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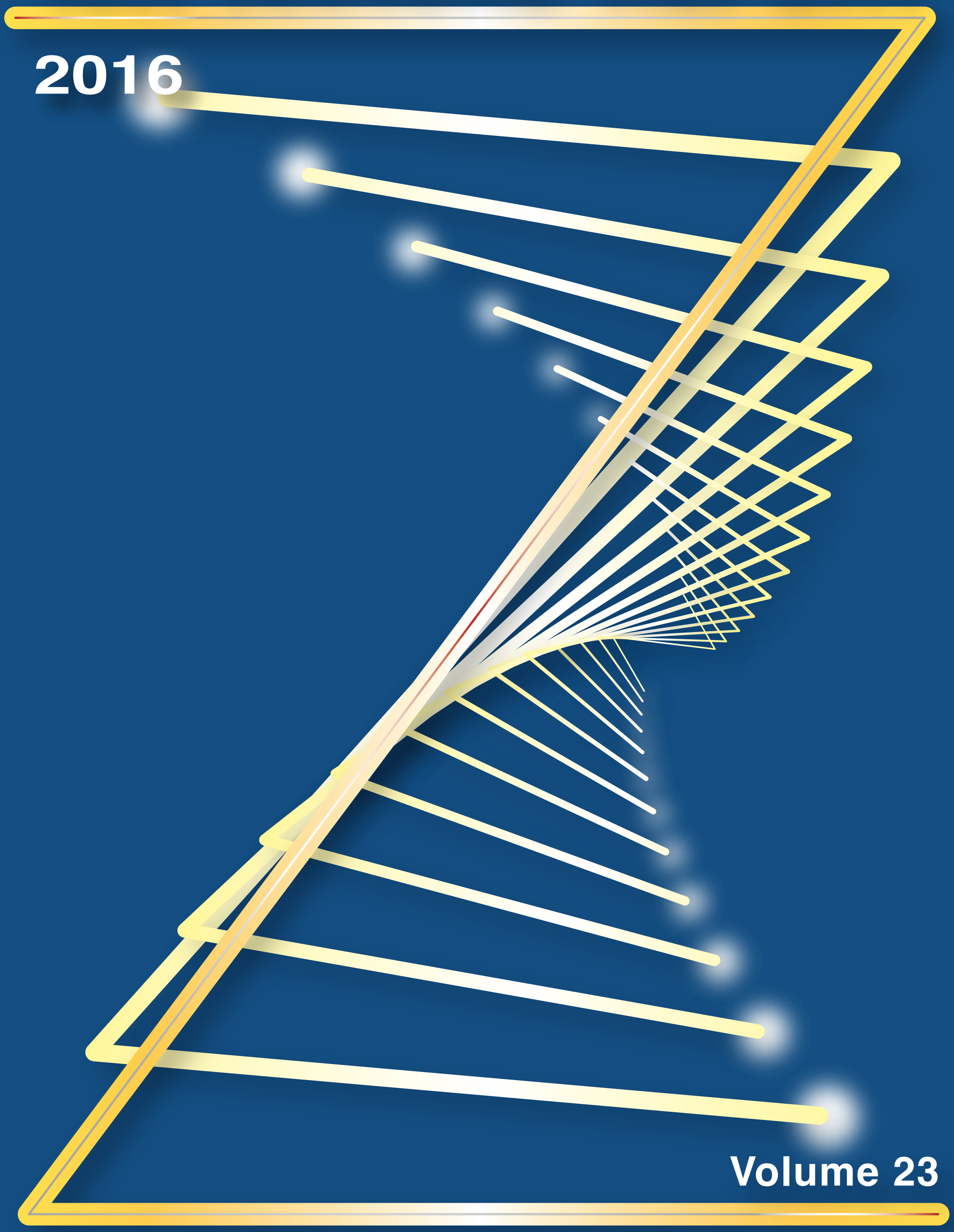
ICR ANNUAL REPORT

2016



Volume 23

Institute for Chemical Research
Kyoto University

ICR ANNUAL REPORT 2016 (Volume 23) - ISSN 1342-0321 -

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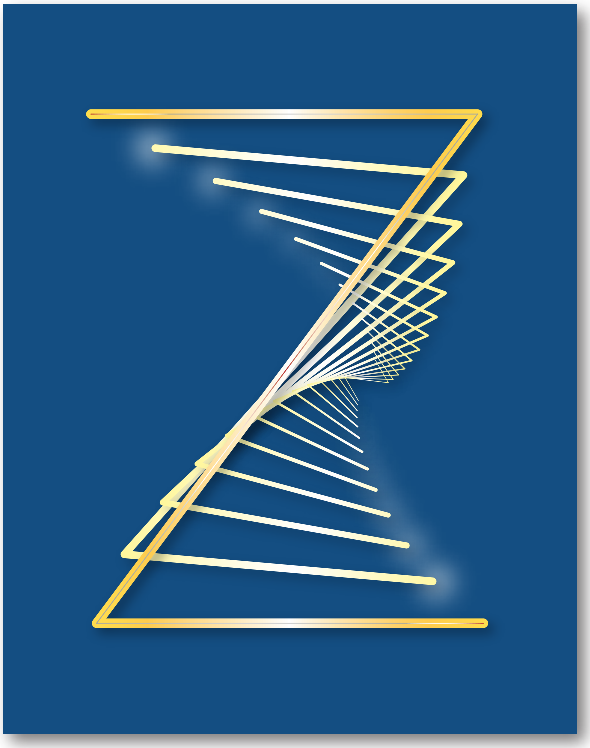


Institute for Chemical Research
Kyoto University
Volume 23

Preface

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

The research within the ICR encompasses the fields of chemistry, physics, biology, and informatics. The chemical studies core covers fields including physical chemistry, inorganic chemistry, organic chemistry, materials chemistry, and biochemistry. The graduate schools encompassing the laboratories accept students in diverse fields of science, engineering, agriculture, pharmaceutical sciences, medicine, and informatics. These laboratories are spearheading leading-edge research, and yielding outstanding results in their own and related research areas with publications such as: *1) Synthesis of a Distinct Water Dimer inside Fullerene* C_{70}*, 2) Formation of Pseudomorphic Nanocages from* Cu_2O *Nanocrystals through Anion Exchange Reactions, 3) Tuning Magnetic Anisotropy by Interfacially Engineering the Oxygen Coordination Environment in a Transition-metal Oxide, 4) Discovery of 12-mer Peptides That Bind to Wood Lignin, and 5) Experimental Observation of Snell's Law for Magnetostatic Spin Waves in Thin Ferromagnetic Permalloy Films*, all achieved last year. The legacy of our founding philosophy continues to the present day and describes the essence of our research activities. The ICR has entrusted its members, with this vision in mind, to choose and pursue research topics at the forefront of advanced chemistry with bottom-up paradigms. Sustainable and sustained growth of the human race is a key issue of this century, and we must reform our country from various perspectives. Hence, the ICR encourages its members to be actively involved in research projects and to value the development of unique interdisciplinary research projects, in order to contribute to the future of our society from materials-related fields.

The ICR also collaborates with domestic and international universities and research organizations (with 70 official international collaboration agreements as of January 1, 2017) and functions as a Joint Usage/Research Center proclaiming the Frontier and Interdisciplinary Research Core for Deepening Investigation and Promoting Collaboration in Chemistry-oriented Fields supported by MEXT (2016–2021); its activity during the former term received high commendation on the term-end assessment in 2016. In addition, the ICR collaborates with the Research Institute for Sustainable Humanosphere and the Institute of Advanced Energy at Kyoto University to start another MEXT-supported joint research project on bio-inspired smart materials as of April 1, 2015. Furthermore, the ICR—IRCELS in particular—is making a significant contribution to the MEXT Project of Integrated Consortium on Chemical Synthesis (2016–2021), in collaboration with the Catalysis Research Center at Hokkaido University, the Research Center for Materials Science at Nagoya University, and the Institute for Materials Chemistry and Engineering at Kyushu University. We also fully strive to foster and secure young researchers through these activities. For instance, we provide an in-house annual grant system named "ICR Grant for Encouraging Promoting Integrated Research." The strong collaboration basis so far constructed in-house and with outside researchers ensures that the Institute will continue to serve as a core of global research propellers in chemistry-oriented fields. With this consideration, we would appreciate your continued encouragement and support.

January 2017

N. Tokitoh

TOKITOH, Norihiro
Director

ICR News 2016

ICR Celebrates 90th Anniversary

Chairperson of ICR 90th Anniversary Committee
Prof KAWABATA, Takeo

Ever since it was formally founded on 4 October 1926 to conduct “fundamental and applied researches on specific subjects in chemistry”, ICR has carried out extensive studies in an extremely wide range of basic and applied chemistry, reaching its 90th anniversary last fall. We celebrated the anniversary on November 11, 2016 by holding Commemorative Lecture Meeting, Ceremony, and Banquet at the Clock Tower Centennial Hall (Centennial Hall and International Conference Hall), Kyoto University. We had another commemorative event, Poster Exhibition showing current activities of ICR. In the Lecture Meeting, lectures were delivered by Director N. Tokitoh on the past, present, and future perspective of ICR and by four ICR members, Professors H. Ogata, Y. Shimakawa, S. Sakabe, and S. Yamago on the frontier science. The Commemorative Ceremony included an address by Director N. Tokitoh and greetings by President J. Yamagiwa, Kyoto University, Director-General Y. Komatsu, Research Promotion Bureau, the Ministry of Education, Culture, Sports, Science and Technology, Dr. M. Sasaki (on behalf of Dr. Z. Matsuura), Council for Research Institutes and Centers of Japanese National Universities, and President. H. Yamamoto, the Chemical Society of Japan. The Lecture Meeting and Ceremony had an approximate total of 500 participants including some 200 guests from academia and industry. The Banquet was also a success with over 300 participants, getting started with greetings by President Y. Hiraki, Joint Usage/Research Center, Director N. Oshiman, Kyoto University Research Coordination Alliance, Dr. K. Tamao, RIKEN, and Dr. K. Soda, Professor Emeritus, Kyoto University, and proceeding in a friendly and enjoyable atmosphere.

Lecture given by Director Tokitoh, ICR

Exhibition of the latest researches at ICR

Commemorative Ceremony for 90th Anniversary

Speech by President Yamagiwa, Kyoto University

Speech by Director-General Komatsu, Research Promotion Bureau, the Ministry of Education, Culture, Sports, Science and Technology

KAGAMIBIRAKI ceremony at the banquet

International Research Network Weeks

■ Prof FUTAKI, Shiroh

ICR has built a community across the world including researchers, students and faculty. A remarkable event "International Research Network Weeks" was held on March 7−11, 2016. ICR invited global researchers and students who have been collaborated with ICR members for a week. The aim of this event is to strengthen partnerships and enhance international collaboration with institutions having MOU (Memorandum of Understanding) with ICR. At the beginning of the event, ICR built new ones with Department of Chemistry and Bioengineering, Notre Dame University (U.S.) and Department of Chemistry and Bioengineering, Ohio State University (U.S.). It is the 68th ICR's faculty level MOU.

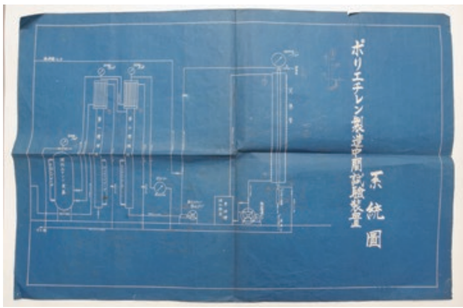
On March 7−8, the opening event -Institute for Chemical Research International Symposium 2016 (ICRIS'16) "Research Network Based on ICR MOU"- was held at Kihada Hall of Uji-Obaku Plaza. 13 investigators from Asia, Europe, and the United State and their Japanese counterparts, 7 investigators having domestic collaboration with ICR members and 6 faculty members of ICR, and 78 posters presented at the symposium. We hope that all presentations stimulated discussion among members of ICR's scientific community.

Materials Related with "Origin of Polyethylene Industry by the High-pressure Process in Japan" in the Institute for Chemical Research Were Approved as Chemical Heritage

■ Prof MURATA, Yasujiro

The engineering drawing, notebook, and reports for the industrial process in Kyoto University and the medal made by the polyethylene celebrating the first actual production in Japan were certified. Polyethylene (PE) is the most common synthetic polymers in petrochemical industry. There are three kinds of PEs depending on the production methods and the density. One of them is the low-density PE produced by high-pressure conditions, and it was industrialized in 1939 in UK. The PE has superior properties for insulation of radiofrequency, and therefore it was an essential material for radar devices during the World War II. In Japan, three groups started research works of PEs. Although one of the group started small industrial process at Minamata in 1945, all facility were destroyed by an air raid. After the World War II, continuous production was conducted in Kyoto University during 1951 to 1953, with which the materials are related.

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 96th Spring Annual Meeting of the Chemical Society of Japan at Doshisha University, Kyotanabe Campus on 26th March 2016.



CONTENTS

International Research Center for Elements Science

Bioinformatics Center

Abbreviations used in the columns

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

Guest Scholar	Guest Scholar
Guest Res Assoc	Guest Research Associate
SPD (JSPS)	Special Post-Doctoral Research Fellow (JSPS)
PD	Post-Doctoral Research Fellow
Res	Researcher
Res Support Staff	Research Support Staff
Proj Res	Project Researcher
RF	Research Fellow
D 1〜3	Doctoral Course (Program) 1〜3
M1〜2	Master’s Course (Program) 1〜2
RS	Research Student
UG	Undergraduate Student
D Sc	Doctor of Science
D Eng	Doctor of Engineering
D Agr	Doctor of Agricultural Science
D Pharm Sc	Doctor of Pharmaceutical Science
D Med Sc	Doctor of Medical Science
D Inf	Doctor of Informatics
D Human & Envirnmtl. Studies	Doctor of Human and Environmental Studies
Ph D	Doctor of Philosophy
(pt)	part-time

ORGANIZATION

Institute for Chemical Research

5 Divisions and 3 Centers | **Laboratories**

Research Divisions

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

Research Centers

- **Advanced Research Center for Beam Science**
  - Particle Beam Science
  - Laser Matter Interaction Science
  - Electron Microscopy and Crystal Chemistry
  - Structural Molecular Biology
- **International Research Center for Elements Science**
  - Synthetic Organotransformation
  - Advanced Solid State Chemistry
  - Organometallic Chemistry
  - Nanophotonics
  - Structural Organic Chemistry
  - Biofunctional Design-Chemistry
- **Bioinformatics Center**
  - Chemical Life Science
  - Mathematical Bioinformatics
  - Bio-knowledge Engineering
  - GenomeNet Project Management Office

- Visiting Divisions
- Joint Usage/Research Center
- Supercomputer System
- Low Temperature Laboratory

TOPICS AND INTRODUCTORY COLUMNS OF LABORATORIES

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


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Scope of Research

Organic chemistry has mainly developed with the use of second-row elements such as carbon, oxygen, and nitrogen, while the synthesis and isolation of the heavier congeners of typical organic molecules as stable compounds has been a dream for organic chemists. Our main research interest is the elucidation of the similarities and differences in structures and reactivities between organic compounds and the corresponding heavier congeners. These studies are interesting and important from the standpoints of fundamental chemistry, and open the way to more extensive application of main group chemistry.

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

Selected Publications

Nagata, K.; Murosaki, T.; Agou, T.; Sasamori, T.; Matsuo, T.; Tokitoh, N., Activation of Dihydrogen by Masked Doubly Bonded Aluminum Species, *Angew. Chem. Int. Ed.*, **55,** 12877-12880 (2016).

Suzuki, Y.; Sasamori, T.; Guo, J.-D.; Nagase, S.; Tokitoh, N., Isolation and Ambident Reactivity of a Chlorogermylenoid, *Chem. Eur. J.*, **22,** 13784-13788 (2016).

Agou, T.; Ikeda, S.; Sasamori, T.; Tokitoh, N., Synthesis and Structure of Lewis-Base-Free Phosphinoalumane Derivatives, *Eur. J. Inorg. Chem.*, **2016,** 623-627 (2016).

Sasamori, T.; Villalba Franco, J. M.; Guo, J.-D.; Sugamata, K.; Nagase, S.; Streubel, R.; Tokitoh, N., Selenium-Substituted Phosphaalkenes Obtained through 1,2-Elimination of Chlorosilanes from Selenenylchlorophosphines, *Eur. J. Inorg. Chem.*, **2016,** 678-684 (2016).

Sugahara, T.; Guo, J.-D.; Sasamori, T.; Karatsu, Y.; Furukawa, Y.; Ferao, A. E.; Nagase, S.; Tokitoh, N., Reaction of a Stable Digermyne with Acetylenes: Synthesis of a 1,2-Digermabenzene and a 1,4-Digermabarrelene, *Bull. Chem. Soc. Jpn.*, **89,** 1375-1384 (2016).

Topics

Activation of Dihydrogen by Masked Doubly Bonded Aluminum Species

Activation of dihydrogen (H_2) with transition-metal complexes is an important fundamental chemical transformation and has been extensively investigated for several decades. In contrast, main-group element compounds had been considered as ineffective for the splitting of H_2 for a long time, until the discoveries of the catalyst-free hydrogenation of heavier Group 14 triply bonded compounds, dimetallynes, and of the frustrated Lewis pair (FLP)-catalyzed hydrogenation. Thereafter, H_2 activation using multiply bonded and low-coordinate compounds of heavier main-group elements have been reported. Among various heavier main-group elements, aluminum is a promising candidate as the key component of the H_2 activation reagents, as shown by the recent reports on small-molecule activation with aluminum-based FLPs.

We have already reported the reactivity of barrelene-type dialumane **1** as the masked form of 1,2-diaryldialumene **2**. At ambient temperature, **1** most certainly undergoes retro [2+4] cycloaddition to generate **2**, which can be trapped by various trapping reagents. These findings are indicative of the possibility of H_2 activation by using **1** as the masked forms of the corresponding dialumenes **2**.

Reactions of **1** with H_2 afforded dihydroalumanes $ArAlH_2$ at room temperature (Ar: bulky aryl groups). These dihydroalumanes form hydrogen-bridged dimers $[ArHAl(\mu\text{-}H)]_2$ **3** in the crystalline state, while a monomer–dimer equilibrium was suggested in solution. Dialumenes **2** generated from **1** are the putative active species in the cleavage of H_2.

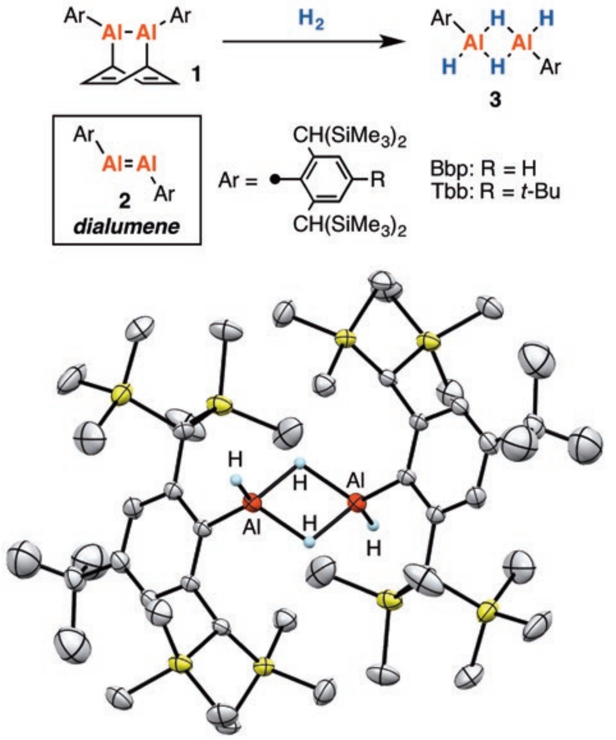

Figure 1. Reactions of barrelene-type dialumane **1** with dihydrogen and the Structure of **3** (Ar = Tbb).

Isolation and Reactivity of a Chlorogermylenoid

Metallylenoids of the general formula R_2EXM (E = group 14 element, X = anionic leaving group, M = metal) represent the silicon analogs of carbenoids (R_2CXM), which may exhibit both carbanion (R_2CX^-) and carbene (R_2C:) character. Silylenoids (R_2SiXM) as well as silylenes (R_2Si:) have been postulated as important intermediates in the reduction of dihalosilanes towards silylenes and/or oligo- and polysilanes. In contrast to the variety and rich chemistry of halosilylenoids, heavier halogermylenoid (R_2GeXM) analogs and their associated chemistry still remains scarce.

Treatment of 2,5-di(3,5-*tert*-butylphenyl)-1-lithioferrocene (Fc*Li) with $GeCl_2$·dioxane afforded the corresponding chlorogermylenoid that exhibited an ambident reactivity in different solvents; it displayed a behavior characteristic for a dichlorogermylene anion in THF, while it exhibited the typical reactivity of a chlorogermylene in toluene. X-Ray diffraction analysis of a single crystal of this chlorogermylenoid, obtained from recrystallization in THF, revealed a separated-ion-pair structure in the solid state.

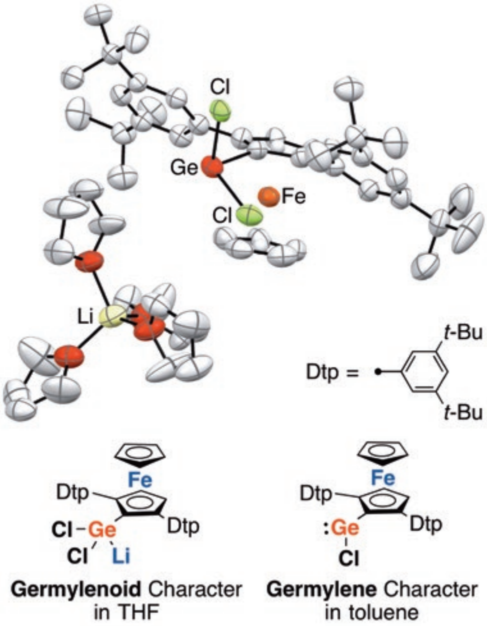

Figure 2. The structure of $[Li^+(thf)_4][Fc^*GeCl_2]^-$.

Division of Synthetic Chemistry
– Structural Organic Chemistry –

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YAKUMARU, Shinya (UG)
OKAMOTO, Shu (UG)

Scope of Research

Fundamental studies are being conducted for the creation of new functional π-systems with novel structures and properties, and for evaluation of their application as organic semi-conducting materials for photovoltaic and electroluminescent devices. The major subjects are: 1) organochemical transformation of fullerenes C_{60} and C_{70} , specifically organic synthesis of endohedral fullerenes by the technique of molecular surgery; 2) generation of ionic fullerene species and their application for the synthesis of functional material; 3) synthesis of new carbon-rich materials by the use of transition metal complex; and 4) creation of new functional π-materials with unique photoelectric properties.

KEYWORDS

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

Selected Publications

Zhang, R.; Murata, M.; Aharen, T.; Wakamiya, A.; Shimoaka, T.; Hasegawa, T.; Murata, Y., Synthesis of a Distinct Water Dimer inside Fullerene C_{70}, *Nat. Chem.*, **8,** 435-441 (2016).

Nishimura, H.; Fukushima, T.; Wakamiya, A.; Murata, Y.; Kaji, H., The Influence of Quasiplanar Structures of Partially Oxygen-Bridged Triphenylamine Dimers on the Properties of their Bulk Films, *Bull. Chem. Soc. Jpn.*, **89,** 726-732 (2016).

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Satou, M.; Nakamura, T.; Aramaki, Y.; Okazaki, S.; Murata, M.; Wakamiya, A.; Murata, Y., Near-Infrared Emissive Donor–Acceptor-Type Molecules Containing Thiazole-Fused Benzothiadiazole as an Electron-Acceptor Moiety, *Chem. Lett.*, **45,** 892-894 (2016).

Murata, M.; Kaji, S.; Nishimura, H.; Wakamiya, A.; Murata, Y., Efficient Synthesis of One- and Two-Dimensional Multimetallic Gold-Bis(dithiolene) Complexes, *Eur. J. Inorg. Chem.*, **2016,** 3228-3232 (2016).

Hashikawa, Y.; Murata, M.; Wakamiya, A.; Murata, Y., Water Entrapped inside Fullerene Cages: A Potential Probe for Evaluation of Bond Polarization, *Angew. Chem. Int. Ed.*, **55,** 13109-13113 (2016).

Synthesis of a Distinct Water Dimer inside Fullerene C_{70}

The water dimer is an ideal chemical species with which to study hydrogen bonds. Owing to the equilibrium between the monomer and oligomer structure, however, selective generation and separation of a genuine water dimer has not yet been achieved. We have developed a synthetic method that leads to the successful encapsulation of one or two water molecules inside fullerene C_{70}. These endohedral C_{70} compounds offer the opportunity to study the intrinsic properties of a single water molecule without any hydrogen bonding, as well as an isolated water dimer with a single hydrogen bond between the two molecules. The structure of $H_2O@C_{70}$ was unambiguously determined by XRD analysis, showing that the H_2O molecule was located at the off-center position of C_{70}. Furthermore, in the case of $(H_2O)_2@C_{70}$, a hydrogen bond was observed between the two H_2O molecules, and their rapid interchange was supported by NMR measurements and theoretical calculations. Infrared spectroscopy suggested the possible qualitative recognition of each water-encapsulating C_{70} species based on their unique and characteristic spectra.

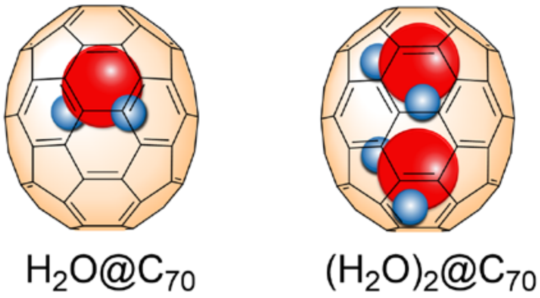

Figure 1. The structures of $H_2O@C_{70}$ and $(H_2O)_2@C_{70}$.

Near-infrared Emissive Donor-Acceptor-type Molecules Containing Thiazole-fused Benzothiadiazole as an Electron-acceptor Moiety

Fluorophores with strong emission in the near-infrared (NIR) region have received attention as NIR organic light-emitting diodes (OLEDs), which find applications in night vision-readable displays and sensors, as well as in fluorescent probes for bioimaging. In addition to conventional dyes, donor (D)−acceptor (A)-type molecules have attracted considerable interest, as their optical properties can be easily tuned by varying the D and A units. In this work, two D–A-type molecules containing thiazole-fused benzothiadiazole (BT) as the acceptor moiety were designed and synthesized. The thiazole-fused BT skeleton enables fine-tuning of the solubility and the electronic structure as well as two-dimensional extension of the π-conjugation. The combination with common donor units such as diphenylaminothiophene or triphenylamine-substituted thiophene resulted in the formation of D–A–D-type molecules, which exhibited fluorescence in the NIR region.

