Japan
“Development of Immuno Modulator, FTY720, from Tochukaso”
26 July 2013

Prof HAINO, Takeharu
Graduate School of Science, Hiroshima University, Hiroshima, Japan
“Supramolecular Structure and its Function Produce by Intermolecular Interaction”
25 January 2013

Dr HARA, Kenji
Hokkaido Univerisy, Japan
“Fabrication of Dense Metal Complex Monolayer on Regulated Surface and Its Application to Catalyst”
9 January 2013

Prof HIRATA, Koichi
Kyushu Institute of Technology, Fukuoka, Japan
“Tai Mapping Hierarchy and Variations of Tree Edit Distance”
9 April 2013

Dr HOSHINA, Hiromichi
Terahertz Sensing and Imaging Laboratory, RIKEN, Japan
“Analysis of Higher-Order Structure of Polymers by Terahertz Spectroscopy”
3 November 2013

Assoc Prof KOGA, Tadanori
Department of Materials Science and Engineering, Stony Brook University, U.S.A.
"Microscope Architecture and Dynamics of Polymer Chains Adsorbed on Flat and Curved Surfaces"
25 July 2013

Dr KOLAR, Michal
Academy of Sciences of the Czech Republic, Prague, Czech R.
"Graph Alignment of Protein-protein Interaction Networks: From Interactions to Functional Annotation"
7 October 2013

Prof KÜNDIG, Peter
Department of Chemistry, University of Geneva, Switzerland
"New Chiral NHC Ligands for the Catalytic Asymmetric Arylation of Amides and the Enantioselective C(sp3)-H Activation"
17 December 2013

Prof LACÔTE, Emmanuel
CPE Lyon, University of Lyon, France
"NHC-Borane Complexes: From Stabilized Reactive Intermediates to Polymer Synthesis"
11 January 2013

Dr LASZLO, Veisz
Laboratory for Attosecond Physics, Max-Planck Institute of Quantum Optics, Germany
"Generation and Applications of Sub-5-fs Multi-10-TW Light Pulses"
3 July 2013

Dr LI, Dazhi
Institute for Laser Technology, Osaka, Japan
"Progress in Smith–Purcell Free-electron Lasers"
15 February 2013

Dr LIMBACH, Michael
BASF, Germany
"A Catalytic Route to Acrylates from Alkenes and CO_2: The Stuff that are Dreams made of "
16 July 2013

Prof LINGAS, Andrzej
Lund University, Sweden
"Counting and Detecting Small Subgraphs via Equations"
7 May 2013

Prof MACLACHLAN, Mark
The University of British Columbia, Canada
"Spramolecular Origami: Transforming Paper into Twisted Shapes"
17 October 2013

Assoc Prof MAEDA, Hiromitsu
Ritsumeikan University, Japan
"Development of π-Conjugated Molecular Assemblies Based on Ionic Recognition"
5 February 2012

Dr MAN, Yi Yim
The University of Hong Kong, China, P.R.
"Impact of Intrinsic Biophysical Diversity on the Activity of Spiking Neurons"
15 October 2013

Dr MANFRED, Grieser
Permanent Researcher, Group Leader of Accelerators, Ion Sources and Storage Rings. Max-Planck Institute für Kernphysik, Germany
"The Storage Rings at MPI for Nuclear Physics in Heidelberg"
13 March 2013

Prof MARGALIT, Hanah
Faculty of Medicine, The Hebrew University, Israel
"The Multifaceted Impact of Post-transcriptional Regulation by Non-coding RNAs"
11 November 2013

Prof MARTIN, Susana Garcia
Professor Titular, Complutense University, Spain
"Materials for Energy"
25 February 2013

Prof MOCEK, Tomas
HiLASE Project & Dept. of Diode-pumped Lasers, Institute of Physics, Czech R.
"The HiLASE Project: A High Average Power DPSSL Development in the Czech Republic"
2 April 2013

Prof MURAKAMI, Masakatsu
Institute of Laser Engineering, Osaka University, Osaka, Japan
"Proton Acceleration Scheme Using Carbon Nanotubes"
14 June 2013

Dr MUROOKA, Yoshie
Advanced Science Institute, RIKEN, Saitama, Japan
"Ultrafast Structural Dynamics Revealed by Femtosecond Time-Resolved Electron Diffraction"
8 February 2013