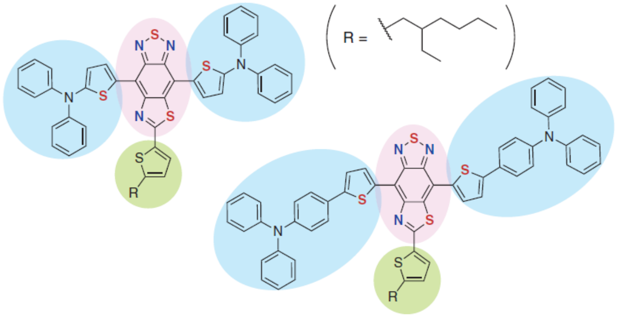

Figure 2. The structures of model compounds for the D–A–D type molecules based on a thiazole-fused BT skeleton.

Efficient Synthesis of One- and Two-Dimensional Multimetallic Gold–Bis (dithiolene) Complexes

Multimetallic complexes having π-conjugated dithiolate ligands have recently received attention because of their unique solid-state properties, which include high conductivity and magnetism, as well as their potential use in organic thermoelectric materials. We demonstrated efficient and versatile methods for the synthesis of 1D and 2D multimetallic gold–bis(dithiolene) complexes with well-defined structures by using a dichlorogold(III) complex having a benzene-1,2-dithiolate ligand as a terminal unit. By using benzene-1,2,4,5-tetrathiolate as a bridging unit, a 1D rod-shaped dimetallic complex was synthesized in good yield. Furthermore, on the basis of this synthetic strategy, we prepared a 2D trimetallic complex with a starburst structure by using a benzenehexathiolate bridging unit. The new synthetic methods can offer a way to prepare a wide variety of unprecedented 1D and 2D multimetallic gold–bis(dithiolene) complexes.

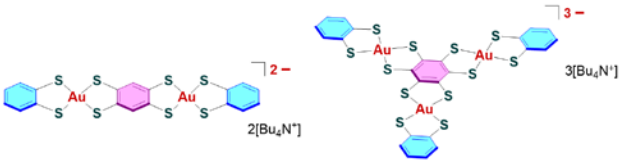

Figure 3. The structures of 1D dimetallic and 2D trimetallic gold–bis(dithiolene) complexes.

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Scope of Research

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

KEYWORDS
Organocatalysis
Regioselective Functionalization
Dynamic Chirality
Unusual Amino Acid
Molecular Recognition

Selected Publications

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

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

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

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

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

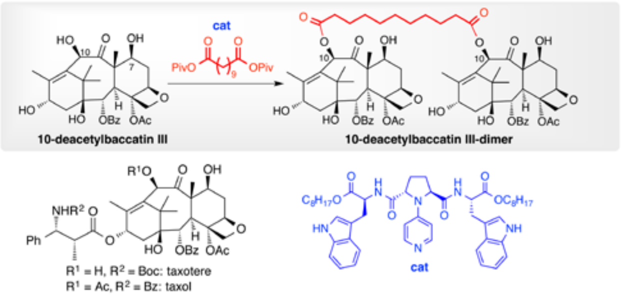
Yoshimura, T.; Tomohara, K.; Kawabata, T., Asymmetric Induction via Short-Lived Chiral Enolates with Chiral C-O Axis, *J. Am. Chem. Soc.*, **135**, 7102-7105 (2013).

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

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

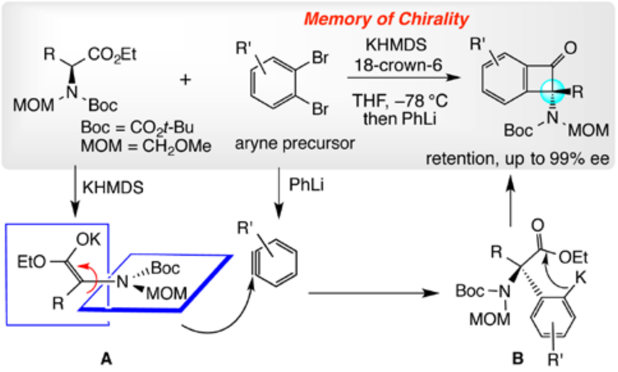
Late-stage Functionalization of Natural Products by Organocatalysis: Site-Selective Dimerization of 10-Deacetylbaccatin III

Late-stage site-selective functionalization of biologically active compounds has been receiving increasing attention because it enables diversification of biologically active compounds retaining their original activity. Here, we report application of our strategy for organocatalytic site-selective acylation to dimerization of 10-deacetylbaccatin III. 10-Deacetylbaccatin III is a natural terpenoid available in a relatively abundant amount and used as a key intermediate for clinically widely used antitumor agents, taxol and taxotere. Dimerization of bioactive compounds is potentially useful strategy toward the discovery of the agents with improved activity profiles including promising activity against the native-compound-resistant infections and cancers. The organocatalytic site-selective acylation of 10-Deacetylbaccatin III with a mixed anhydride prepared from undecanedioic acid and pivaloyl chloride took place at C(10)-OH in the presence of an organocatalyst to provide its dimer as a pure regioisomer in 40% yield. The site-selectivity was assumed to be controlled by the catalyst because the C(7)-OH has been known to be intrinsically more reactive hydroxy group.



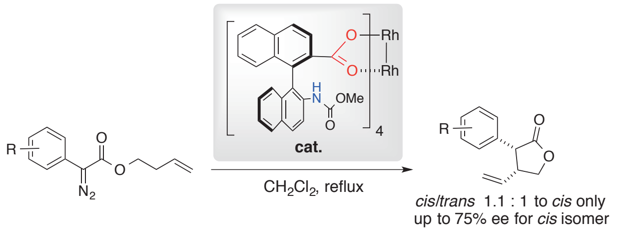
Asymmetric α-Arylation of α-Amino Acid Derivatives via Memory of Chirality

We have studied asymmetric synthesis via memory of chirality (MOC). A salient feature of the MOC strategy is that asymmetric reactions take place via axially chiral enolates with limited half-lives of racemization. Because the rate of enolate-racemization strongly depends on the reaction temperature, the reactions via MOC are usually performed at low temperatures to minimize the enolate racemization. While we have successfully developed several intermolecular asymmetric reactions and *intramolecular* asymmetric α-arylation of α-amino acid derivatives via the MOC strategy, the development of asymmetric *intermolecular α-arylation* has been unsuccessful so far. This was assumed to be because usual methods for α-arylation of enolates often requires long reaction times at high temperature, which should cause significant racemization of the intermediary chiral enolates. We describe here a solution to this long-standing problem in the MOC study. We employed arynes as reactive electrophilic aryl species at low temperatures, and successfully developed the target reaction. Treatment of a solution of the amino acid derivative and the aryne precursor with potassium hexamethyldisilazide (KHMDS) followed by phenyl lithium (PhLi) at –78 °C gave benozocyclobutenones with tetra-substituted carbon with retention of configuration in up to 99% ee. The reaction was assumed to proceed via intermolecular asymmetric α-arylation of axially chiral enolate **A** generated by the amino acid derivative and KHMDS with arynes generated by the aryne precursors and PhLi, followed by intramolecular C-acylation of resulting aryl metallic species **B**.



Asymmetric Intramolecular C–H Insertion Promoted by Dirhodium(II) Carboxylate Catalyst Bearing Axially Chiral Amino Acid Derivatives

The asymmetric intramolecular C–H insertion of a rhodium carbenoid intermediate has attracted much attention as a powerful synthetic tool for constructing chiral cyclic compounds. A dirhodium(II) carboxylate catalyst bearing axially chiral amino acid derivatives is prepared. This catalyst is effective in the asymmetric intramolecular C–H insertion of α-aryl-α-diazoacetates to α-aryl-β-substituted γ-lactones with a reasonable level of diastereo- and enantioselectivity, especially in the reaction of phenyl and β-naphthyl substituted substrates.



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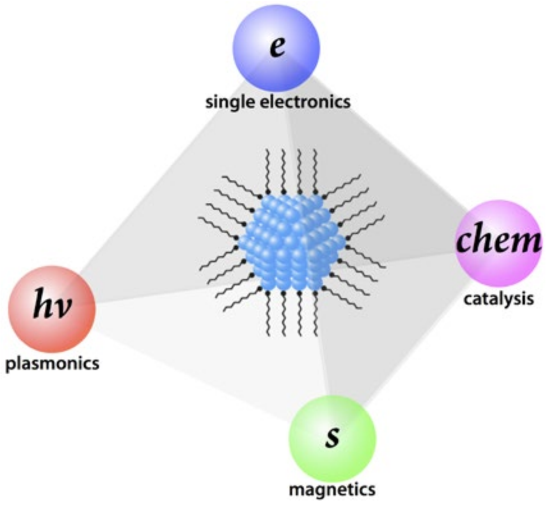
Scope of Research

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



KEYWORDS
Inorganic Nanoparticles
Single Electronics
Plasmonics
Nanocomposite Magnet
Photocatalysts

Selected Publications

Sakamoto, M.; Inoue, K.; Okano, M.; Saruyama, M.; Kim, S.; So, Y.-G.; Kimoto, K.; Kanemitsu, Y.; Teranishi, T., Light-Stimulated Carrier Dynamics of $CuInS_2$/CdS Heterotetrapod Nanocrystals, *Nanoscale*, **8,** 9517-9520 (2016).
Wu, H.-L.; Sato, R.; Yamaguchi, A.; Kimura, M.; Haruta, M.; Kurata, H.; Teranishi, T., Formation of Pseudomorphic Nanocages from Cu_2O Nanocrystals through Anion Exchange Reactions, *Science*, **351,** 1306-1310 (2016).

Nano-pseudomorphic Chemistry: Anionic Frameworks Dictate Crystal Systems in Sequential Ion Exchange Reactions

Ionic crystals have been widely used as photo-functional materials such as photocatalysts and photoelectric conversion materials, which are determined by the constituent elements, morphologies, and crystal structures. Because the stable crystal structures of the ionic crystals follow their phase diagrams, it has been difficult to chemically synthesize the high-temperature stable phases. In contrast to the bulk form, chemical conversion of ionic nanocrystals (NCs) via ion exchange reactions can overcome the difficulties associated with controlling the size, shape, chemical composition, and crystal structure in conventional syntheses. In our research, we discovered that the retained shape of the parent-NCs in sequential ion exchange reactions provided an opportunity to obtain non-equilibrium unique structures and even new structures of ionic NCs, these morphologically retained products being known as "pseudomorphs".

We investigated the crystal structures of the pseudomorphic nanocages, which were formed by the anion exchange ($O^{2-} \rightarrow S^{2-}$) of hexahedral Cu_2O NCs enclosed with {100} planes and rhombic dodecahedral Cu_2O NCs enclosed with {110} planes at ambient conditions. It was discovered that the shape-dependent anionic framework (surface anion sublattice and stacking pattern) of Cu_2O NCs determined the crystal system of anion-exchanged products (Figure 1). In other words, the cubic system can transform into not only the cubic system but also the triclinic and hexagonal systems. Furthermore, we found that the resulting nanocages have the multiply-twinned structure. A high-temperature stable phase such as wurtzite ZnS (> 1020 °C) was also obtained with this method at ambient conditions. We envisage that this pseudomorphic transformation method could be applicable to a number of other ionic NCs and thin films at ambient temperatures to find the novel properties and functions.

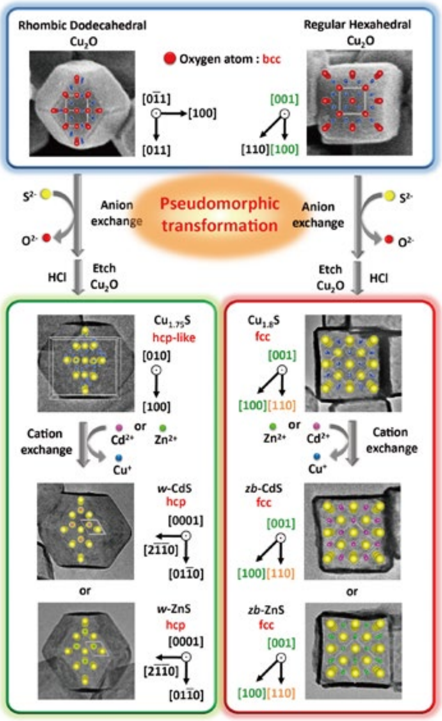


Figure 1. (Left hand) The rhombic dodecahedral $Cu_{1.75}S$ nanocages with a triclinic phase are formed by the anion exchange ($O^{2-} \rightarrow S^{2-}$) and the subsequent etching of rhombic dodecahedral Cu_2O NCs enclosed with {110} planes at ambient conditions. Further cation exchange ($Cu^+ \rightarrow Cd^{2+}$, Zn^{2+}) gives the hexahedral CdS or ZnS with a hexagonal phase. (Right hand) The hexahedral $Cu_{1.8}S$ nanocages with a cubic phase are formed by the anion exchange ($O^{2-} \rightarrow S^{2-}$) and the subsequent etching of hexahedral Cu_2O NCs enclosed with {100} planes at ambient conditions. Further cation exchange ($Cu^+ \rightarrow Cd^{2+}$, Zn^{2+}) gives the hexahedral CdS or ZnS with a cubic phase.

Porphyrin Derivative-Protected Gold Cluster with a Pseudo-Tetrahedral Shape

The shape of a nanomaterial plays an important role in controlling the packing arrangement and properties of the assembly that it forms. In the case of metal clusters, the shape of the metal core is veiled by a flexible organic ligand with a comparable size to that of the metal core. Here, we controlled the overall shape of ligand-protected gold clusters (AuCs) using a rigid, planar molecule as a ligand by following a simple geometrical relationship between an inscribed sphere and a circumscribed polyhedron.

For the rigid, planar molecule, we synthesized a new porphyrin derivative that could strongly attach to the AuCs in a face-coordination fashion (Figure 2a). We synthesized AuCs face-coordinated by four $ZnSC_2P$-SS ligands with a core size of 1.0±0.2 nm. Structural assignment using MALDI-TOF MS, ICP-AES, and UV-vis-NIR absorption spectra indicated that the $ZnSC_2P$-SS/AuCs have a pseudo-tetrahedral shape (Figure 2b). Thus, we have demonstrated that a simple geometrical relationship between an inscribed sphere and a circumscribed polyhedron can be applied to control the shape (symmetry) of metal clusters with a size of less than 2 nm. The present results pave the way to a new concept for controlling the pseudo-symmetry of ligand-protected metal clusters.

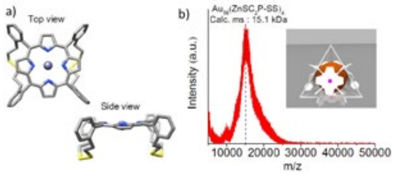


Figure 2. (a) single X-ray crystal structures of SC_2P and $ZnSC_2P$-SS from top view and side view. Hydrogen atoms have been omitted for clarity. (b) MALDI-TOF spectrum of $ZnSC_2P$-SS/AuCs. Insert is schematic illustration of the $ZnSC_2P$-SS/AuCs with pseudo-tetrahedron shape.

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Scope of Research

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

KEYWORDS
Precision Polymerization
Hybrid Materials
Living Radical Polymerization
Biointerface
Polymer Brush

Selected Publications

Tsujii, Y.; Nomura, Y.; Okayasu, K.; Gao, W.; Ohno, K.; Fukuda, T., AFM Studies on Microtribology of Concentrated Polymer Brushes in Solvents, *J. Phys.: Conf. Ser.*, **184,** 012031 (2009).
Arita, T.; Kayama, Y.; Ohno, K.; Tsujii, Y.; Fukuda, T., High-Pressure Atom Transfer Radical Polymerization of Methyl Methacrylate for Well-Defined Ultrahigh Molecular-Weight Polymers, *Polymer*, **49,** 2426-2429 (2008).
Tsujii, Y.; Ohno, K.; Yamamoto, S.; Goto, A.; Fukuda, T., Structure and Properties of High-Density Polymer Brushes Prepared by Surface-Initiated Living Radical Polymerization, *Adv. Polym. Sci.*, **197,** 1-45 (2006).
Ohno, K.; Morinaga, T.; Takeno, S.; Tsujii, Y.; Fukuda, T., Suspension of Silica Particles Grafted with Concentrated Polymer Brush: Effects of Graft Chain Length on Brush Layer Thickness and Colloidal Crystallization, *Macromolecules*, **40,** 9143-9150 (2007).
Ohno, K.; Morinaga, T.; Koh, K.; Tsujii, Y.; Fukuda, T., Synthesis of Monodisperse Silica Particles Coated with Well-Defined, High-Density Polymer Brushes by Surface-Initiated Atom Transfer Radical Polymerization, *Macromolecules*, **38,** 2137-2147 (2005).

Structure Analysis of Composite Membranes of Polymer-brush-afforded Nanoparticles and Ionic Liquid

Previously, we succeeded in fabricating a solid membrane of high ionic conductivity using self-assembled nanoparticles with CPBs in an ionic liquid (IL) and in developing a novel bipolar-type 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-dense segmental density in a solvent. In this study, we achieved in analyzing the higher-order structure of the composite membranes using concentrated ionic liquid-type polymer brush-modified nanoparticles (PSiP) and IL by ultra-small angle X-ray scattering (USAXS). The results showed that the higher-order structure of PSiP/IL composites changed from disorder to random hexagonal-closed-packing (rhcp), and face-centered-cubic (fcc) as the concentration of PSiP increased. As concentrated polymer brushes have unique properties such as high elasticity in a good solvent, it can be concluded that these results are applied to the model for particle assemblies with high-elasticity.

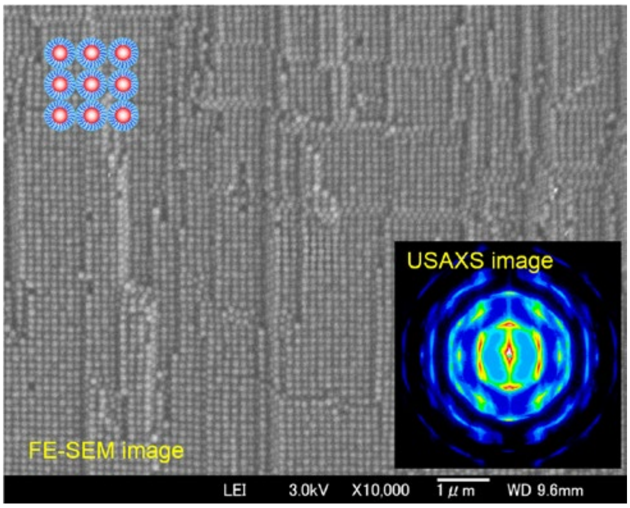

Figure 1. USAXS and FE-SEM images of composite membranes of concentrated ionic liquid-type polymer brush-modified nanoparticles and ionic liquid.

Surface Engineering of Cellulose Nanofiber by Adsorption of Diblock Copolymer Dispersant for Green Nanocomposite Materials

An effective approach for the dispersion of hydrophilic cellulose nanofiber (CNF) in hydrophobic high-density polyethylene (HDPE) is presented using adsorption of a diblock copolymer dispersant. The dispersant consists of both resin compatible poly(lauryl methacrylate) (PLMA) and cellulose interactive poly(2-hydroxyethyl methacrylate) blocks. The PLMA-adsorbed CNFs are characterized by FT-IR and contact angle measurement, revealing successful hydrophobization. X-ray CT imaging shows there are apparently less CNF aggregates in the nanocomposites if adding amount of the dispersant was enough. The good dispersion results in a high mechanical reinforcement, corresponding to 140 % higher Young's modulus and 84 % higher tensile strength than the neat HDPE. This study represents a potential approach to mediate CNF-CNF and CNF-resin interactions and to influence the CNF dispersion significantly without chemical functionalization, which may be compatible with a low-cost and environmentally green process and therefore an industrial application. Based on this concept, simultaneous nano-fibrillation compounding (SFC) process has been developed.

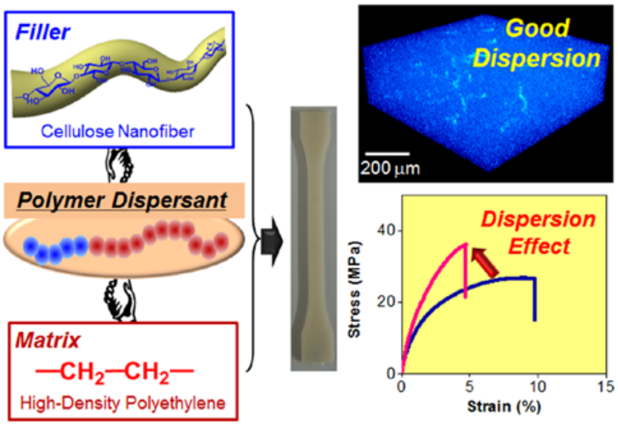

Figure 2. X-ray CT image and strain-stress curve of CNF-reinforced HDPE nanocomposite materials.

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Scope of Research

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

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

Selected Publications

Fan, W.; Nakamura, Y.; Yamago, S., Synthesis of Multivalent Organotellurium Chain Transfer Agents by Post-modification and Their Applications in Living Radical Polymerization, *Chem. Eur. J.*, **22,** 17006-17010 (2016).

Nakamura, Y.; Lee, R.; Coote, M.; Yamago, S., Termination Mechanism of the Radical Polymerization of Acrylates: Elucidation of the Reactivity of Polymer-end and Mid-chain Radicals, *Macromol. Rapid Commun.*, **37,** 506-513 (2016).

Kayahara, E.; Patel, V. K.; Mercier, A.; Kündig, E. P.; Yamago, S., Regioselective Synthesis and Characterization of Multinuclear Convex-bounded Ruthenium-[n]Cycloparaphenylene (n = 5 and 6) Complexes, *Angew. Chem. Int. Ed.*, **55,** 302-306 (2016).

Kayahara, E.; Fukayama, K.; Nishinaga, T.; Yamago, S., Size Dependence of [N]Cycloparaphenylenes (N = 5-12) in Electrochemical Oxidation, *Chem. Asian J.*, **11,** 1793-1797 (2016).

Kayahara, E.; Kouyama, T.; Kato, T.; Yamago, S., Synthesis and Characterization of [*n*]CPP (*n* = 5, 6, 8, 10, and 12) Radical Cation and Dications: Size-Dependent Absorption, Spin, and Charge Delocalization, *J. Am. Chem. Soc.*, **138,** 338-344 (2016).

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

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

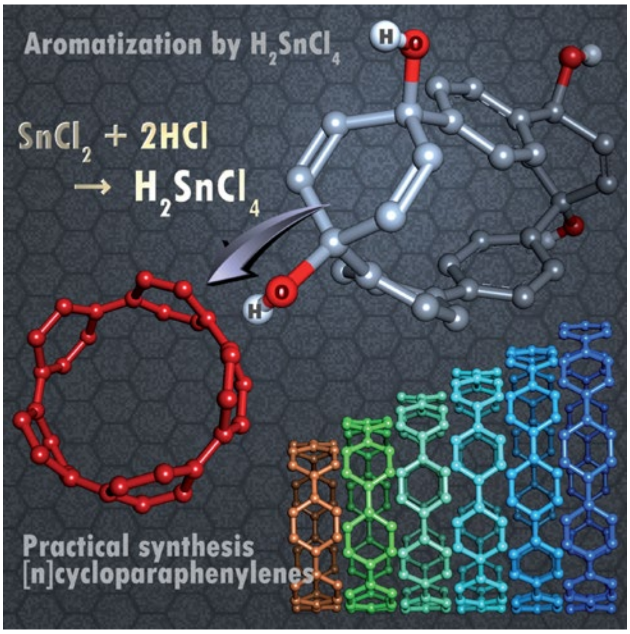
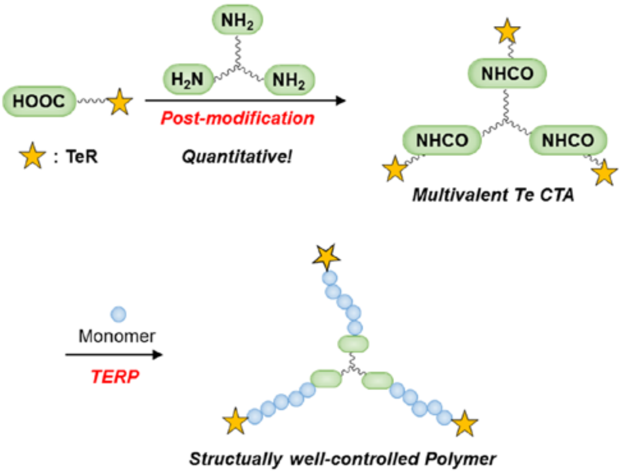


Figure 1. Synthesis of [*n*]Cycloparaphenylenes (*n* = 5, 7–12).

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

Multivalent or functionalized organotellurium chain-transfer agents (CTAs) for living radical polymerization were synthesized by post-modification. The synthesis involving the condensation between a carboxylic-acid-functionalized CTA and various amines proceeded in excellent yields without affecting the reactive tellurium moiety. The CTAs exhibited high synthetic versatility for radical polymerization and gave structurally well-controlled polymers, such as multiarmed polymers, from various monomers. Because all new CTAs are easily available on a large scale by simple purification, the current method significantly facilitates macromolecular engineering based on organotellurium-mediated radical polymerization (TERP).



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Scope of Research

NV center in diamond has been extensively interested because the single spin of it can be manipulated and detected at room temperature. Furthermore, spin coherence time of the NV center is very long. The coherence time is the time to retain coherence (superposition state) and directly relates to the sensitivity of sensor of magnetic field, electric field and temperature. Therefore, the unique and excellent properties of the NV center are expected to be applied for quantum computing, quantum communication, bio-imaging, and high-sensitive sensor with nano-scale resolution.

KEYWORDS

Diamond
Quantum Materials
NV Center
Quantum Sensing
Quantum Information Science

Selected Publications

Fukui, T.; Doi, Y.; Miyazaki, T.; Miyamoto, R.; Kato, H.; Matsumoto, T.; Makino, T.; Yamasaki, S.; Morimoto, R.; Tokuda, N.; Hatano, M.; Sakagawa, Y.; Morishita, H.; Tashima, T.; Miwa, S.; Suzuki, Y.; Mizuochi, N., Perfect Selective Alignment of Nitrogen-vacancy Center in Diamond, *Appl. Phys. Express*, **7,** 055201 (2014).

Doi, Y.; Makino, T.; Kato, H.; Takeuchi, D.; Ogura, M.; Okushi, H.; Morishita, H.; Tashima, T.; Miwa, S.; Yamasaki, S.; Wrachtrup, J.; Suzuki, Y.; Mizuochi, N., Deterministic Electrical Charge State Initialization of Single Nitrogen-vacancy Center in Diamond, *Phys. Rev. X*, **4,** 011057 (2014).

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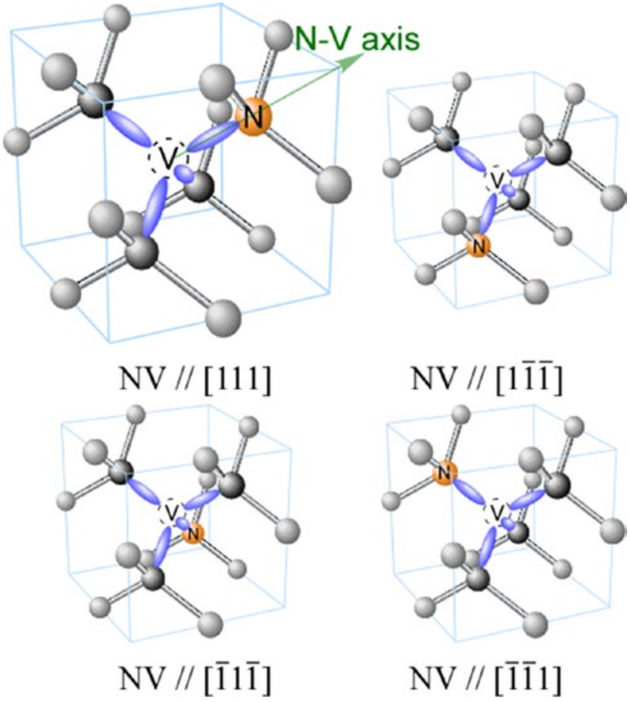
Neumann, P.; Mizuochi, N.; Rempp, F.; Hemmer, P.; Watanabe, H.; Yamasaki, S.; Jacques, V.; Gaebel, T.; Jelezko, F.; Wrachtrup, J., Multipartite Entanglement Among Single Spins in Diamond, *Science*, **320,** 1326 (2008).

Perfect Selective Alignment of Nitrogen-vacancy Center in Diamond

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



NV // [111] NV // $[1\bar{1}\bar{1}]$

NV // $[\bar{1}1\bar{1}]$ NV // $[\bar{1}\bar{1}1]$

Figure 1. Four possible orientations of NV centers in diamond crystal.

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

Pure Negatively Charged State of NV Center in n-type Diamond

For the applications of NV center, controlling the charge state is crucial, because optical initialization and readout of the spin state of the NV centers are only possible in negatively charged one (NV^-). However, upon illumination, the NV centers undergo stochastic charge-state transitions between NV^- and a dark state of a neutral charge state of the NV center (NV^0) as shown in Fig. 2. For example, upon excitation around 580 nm, where NV^- has the highest absorption, NV^- easily turns into the dark state of NV^0 and the steady-state-population of NV^- decreases to about 10%, which could be revealed from single-shot charge-state measurements. Therefore, illumination at 532 nm is usually used in the experiment of NV^-. This charge-state interconversion occurs upon illumination at any wavelength, so the steady-state NV^- population is always less than 75%–80%. We experimentally showed Fermi level control by phosphorus doping generates 99.4 ± 0.1% NV^- under 1 μW and 593 nm excitation which is close to maximum absorption of NV^-. The pure NV^- shows a five-fold increase of luminescence and a four-fold enhancement of an optically detected magnetic resonance under 593 nm excitation compared with those in intrinsic diamond. These results are expected to significantly enhance the versatile potential of NV centers.

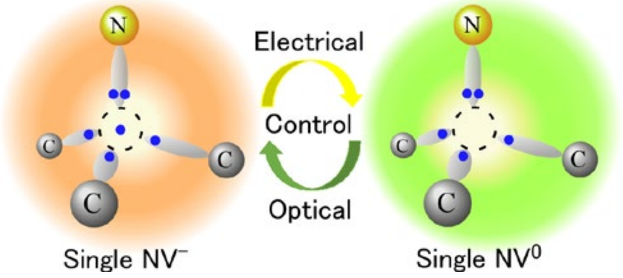


Figure 2. Stochastic charge-state transitions between NV^- and a dark state of a neutral charge state of the NV center.

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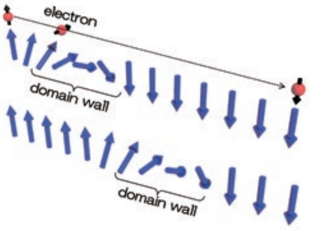
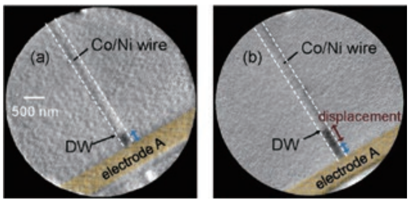
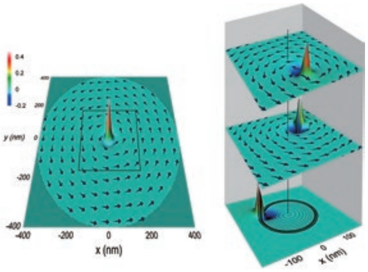
Scope of Research

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

KEYWORDS
Spintronics
Quantum Transport
Nano-fabrication
Artificial Materials







Selected Publications

Moriyama, T.; Takei, S.; Nagata, M.; Yoshimura, Y.; Matsuzaki, N.; Terashima, T.; Tserkovnyak, Y.; Ono, T., Anti-damping Spin Transfer Torque through Epitaxial Nickel Oxide, *Appl. Phys. Lett.*, **16,** 162406 (2015).

Yoshimura, Y.; Kim, K.-J.; Taniguchi, T.; Tono, T.; Ueda, K.; Hiramatsu, R.; Moriyama, T.; Yamada, K.; Nakatani, Y.; Ono, T., Soliton-like Magnetic Domain Wall Motion Induced by the Interfacial Dzyaloshinskii-Moriya Interaction, *Nat. Phys.*, **12,** 157-161 (2016).

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

Stigloher, J.; Decker, M.; Korner, H. S.; Tanabe, K.; Moriyama, T.; Taniguchi, T.; Hata, H.; Madami, M.; Gubbiotti, G.; Kobayashi, K.; Ono, T.; Back, C. H., Snell's Law for Spin Waves, *Phys. Rev. Lett.*, **117,** 037204 (2016).

Ando, F.; Kakizakai, H.; Koyama, T.; Yamada, K.; Kawaguchi, M.; Kim, S.; Kim, K.-J.; Moriyama, T.; Chiba, D.; Ono, T., Modulation of the Magnetic Domain Size Induced by an Electric Field, *Appl. Phys. Lett.*, **109,** 022401 (2016).

Modulation of the Magnetic Domain Size Induced by an Electric Field

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

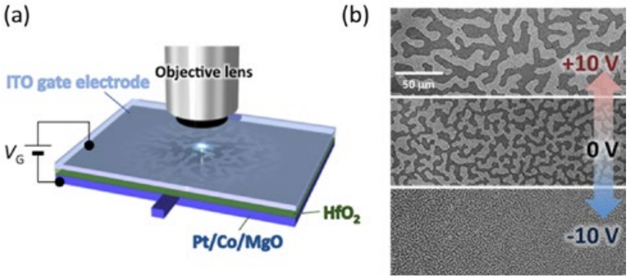


Figure 1. (a) Schematic illustration of the experimental setup (b) Modulation of the magnetic domain size with the electric field of ±10V.

Anti-damping Spin Transfer Torque through Antiferromagnetic Material

Spin transfer torque (STT) has been an efficient and promising technique to control magnetization of ferromagnetic materials in modern spintronic devices. This novel technique is based on an interaction between electron spin and local magnetic moments. The same interaction should be conserved in antiferromagnets in which there are microscopic local magnetic moments that compensate each other to exhibit no net magnetization. In this work, we prepared MgO(001) substrate / Pt 5 nm / NiO 10 nm / FeNi 3 nm / SiO_2 5 nm multilayers, in which the films are epitaxially grown until the NiO layer, and performed a spin torque ferromagnetic resonance (ST-FMR) measurement to quantify the anti-damping spin torque transported between the Pt and the FeNi through the antiferromagnetic NiO layer. A pure spin current is created by the spin Hall effect of the Pt and injected into the NiO. As shown in Figure 2(a), we found that the FMR linewidth monotonously varies with the spin current injection. As the ST-FMR measurement is only sensitive to the linewidth (i.e., magnetic damping) of the FeNi layer, this change in the linewidth in Pt/NiO/FeNi can be interpreted in a way that the spin current is transferred through the NiO and interacts with the FeNi. This intriguing spin current transport can be explained by the angular-momentum transfer mediated by the antiferromagnetic magnons as shown in Figure 2(b). Our results assure that the spin current exerts a spin torque on the NiO magnetic moments and excites their dynamics. The results open up a new field of antiferromagnetic spintronics.

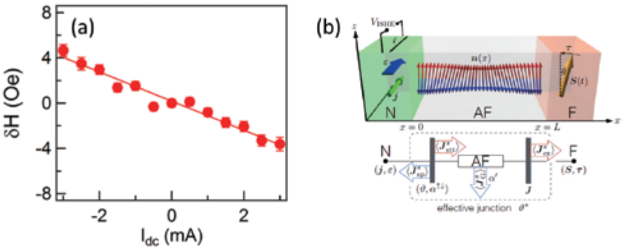


Figure 2. (a) FMR linewidth *δH* as a function of the dc current. Due to the spin Hall effect of Pt, the spin current injection is proportional to the dc current. (b) Schematic illustration of the N (Pt) / AF (NiO) / F (FeNi) structure in which the anti-damping spin transfer torque takes place. N (Pt)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

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Scope of Research

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

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

Selected Publications

Kawaguchi, Y.; Takeuchi, T.; Kuwata, K.; Chiba, J.; Hatanaka, Y.; Nakase, I.; Futaki, S., Syndecan-4 Is a Receptor for Clathrin-Mediated Endocytosis of Arginine-Rich Cell-Penetrating Peptides, *Bioconjug. Chem.*, **27,** 1119-1130 (2016).

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Azuma, Y.; Kükenshöner, T.; Ma, G.; Yasunaga, J.; Imanishi, M.; Tanaka, G.; Nakase, I.; Maruno, T.; Kobayashi, Y.; Arndt, K. M.; Matsuoka, M.; Futaki, S., Controlling Leucine-Zipper Partner Recognition in Cells through Modification of a-g Interactions, *Chem. Commun.*, **50,** 6364-6367 (2014).

Use of Calmodulin EF-Hand Peptides as Ca^{2+} -Switchable Recognition Tags

Peptide motifs specifically recognizing each other are useful molecular tags to detect specific proteins and to control protein interactions. Calmodulin is a representative calcium-binding protein composed of four Ca^{2+}-binding motifs with a helix-loop-helix structure called EF-hands, in which two helices pack together at an angle of approximately 90 degrees. The two helices are separated by a calcium-binding loop region. Here, we revealed the potential of peptide segments derived from the third and fourth EF-hands (EF3 and EF4) to act as recognition tags. An analysis of the disulfide formation mode among cysteines inserted at the N- or C-terminus of these peptide segments suggested that EF3 and EF4 peptides form a heterodimer with a topology similar to that in the wild-type protein. Heterodimer formation was shown to be a function of the Ca^{2+} concentration, indicating that these structures can be used as Ca^{2+} -switchable recognition tags. Using this EF-tag system, membrane fusion of liposomes decorated with EF3 and EF4 peptides was successfully induced. Because the EF-tags have different modes of mutual recognition and dimer formation from conventional peptide tags, this system would be used as an orthogonal recognition system to conventional ones.

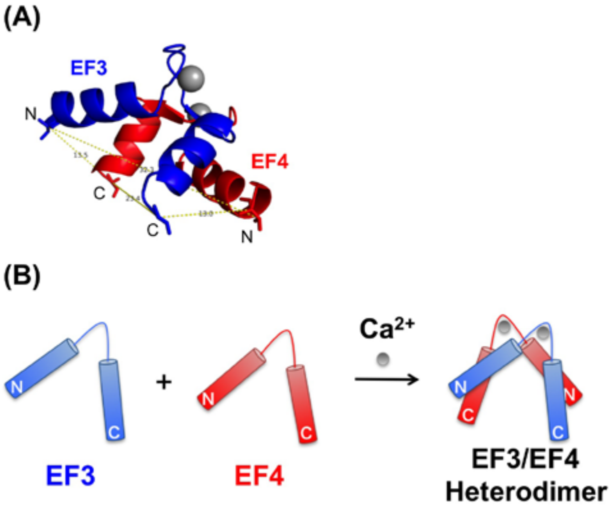

Figure 1. (A) A possible structure of EF3 and EF4 dimers in the presence of Ca^{2+}. (B) Schematic representation of complex formation by EF3 with EF4 dependent on Ca^{2+}.

Identifying Membrane Proteins Responsible for Cellular Uptake of Octaarginine by Photocrosslinking

Arginine-rich cell-penetrating peptides (CPPs) have been widely used as carriers for intracellular delivery of bioactive molecules. In spite of increasing evidence for involvement of endocytosis in the cellular uptake of arginine-rich CPPs, the primary cell-surface receptors for these peptide carriers that would initiate endocytic processes have remained unknown. Our previous effort to identify membrane receptors for octa-arginine (R8) peptide using the photo-cross-linking probe bearing a photoreactive diazirine was unsuccessful due to substantial amounts of cellular proteins nonspecifically bound to the affinity beads. To address this issue, here a photo-cross-linking probe was developed, in which a cleavable linker of a diazobenzene moiety was employed to selectively elute cross-linked proteins by reducing agent-mediated cleavage. It was demonstrated that introduction of the diazobenzene moiety into the photoaffinity probe results in efficient purification of cross-linked proteins with remarkable reduction of nonspecific binding proteins, leading to successful identification of 17 membrane-associated proteins that would interact with R8 peptide. Among the proteins identified, syndecan-4, one of the heparan sulfate proteoglycans, was revealed to be an endogenous membrane-associated receptor for the cellular uptake of R8 peptide via clathrin-mediated endocytosis. It was also clarified that the intracellular delivery of bioactive proteins mediated by R8 peptide this syndecan-4-dependent pathway was also involved in. These results reveal that syndecan-4 is a primary cell-surface target for R8 peptide that allows intracellular delivery of bioactive cargo molecules via clathrin-mediated endocytosis.

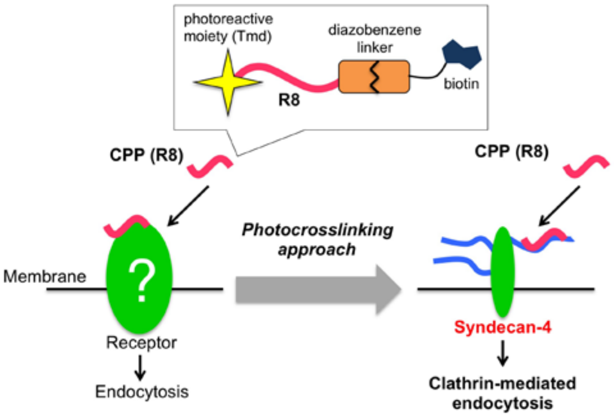

Figure 2. Identification of cell-surface receptors bound to R8 using photo-cross-linking reaction.

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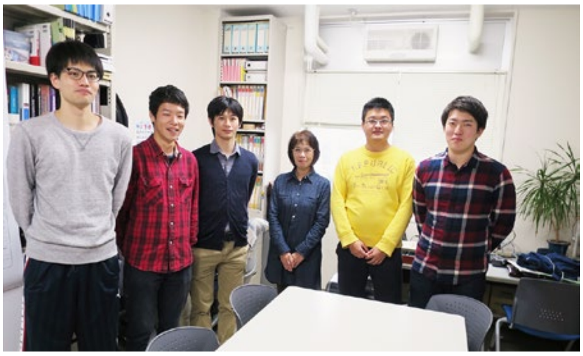
Scope of Research

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

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



Selected Publications

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

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

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

Hayashi, K.; Watanabe, B.; Nakagawa, Y.; Minami, S.; Morita, T., RPEL Proteins are the Molecular Targets for CCG-1423, an Inhibitor of Rho Signaling, *PLOS ONE*, **9,** [e89016-1]-[e89016-12] (2014).

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

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

Substrate-Analog Fructosyl Peptide Oxidase Inhibitors

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

Molecular Mechanism of Myocardin-Related Transcription Factor A Inhibitors

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

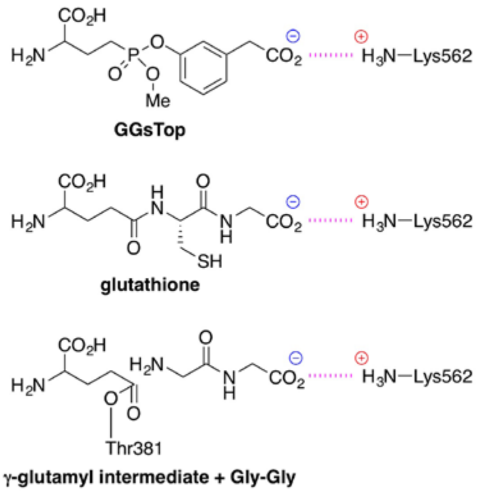

Figure 1. Proposed binding mode of GGsTop, glutathione, and acceptor substrate (Gly-Gly) to Lys562.

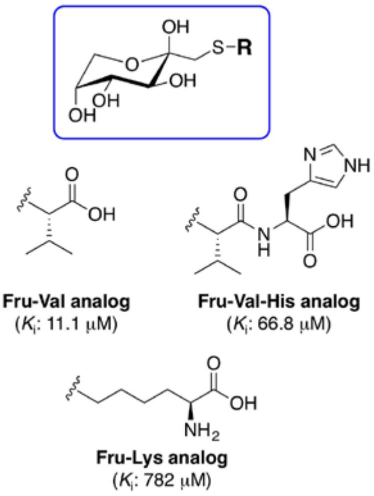

Figure 2. Chemical structures and inhibitory activity of FPOX inhibitors.

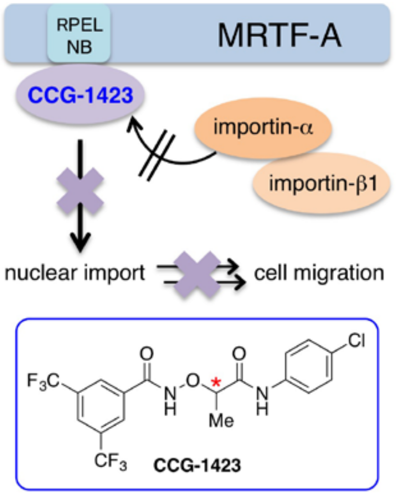

Figure 3. Molecular mechanism of MRTF-A inhibitor CCG-1423.

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Guest Res Assoc

LIN, Xiaoya	Peking University, China, P.R., 16 September–15 December

Scope of Research

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

KEYWORDS

Morphogenesis
Phospholipid Signaling
RNA
Signal Transduction
COP9 Signalosome

Selected Publications

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

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

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

Kato, M.; Aoyama, T.; Maeshima, M., The 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).

Genetic Analysis of RNA-Binding Protein Genes in *Arabidopsis thaliana*

Some classes of RNA binding proteins (RBPs) play pivotal roles in regulating gene expression, both co-transcriptionally and post-transcriptionally. The *Arabidopsis thaliana* genome encodes more than 600 putative RBPs, but the detailed functions of the vast majority of these RBPs remain unclear. Serine/arginine-rich (SR) proteins belong to a group of RBPs. Among the 19 SR proteins in *Arabidopsis*, only a few have been studied functionally. Gain-of-function analyses of SR protein genes RS2Z33 and SR30, as well as loss-of-function analyses of SR45, SCL33, SCL33a, RS40, and RS41, have revealed that the proteins encoded by these genes regulate alternative splicing of their own pre-mRNA and that of other SR genes. Glycine-rich RNA binding proteins (GRPs), a small group of plant RBPs, contain an N-terminal RRM domain and a C-terminal glycine-rich stretch. GRPs in *Arabidopsis* include GRP1-8 and RZ-1A-C (Fig 1). GRP7 and GRP8 are important regulators of circadian oscillations, flowering time, responses to plant pathogens, and cold stress. RZ-1A-C has a zinc finger motif between the RRM domain and C terminus. RZ-1, which was first reported in the tobacco, belongs to a subgroup of GRPs and binds to a large ribonucleoprotein particle localized in the nucleus. Homologs of RZ-1 in *Arabidopsis* were shown to have RNA chaperone activity in *Escherichia coli*. Overexpression of RZ-1A, but not homologous genes RZ-1B and RZ-1C, confers freezing tolerance in transgenic *Arabidopsis*. However, there is no direct genetic evidence to support the apparently important roles of these GRPs in plant growth and development and in responses to environmental stimuli.

In this study, we provide functional evidence that *Arabidopsis* RZ-1B and RZ-1C represent a unique group of GRPs. rz-1b rz-1c double mutants displayed a wide variety of defects, including delayed germination, retarded development of root and shoot meristems, late flowering, reduced stature, and serrated leaves (Fig 2). RZ-1B and RZ-1C interact with SR proteins through their C-terminal domains, which are also essential for nuclear speckle localization. High-throughput RNA-seq analysis of rz-1b rz-1c double mutants revealed perturbation of the splicing of many genes. Defective splicing was also observed in plants overexpressing the C-terminal domain of RZ-1C, confirming that RZ-1B/1C regulates splicing via interaction with SR proteins. RZ-1B and RZ-1C were found to be required for maintaining the optimal expression levels of more than 3000 genes, including many developmental regulators. Taken together, these findings reveal the essential roles of RZ-1B and RZ-1C as regulators of plant development, splicing, and general gene expression via interaction with proteins including SR proteins.

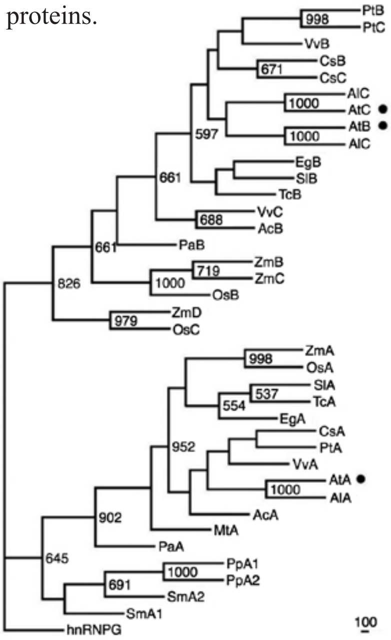

Figure 1. Phylogenetic tree of At RZ-1-related proteins from different plant species.
The tree consists of two large clades. The number at each node indicates the bootstrap value (1000 replicates). Three At RZ-1 proteins are marked with black circles. At A, At B, and At C refer to At RZ-1A, At RZ-1B, and At RZ-1C, respectively.

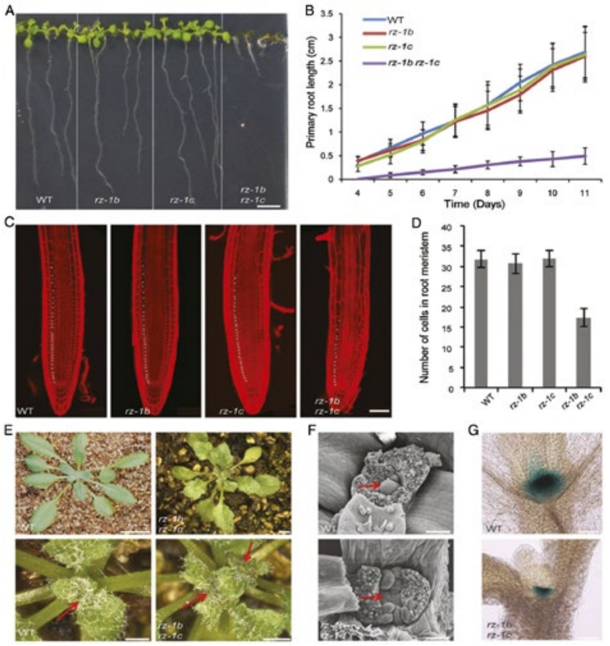

Figure 2. Pleotropic Defects of the rz-1b rz-1c Double Mutant.
(A) Image of seedlings grown vertically for 10 d after germination. Bar = 0.5 cm. (B) Statistics of the primary root length from day 4 to day 11 after germination. Error bars represent SD (n = 20). (C) Confocal image of root meristems from different genotypes. The image shows the representative root meristems from seedlings at 4 d after germination. The roots were stained with propidium iodide. Asterisks indicate the dividing cells in the endodermis. Bar = 50 mm. (D) Statistics of endodermal cells from different genotypes within the meristematic regions. Error bars represent SD (n = 15). (E) rz-1b rz-1c generates multiple SAMs during vegetative growth. The images show wild-type and rz-1b rz-1c seedlings 3 weeks after germination. The lower panels show magnified images of the upper panels. Arrows indicate the positions of SAMs. Bars = 5 mm (upper panel) and 1 mm (lower panel). (F) Scanning electron microscopy images of the SAMs of the wild type and rz-1b rz-1c. Arrows indicate the SAM in the wild type and the corresponding region in rz-1b rz-1c. Bar = 50 mm. (G) Histochemical staining of CLAVATA3:GUS reporter in wild-type and rz-1b rz-1c backgrounds. Bar = 80 mm.

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Scope of Research

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

KEYWORDS
Cell Therapy
Chemical Biology
Small Molecules
Chemical Library
Chemical Genetics

Selected Publications

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

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

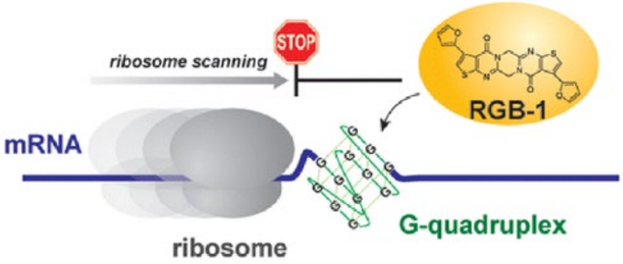
Parvatkar, P.; Kato, N.; Uesugi, M.; Sato, S.; Ohkanda, J., Intracellular Generation of a Diterpene-Peptide Conjugate that Inhibits 14-3-3-Mediated Interactions, *J. Am. Chem. Soc.*, **137,** 15624-15627 (2015).