Prof NAGASHIMA, Hideo
Institute for Materials Chemistry and Engineering, Kyushu University, Fukuoka, Japan
"Living Radical Polymerization and Hyper-branched Polymer; Homogeneous Catalytic System Inspired by Industry-Academia Partnership"
23 May 2013
"Iron Carbonyl Complexes which Easily Generate Active Species; Utilization in Catalytic Reactions"
27 November 2013

Dr NAITO, Masanobu
National Institute for Materials Science, Japan
"σ-Conjugated Polysilane: Interface, Chiral, and Exotic Self-Assembly"
5 February 2012

Dr NEDELA, Vilem
Institute of Science Instruments of the ASCR, Czech R.
"Environmental Scanning Electron Microscope for Observation of Live Nature"
16 May 2013

Prof NEIDIG, Michael
University of Rochester, U.K.
"Mössbauer and Magnetic Circular Dichroism Spectroscopy of Iron Coordination Complexes: Theory and Application"
11 March 2013

Vis Assoc Prof NISHIOKA, Jun
Pan-Okhotsk Research Center, Institute of Low Temperature Science, Hokkaido University, Japan
“The Role of the Subpolar Region in the Material Cycle and Biological Productivity in the North Pacific Ocean”
11 October 2013

Dr NUSS, Jurgen
Max Planck Institute for Solid State Research Stuttgart, Germany
“Structure Systematics and Geometric Variations in La2Sb and Related Compounds”
24 June 2013

Prof OCHIAI, Masahito
Faculty of Pharmaceutical Sciences, The University of Tokushima, Tokushima, Japan
“Chemistry of Hypervalent Bromine: A New Frontier”
15 March 2013

Prof OHFUNE, Yasufumi
Emeritus Professor, Osaka City University, Japan
“Chemistry of Glutamate Receptor Ligands”
25 October 2013

Prof RICE, David
The University of Sheffield, U.K.
“Discovery of a Lethal Toxin from the Bacterial Pathogen *Burkholderia pseudomallei*”
2 April 2013

Dr SARAKONSRI, Thapanee
Faculty of Science, Chiang Mai University, Thailand
“Chemically Prepared Chalcogenide Compounds for Used as Thermoelectric Materials”
8 July 2013

Dr SCHAPER, Andreas Karl.
Materials Science Center, Philipps University Marburg, Germany
“Microscopy of Organic Fibers and Nanotubes”
19 April 2013

Prof SHINSHIDO, Kozo
Faculty of Pharmaceutical Sciences, The University of Tokushima, Tokushima, Japan
“Synthesis of Highly Functionalized Bioactive Natural Products”
15 March 2013

Dr SIRITANON, Theeranun
School of Chemistry, Institute of Science, Suranaree University of Technology, Thailand
“First Observation of electronic Conductivity in Mixed Valence Tellurium Oxides”
20 May 2013

Dr SUGIMOTO, Kunihisa
Japan Synchrotron Radiation Institute, Japan
“Introduction to Single Crystal Analysis in BL02B1/SPring-8 and Recent Research Topics”
4 March 2012

Prof SWAGTEN, Henk
Eindhoven University of Technology, Netherlands
“Domain-wall Physics in Perpendicularly Magnetized Devices: Some Recent Developments”
28 May 2013

Prof ULRICH, Gilles
The National Center for Scientific Research (CNRS), France
“BODIPY and Related Boron Complexes: Versatile Functional Fluorescent Dyes”
21 November 2013

Dr VERT, Jean-Philippe
The Diretcor of Centre for Computational Biology, Mines ParisTech and the Adjunct Director of Mines ParisTech–Curie Institute–INSERM U900 Joint Laboratory on Bioinformatics and Computational Systems Biology of Cancer, France
“Flip-Flop: Fast Lasso-based Isoform Prediction from RNA-Seq Data”
12 July 2013

Prof VILA, Laurent
Institut Nanosciences et Cryogénie, CEA Grenoble, France
“Dimensionality Effects on the Magnetization Reversal, Magnetoresistance and Domain Wall Depinning Process in Nanowires”
9 August 2013

Prof VLASSOPOULOS, Dimitris
IESL-FORTH and Department of Materials Science and Technology, University of Crete, Heraklion, Crete, Greece
“Entanglement Dynamics in Ring Polymers: Recent Progress and Open Challenges”
14 May 2013

Prof VOLLHARDT, K. Peter C.
University of California at Berkeley, U.S.A.
“Saving the Planet: Toward a Sun-charged Thermal Molecular Battery”
20 May 2013

Prof WILLIAMS, Robert M.
Colorado State University, U.S.A.
“Asymmetric Synthesis of Amino Acids: Gateway to Alkaloids and Peptides”
18 April 2013