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

Topics

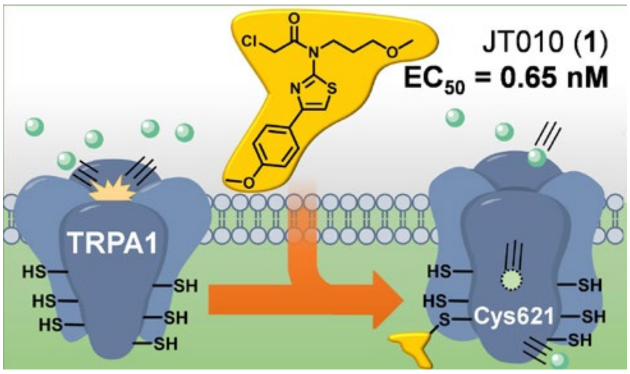
A Small Molecule That Represses Translation of G-Quadruplex-Containing mRNA

The G-quadruplexes form highly stable nucleic acid structures, which are implicated in various biological processes in both DNA and RNA. Although DNA G-quadruplexes have been studied in great detail, biological roles of RNA G-quadruplexes have received less attention. In this study, a screening of a chemical library permitted identification of a small-molecule tool that binds selectively to RNA G-quadruplex structures. The polyaromatic molecule, RGB-1, stabilizes RNA G-quadruplex, but not DNA versions or other RNA structures. RGB-1 intensified the G-quadruplex-mediated inhibition of RNA translation in mammalian cells, decreased expression of the NRAS proto-oncogene in breast cancer cells, and permitted identification of a novel sequence that forms G-quadruplex in NRAS mRNA. RGB-1 may serve as a unique tool for understanding cellular roles of RNA G-quadruplex structures.



A Potent and Site-Selective Agonist of TRPA1

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



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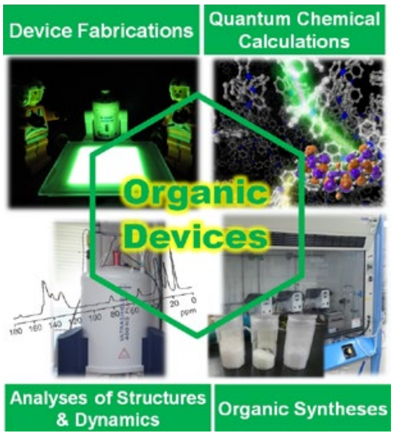
Scope of Research

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

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



Selected Publications

Uratani, H.; Kubo, S.; Shizu, K.; Suzuki, F.; Fukushima, T.; Kaji, H., Detailed Analysis of Charge Transport in Amorphous Organic Thin Layer by Multiscale Simulation without Any Adjustable Parameters, *Sci. Rep.*, **6,** 39128 (2016).

Shizu, K.; Kaji, H., Organic Electroluminescent Materials Realizing Efficient Conversion from Electricity to Light, *J. Photopolym. Sci. Technol.*, **29,** 305-310 (2016).

Nishimura, H.; Fukushima, T.; Wakamiya, A.; Murata, Y.; Kaji, H., The Influence of Quasiplanar Structures of Partially Oxygen-Bridged Triphenylamine Dimers on the Properties of Their Bulk Films, *Bull. Chem. Soc. Jpn.*, **89,** 726-732 (2016).

Hayase, G.; Nonomura, K.; Kanamori, K.; Maeno, A.; Kaji, H.; Nakanishi, K., Boehmite Nanofiber-Polymethylsilsesquioxane Core-Shell Porous Monoliths for a Thermal Insulator under Low Vacuum Conditions, *Chem. Mater.*, **28,** 3237-3240 (2016).

Wada, Y.; Shizu, K.; Kubo, S.; Fukushima, T.; Miwa, T.; Tanaka, H.; Adachi, C.; Kaji, H., Highly Efficient Solution-Processed Host-Free Organic Light-Emitting Diodes Showing an External Quantum Efficiency of Nearly 18% with a Thermally Activated Delayed Fluorescence Emitter, *Appl. Phys. Express*, **9,** 032102-1-032102-3 (2016).

Hayase, G.; Kanamori, K.; Maeno, A.; Kaji, H.; Nakanishi, K., Dynamic Spring-Back Behavior in Evaporative Drying of Polymethylsilsesquioxane Monolithic Gels for Low-Density Transparent Thermal Superinsulators, *J. Non-Cryst. Solids*, **434,** 115-119 (2016).

Highly Efficient Solution-processed Host-free Organic Light-emitting Diodes using a Thermally Activated Delayed Fluorescence Emitter

Organic light-emitting diodes (OLEDs) have attracted great interest as a promising technique for developing solid-state lighting source and flexible flat-panel displays. To date, vacuum vapor deposition has been widely used to fabricate OLEDs. However, it has drawbacks, including high production cost and difficulty in fabricating multi-dopant OLEDs. Solution processing is an alternative method to vacuum vapor deposition for fabricating OLEDs. It has an advantage of lowering the production cost and realizing large-area high-resolution displays. An emitting layer of an OLED is generally a doped film composed of an emitting dopant and a host material. To realize a high-performance OLED, the host material is required to have high excited-state energies, ambipolar transport properties, and suitable HOMO and LUMO energy levels. Host-free OLEDs contain a neat film as an emissive layer (that is, the emissive layer consists of an emitting material alone), which can remove the limitations of host materials. In this study, using a spin-coated neat film of a thermally activated delayed fluorescence emitter (DMAC-TRZ) as an emissive layer, we fabricated a solution-processed OLED. The OLED exhibited a maximum external quantum efficiency (EQE) of 17.6% (Figure 1), which is the highest value obtained for solution-processed host-free OLEDs, including phosphorescent systems. By further optimizing the device structure, we achieved an EQE of 16.8% at high luminance.

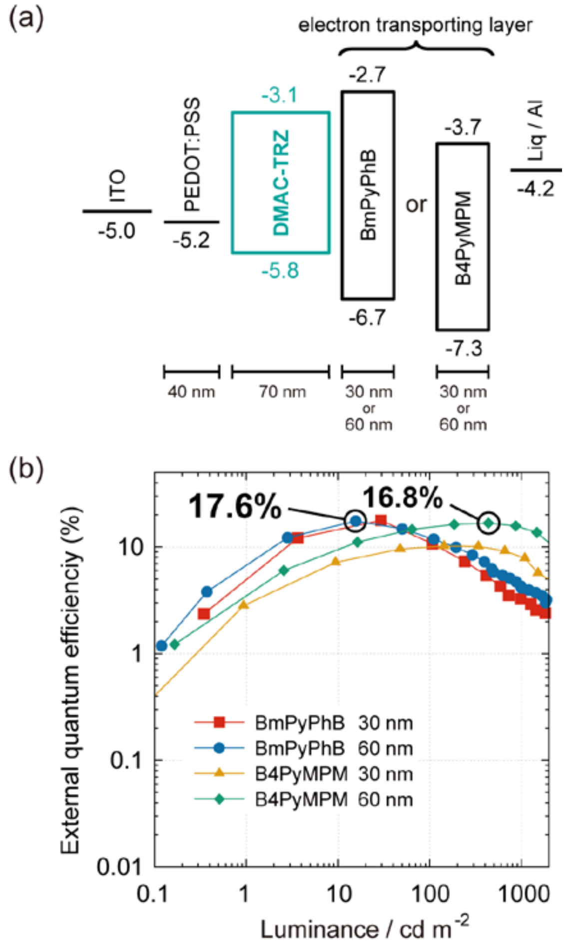


Figure 1. (a) Energy diagram of solution-processed host-free OLEDs containing DMAC-TRZ as an emitter. (b) Luminance–EQE characteristics of the solution-processed host-free OLEDs.

Charge Transport Simulations in Amorphous Thin Films for OLEDs

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

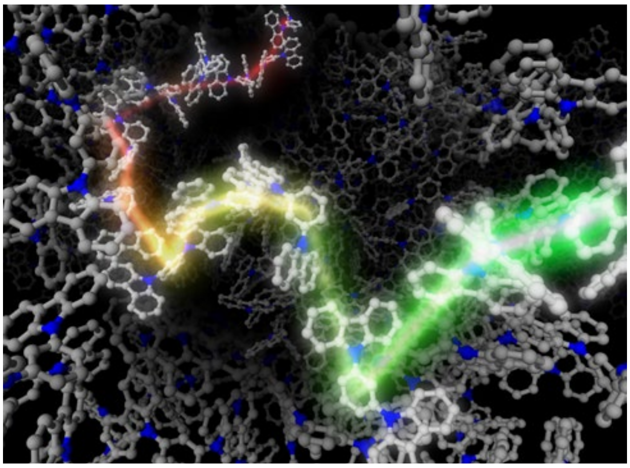


Figure 2. Image of charge transport in amorphous mCP films.

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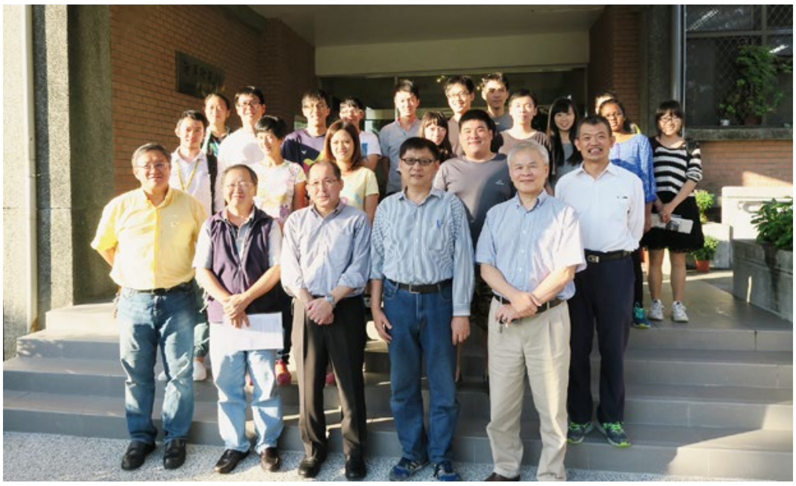
Scope of Research

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



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

Selected Publications

Nakashima, Y.; Shimizu, A.; Maruo, M.; Sohrin, Y., Trace Elements Influenced by Environmental Changes in Lake Biwa: (I) Seasonal Variations under Suboxic Hypolimnion Conditions during 2007 and 2009, *Limnol.*, **17,** 151-162 (2016).
Sohrin, Y.; Nakashima, Y.; Maruo, M., Trace Elements Influenced by Environmental Changes in Lake Biwa: (II) Chemical Variations in the Hypolimnion over the Last Half-century, *Limnol.*, **17,** 163-173 (2016).
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Takano, S.; Tanimizu, M.; Hirata, T.; Sohrin, Y., Isotopic Constraints on Biogeochemical Cycling of Copper in the Ocean, *Nat. Commun.*, **5,** [5663-1]-[5663-7] (2015).
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Firdaus, M. L.; Minami, T.; Norisuye, K.; Sohrin, Y., Strong Elemental Fractionation of Zr-Hf and Nb-Ta across the Pacific Ocean, *Nature Geosci.*, **4,** 227-230 (2011).

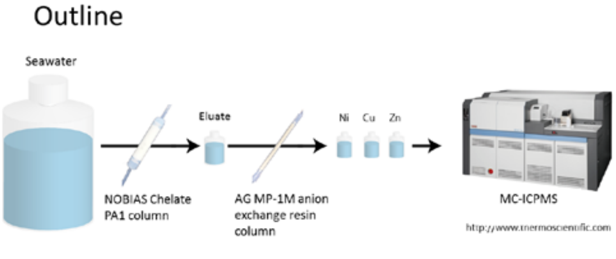
Stoichiometry of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb in Seawater around the Juan de Fuca Ridge

We have studied the distributions of Al, Mn, Fe, Co, Ni, Cu, Zn, Cd, and Pb around the Juan de Fuca Ridge (JdFR) in total dissolvable (td), dissolved (d), and labile particulate (lp) fractions, which represent a fraction in unfiltered samples, filtered samples through an AcroPak capsule filter, and the difference between td and d, respectively. Al and Fe were dominated by lp-species, while Ni, Zn, and Cd were dominated by d-species with undetectable amounts of lp-species. Major findings in this study are as follows: (i) The continental margin (CM) provided large sources of Al, Mn, Fe, and Co from the surface to ~2000 m in depth. The supply from CM caused high surface concentrations of dMn and dCo, a subsurface (100–300 m depth) maximum of dCo, and intermediate (500–2000 m depth) maxima of lpAl and lpFe. The supply of dFe from CM was ~10 times that from the high-temperature hydrothermal activity at station BD21, which is located at ~3 km from the Middle Valley venting site and ~200 km from Vancouver Island. (ii) DPb was maximum at the top layer of North Pacific Intermediate Water, probably owing to isopycnal transport of anthropogenic Pb via advection of subducted surface waters. Although dCo and dPb had different sources in the upper water, they showed a strong linearity below 300 m ($r^2 = 0.95$, $n = 38$), indicating concurrent scavenging. (iii) A high-temperature hydrothermal plume occurred at a depth of 2300 m at BD21, accounting for maxima of dAl, dMn, dFe, lpCu, and lpPb and a minimum of dCu. (iv) Strong bottom maxima of lpAl, lpMn, lpFe, lpCo, and lpPb occurred above the abyssal plain at the western foot of the JdFR, indicating resuspension of sediments. However, bottom maxima of d-species were apparent only for dAl and dCu.

A Simple and Rapid Method for Isotopic Analysis of Nickel, Copper, and Zinc in Seawater Using Chelating Extraction and Anion Exchange

Stable isotope ratios of Ni, Cu, and Zn are powerful tools to elucidate biogeochemical cycling of the trace metals in the ocean. However, analytical difficulties have retarded development of isotopic study of these metals. Especially, isotopic analysis of seawater Ni is troublesome, because Ni is not retained on anion exchange resin and passed through the column with seawater matrix. We have developed a simple and rapid method for simultaneous analyses of Ni, Cu, and Zn isotope ratio in seawater using NOBIAS Chelate-PA1 resin and anion exchange resin. A NOBIAS Chelate-PA1 resin column quantitatively collected Ni, Cu, and Zn from seawater and effectively removed seawater matrix. Subsequent anion exchange purified Ni, Cu, and Zn from each other. The blanks of this method (0.22 ng for Ni, 0.29 ng for Cu, and 0.53 ng for Zn) were sufficiently low to determine isotope ratios of Ni, Cu, and Zn in surface seawater. Using this method, we analyzed GEOTRACES reference seawater samples, i.e., SAFe D1 and SAFe D2, and seawater samples collected from some depths in the subarctic North Pacific. The results were consistent with reported values.

Figure 1. Members of the Hakuho-Maru KH-12-4 cruise, during which samples for this work were collected.



Takano et al., (in preparation)

Figure 2. Outline of the analytical method.

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Scope of Research

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

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

Selected Publications

Wakai, C.; Shimoaka, T.; Hasegawa, T., Characterization of Adsorbed Molecular Water on the Surface of a Stretched Polytetrafluoroethylene Tape Analyzed by ^{1}H NMR, *J. Phys. Chem. B*, **120,** 2538-2543 (2016).

Shimoaka, T.; Tanaka, Y.; Shioya, N.; Morita, K.; Sonoyama, M.; Amii, H.; Takagi, T.; Kanamori, T.; Hasegawa, T., Surface Properties of a Single Perfluoroalkyl Group on Water Surfaces Studied by Surface Potential Measurements, *J. Colloid Interf. Sci.*, **483,** 353-359 (2016).

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Shimoaka, T.; Hasegawa, T., Molecular Structural Analysis of Hydrated Ethylene Glycol Accounting for the Antifreeze Effect by Using Infrared Attenuated Total Reflection Spectroscopy, *J. Mol. Liquids*, **223,** 621-627 (2016).

Iwasa, J.; Kumazawa, K.; Aoyama, K.; Suzuki, H.; Norimoto, S.; Shimoaka, T.; Hasegawa, T., In Situ Observation of a Self-Assembled Monolayer Formation of Octadecyltrimethoxysilane on a Silicon Oxide Surface Using a High-Speed Atomic Force Microscope, *J. Phys. Chem. C*, **120,** 2807-2813 (2016).

Characterization of Adsorbed Molecular Water on the Surface of a Stretched Polytetrafluoroethylene Tape Analyzed by ^{1}H NMR

A single molecule often exhibits a largely different material character from a bulk matter. Although a perfluoroalkyl (Rf) compound is a representative one, many interests have mostly been devoted to the bulk character only thus far, leaving the single molecular character unclear. Recently, a new theoretical framework, stratified dipole-arrays (SDA) theory, has appeared for comprehensive understanding of Rf compounds in terms of both single and bulk systems. On this theory, a mechanically stretched polytetrafluoroethylene (PTFE) is expected to exhibit a single-molecular character having dipole-driven properties, which should attract molecular water. In the present study, a stretched PTFE tape is revealed to attract molecular water (not water droplet) in fact, and the adsorbed water molecules are highly restricted in motion by the dipole−dipole interaction studied by using ^{1}H NMR, which agrees with the prediction by the SDA theory.

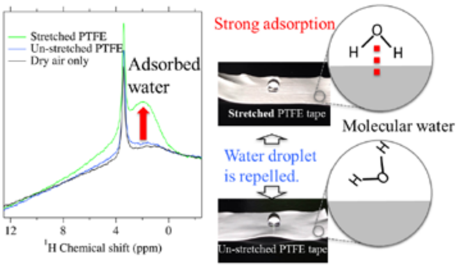

Figure 1. ^{1}H NMR spectra of strongly adsorbed molecular water on a stretched PTFE tape.

Surface Properties of a Single Perfluoroalkyl Group on Water Surfaces Studied by Surface Potential Measurements

A discriminative study of a single perfluoroalkyl (Rf) group from a bulk material is recently recognized to be necessary toward the total understanding of Rf compounds based on a primary chemical structure. The single molecule and the bulk matter have an interrelationship via an intrinsic two-dimensional (2D) aggregation property of an Rf group, which is theorized by the stratified dipole-arrays (SDA) theory. Since an Rf group has dipole moments along many C–F bonds, a single Rf group would possess a hydrophilic-like character on the surface. To reveal the hydration character of a single Rf group, in the present study, surface potential (ΔV) measurements are performed for Langmuir monolayers of Rf-containing compounds. From a comparative study with a monolayer of a normal hydrocarbon compound, the hydration/dehydration dynamics of a lying Rf group on water has first been monitored by ΔV measurements, through which a single Rf group has been revealed to have a unique “dipole-interactive” character, which enables the Rf group interacted with the water ‘surface.’ In addition, the SDA theory proves to be useful to predict the 2D aggregation property across the phase transition temperature of 19 °C by use of the ΔV measurements.

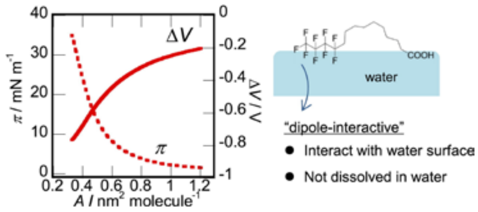

Figure 2. Schematic image of a dipole-interactive Rf group on the water surface and a fairly large negative surface potential.

Comprehensive Understanding of Structure-Controlling Factors of a Zinc Tetraphenylporphyrin Thin Film Using pMAIRS and GIXD Techniques

The performance of an organic electronic device is significantly influenced by the anisotropic molecular structure in the film, which has long been difficult to predict especially for a solution process. In the present study, a zinc tetraphenylporphyrin (ZnTPP) thin film prepared by a solution process was chosen to comprehensively explore the molecular-arrangement mechanism as a function of representative film-preparation parameters: solvent, film-preparation technique, and thermal annealing. The anisotropic structure was first analyzed by using a combination of infrared p-polarized multiple-angle incidence resolution spectrometry (pMAIRS) and grazing incidence X-ray diffraction (GIXD), which readily revealed the molecular orientation and crystal structure, respectively. As a result, the real dominant factor was found to be the evaporation time of the solvent that determines the initial two different molecular arrangements, types-I and -II, while the thermal annealing was found to play an additional role of improving the molecular order. The correlation between the molecular orientation and the crystal structure was also revealed through the individual orientation analysis of the porphyrin and phenyl rings.

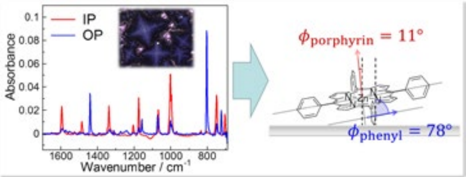

Figure 3. pMAIRS spectra of a ZnTPP thin film and a schematic image of the two conjugated rings on the surface.

Division of Environmental Chemistry
– Molecular Microbial Science –

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

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Scope of Research

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

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

Selected Publications

Ito, T.; Gong, C.; Kawamoto, J.; Kurihara, T., Development of a Versatile Method for Targeted Gene Deletion and Insertion by Using the *pyrF* Gene in the Psychrotrophic Bacterium, *Shwanella livingstonensis* Ac10, *J. Biosci. Bioeng.*, **122,** 645-651 (2016).
Ohke, Y.; Maruyama, S.; Tarui, J.; Wang, Y.; Kawamoto, J.; Kurihara, T., A Phosphoporin Homolog Plays a Critical Role in the Dissimilatory Iron-Respiration Linked to Iron (III) Reduction by a Cold-adapted Bacterium, *Shewanella livingstonensis* Ac10, *Trace Nutr. Res.*, **33,** 35-42 (2016).
Sugiura, M.; Park, J.; Kawamoto, J.; Esaki, N.; Kurihara, T., Regulatory Mechanism of Membrane Protein Production in an EPA-Producing Bacterium, *Shewanella livingstonensis* Ac10, *Trace Nutr. Res.*, **33,** 63-72 (2016).

Purification and Enzymatic Characterization of Bacterial 1-Acyl-*sn*-glycerol-3-phosphate Acyltransferase PlsC

A cold-adapted bacterium *Shewanella livingstonensis* Ac10 produces phospholipids esterified at the *sn*-2 position with eicosapentaenoic acid (EPA), which are important biomembrane components to survive in a cold environment. It is known that, in a bacterial *de novo* phospholipid synthesis, acylation at the *sn*-2 position is catalyzed by 1-acyl-*sn*-glycerol-3-phosphate acyltransferase PlsC. We previously carried out gene deletion experiments to find that the microbe has five PlsC homologs (PlsC1-5), among which PlsC1 is exclusively responsible for the production of the EPA-containing phospholipids. To gain further insights into the enzymatic properties of PlsC1, we attempted to purify and characterize the enzyme. After careful investigation of purification conditions, we finally succeeded in purifying PlsC1 in an active form and revealed its enzymatic features such as optimal reaction conditions and substrate specificity. It is notable that PlsC1 showed a higher activity toward unsaturated fatty acids including EPA than saturated ones. These findings will enable us to investigate a protein interaction network underlying the cold adaptation of *S. livingstonensis* Ac10 and to analyze as yet unidentified reaction mechanism of PlsC.

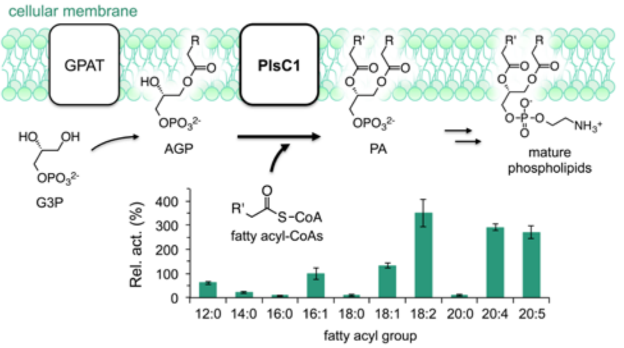

Figure 1. Schematic view of PlsC1-catalyzed reaction. PlsC1 showed a higher activity toward unsaturated fatty acids including EPA (20:5) and hexadecenoic acid (16:1) than saturated ones such as hexadecanoic acid (16:0). G3P, *sn*-glycerol 3-phosphate; AGP, 1-acyl-*sn*-glycerol 3-phosphate; PA, phosphatidic acid; GPAT, G3P acyltransferase.

Characterization of Membrane Vesicles Produced by *Shewanella* Species

It is known that most bacteria secrete membrane vesicles (MVs), which are composed of lipid membrane and contain nucleic acids, proteins and periplasmic solutes, to outer milieu. Though much attention has been paid to their physiological roles as well as the application to biotechnology, the molecular mechanism for MV secretion remains largely unknown. To better understand the mechanism, we characterized MVs from two cold-adapted *Shewanella* species. By using cryo-electron microscopy techniques, an EPA-producing bacterium *S. livingstonensis* Ac10 was shown to secrete MVs that mainly have a spherical single-bilayered structure with diameter of approximately 100 nm. Fatty acid profiling showed that specific fatty acids, e.g. hexadecanoic acid, are predominantly loaded onto MVs. Moreover, it was notable that the deletion of EPA biosynthetic genes altered the size and productivity of MVs. On the other hand, we found that *Shewanella* sp. HM13 secretes a much larger amount of MVs than *S. livingstonensis* Ac10. The MVs from this novel strain were found to include a single major protein. These features will be suitable for developing a new low-temperature protein production system where a protein of interest is concentrated in secreted MVs.

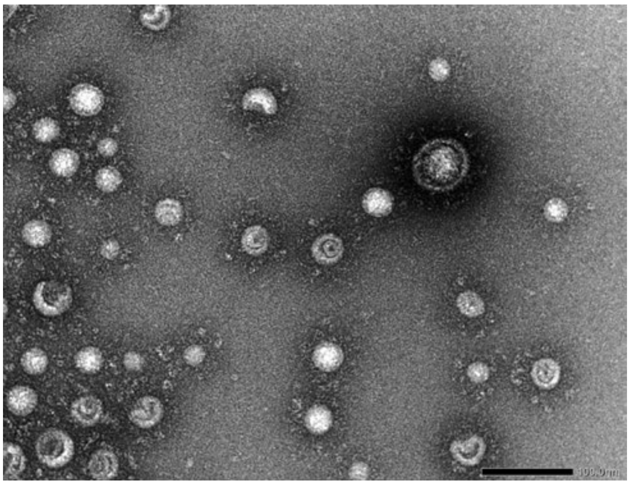

Figure 2. Electron microscopic image of MVs from *Shewanella* sp. HM13. The bar indicates 100 nm.

Division of Multidisciplinary Chemistry
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Scope of Research

The structure and molecular motion of polymer substances are studied, mainly using scattering methods such as X-ray, neutron, and light with intent to solve fundamentally important problems in polymer science. The main project are studied on 1) the morphologies and the dynamics of self-assembling processes in block copolymers, 2) the hierarchical structures in crystalline polymers, 3) the viscoelastic effects in glassy materials, 4) formation processes and structure of polymer gels, and 5) the structure ad molecular motion of polyelectrolyte solutions.

KEYWORDS
Polymer Physics
Polymer Properties
Self Assembly
Softmatter
Hierarchical Structure

Selected Publications

Wang, Y. C.; Kim, M. I.; Akasaka, S.; Saijo, K.; Hasegawa, H.; Hikima, T.; Takenaka, M., Fddd Structure in Polystyrene-block-polyisoprene Diblock Copolymer/Polystyrene Homopolymer Blends, *Macromolecules*, **49 (6),** 2257-2261 (2016).
Matsumoto, K.; Terashima, T.; Sugita, T.; Takenaka, M.; Sawamoto, M., Amphiphilic Random Copolymers with Hydrophobic/Hydrogen-Bonding Urea Pendants: Self-Folding Polymers in Aqueous and Organic Media, *Macromolecules*, **49 (20),** 7917-7927 (2016).
Ogawa, H.; Takenaka, M.; Miyazaki, T.; Fujiwara, A.; Lee, B.; Shimokita, K.; Nishibori, E.; Takata, M., Direct Observation on Spin-Coating Process of PS-*b*-P2VP Thin Films, *Macromolecules*, **49,** 3471-3477 (2016).
Ishige, R.; Ohta, N.; Ogawa, H.; Tokita, M.; Takahara, A., Fully Liquid-Crystalline ABA Triblock Copolymer of Fluorinated Side-Chain Liquid-Crystalline A Block and Main-Chain Liquid-Crystalline, B Block: Higher Order Structure in Bulk and Thin Film States, *Macromolecules*, **49,** 6061-6074 (2016).

Formation of OBDD Structure in PS-PI-PDMS

Ordered bicontinuous double-diamond morphology (OBDD) was formed in cast film of polystyrene-*block*-polyisoprene-*block*-polydimethylsiloxiane (SID) triblock copolymer from toluene solution. The following two step phase separation was found to occurs during solvent cast: In the early stage of the cast process, hexagonally-packed polydimethylsiloxiane (PDMS) cylinders were self-assembled in polystyrene (PS)/polyisoprene (PI) matrix order-order transition, then order-order transition was induced by microphase separation between PS and PI association with the increase of concentration.

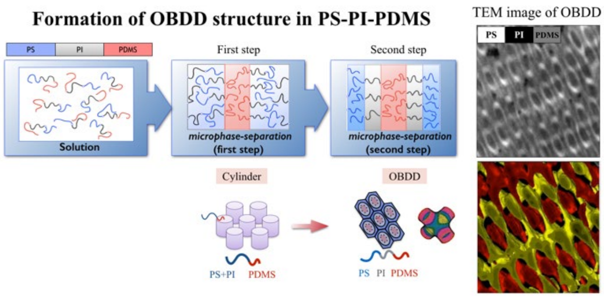

Figure 1. Formation of OBDD structure in PS-PI-PDMS.

Quasi-Equilibrium Gelation Temperature of Aqueous Methylcellulose

Aqueous methylcellulose (MC) forms hydrogel upon heating and the gel dissolves upon cooling i.e. thermo-reversible gelation. However, the values of the gelation temperature differ depending on the sources of MC samples and on the methods of determination as well. In this study, we have obtained a lower limit of the gelation temperature for a specific MC below which aqueous MC does not form the gel, by dually extrapolating the holding time for gelation to infinite and the mechanical probing force to zero. The gelation temperature obtained in this manner decreased with increasing concentration of the MC; to cite a case, it was located at ca. 21 °C for 10 wt%, which is ca. 10 °C lower than a conditional value estimated after holding 1 h without these dual extrapolations.

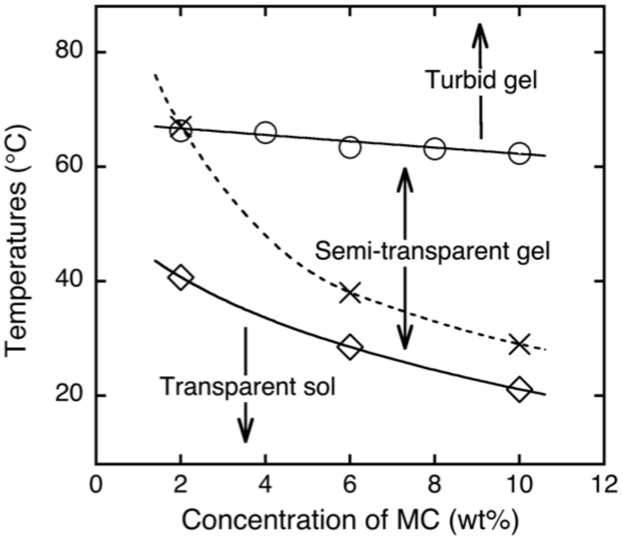

Figure 2. Lower limit of gelation temperature (diamond marks), lower limit of cloud point (open-circle marks) and conditional gelation temperature estimated by employing a stainless-steel ball after holding 1 h (cross marks). Lines are guide for eyes.

Direct Observation on Spin-coating Process of PS-*b*-P2VP Thin Films

During the spin-coating process of symmetric poly(styrene-*b*-2-vinylpyridine) (PS-*b*-P2VP) block copolymers, after the formation of the micelles in dilute solution, the selective solvent induced two kinds of the morphological transition. Firstly, the disordered spherical micelles were transformed into a BCC lattice of spheres of which the (110) plane was oriented perpendicularly to the substrate surface. Secondly, further evaporation induced a transition from spheres on the BCC lattice into cylindrical structures. The orientation of the cylinders perpendicular to the substrate surface was induced by solvent convection perpendicular to the substrate, which occurs during rapid solvent evaporation. After this transition, vitrification of PS and P2VP prevented any further transition from cylinders to the more thermodynamically stable lamellar structures, as are generally observed as the bulk equilibrium state.

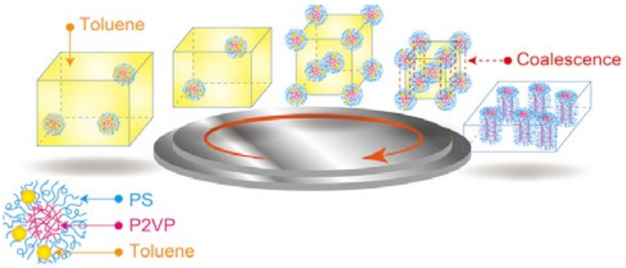

Figure 3. Spin-coating process of PS-P2VP thin film.

Division of Multidisciplinary Chemistry
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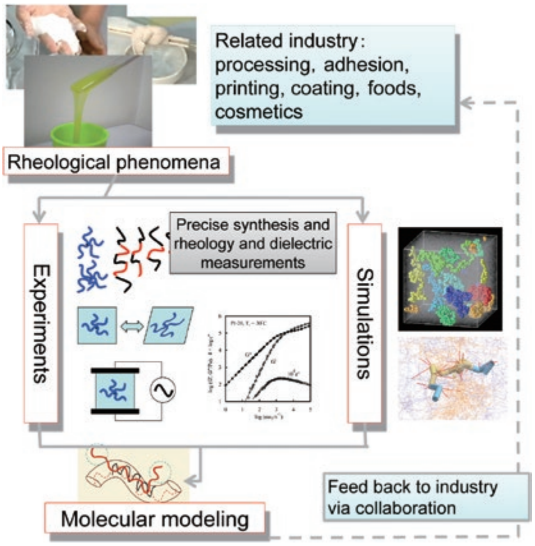
Guest Res Assoc

RAKKAPAO, Natthida (Ph D)	Prince of Songkla University, Thailand, 11 July−13 August
KWON, Oh Min	Seoul National University, Korea, R., 14 April−31 August

Scope of Research

Research focus is placed on the molecular origin of rheological properties of various materials. Depending on time and temperature, homogeneous polymeric materials exhibit typical features of glass, rubber, and viscous fluid while heterogeneous polymeric systems exhibit plasticity in addition to these features. For basic understanding of these features, the molecular motion and structures at various scales are studied for polymeric systems in deformed state. Rheological measurements are performed with various rheometers. Auto-correlation of the molecular orientation is also investigated with dynamic dielectric spectroscopy. Analysis of rheological and dielectric behavior elucidates new aspect of softmatter physics.



KEYWORDS
Rheology
Dielectric Spectroscopy
Softmatter

Selected Publications

Ankiewicz, S.; Orbey, H.; Watanabe, H.; Lentzakis, H.; Dealy, J., On the Use of Continuous Relaxation Spectra to Characterize Model Polymers, *J. Rheol.*, **60,** 1115-1120 (2016).

Matsumiya, Y.; Watanabe, H.; Urakawa, O.; Inoue, T., Experimental Test for Viscoelastic Relaxation of Polyisoprene Undergoing Monofunctional Head-to-Head Association and Dissociation, *Macromolecules*, **49(18),** 7088-7095 (2016).

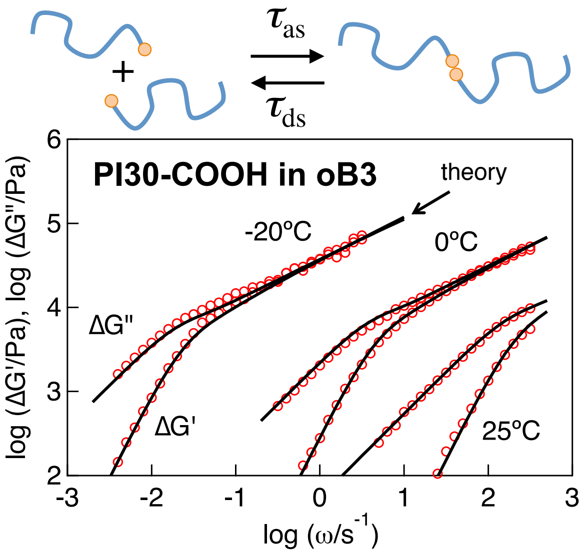
Matsumiya, Y.; Watanabe, H., Nonlinear Stress Relaxation of Miscible Polyisoprene/Poly(p-tert-butylstyrene) Blends in Pseudomonodisperse State, *Macromolecules*, **49(12),** 4544-4556 (2016).

Kwon, Y.; Matsumiya, Y.; Watanabe, H., Viscoelastic and Orientational Relaxation of Linear and Ring Rouse Chains Undergoing Reversible End-Association and Dissociation, *Macromolecules*, **49(9),** 3593-3607 (2016).

Doi, Y.; Iwasa, Y.; Watanabe, K.; Nakamura, M.; Takano, A.; Takahashi, Y.; Matsushita, Y., Synthesis and Characterization of Comb-Shaped Ring Polystyrenes, *Macromolecules*, **49,** 3109-3115 (2016).

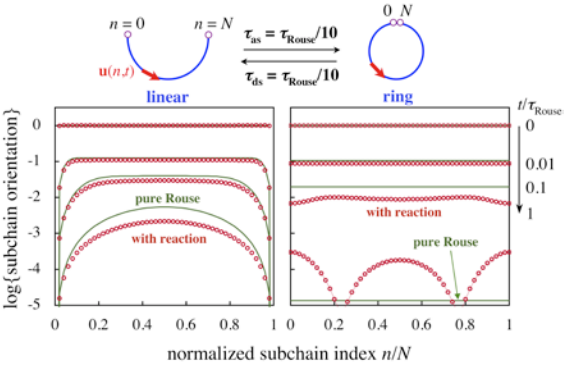
Experimental Test for Viscoelastic Relaxation of Polyisoprene Undergoing Monofunctional Head-to-Head Association and Dissociation

A viscoelastic test was made for end-carboxylated polyisoprene (PI-COOH) of the molecular weight $M = 30._5 \times 10^3$ that underwent the interchain association and dissociation through hydrogen bonding of the COOH groups at the chain end. As a reference, the test was made also for neat PI unimer (with no COOH group at the chain end) and for PI$_2$ dimer (with $M = 61.0 \times 10^3$), the latter being synthesized through end-coupling of PI$^-$ anions (precursor of the PI-COOH sample). The PI-COOH, neat unimer, and dimer samples were diluted in oligomeric butadiene (oB) to a concentration of 10 wt %. The neat unimer and dimer exhibited nonentangled Rouse behavior at this concentration, as expected from their molecular weights. At low temperatures ($T \leq 0$ °C) the PI-COOH sample relaxed slower than the reference unimer but faster than the dimer, whereas the relaxation of PI-COOH approached that of the unimer with increasing $T > 0$ °C, and this change of the relaxation time of PI-COOH was associated with changes in the angular frequency (ω) dependence of the dynamic modulus. This behavior of PI-COOH was well described by a recently proposed theory considering motional coupling between the end-associating unimer and its dimer at chemical equilibrium. On the basis of this result, an effect of the polymeric character of PI-COOH chain on the viscoelastically detected association/dissociation of the hydrogen bonding of the COOH groups was discussed.



Viscoelastic and Orientational Relaxation of Linear and Ring Rouse Chains Undergoing Reversible End-Association and Dissociation

For dilute telechelic linear and ring Rouse chains undergoing reversible end-association and dissociation, the time (t) evolution equation was analytically formulated for the bond vector of the subchain (or segment), $\mathbf{u}^{[c]}(n,t)$ with n being the subchain index and the superscript c specifying the chain (c = L and R for the linear and ring chains). The end-association of the linear chain (i.e., ring formation) occurs only when the ends of the linear chain come into close proximity. Because of this constraint for the ring formation, the time evolution equation for $\mathbf{u}^{[L]}(n,t)$ of the linear chain was formulated with a conceptually new, two-step expansion method: $\mathbf{u}^{[L]}(n,t)$ was first expanded with respect to its sinusoidal Rouse eigenfunction, $\sin(p\pi n/N)$ with p = integer and N being the number of subchains *per* chain, and then the series of odd sine modes is re-expanded with respect to cosine eigenfunctions of the ring chain, $\cos(2\alpha\pi n/N)$ with α = integer, so as to account for that constraint. This formulation allowed analytical calculation of the orientational correlation function, $S^{[c]}(n,m,t) = b^{-2}\langle u_x^{[c]}(n,t)u_y^{[c]}(m,t)\rangle$ (c = L, R) with b being the subchain step length, and the viscoelastic relaxation function, $g^{[c]}(t) \propto \int_0^N S^{[c]}(n,n,t)\,\mathrm{d}n$. It turned out that the terminal relaxation of $g^{[R]}(t)$ and $g^{[L]}(t)$ of the ring and linear chains is retarded and accelerated, respectively, due to the motional coupling of those chains occurring through the reaction. This coupling breaks the ring symmetry (equivalence of all subchains of the ring chain in the absence of reaction), thereby leading to oscillation of the orientational anisotropy $S^{[R]}(n,n,t)$ of the ring chain at long t with the subchain index n. The coupling also reduces a difference of the anisotropy $S^{[L]}(n,n,t)$ of the linear chain at the middle ($n \sim N/2$) and end ($n \sim 0$).



Division of Multidisciplinary Chemistry
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http://www.em2.kuicr.kyoto-u.ac.jp/index.html

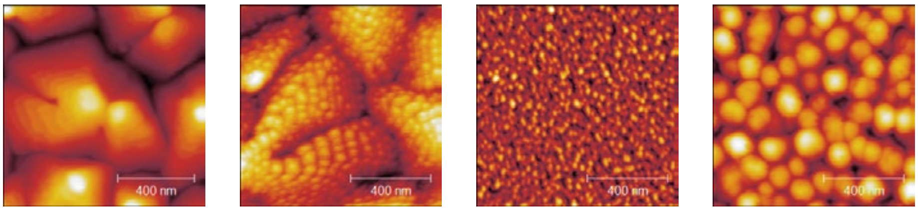
Assist Prof
MURDEY, Richard James
(Ph D)

Scope of Research

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

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

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



10 nm pentacene

10 nm pentacene
+ 10 nm C_{60}

10 nm C_{60}

10 nm C_{60}
+ 10 nm pentacene

Selected Publications

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

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

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

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

Nonlinear Photocurrent Spectroscopy

As photocurrent is proportional to the quantity of absorbed radiation it is possible in principle to extract an optical absorption spectrum using the photocurrent recorded at different wavelengths. Photocurrent in this instance can be considered as a measure of the absorbed light.

If the relationship between photocurrent, I, and the absorbed light intensity, F, is not linear, however, the incident light intensity for each data point must be attenuated such that the photocurrent remains constant – unless a mathematical function can be found to transform the photocurrent into a linear function of absorbance. We have determined that this linearization function, called the current response function, can be expressed as,

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

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

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

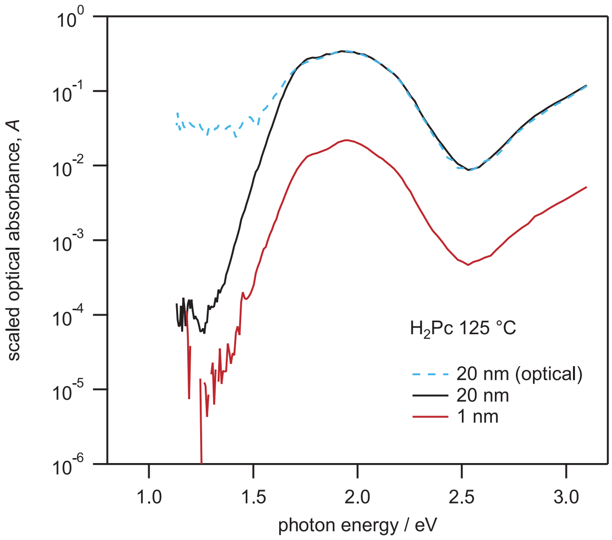


Figure 1. Absorbance spectra of 20 nm and 1 nm free base phthalocyanine thin films derived from photocurrent measurements after application of the nonlinear current response function and scaled to an optical reference. The reference optical spectra for the 20 nm film measured with the transmitted beam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

Conductance in Organic Radical Solids

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

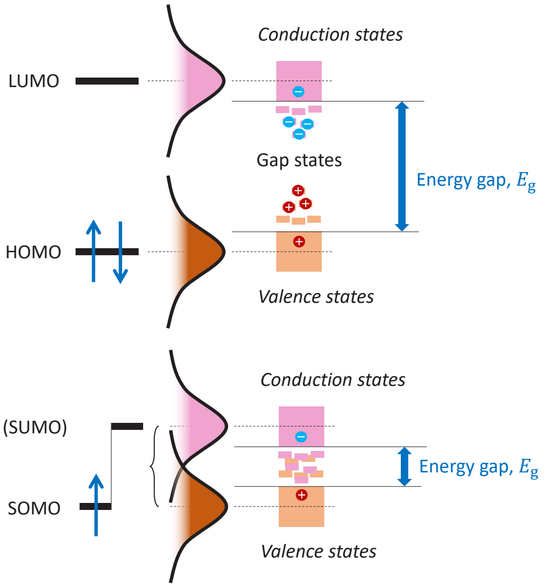


Figure 2. The relation between the molecular orbitals and the solid state energy gap E_g in a) typical closed shell organic semiconductors, and b) open shell organic radicals. Charge held in gap states is said to be “trapped”.

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

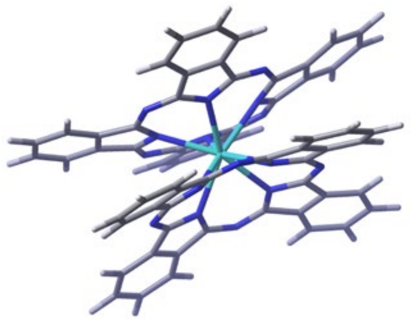


Figure 3. Molecular structure of the phthalocyanine sandwich complex bis(phthalocyanininato)terbium(III) ($TbPc_2$). A single unpaired electron is shared between the two phthalocyanine ligands.

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

Advanced Research Center for Beam Science
– Particle Beam Science –

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

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Researcher(pt)

HOKONOHARA, Hisao

Lect (pt)

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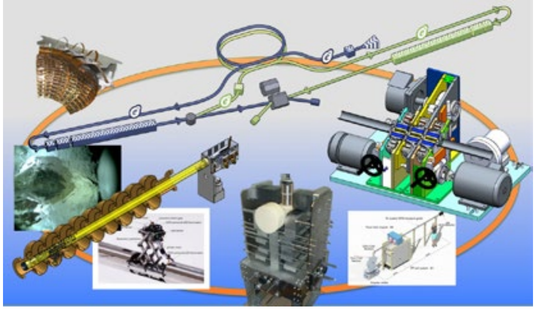
FUWA, Yasuhiro (D3)
KITAHARA, Ryunosuke (D3)
IKEDA, Hideki (M2)
MIYAWAKI, Eisuke (M1)

Guest Scholar

JAMESON, Robert A. (Ph D) Goethe University, Frankfurt Germany, 3−29 November

Scope of Research

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



KEYWORDS

Beam Physics
Accelerator Physics
Neutron Optics
Phase Rotation
International Linear Collider

Selected Publications

Imajo, S.; Mishima, K.; Kitaguchi, M.; Iwashita, Y.; Yamada, N. L.; Hino, M.; Oda, T.; Ino, T.; Shimizu, H. M.; Yamashita, S.; Katayama, R., Pulsed Ultra-cold Neutron Production Using a Doppler Shifter at J-PARC, *Prog. Theor. Exp. Phys.*, **2016-1,** 013C02-1-22 (2016).

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

Fuwa, Y.; Iwashita, Y.; Tongu, H.; Inoue, S.; Hashida, M.; Sakabe, S.; Okamura, M.; Yamazaki, A., RF Synchronized Short Pulse Laser Ion Source, *Rev. Sci. Instrum.*, **87,** 02A911-1-02A911-4 (2016).

Arimoto, Y.; Higashi, N.; Igarashi, Y.; Iwashita, Y.; Ino, T.; Katayama, R.; Kitaguchi, M.; Kitahara, R.; Matsumura, H.; Mishima, K.; Nagakura, N.; Oide, H.; Otono, H.; Sakakibara, R.; Shima, T.; Shimizu, H. M.; Sugino, T.; Sumi, N.; Sumino, H.; Taketani, K.; Tanaka, G.; Tanaka, M.; Tauchi, K.; Toyoda, A.; Tomita, T.; Yamada, T.; Yamashita, S.; Yokoyama, H.; Yoshioka, T., Development of Time Projection Chamber for Precise Neutron Lifetime Measurement Using Pulsed Cold Neutron Beams, *Nucl. Instr. Meth. Phys. Res. A*, **799,** 187-196 (2015).

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

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

Measurement of Thermal Cross Section of $^{14}N(n,p)^{14}C$ Using Cold Neutron Beam at J-PARC

The cross section of the $^{14}N(n,p)^{14}C$ reaction is one of the key parameters in the slow-neutron capture process of stellar nucleosynthesis occurring in the helium burning shells whose typical temperature is ~25 keV. In late 1980s, the $^{14}N(n,p)^{14}C$ reaction cross section at around 30 keV have been measured by two groups, and their results deviated from each other by a factor of more than two. One of them has been supported by later measurements, but the extrapolated cross section of their results assuming the 1/v law differs from the recent evaluated cross section with the deviation of more than 1.6 σ.

To improve the reliability of the evaluated cross section data, we measured the thermal cross section of the $^{14}N(n,p)^{14}C$ reaction using a pulsed cold neutron beam at J-PARC (Japan Proton Accelerator Research Complex). Our experiment has a feature that the $^{14}N(n,p)^{14}C$ and $^{3}He(n,p)^{3}H$ reactions are measured simultaneously by Time Projection Chamber (TPC), where the cross section of the latter reaction has been measured within the error of 0.13% as 5333(7) barn. The TPC, which was originally developed for a neutron lifetime measurement by the NOP (Neutron Optics and Physics) collaborators at J-PARC (Figure 1), consisted of a drift cage with a multi-wire proportional chamber (MWPC) inside the seal-off vacuum vessel (Figure 2). An operational gas was the mixture of 80 kPa ^{4}He, 20 kPa N_2, and a few Pa ^{3}He, where the partial pressures were measured by the gas injection system.

Pulsed cold neutron beams in the energy range of 1~20 meV are produced by the nuclear spallation reaction of Hg target using a 3 GeV pulsed proton beam at MLF (the Materials and Life Science Facility). Since the length of a neutron bunch is 40 cm which is shorter than the length of the TPC sensitive volume, background events caused by neutron capture reactions in materials of inner walls or frames of the TPC could be reduced by selecting only the events whose particle tracks were fully contained in the sensitive volume. Since the Q-values of the $^{14}N(n,p)^{14}C$ and $^{3}He(n,p)^{3}H$ reactions are 626 keV and 764 keV, respectively, they were able to be separately detected by the deposit energy difference of the reactions (Figure 3). Thus we could deduce the thermal cross section of $^{14}N(n,p)^{14}C$ relative to the thermal cross section of $^{3}He(n,p)^{3}H$ by using the known ratios of the target densities of ^{14}N and ^{3}He and the detection efficiencies for (n,p) reactions on those nuclei.

To check the quality of the separation between the $^{14}N(n,p)^{14}C$ and $^{3}He(n,p)^{3}H$ reactions in the energy spectrum, we made measurements using the operational gases with three different partial pressures of ^{3}He, and obtained a preliminary result on the thermal cross section of the $^{14}N(n,p)^{14}C$ reaction as 1.864(3) barn with the world best accuracy of 0.3%.

The method of our experiment is in principle applicable to the measurements of other (n,p) and (n,α) reaction cross sections, for example, $^{10}B(n,p)^{10}Be$, which is also one of the important reactions in astrophysics. We are considering a measurement of the thermal cross section of the $^{10}B(n,p)^{10}Be$ reaction in a near future.

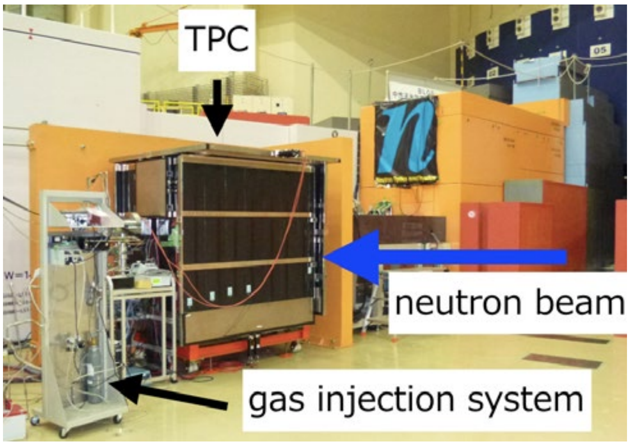


Figure 1. Experimental set up at J-PARC/MLF Beam Line 05.