Prof WILLIARD, Paul
Brown University, Rhode Island, U.S.A.
“Discovery of New Organolithium Aggregates”
27 September 2013

Prof WINTNER, Ernst
Photonics Institute, Vienna University of Technology, Austria
“Laser Ignition of Engines–Application of Most Recent Laser Development”
26 April 2013

Prof YAO, Zhu-Jun
School of Chemistry and Chemical Engineering, Nanjing University, Nanjing, China, P.R.
“Natural Product-like Mimicry of Annonaceous Acetogenins”
29 November 2013

Dr YASUDA, Nobuhiro
Japan Synchrotron Radiation Institute, Japan
“Introduction to Micro-Single Crystal Analysis in BL40XU/SPring-8”
4 March 2012

Dr YASUDA, Nobuyoshi
Merck Research Laboratories, U.S.A.
“The Art of Process Chemistry”
8 April 2013

Dr YOSHIKAI, Naohiko
Nanyang University, Japan
“C–H Bond Functionalization Catalyzed by Cobalt Complexes”
13 February 2013

Prof YU, Jaehoon
Department of Chemistry & Education, Seoul National University, Korea, R.
“An Apolipoprotein A-I mimetic Peptide Containing a Naphthylalanine Residue Enhances Cholesterol Efflux from Macrophage Cells and Sequesters Oxidized LDL”
18 November 2013

MEETINGS AND SYMPOSIA

Asian Chemical Biology Initiative 2013 Bangkok Meeting
Organized by UESUGI, Motonari
26-27 January 2013 (Bangkok, Thailand)

The 93rd Annual Meeting of The Chemical Society Japan "Introduction of Synchrotron to Chemists ~From Basic Theory to Advanced Application of XAFS Analysis~"
Organized by TAKAYA, Hikaru; ISOZAKI, Katsuhiro
22 March 2013 (Shiga, Japan)

The 93rd Annual Meeting of The Chemical Society Japan "Important Points in X-ray Single Crystal Analysis ~Practical Use of CheckCIF before Paper Submittion~"
Organized by TAKAYA, Hikaru
25 March 2013 (Shiga, Japan)

The 133rd Meeting of the Pharmaceutical Society of Japan "Chemistry Challenge to Mystery of Life" Symposium
Organized by SASAKI, Shigeki; FUTAKI, Shiroh
29 March 2013 (Yokohama, Japan)

KUBIC-NII Joint Seminar on Bioinformatics 2013
Organized by Bioinformatics Center, Institute for Chemical Research, Kyoto University and National Institute of Informatics
19 April 2013 (Uji, Japan)

The 8th International Symposium on Metallic Multilayers
Chaired by ONO, Teruo
19-24 May 2013 (Kyoto, Japan)

1st Investigation Expert Committee on Light and Particle Beam toward Nanomedicine
Organized by TERANISHI, Toshiharu
20 May 2013 (Uji, Japan)

International Discussion Meeting on Polymer Crystallization 2013 (IDMPC2013)
Co-organized by ICR, JSPS and other facilities (Conference Chairs are KANAYA, Toshiji; TODA, Akihiko)
30 June-4 July 2013 (Kyoto, Japan)

The 13th Annual International Workshop on Bioinformatics and Systems Biology
"International Research and Training Program of Bioinformatics and Systems Biology"
Organized by JSPS-International Training Program (ITP)
31 July-2 August 2013 (Uji, Japan)

2013 Sapporo Workshop on Machine Learning and Applications to Biology (MLAB Sapporo 2013)
Organized by MAMITSUKA, Hiroshi
5-6 August 2013 (Sapporo, Japan)

The Seventh International Conference on Advanced Vibrational Spectroscopy (ICAVS-7)
Contributed by HASEGAWA, Takeshi as Program Chair
25-30 August 2013 (Kobe, Japan)

The 62nd Conference of The Japan Society of Coordination Chemistry
"Catalysis Research Innovation on Supramolecular Materials"
Organized by TAKAYA, Hikaru; UENO, Takafumi
21 October 2012 (Toyama, Japan)

The 9th Organoelement Chemistry Seminar
Organized by TOKITOH, Norihiro; SASAMORI, Takahiro; MIZUHATA, Yoshiyuki; AGOU, Tomohiro
29-30 November 2013 (Uji, Japan)

INDEX

NAME INDEX

KEYWORD INDEX

Institute for
Chemical
Research

Kyoto University