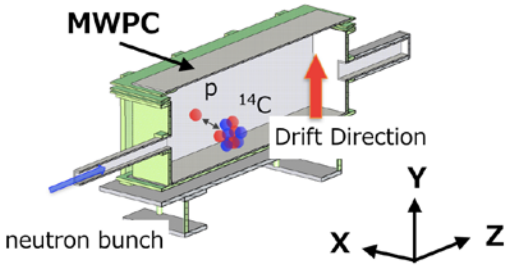


Figure 2. Schematic drawing of the Time Projection Chamber (TPC). Electrons ionized by a charged particle in the operational gas drift to the multi-wire proportional counter (MWPC). Deposit energy in the TPC is determined by measuring an amount of the electrons detected by MWPC.

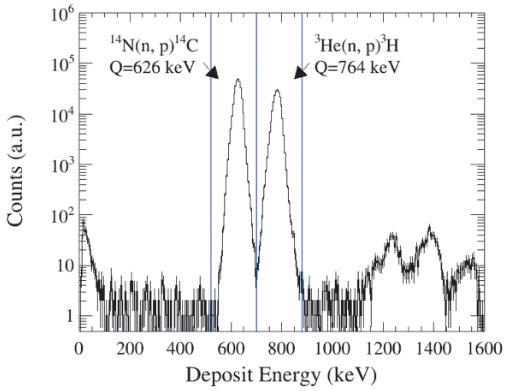


Figure 3. Deposit energy distribution in the measurement with the ^{3}He partial pressure of 9 Pa. The peaks corresponding to the $^{14}N(n,p)^{14}C$ and $^{3}He(n,p)^{3}H$ reactions are found in the energy regions of 520~700 keV and 700~880 keV, respectively, and are well separated with the threshold level of 700 keV (blue line).

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

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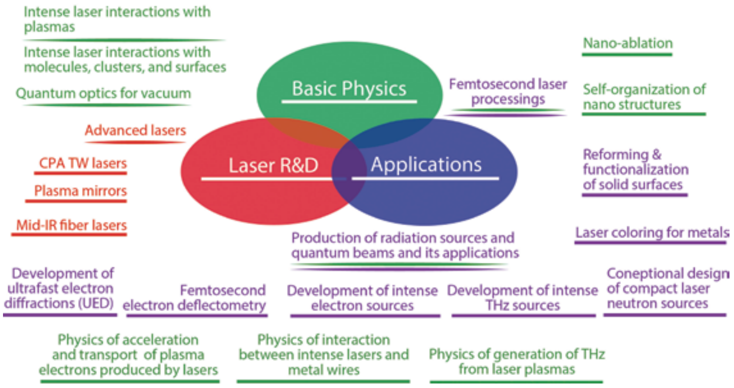
Scope of Research

The interaction of femtosecond laser pulses with matter involves interesting physics not seen with nanosecond laser pulses. Through investigation of the interaction physics, the potential of intense femtosecond lasers for new applications is being developed (e.g., laser-produced radiation and laser processing). Ultra-intense lasers can produce intense radiations (e.g., electrons, ions, and THz), which are promising as next-generation radiation sources. Ultra-short lasers can process any matter without thermal dissociation. Femtosecond laser processing is also the next-generation of laser processing. Our laboratory is equipped with an ultra-intense femtosecond laser named T6, to study the physics of intense laser–matter interactions and its applications.



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

Selected Publications

Gouda, A. M.; Sakagami, H.; Ogata, T.; Hashida, M.; Sakabe, S., The Formation Mechanism of the Periodic Nanograting Structure by the Weibel Instability, *Appl. Phys. A*, **122,** 454-1-454-6 (2016).

Hashida, M.; Nishii, T.; Miyasaka, Y.; Sakagami, H.; Shimizu, M.; Inoue, S.; Sakabe, S., Orientation of Periodic Grating Structures Controlled by Double-pulse Irradiation, *Appl. Phys. A*, **122,** 484-1-484-5 (2016).

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

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

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

Highly Intensified Emission of the Laser Accelerated Fast Electrons by Using Solid-plasma Composite Target

Intense ultrashort electrons pulses are driven by the interaction of intense short laser pulses with solid targets. These laser-accelerated fast electrons have many possible applications such as fast ignition for inertial confinement fusion, ultrafast electron diffraction measurement, and ultrafast transient field measurement. For these applications using fast electrons as probe pulses with high temporal resolution, it is desirable for a greater number of electrons to be emitted from the laser plasma. However, most laser-accelerated electrons cannot escape from the laser plasma because they are trapped by a strong quasi-static electric field, called the sheath field, produced around the steep density gradient boundary between the solid/plasma and the vacuum. Almost all electrons are bound within the solid target, and only about 1% of the hot electrons can escape. Therefore, only a small fraction of electrons accelerated by intense short-pulse laser escapes from the laser plasma, and the most of electrons expend their energy heating the target or producing other types of radiation.

We demonstrate the intensification of electrons escaping from an intense laser plasma by using double femtosecond laser pulses. An intense pulse from a chirped pulse amplification laser (CPA1) for driving fast electrons is used to irradiate a foil target, the rear of which is pre-irradiated with another laser pulse (CPA2). Pre-irradiation with CPA2 controls the electron density distributions in the target to suppress sheath field growth and expand the target plasma into which the fast electrons are released. The number of escaping electrons increases greatly when the target is irradiated with CPA2 540 ps prior to CPA1. The number of electrons released is 7 times that for single pulse irradiation. These results are supported by two-dimensional (2D) particle-in-cell (PIC) simulations of plasma produced by CPA2 and analytical evaluation considering the expansion of the plasma.

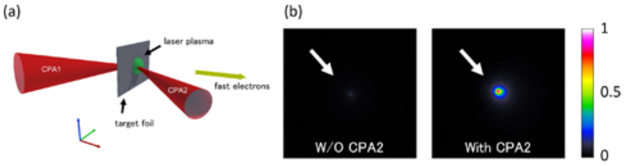


Figure 1. (a) schematic of the experimental setup. (b) Images of fast electrons emitted from laser plasma.

Threshold Fluence of Femtosecond Laser Nano-Ablation for Metals

Femtosecond laser nano-ablation of Ti by short-pulse laser irradiation (800 nm/40 fs) is studied in the laser fluence range of 0.07 – 0.5 J/cm^2. To determine the ablation threshold, the ablation rate dependence on laser fluence is precisely measured. Multi-shot ablation threshold of titanium is found to be 0.074 J/cm^2 in which value is good agreement with that reported previously by other group. To discuss the ablation mechanism, all the ablation thresholds for metals previously published are plotted as a function of work function and melting temperature. We found that the ablation thresholds correlated with work function of metals. Experimental data suggested that the femtosecond laser ablation is mainly due to multi-photon absorption and optical field ionization.

Reduction of Ablation Rate by Double-Pulse Laser Irradiation on Titanium

Reduction of ablation rate is demonstrated on a titanium surface irradiated by a double-pulse beam parallel-polarized at time delays from $\Delta t = 0.16 – 1280$ ps. The first-pulse fluence F_1 and the delayed pulse fluence F_2 are kept below or above the ablation threshold $F_{TH} \sim 100$ mJ/cm^2 of Ti. A pair of laser pulses with fluences of 70 and 140 mJ/cm^2 is used for ablation rate experiment. Figures 1 show the dependence of ablation rate on interval Δt for the fluences $(F_1, F_2) = (70, 140)$. The maximum and minimum ablation rates are 15.5 nm for $\Delta t = 0.16$ ps and 4.4 nm for $\Delta t = 80$ ps, respectively. The maximum is as much as that (17.1 nm) for a single pulse of 210 mJ/cm^2 ; the minimum (4.4 nm) is half of that for a 140 mJ/cm^2 single pulse. Thus, the first pulse modifies the surface to suppress ablation even if its fluence is below the ablation threshold. The experimental results suggest that the first pulse influences the surface, suppressing ablation by the following pulse even though no laser plasma is produced on the surface, and that this influence continues for rather a long time (several hundred picoseconds). Double-pulse irradiation certainly has significant potential for future applications of laser nano-processing.

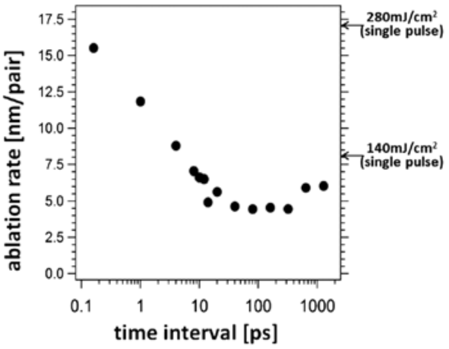


Figure 2. Dependence of ablation rate on time interval for fluences $(F_1, F_2) = (70,140)$.

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

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SCHAPER, Andreas Karl (Ph D) Phillips University of Marburg, Germany, 26 September–17 October

Scope of Research

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

KEYWORDS
EELS
STEM
Elemental Ratio
Surface Plasmon
Electronic Structure

Selected Publications

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

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

Saito, H.; Kurata, H., Formation of a Hybrid Plasmonic Waveguide Mode Probed by Dispersion Measurement, *J. Appl. Phys.*, **117,** [133107-1]-[133107-7] (2015).

Haruta, M.; Hosaka, Y.; Ichikawa, N.; Saito, T.; Shimakawa, Y.; Kurata, H., Determination of Elemental Ratio in an Atomic Column by Electron Energy-Loss Spectroscopy, *ACS Nano*, **10,** 6680-6684 (2016).

Determination of Elemental Ratio in an Atomic Column by Electron Energy Loss Spectroscopy

Elemental mapping with atomic-column resolution can be obtained using electron energy loss spectroscopy (EELS) combined with scanning transmission electron microscopy (STEM). One step in STEM−EELS is quantitative determination of elemental ratio in an atomic column. However, during elemental mapping using STEM−EELS, the elemental signals do not necessarily localize at atomic-column positions. The spatial resolution of an EELS signal is constrained by the delocalization of inelastic scattering. Careful attention to the mixing of signals from neighboring atomic-columns is required to analyze a spectrum at a single point. In the present study, the elemental ratio of Fe to Mn at octahedral and tetrahedral sites in brownmillerite $Ca_2Fe_{1.07}Mn_{0.93}O_5$ was determined quantitatively with atomic resolution using STEM−EELS. This study presents the experimental criteria for semiquantitative analysis of the $L_{2,3}$-edges of Fe and Mn in a perovskite-related structure.

A HAADF image along the [101] direction and an EELS data cube for the Fe and Mn $L_{2,3}$-edges were simultaneously collected using an aberration-corrected JEM ARM-200F operating at 80 kV with a probe-forming aperture of 21.3 mrad. Spectra were recorded as line scans along the 〈010〉 direction. The scan step was 0.19 Å/pixel, which corresponded to 20 segment divisions in the B−B' cation distance. In the present research, the line-profiling method was used instead of two-dimensional mapping to avoid some practical problems (damage and stability) due to oversampling conditions.

Figure 1 shows a HAADF image with the projected structure overlaid. The cation $L_{2,3}$-edge intensities after background-subtraction are shown in Figure 2b. The individual spectra extracted from the octahedral and tetrahedral sites contain a weak intensity from the nonpreferred cation at both polyhedral sites, as shown in Figure 2d. The delocalization factors of the Fe and Mn $L_{2,3}$-edge excitations were approximately 1.2 and 1.3 Å, respectively, which are small enough to resolve the atomic distance (3.8 Å) between B and B' cations. The relative composition profiles obtained by quantifying the intensity at each spatial increment in the elemental profiles of Figure 2b are shown in Figure 2c. The relative composition profiles resembled wide isosceles trapezoids. The elemental profile reflects the one-dimensional distribution of excitation probabilities for a specific energy loss; a maximal excitation should occur just above each atomic position. In contrast, the relative composition profile should be constant near each atomic position if the spectra contain only the contribution from illuminated atomic columns. The flat region of the relative composition profile (Figure 2c) indicates very little contribution from nearest neighbor columns and the quantitative analysis is achieved near-atomic resolution. Such a profile can be obtained only by oversampling of spectral data. The present experiment found that the relative composition profile was nearly constant within a 1.2 Å radius around the atomic position of each polyhedral site. The average ratio of Fe to Mn in this flat region (Figure 2c) was (17.5:82.5) ± 5.9 in octahedral sites and (81.6:18.4) ± 6.0 in tetrahedral sites. The result at octahedral sites roughly agreed with previous results from neutron diffraction, (14.4:85.6) ± 0.2. Simple multislice calculations were used to estimate the error due to electron dechanneling combined with a delocalization factor. The Mn atomic fraction profile derived from EELS intensity ratio was calculated by assuming "true fractions" of Mn at octahedral site, x=0.87. The simulated profile accurately reproduced the flat region near an octahedral site, as expected, with a radius of 0.9 Å, which agreed well with the experimental value. For a thin sample ($t < 10$ nm), the estimated error was negligibly small.

Results showed that relative composition profiles with an isosceles trapezoid-shape are useful for quantifying the resolution of measurements. An area with a radius of about 1.2 Å surrounded both atomic sites and provided information at near-atomic resolution. This study demonstrates that the experimental spectra at the $L_{2,3}$-edge, obtained from octahedral atomic columns of 3d transition metals in perovskite-like structures, can be quantitatively interpreted with an uncertainty of 10% (accuracy of calculated partial cross sections of L-shell using Hartree-Slater model) without full quantum mechanical simulation.

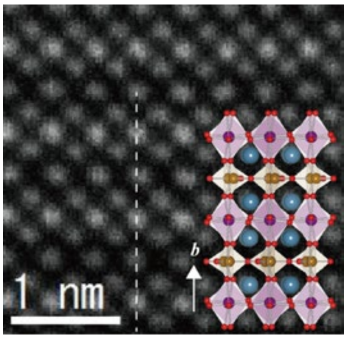

Figure 1. HAADF image of the [101] direction in $Ca_2Fe_{1.07}Mn_{0.93}O_5$. Inset shows the corresponding structure. Spectral imaging was performed along the dashed line.

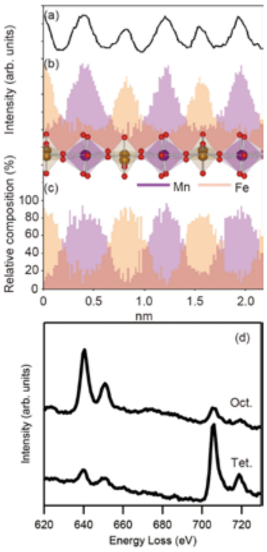

Figure 2. Line profiles and spectra for $Ca_2Fe_{1.07}Mn_{0.93}O_5$: (a) HAADF profiles; (b) EELS elemental 〈010〉 line profiles for the $L_{2,3}$-edges of Fe and Mn; (c) profile of the relative compositions of Fe and Mn; (d) spectra measured above the octahedral and tetrahedral cations.

Advanced Research Center for Beam Science
– Structural Molecular Biology –

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FUJII, Tomomi
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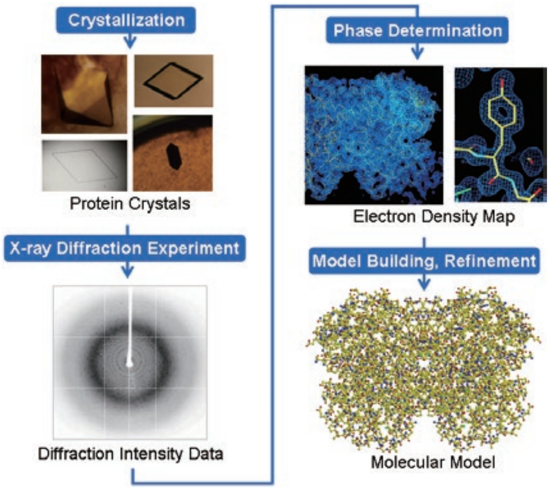
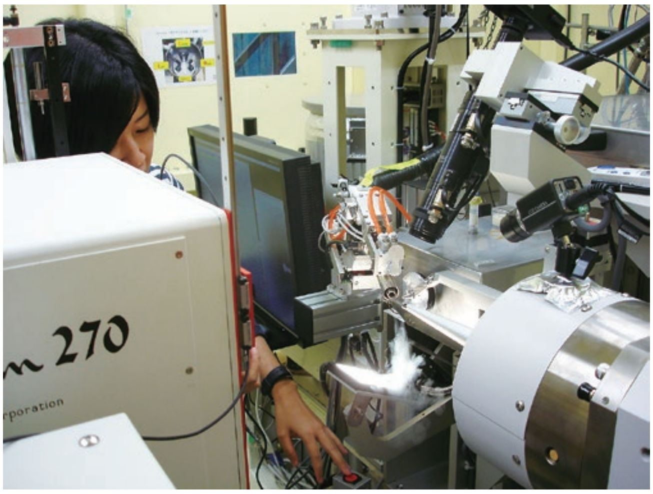
Scope of Research

Our laboratory analyzes the electronic state of atomic or molecular structure in materials, which are obtained from diffraction images and spectra observed by X-ray irradiation of these substances, respectively, to elucidate the relationships between the structure and functions or physical properties. Our main themes are (1) high-resolution experimental and theoretical studies on the natural width of elements in materials, (2) the development in the measurements of the diagram lines in soft X-rays region, (3) structural determination of novel protein molecules and their complexes, and (4) studies on the structural basis of functions, physical properties, and intermolecular interactions.

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





Selected Publications

Fujii, T.; Sato, A.; Okamoto, Y.; Yamauchi, T.; Kato, S.; Yoshida, M.; Oikawa, T.; Hata, Y., The Crystal Structure of Maleylacetate Reductase from *Rhizobium* sp. Strain MTP-10005 Provides Insights into the Reaction Mechanism of Enzymes in Its Original Family, *Proteins: Structure, Function, and Bioinformatics*, **84,** 1029-1042 (2016).

Fujii, T.; Yamauchi, T.; Ishiyama, M.; Gogami, Y.; Oikawa, T.; Hata, Y., Crystallographic Studies of Aspartate Racemase from *Lactobacillus sakei* NBRC 15893, *Acta Crystallogr. Sect. F Struct. Biol. Cryst. Commun.*, **71,** 1012-1016 (2015).

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

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

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

Structural Features and Low-temperature Adaptation of Aspartate Racemase

Amino-acid racemases are responsible for the racemization of amino acids and can be mainly grouped into two families, pyridoxal 5’-phosphate (PLP) dependent and PLP independent. Aspartate racemase (AspR) catalyzes the interconversion between L- and D-aspartate and belongs to the PLP-independent racemase group. The enzyme is thought to employ a two-base mechanism to catalyze both the directions of racemization and utilize two cysteine residues as the conjugated catalytic acid and base in the catalytic reaction. The only crystal structure of the PLP-independent amino-acid racemase is now available from a hyperthermophilic archaeon. To elucidate the structure and the low-temperature adaptation of the racemase group, we determined the crystal structures of AspR from *Lactobacillus sakei* NBRC 15893 (LsAspR), which works in the low-to-medium temperature range, and for comparison AspR from *Thermococcus litoralis* DSM 5473 (TlAspR), which has the maximum activity at 95 °C.

LsAspR and TlAspR were crystallized at 20 °C by the sitting-drop vapour-diffusion method using a precipitant solution of 25% (v/v) PEG-MME 550, 5% (v/v) 2-propanol and 0.1 M sodium acetate pH 4.8 and a precipitant solution of 24% (w/v) PEG1500, 0.2 M L-proline and 0.1 M HEPES pH 7.5, respectively. Diffraction experiments were performed at beamlines NE-3A of Photon Factory AR, and BL-5A of Photon Factory, Tsukuba, Japan. The crystals were flash-cooled in a nitrogen stream at 100 K. Diffraction data were collected at a wavelength of 1.000 Å using Quantum 270 and 315r CCD detectors. The crystals belonged to space groups $P3_121$ with unit cell parameters of $a = b = 105.5$ Å and $c = 96.5$ Å, and $P2_12_11$ with unit cell parameters of $a = 90.26$, $b = 125.78$, $c = 40.64$ Å, respectively. The structures of LsAspR and TlAspR were determined by molecular replacement and refined at 2.6 Å resolution ($R = 23.8\%$, $R_{\text{free}} = 31.6\%$) and 2.0 Å resolution ($R = 18.7\%$, $R_{\text{free}} = 25.0\%$), respectively.

Both LsAspR and TlAspR molecules are homodimers with molecular two-fold axis. The subunit of each enzyme molecule comprises the N-terminal and C-terminal domains. In each domain, a central four-stranded parallel β-sheet is flanked by six α-helices. The molecules are formed mainly by intersubunit interactions between the N-terminal α-helices and intersubunit hydrogen-bonds between the N-terminal β-sheets in the dimer interface. The active-site cleft exists between both the domains. The spatial arrangement of the strictly conserved cysteine residues in the cleft reveals the Cys residues involved in the enzymatic catalysis: Cys84 and Cys196 of LsAspR and Cys83 and Cys194 of TlAspR.

A structural comparison of LsAspR and TlAspR reveals structural factors probably involved in thermostability of AspR. The molecular volume, intersubunit interaction, and the number of ion pairs suggest that the LsAspR molecule is more loose than that of TlAspR (Fig. 1). Most characteristic difference at the dimer interface between LsAspR and TlAspR is the interactions between α1 helices (Fig. 2). Moreover, π-π interaction between indole rings of Trp74 is found at the dimer interface of TlAspR (Fig. 3). In LsAspR, Leu75 corresponds to Trp74 in TlAspR and does not make an intersubunit interaction.

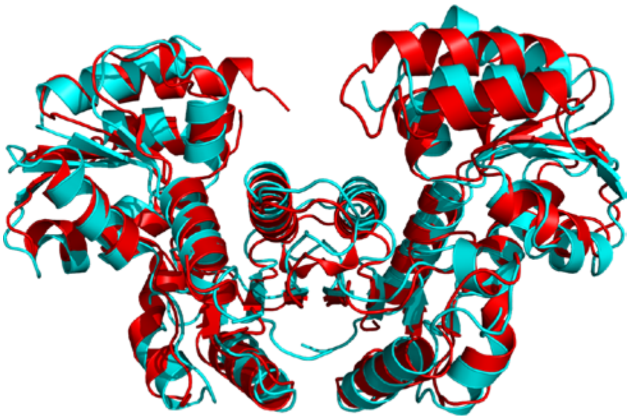


Figure 1. Superposition of LsAspR and TlAspR dimers. Cyan, LsAspR; Red, TlAspR.

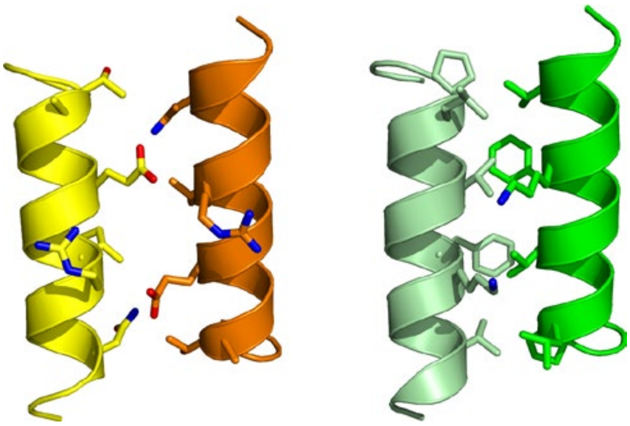


Figure 2. Interactions between α1 helices in dimer interface. (Left panel) LsAspR. (Right panel) TlAspR.

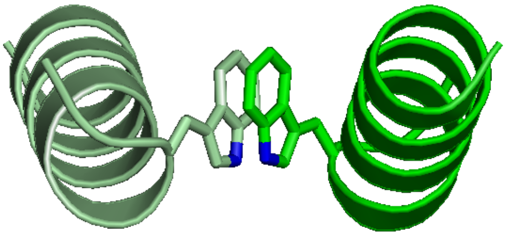


Figure 3. π-π Interaction between indole rings of Trp74 at dimer interface of TlAspR.

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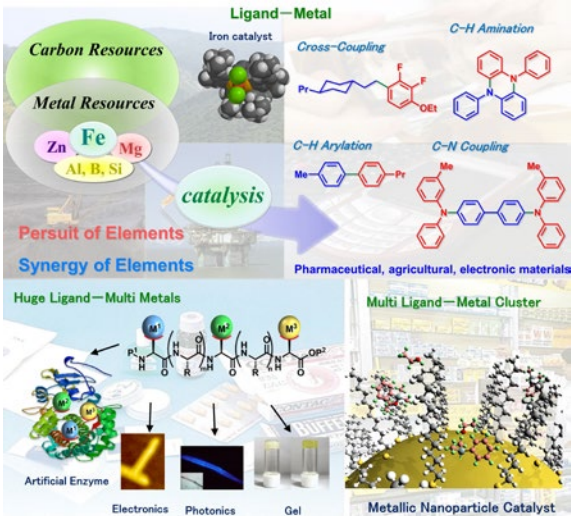
Scope of Research

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



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

Selected Publications

Yoshida, R.; Isozaki, K.; Yokoi, T.; Yasuda, N.; Sadakane, K.; Iwamoto, T.; Takaya, H.; Nakamura, M., ONO-pincer Ruthenium Complex-bound Norvaline for Efficient Catalytic Oxidation of Methoxybenzenes with Hydrogen Peroxide, *Org. Biomol. Chem.*, **14,** 7468-7479 (2016).

Yamaguchi, A.; Isozaki, K.; Nakamura, M.; Takaya, H.; Watanabe, T., Discovery of 12-mer Peptides that Bind to Wood Lignin, *Scientific Reports*, **6,** 21833 (2016).

Isozaki, K.; Yokoi, T.; Yoshida, R.; Ogata, K.; Hashizume, D.; Yasuda, N.; Sadakane, K.; Takaya, H.; Nakamura, M., Synthesis and Functions of ONO-Pincer Ruthenium-Complex-Bound Norvalines, *Chemistry an Asian Journal*, **11,** 1076-1091 (2016).

Iron-Catalyzed Cross-Coupling Reactions

Transition-metal-catalyzed carbon–carbon and carbon–heteroatom bond forming reactions are powerful tools for the synthesis of functional molecules. Our group focuses on use of iron as a catalyst, and so far developed a variety of iron-catalyzed cross-coupling reactions, some of which can't be achieved by conventional transition-metal catalysts such as palladium. For example, we recently developed iron-catalyzed enantioselective cross-coupling reaction of α-chloroesters with aryl Grignard reagents, which is the first iron-catalyzed enantioselective coupling reaction. In addition, we found a novel intermolecular and intramolecular C-H amination of diarylamines to provide dihydrophenazine derivatives. Importantly, these rections enable facile access to several important pharmaceutical and functional molecules. Furthermore we clarified the mechanisms of these reactions by using synchrotron X-ray absorption spectroscopy combined with theoretical calculations.

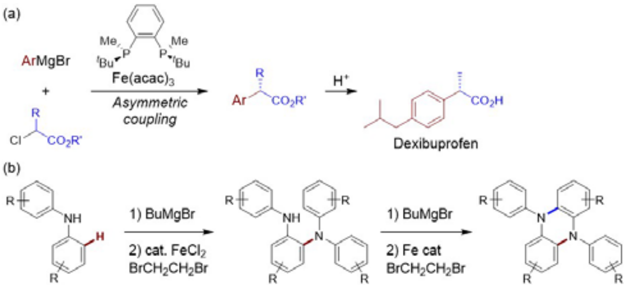


Figure 1. (a) Iron-catalyzed enantioselective cross-coupling reaction of α-chloroesters with aryl Grignard reagents, and (b) intermolecular and intramolecular C-H amination of diarylamines.

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

This project focuses on development of smart materials based on synergistic effect of various metals on artificial peptides. Based on this concept, novel ruthenium catalysts bound with norvaline have been developed, achieving efficient and selective oxidation of several methoxy-benzene analogues to quinones. In this reaction, norvaline act as a mediator inducing micelle-like aggregates, which is the origin of high efficiency and selectivity. Now we are trying further modification of the catalysts to oxidize much challenging aromatic substrate toward investigation of future chemical resources.

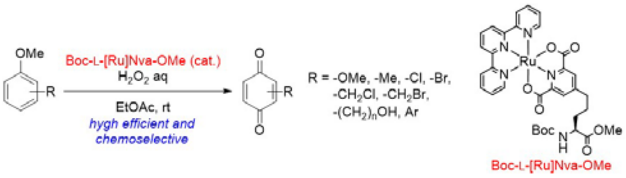


Figure 2. Efficient catalytic oxidation of methoxybenzenes with ruthenium catalyst bound with norvaline.

Supramolecular Approach for Creating Enhanced Catalysis of Metallic Nanoparticles

This project focuses on the development of highly active and selective metallic nanoparticle and cluster catalysts. To achieve this purpose, four key methodologies have been developed: 1) creation of reaction field with advanced self-assembly, 2) design of selective molecular transformation with multi-points intermolecular interaction, 3) size selective synthesis of metallic nanoparticles and clusters, and 4) utilization of plasmonic resonance with light.

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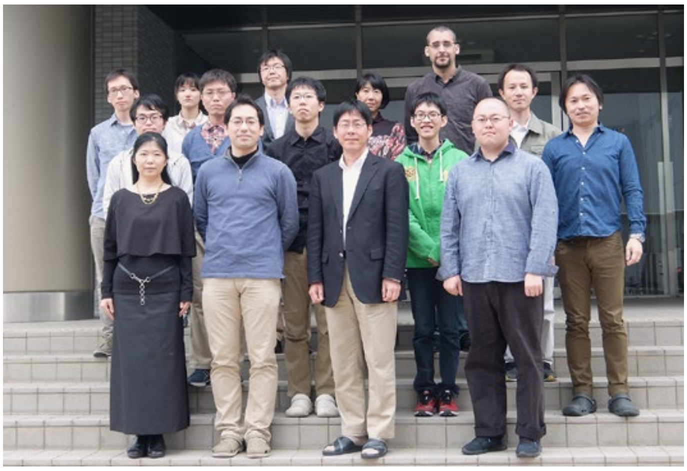
Scope of Research

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

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



Selected Publications

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

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

Matsumoto, K.; Haruta, M.; Kawai, M.; Sakaiguchi, A.; Ichikawa, N.; Kurata, H.; Shimakawa, Y., Selective Reduction of Layers at Low Temperature in Artificial Superlattice Thin Films, *Sci. Rep.*, **1,** [27-1]-[27-14] (2011).

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

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

Ferromagnetism Induced by Substitution of the Iron(IV) Ion by an Unusual High-Valence Nickel(IV) Ion in Antiferromagnetic $SrFeO_3$

In addition to the usual valence states of 3d transition-metal cations in oxides, such as Fe^{II}/Fe^{III} for Fe and Ni^{II} for Ni, unusual high-valence states, such as Fe^{IV} and Ni^{IV}, can be stabilized in a strongly oxidizing atmosphere. Iron(IV) is stabilized in the cubic perovskite $SrFeO_3$, which is synthesized at high pressure and temperature. The iron(IV) ion in the perovskite, having a nominal d^4 electron configuration in the corner-sharing FeO_6 octahedron, has a spin of S=2, and at low temperatures the compound shows a helical magnetism as a result of competing ferromagnetic and antiferromagnetic interactions between the spins. Ni^{IV}, on the other hand, is stabilized in hexagonal perovskites such as $SrNiO_3$ and $BaNiO_3$ and is expected to have a low spin state (S=0). Indeed, $BaNiO_3$ is nonmagnetic.

In the course of preparing a solid solution of $SrFeO_3$ and $SrNiO_3$, we found that Ni^{IV} is stabilized in the $SrFeO_3$-type cubic perovskite $Sr(Fe^{IV}{}_{1-x}Ni^{IV}{}_x)O_3$ with x up to 0.5. Interestingly, the substitution of Fe^{IV} ions by Ni^{IV} ions in the helical antiferromagnetic $SrFeO_3$ induces ferromagnetism with a transition temperature (T_c) higher than room temperature. X-ray absorption spectroscopy and x-ray magnetic circular dichroism spectroscopy imply that substantial magnetic moments of the Ni^{IV} ion were induced by the large magnetic moments of Fe^{IV} through orbital hybridization with oxygen and as a result of this orbital hybridization, ferromagnetism, with the transition temperature above room temperature, is achieved.

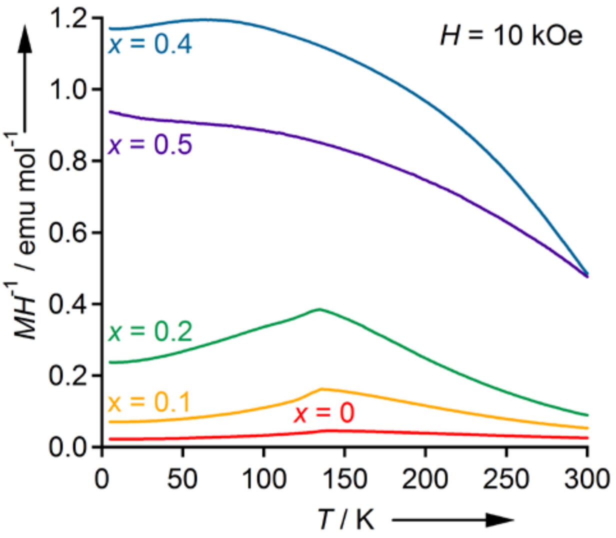


Figure 1. Temperature dependence of magnetic susceptibility for $Sr(Fe_{1-x}Ni_x)O_3$ measured under 10 kOe magnetic field upon heating after zero-field cooling.

Interface Engineering of Oxygen Coordination Environment as a New Route for Exploring Functional Properties of Transition Mental Oxides

The oxygen coordination environments of the transition metals in transition metal oxides often underpin a wide variety of functional properties through crystal field splitting and magnetic interactions. It has been demonstrated that artificial heterostructures and superlattices consisting of dissimilar oxides provide a good platform on which structural distortions associated with changes in metal-oxygen bonds, namely, the oxygen coordination environments, can be engineered. We show that the oxygen coordination environment (or the Ru-O-Ru bond angle) in SRO can be interfacially controlled by inserting a very thin CSTO layer (0-4 monolayers thick) into the SRO/GSO heterointerface. Our aberration-corrected scanning transmission electron microscopy (STEM) observations reveal that the Ru-O-Ru bond angle in the entire SRO layer is controlled through the Ru-O-Ti bond angle, which is determined by the oxygen position at the SRO/CSTO interface. More importantly, the Ru-O-Ti bond angle (or the interfacial oxygen position) can be engineered by layer-by-layer control of the thickness of the CSTO buffer layer that stabilizes the oxygen coordination environment, a Ru-O-Ru bond angle not seen in bulk SRO. Our magneto-transport characterization of the SRO/CSTO/GSO heterostructures also shows that the Ru-O-Ti bond angle plays a decisive role in magnetic anisotropy with the uniaxial magnetic easy axis of the SRO layer, highlighting the significant effect of the interfacially engineered oxygen coordination environment on the spin-orbit interaction of the SRO layer.

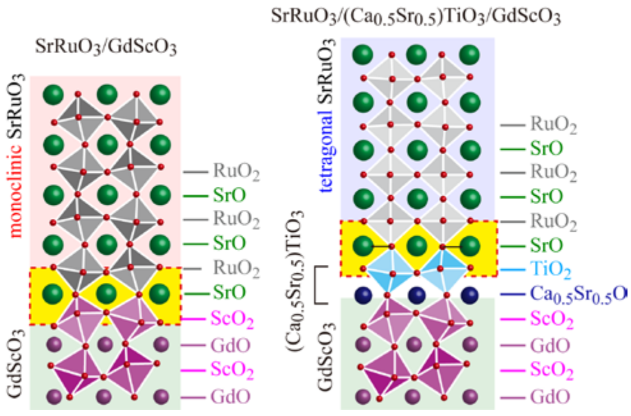


Figure 2. Interface engineering of oxygen coordination environments of perovskite $SrRuO_3$.

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Scope of Research

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

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

Selected Publications

Takeuchi, K.; Taguchi, H.; Tanigawa, I.; Tsujimoto, S.; Matsuo, T.; Tanaka, H.; Yoshizawa, K.; Ozawa, F., A Square Planar Complex of Platinum(0), *Angew. Chem. Int. Ed.*, **55,** 15347-15350 (2016).

Ozawa, F.; Nakajima, Y., PNP-Pincer Type Phosphaalkene Complexes of Late Transition Metals, *Chem. Rec.*, **16,** 2314-2323 (2016).

Taguchi, H.; Sasaki, D.; Takeuchi, K.; Tsujimoto, S.; Matsuo, T.; Tanaka, H.; Yoshizawa, K.; Ozawa, F., Unsymmetrical PNP-Pincer Type Phosphaalkene Ligands Protected by a Fused-Ring Bulky Eind Group: Synthesis and Applications to Rh(I) and Ir(I) Complexes, *Organometallics*, **35,** 1526-1533 (2016).

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

Nakajima, Y.; Tsuchimoto, T.; Chang, Y.-H.; Takeuchi, K.; Ozawa, F., Reactions of [Cu(X)(BPEP-Ph)] (X = PF_6, SbF_6) with Silyl Compounds. Cooperative Bond Activation Involving Non-coordinating Anions, *Dalton Trans.*, **45,** 2079-2084 (2016).

A Square Planar Complex of Platinum(0)

The Pt(0) complex [Pt(PPh$_3$)(Eind$_2$-BPEP)] with a pyridine-based PNP-pincer-type phosphaalkene ligand (Eind$_2$-BPEP) has a highly planar geometry around Pt with Σ(Pt) = 358.6°. This coordination geometry is very uncommon for formal d^{10} complexes, and the Pd and Ni homologues with the same ligands adopt distorted tetrahedral geometries. DFT calculations reveal that both the Pt and Pd complexes are M(0) species with nearly ten valence electrons on the metals whereas their atomic orbital occupancies are evidently different from one another. The Pt complex has a higher occupancy of the atomic 6s orbital because of strong s–d hybridization due to relativistic effects, thereby adopting a highly planar geometry reflecting the shape and orientation of the partially unoccupied d$_{x2–y2}$ orbital.

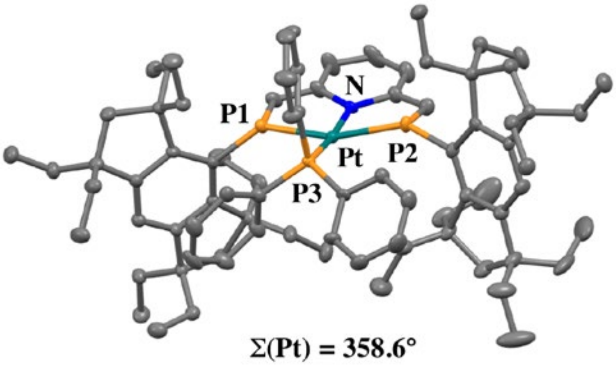


Figure 1. Molecular Structure of [Pt(PPh$_3$)(Eind$_2$-BPEP)].

Unsymmetrical PNP-Pincer Type Phosphaalkene Ligands Protected by a Fused-Ring Bulky Eind Group: Synthesis and Applications to Rh(I) and Ir(I) Complexes

Unsymmetrical PNP-pincer type phosphaalkene ligand 2-(Phospholanylmethyl)-6-(2-phosphaethenyl)pyridine (Eind-PPEP) protected by an octaethyl-*s*-hydrindacen-4-yl (Eind) group was synthesized. The fused-ring bulky Eind group successfully prevents the loss of the P=C bond and enables us to compare the reactivity of Rh(I) and Ir(I) complexes toward ammonia. The complex K[RhCl(Eind-PPEP*)], bearing a dearomatized Eind-PPEP* ligand, undergoes simple ligand displacement to give [Rh(NH$_3$)(Eind-PPEP*)], whereas the iridium analogue K[IrCl(Eind-PPEP*)] causes N–H bond cleavage to form [Ir(NH$_2$)(Eind-PPEP)]. DFT calculations indicate a thermodynamic cause of the metal-dependent product change.

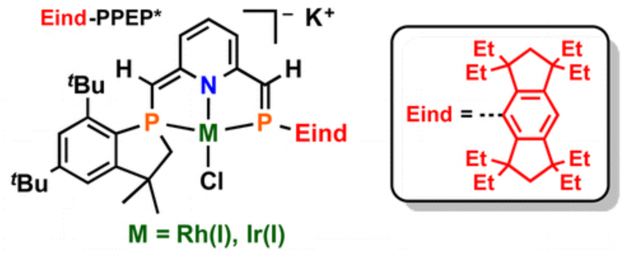
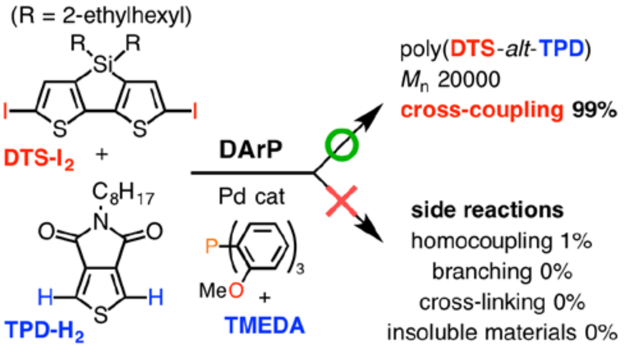


Figure 2. Non-innocent PNP-pincer type phosphaalkene ligand protected by a fused-bulky Eind group.

Mixed-Ligand Approach to Palladium-Catalyzed Direct Arylation Polymerization: Effective Prevention of Structural Defects Using Diamines

We found a novel mixed ligand catalyst for palladium-catalyzed direct arylation polymerization (DArP) of 2,6-diiododithienosilole (DTS-I$_2$) and thienopyrroledione (TPD-H$_2$) to give poly(DTS-*alt*-TPD). It has been documented that this monomer combination has a marked tendency to form homocoupling and branching defects in polymer chains, and the latter defects eventually lead to the formation of insoluble materials. In this study, we demonstrated that the combined use of P(*o*-MeOC$_6$H$_4$)$_3$ and TMEDA ligands effectively prevents the defect formation. The side reactions that afford structural defects constitute a sequential process triggered by the reduction of DTS-I units. TMEDA as a simple diamine effectively inhibits the reduction of DTS-I units, giving poly(DTS-*alt*-TPD) (M_n^{GPC} = 20,000) in high cross-coupling selectivity (99%).



Scheme 1.

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Scope of Research

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

KEYWORDS
Femtosecond Laser Spectroscopy
Single Photon Spectroscopy
Semiconductor Nanoparticles
Solar Cells
Perovskites

Selected Publications

Yamashita, D.; Handa, T.; Ihara, T.; Tahara, H.; Shimazaki, A.; Wakamiya, A.; Kanemitsu, Y., Charge Injection at the Heterointerface in Perovskite $CH_3NH_3PbI_3$ Solar Cells Studied by Simultaneous Microscopic Photoluminescence and Photocurrent Imaging Spectroscopy, *J. Phys. Chem. Lett.*, **7,** 3186-3191 (2016).

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

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

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

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

Biexciton Cascade Emission and Absorption Cross Section of Single Semiconductor Nanocrystals

The sequential two-photon emission process known as biexciton cascade emission is a characteristic phenomenon that occurs in photoexcited semiconductor nanocrystals (NCs). This process occurs when a biexciton state is created in the NCs; thus, the occurrence of the process is related to the photoabsorption properties of the NCs. We presented a simple equation that connects the photoabsorption of single NCs and the biexciton cascade emission. The equation is found to be independent of the quantum yields of photoluminescence (PL). With this equation and using an analysis of second-order photon correlation, the absolute absorption cross section of the single NCs could be evaluated, obtaining values on the order of 10^{-14} cm^2.

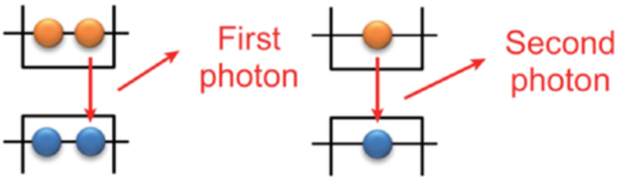

Figure 1. Schematic of the biexciton cascade emission process.

Microscopic Photoluminescence and Photocurrent Imaging of $CH_3NH_3PbI_3$ Perovskite Solar Cells

Metal halide perovskite semiconductors are attracting much attention owing to their high photovoltaic properties in solution-processed solar cells. Detailed understanding of carrier recombination and transport processes is needed to further improve the power conversion efficiency. We analyzed these processes in perovskite solar cells by microscopic imaging of time-resolved photoluminescence (TR-PL) and photocurrent (PC). Simultaneous measurements of TR-PL and PC show a positive correlation between PL intensity and PL lifetime, and a negative correlation between PL and PC intensities. We found that these correlations are caused by the competition between the photocarrier injection from the perovskite layer to the charge transport layer and the photocarrier recombination in the perovskite layer.

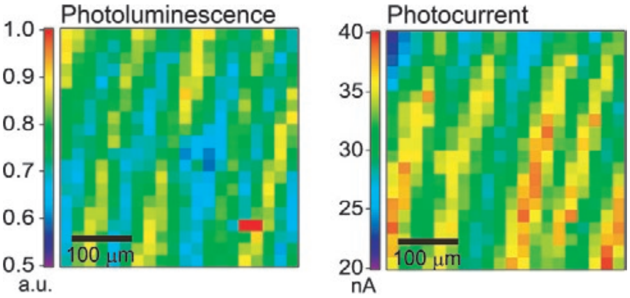

Figure 2. Microscopic image of photoluminescence and photocurrent intensities in perovskite solar cell.

Free Carriers Versus Excitons in $CH_3NH_3PbI_3$ Perovskite Thin Films at Low Temperatures

Organometal halide perovskites are an excellent class of materials for developing cost-effective electronic devices including solar cells, light-emitting diodes, and lasers. Therefore, insightful knowledge of photocarrier recombination dynamics in perovskites, which determines fundamentally performance of perovskite-based devices, is important. We investigated the dynamic responses of photocarriers in $CH_3NH_3PbI_3$ ($MAPbI_3$) thin films at low temperatures using various time-resolved laser spectroscopy. The spectroscopic data consistently indicate that the high-temperature tetragonal phase remains in $MAPbI_3$ films. We observed a fast charge transfer from the major orthorhombic phase to the minor tetragonal phase, which likely prevents the formation of excitons in the orthorhombic phase. Thus, the photocarrier recombination dynamics in two phases could be described by a free-carrier model, rather than an exciton model, even at low temperatures.

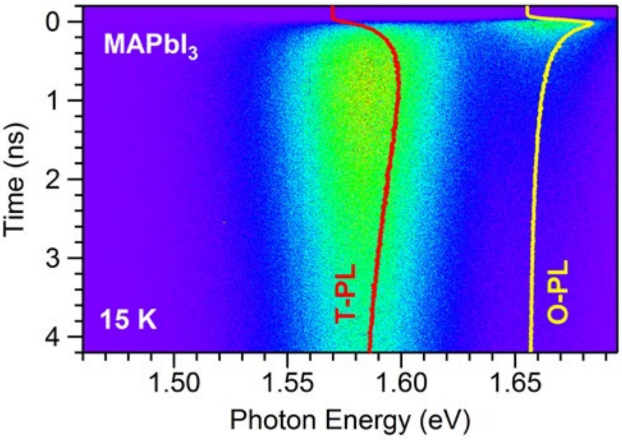

Figure 3. Two-dimensional contour image of a time-resolved photoluminescence spectrum of $MAPbI_3$ thin films at 15 K.

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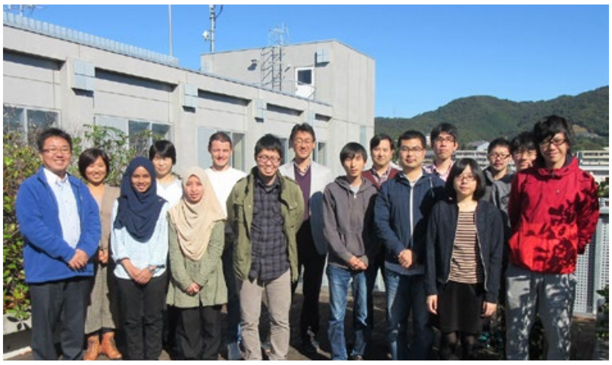
Scope of Research

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



KEYWORDS
GenomeNet
Environmental Genomics
Molecular Evolution
Bioinformatics
Virology

Selected Publications

Blanc-Mathieu, R.; Ogata, H., DNA Repair Genes in the Megavirales Pangenome, *Curr. Opin. Microbiol.*, **31,** 94-100 (2016).
Mihara, T. *et al.*, Linking Virus Genomes with Host Taxonomy, *Viruses*, **8,** 66 (2016).
Moriya, Y. *et al.*, Identification of Enzyme Genes Using Chemical Structure Alignments of Substrate-product Pairs, *J. Chem. Inf. Model.*, **56,** 510-516 (2016).
Guidi, L. *et al.*, Plankton Networks Driving Carbon Export in the Oligotrophic Ocean, *Nature*, **532,** 465-470 (2016).

Diversity of the Giant Virus Family Megaviridae

Megaviridae is a proposed family of eukaryotic viruses classified in the group of nucleocytoplasmic large double-stranded DNA viruses (NCLDVs). They possess large genomes and atypical gene contents as compared to other viruses. Genomic data suggest that the diversity of Megaviridae is vast and perhaps greater than that of cellular organisms. In the present work, we aimed at characterizing the diversity of Megaviridae at a single site using high-throughput sequencing analysis of PCR-amplified DNA polymerase family B (PolB) gene.

PolB was chosen as a marker gene for PCR amplification. PolB is encoded in all available Megaviridae genome sequences. Its high level of divergence makes it impossible to design a single PCR primer pair that would amplify all Megaviridae PolB sequences observed in current metagenomic data. To overcome this limitation we designed 82 degenerate primer pairs that target a conserved domain of PolB based on 923 PolB sequences from isolated Megaviridae and environmental Megaviridae. *In silico* tests demonstrated that this set of primer pairs specifically covers 97.4% of the 923 PolB sequences.

We first experimentally tested a subset of 34 primer pairs on environmental DNA extracted from water samples collected at the sea surface of Osaka bay. PCR-products (n=34) were sequenced with Illumina MiSeq to produce paired-end reads. The reads were quality trimmed, merged and clustered by 100% identity threshold. Representative sequences of the clusters were then searched for homology against a reference database containing PolB sequences of cellular organisms and viruses. Then, PolB sequences from all primer pairs were pooled together and aligned. The alignment was trimmed so that the amplicon sequences were well aligned at their both ends. As a result, we obtained 3,400,247 high quality merged reads. All the PolB fragments were predicted to be of Megaviridae origin by a phylogenetic analysis using pplacer.

We clustered all PolB amplicon sequences into operational taxonomic units (OTUs) at 97% identity cutoff. The number of OTUs reached near saturation at 5,000 OTUs (Figure 1), suggesting that even a single sea water sample contains diverse viruses of Megaviridae.

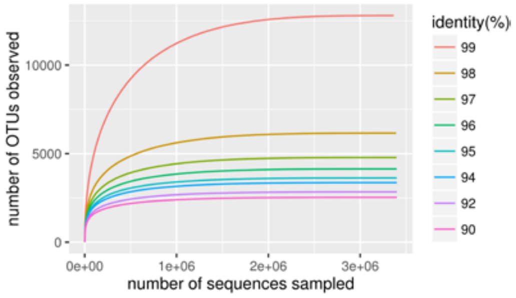


Figure 1. Rarefaction curve for the number of OTUs. Singleton OTUs are excluded.

A Characterization of the Genome of XacN1, a Jumbo Phage Infecting the Citrus Canker Agent Xanthomonas Citri

There is an increasing interest in the use of phages for controlling plant-pathogenic bacteria in agricultural activities. *Xanthomonas citri* is the bacterial pathogen of citrus canker disease, which is one of the serious citrus plant diseases and leads to significant economic damages worldwide. XacN1 is a bacteriophage that infects *X. citri.* Electron microscopic analysis revealed XacN1 is a large myovirus composed of an icosahedral head of 140 nm in diameter with a 145 nm contractile tail. XacN1 has the second largest double stranded DNA genome (384 kb) among sequenced phages. Its interesting structural feature is the presence of 65 kb direct repeats at the extremities of the linear genome, likely serving for genome replication.

We predicted 592 open reading frames (ORFs) in the XacN1 genome. Homology search revealed that the ORFs include important genes such as genes involved in replication, translation system, and those encoding structural proteins. The genome was found to encode a surprisingly large number of tRNA genes, i.e., 58 tRNAs corresponding to all the twenty amino acids and suppressor tRNAs. The tRNAs showed a significant tendency: codons highly used by the phage were less frequently used by the host bacterium and vice versa. Phylogenetic tree reconstructions of structural proteins indicate that four myoviruses and XacN1 with genome size >300 kb form a clade (Figure 2). Further analysis of the XacN1 genome will lead to uncover yet unidentified unique evolutionary and functional properties of giant phages.

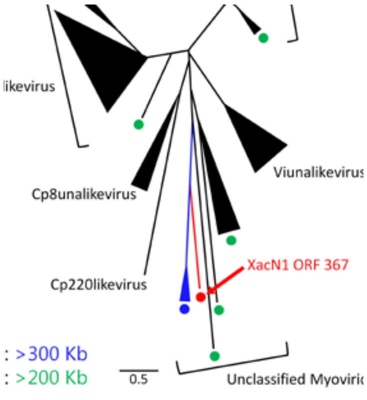


Figure 2. Maximum likelihood phylogenetic tree of tail sheath proteins. Blue and green circles indicate phages with a genome greater than 300 kb and 200 kb, respectively.

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JIRA, Jindalertudomdee
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LI, Ruiming (M1)
CAO, Yu (RS)
PI, Wenya (RS)

Guest Scholars

VINCHENT, Alexandra	University of Montpellier, France, 20 April−16 July
HOU, Wenpin (Ph D)	The University of Hong Kong, China, P.R., 23 May−22 August

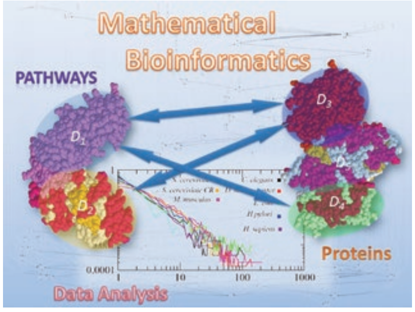
Guest Res Assoc

YANG, Jinn-Moon (Ph D)	National Chiao Tung University, Taiwan, 4 February−4 May
CHENG, Xiaoqing (Ph D)	The University of Hong Kong, China, P.R., 6 March−3 April

Scope of Research

Due to rapid progress of genome sequencing technology, whole genome sequences of organisms ranging from bacteria to human have become available. In order to understand the meaning behind the genetic code, we have been developing algorithms and software tools for analyzing biological data based on advanced information technologies such as theory of algorithms, artificial intelligence, and machine learning. We are currently studying the following topics: systems biology, scale-free networks, protein structure prediction, inference of biological networks, chemo-informatics, and discrete and stochastic methods for bioinformatics.

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



Selected Publications

Hou, W.; Tamura, T.; Ching, W. K.; Akutsu, T., Finding and Analyzing the Minimum Set of Driver Nodes in Control of Boolean Networks, *Advances in Complex Systems*, **19,** 1650006 (2016).

Takemoto, K.; Akutsu, T., Analysis of the Effect of Degree Correlation on the Size of Minimum Dominating Sets in Complex Networks, *PLoS ONE*, **11,** e0157868 (2016).

Jindalertudomdee, J.; Hayashida, M.; Akutsu, T., Enumeration Method for Structural Isomers Containing User-defined Structures Based on Breadth-first Search Approach, *J. Comput. Biol.*, **23,** 625-640 (2016).

Ishitsuka, M.; Akutsu, T.; Nacher, J. C., Critical Controllability in Proteome-wide Protein Interaction Network Integrating Transcriptome, *Sci. Rep.*, **6,** 23541 (2016).

Enumeration Method for Structural Isomers Containing User-defined Structures Based on Breadth-first Search Approach

Enumeration of chemical structures is useful for discovering new compounds and drugs, and elucidating chemical structures from mass spectrometry. We previously developed efficient algorithms, BfsSimEnum, BfsMulEnum, BfsBenNaphEnum for enumerating tree-like chemical compounds without and with multiple bonds, and compounds containing rings such as benzene and naphthalene, respectively. For many instances, the algorithms were able to enumerate chemical structures faster than other existing methods.

In this study, we propose a novel efficient enumeration algorithm, BfsStructEnum, which allows users to define desired cyclic structures and enumerates all nonredundant chemical compounds containing only user-defined structures as cyclic structures from a given chemical formula.

For evaluating the performance, we confirmed that the number of enumerated structures of BfsStructEnum was the same as that of an existing method, MOLGEN for several instances. Furthermore, we also found that BfsStructEnum was significantly faster than MOLGEN. It implies that compression of cyclic structures into single nodes makes the enumeration more efficiently.

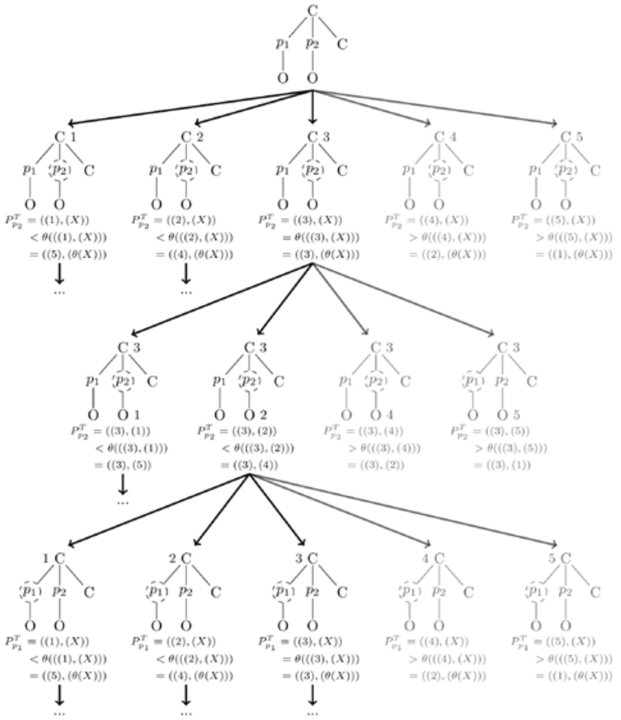


Figure 1. Example of the assignment process of atom position lists to pyridine nodes (denoted by p1 and p2).

Finding Influential Genes using Gene Expression Data and Boolean Models of Metabolic Networks

Selection of influential genes using gene expression data from normal and disease samples is an important topic in bioinformatics. In this research, we propose a novel computational method for the problem, which combines gene expression patterns from normal and disease samples with a mathematical model of metabolic networks. This method seeks a set of *k* genes knockout of which drives the state of the metabolic network towards that in the disease samples. We adopt a Boolean model of metabolic networks and formulate the problem as a maximization problem under an integer linear programming framework. We applied the proposed method to selection of influential genes using gene expression data from normal samples and disease (head and neck cancer) samples. The result suggests that the proposed method can select more biologically relevant genes than an existing *P* -value based ranking method can.

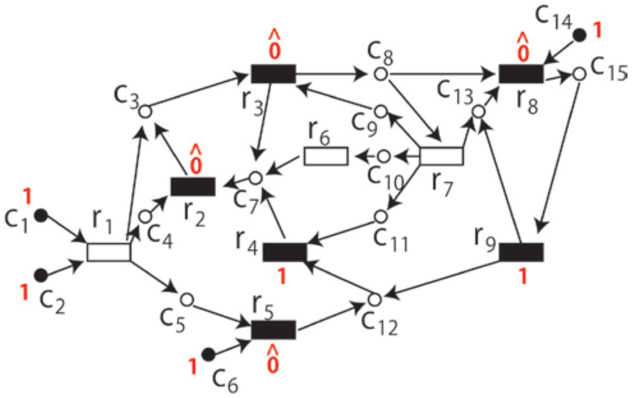


Figure 2. In Boolean metabolic networks, rectangles and circles represent reactions and metabolites, respectively. Each node is assigned either 0 or 1 to represent the status of the node.

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Assist Prof
YAMADA, Makoto
(D Statistical Science)

Program-Specific Res
WIMALAWARNE, Kishan
(D Eng)

Students

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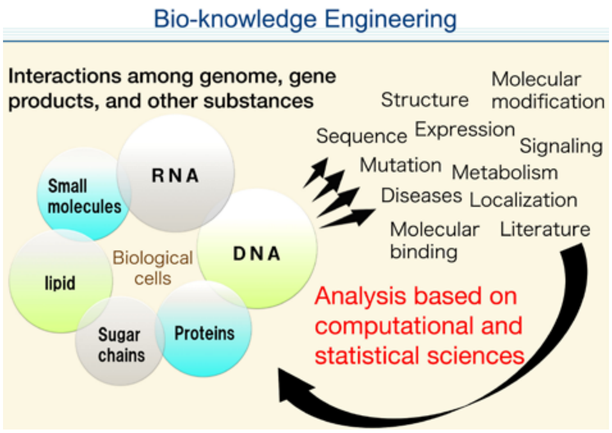
KIRIHATA, Tatsuro (UG)

Scope of Research

We are interested in graphs and networks in biology, chemistry, and medical sciences, including metabolic networks, protein-protein interactions and chemical compounds. We have developed original techniques in machine learning and data mining for analyzing these graphs and networks, occasionally combining with table-format datasets, such as gene expression and chemical properties. We have applied the techniques developed to real data to demonstrate the performance of the methods and find new scientific insights.

KEYWORDS
Bioinformatics
Computational Genomics
Data Mining
Machine Learning
Systems Biology



Selected Publications

Gao, J.; Yamada, M.; Kaski, S.; Mamitsuka, H.; Zhu, S., A Robust Convex Formulations for Ensemble Clustering, *Proceedings of the 25th International Joint Conference on Artificial Intelligence (IJCAI 2016)*, 1476-1482 (2016).

Peng, S.; You, R.; Wang, H.; Zhai, C.; Mamitsuka, H.; Zhu, S., DeepMeSH: Deep Semantic Representation for Improving Large-scale MeSH Indexing, *Bioinformatics 32 (12) (Proceedings of the 24th International Conference on Intelligent Systems for Molecular Biology (ISMB 2016))*, i70-i79 (2016).

Yuan, Q.-J.; Gao, J.; Wu, D.; Zhang, S.; Mamitsuka, H.; Zhu, S., DrugE-Rank: Improving Drug-Target Interaction Prediction of New Candidate Drugs or Targets by Ensemble Learning to Rank, *Bioinformatics 32 (12) (Proceedings of the 24th International Conference on Intelligent Systems for Molecular Biology (ISMB 2016))*, i18-i27 (2016).

Mohamed, A.; Nguyen, C. H.; Mamitsuka, H., NMRPro: An Integrated Web Component for Interactive Processing and Visualization of NMR Spectra, *Bioinformatics*, **32,** 2067-2068 (2016).

Shinkai-Ouchi, F.; Koyama, S.; Ono, Y.; Hata, S.; Ojima, K.; Shindo, M.; duVerle, D.; Kitamura, F.; Doi, N.; Takigawa, I.; Mamitsuka, H.; Sorimachi, H., Predictions of Cleavability of Calpain Proteolysis by Quantitative Structure-Activity Relationship Analysis Using Newly Determined Cleavage Sites and Catalytic Efficiencies of an Oligopeptide Array, *Mol. Cell. Proteomics*, **15,** 1262-1280 (2016).

Nguyen, C. H.; Mamitsuka, H., New Resistance Distances with Global Information on Large Graphs, *Proceedings of the Nineteenth International Conference on Artificial Intelligence and Statistics (AISTATS 2016) (JMLR Workshop and Conference Proceedings,51)*, 639-647 (2016).

Ultra High-Dimensional Nonlinear Feature Selection for Big Biological Data

Life sciences are going through a revolution thanks to the possibility to collect and learn from massive biological data. Efficient processing of such “big data” is extremely important for many medical and biological applications, including disease classification, biomarker discovery, and drug development. The complexity of biological data is dramatically increasing due to improvements in measuring devices such as next-generation sequencers, microarrays and mass spectrometers. As a result, we must deal with data that includes many observations (hundreds to tens of thousands) and even larger numbers of features (thousands to millions). Machine learning algorithms are charged with learning patterns and extracting actionable information from biological data. These techniques have been used successfully in various analytical tasks, such as genome-wide association studies and gene selection.

However, the scale and complexity of big biological data pose new challenges to existing machine learning algorithms. There is a trade-off between scalability and complexity: linear methods scale better to large data, but cannot model complex patterns. Nonlinear models can handle complex relationships in the data but are not scalable to the size of current datasets. In particular, learning nonlinear models requires a number of observations that grows exponentially with the number of features. Biological data generated by modern technology has as many as millions of features, making the learning of nonlinear models unfeasible with existing techniques. To make matters worse, current nonlinear approaches cannot take advantage of distributed computing platforms.

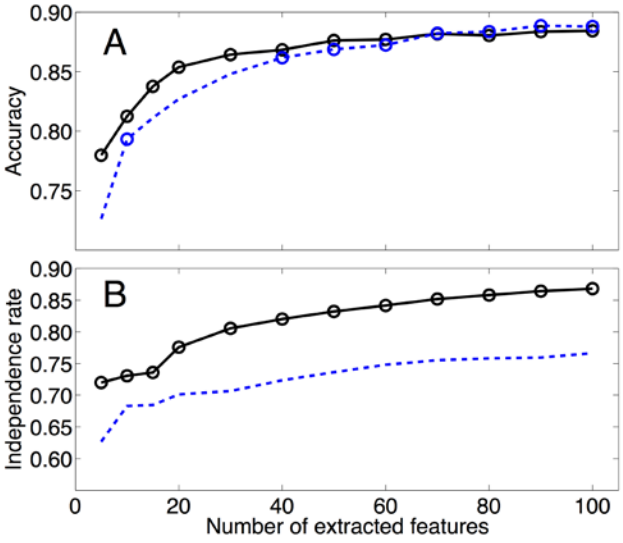


Figure 1. Results for the enzyme dataset. Circles indicate best accuracy/ independence rate according to t-tests ($p<0.05$). Differences in accuracy are significant for m=5,20,30,40. (B)~Independence rate vs. m: all differences are significant.

A promising approach to make nonlinear analysis of big biological data computationally tractable is to reduce the number of features. This method is called feature selection. Biological data is often represented by matrices where rows denote features and columns denote observations. Feature selection aims to identify a subset of features (rows) to be preserved, while eliminating all others.

Here we propose a novel feature selection framework for big biological data that makes it possible for the first time to identify very few relevant, non-redundant features among millions. The proposed method is based on two components: Least Angle Regression (LARS), an efficient feature selection method, and the Hilbert-Schmidt Independence Criterion (HSIC), which enables the selection of features that are non-linearly related. These properties are combined to obtain a method that can exploit nonlinear feature dependencies efficiently, and furthermore enables distributed implementation on commodity cloud computing platforms. We name our algorithm Least Angle Nonlinear Distributed (LAND) feature selection. Through experiment on a large and high-dimensional dataset (million features with tens of thousand samples), we show that our approach can find a set of independent features without losing classification accuracy (Figure 1 A and B). Moreover, the result is achieved in hours of cluster computing time (Figure1 C). The selected features are relevant and non-redundant, making it possible to obtain accurate and interpretable models that can be run on a laptop computer.

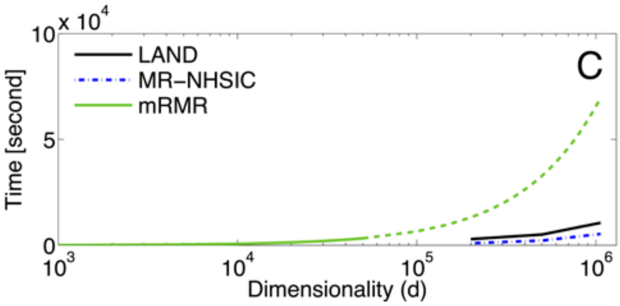


Figure 2. Computation time of feature selection algorithms. We ran the algorithms on reduced-dimensionality datasets. We estimated the mRMR runtime for d> 50,000, given that it scales linearly with d (dotted line).

HAKUBI RESEARCHERS' ACTIVITIES IN ICR

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

Research Topic

Algorithmic Graph Theory with Applications to Bioinformatics

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JANSSON, Jesper
(Ph D)

Host Laboratory Laboratory of Mathematical Bioinformatics
Host Professor AKUTSU, Tatsuya

Outline of Research

This year, my research collaborators and I have continued our work on efficient algorithms for computing different types of consensus trees. Given an input consisting of k phylogenetic trees with n leaves each and with identical leaf label sets, the running times of our algorithms are:

- O(k n) time [majority rule consensus tree],
- O(k n) time [loose consensus tree],
- O(k n^2) time [greedy consensus tree],
- min{O(k n^2), O(k n (k + log^{2} n))} time [frequency difference consensus tree],
- O(k n log n) [Adams consensus tree],
- O(n^2) [R* consensus tree with k=2],
- O(n^2 log^{4/3} n) [R* consensus tree with k=3],
- O(n^2 log^{k+2} n) [R* consensus tree with k>3],
- O(k n^3 + 2.733^n) [minimally resolved local consensus tree], and
- O(k n^3 + 4^n poly(n)) [minimally rooted-triplet-inducing consensus tree].

ACTIVITIES OF JOINT USAGE/RESEARCH CENTER

JURC Cooperative Research Subjects 2016

(1 April 2016 ~ 31 March 2017)

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

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

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

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

Feasibility Study of Deuteron Beam for Compact Neutron Sources
HIROTA, Katsuya, Graduate School of Science, Nagoya University
Host in JURC IWASHITA, Yoshihisa

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

Fundamental Research on Compact Neutron Source with Permanent Magnet
OHNUMA, Masato, Division of Quantum Science and Engineering Faculty of Engineering, Hokkaido University
Host in JURC IWASHITA, Yoshihisa

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

Development of a Novel 3d Metal Catalyst Bearing a M-E Bond as a Key Active Site
NAKAJIMA, Yumiko, Interdisciplinary Research Center for Catalytic Chemistry, National Institute of Advanced Industrial Science and Technology
Host in JURC OZAWA, Fumiyuki F

Dielectric Function and Excitonic Effect of Dynamical Screening in Semiconducting Materials for Photoelectric Conversion
SUZUURA, Hidekatsu, Graduate School of Engineering, Hokkaido University
Host in JURC KANEMITSU, Yoshihiko

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

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

Development of Synthetic Organic Reactions Mediated by Low-valent Fe Complexes of N-heterocyclic Carbenes
OHKI, Yasuhiro, Department of Chemistry, Graduate School of Science, Nagoya University
Host in JURC NAKAMURA, Masaharu

Development of Transition metal Complexes Based on Controlled Coordination Ability of NHC
YAMAGUCHI, Yoshitaka, Faculty of Engineering, Division of Materials Science and Chemical Engineering, Yokohama National University
Host in JURC NAKAMURA, Masaharu

Precise Separation and Characterization of Novel Thiolate Protected Metal Clusters by Using LC/MS
NEGISHI, Yuichi, Faculty of Science, Department of Applied Chemistry, Tokyo University of Science
Host in JURC TAKAYA, Hikaru

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

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

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

Biological Molecular Interaction Data Analysis Using Auxiliary Information
SHIGA, Motoki, Informatics Course, Department of Electrical, Electronic and Computer Engineering, Faculty of Engineering, Gifu University
Host in JURC MAMITSUKA, Hiroshi I

I : International Joint Research
F : Female PI

Total Synthesis of Dendrochrysanene
KURAMOCHI, Koji, Graduate School of Life and Environmental Sciences, Kyoto Prefectural University
Host in JURC KAWABATA, Takeo

Polymer Nano-architectonics for Bridging a Gap between Macroscopic Interfacial Phenomena and Molecular Function
NAKANISHI, Waka, MANA, National Institute for Materials Science
Host in JURC SAKAKIBARA, Keita F

Precursor Approach towards Controlled Preparation of Organic Heterojunction Layers
SUZUKI, Mitsuharu, Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST)
Host in JURC MURATA, Yasujiro

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

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

Simulation of Photoacoustic Signals Generated by Gold Nanoparticles
OKAWA, Shinpei, National Defense Medical College
Host in JURC TERANISHI, Toshiharu

Kinetic Analysis of Hydrogen Absorption Process Observed on Shape-controlled Pd Nanoparticles
YAMAUCHI, Miho, International Institute for Carbon-Neutral Energy Research, Kyushu University
Host in JURC TERANISHI,Toshiharu F

Preparation and Evaluation of Colorful Dye-Sensitized Solar Cell Devices Using Designed Anthocyanins and Their Theoretical Studies toward Improvement of the Efficiency
YOSHIDA, Kumi, Department of Complex Systems Science, Graduate School of Information Science, Nagoya University
Host in JURC MURATA, Yasujiro; WAKAMIYA, Atsushi F

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

EXPANDING SUBJECTS (IN SPECIFIC FIELDS CHOSEN BY JURC)

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

Study for High-repetition Electron/Ion Generation with High Power Laser
ARIKAWA, Yasunobu, Institute of Laser Engineering, Osaka University
Host in JURC INOUE, Shunsuke

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

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

X-ray Structural Biology Study of Flavin Reductase Involved in Resorcinol Catabolism
OIKAWA, Tadao, Faculty of Chemistry, Materials and Bioengineering, Kansai University
Host in JURC FUJII, Tomomi

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

Construction and Functionality of Phosphasilene and Silanethione at Transition-metals
OKAZAKI, Masaaki, Graduate School of Science and Technology, Hirosaki University
Host in JURC OZAWA, Fumiyuki

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

Development of Cooperative Asymmetric Pincer-Fe Catalyst
ARAI, Takayoshi, Department of Chemistry, Graduate School of Science, Chiba University
Host in JURC NAKAMURA, Masaharu

Elucidation of Electronic Structures of Cycloparaphenylenes and Their Application to Materials Science
UCHIYAMA, Masanobu, Graduate School of Pharmaceutical Science, The University of Tokyo
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

MiSeq Amplicon Analysis of Megaviridae DNA Polymerase
YOSHIDA, Takashi, Graduate School of Agriculture, Kyoto University
Host in JURC OGATA, Hiroyuki

Comparative Population Genomics of Parmales
KUWATA, Akira, Tohoku National Fisheries Research Institute
Host in JURC OGATA, Hiroyuki

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

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

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

Exploration of Novel Charge Transport Materials for Perovskite Solar Cell via Direct Evaluation of Charge Transfer Process
SAEKI, Akinori, Graduate School of Engineering, Osaka University
Host in JURC WAKAMIYA, Atsushi

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

A Study of Roll-off Mechanisms of External Quantum Efficiency of Organic Light-emitting Diodes Based on Thermally-assisted Delayed Fluorescent Materials
NAITO, Hiroyoshi, Department of Electronics, University of Osaka Prefecture
Host in JURC KAJI, Hironori

Making of the Vertical Cross Section of Bioactive Trace Metals in the East China Sea
NAKAGUCHI, Yuzuru, Faculty of Science and Engineering, Kindai University
Host in JURC SOHRIN, Yoshiki

Structural Analysis of Mixed Oxide Nanoparticles Protected by Organic Compounds and Their Magnetic Properties
HARADA, Masafumi, Faculty of Human Life and Environment, Nara Women’s University
Host in JURC TERANISHI, Toshiharu

Examination of Randomness of Lithium Silicate Glasses using Light-scattering Spectroscopy
KOREEDA, Akitoshi, Department of Physical Science, College of Science and Engineering, Ritsumeikan University
Host in JURC MASAI, Hirokazu

Stress-Optical Law for Polymeric Liquids under High Shear
MASUBUCHI, Yuichi, National Composite Center, Nagoya University
Host in JURC MATSUMIYA, Yumi I

Dynamics of Entanglements between Polymer Networks by Contrast Variation Optical-rheometry
KATASHIMA, Takuya, Graduate School of Science, Osaka University
Host in JURC MATSUMIYA, Yumi

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

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

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

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

Chemical Biology of Endogenous Vitamin D Derivatives
KITTAKA, Atsushi, Faculty of Pharma Sciences, Teikyo University
Host in JURC UESUGI, Motonari

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

Study of Tunnel Magnetoresistance Effect of the Magnetic Insulator Films with Perpendicular Magnetic Anisotropy for Development of High Spin Polarized Current Source
TANAKA, Masaaki, Department of Engineering Physics, Electronics and Mechanics, Nagoya Institute of Technology
Host in JURC ONO, Teruo

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

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

Precise Analysis for Brill Transition of Polyurea
MATSUBA, Go, Graduate School of Science and Engineering, Yamagata University
Host in JURC NISHIDA, Koji

Physical and Structural Properties of Glass-ceramics Fabricated at High Temperatures and High Pressures
MASUNO, Atsunobu, Institute of Industrial Science, The University of Tokyo
Host in JURC SHIMAKAWA, Yuichi

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

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

Au Nanoparticle Single-electron Transistors by Using Four-legs Sb-porphyrin and Three-legs Phenol as Ligand and Anchor and Vice Versa
MAJIMA, Yutaka, Materials and Structures Laboratory, Tokyo Institute of Technology
Host in JURC TERANISHI, Toshiharu

Molecular Structure Determination by Combination of Spectroscopy and Chemometrics
SHIMADA, Toru, Faculty of Education, Hirosaki University
Host in JURC HASEGAWA, Takeshi

In-situ Observation of Interfacial Chemical Reaction Using Polarization Modulation Infrared Reflection Adsorption Spectroscopy
HAMA, Tetsuya, Institute of Low Temperature Science, Hokkaido University
Host in JURC HASEGAWA, Takeshi

Development of a Prediction Method Using Cell Penetrating Peptides for Anticancer Effects on a New Anticancer Drug "PARP inhibitors"
OKUDA, Akiko, Graduate School of Health Sciences, Niigata University
Host in JURC FUTAKI, Shiroh F

Construction of Novel Cell-penetrating Peptides that Have Retentivity in Blood
KUWATA, Keiko, Institute of Transformative Bio-Molecules, Nagoya University
Host in JURC FUTAKI, Shiroh F

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

Preparation of Sm-doped Amorphous Materials for Radiophotoluminescence Applications
OKADA, Go, Graduate School of Materials Science, Nara Institute of Science and Technology
Host in JURC MASAI, Hirokazu

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

Viscoelastic Relaxation of Linear and Ring Rouse Chains at Association/Dissociation Equilibrium
KWON, Youngdon, School of Chemical Engineering, Sungkyunkwan University
Host in JURC MATSUMIYA, Yumi I

Preparation and Mechanical Properties of Noncovalent-Bonded Soft Elastomers
NORO, Atsushi, Graduate School of Engineering, Nagoya University
Host in JURC WATANABE, Hiroshi

Synthesis of Metal Complexes Bearing Chiral Multidentate Carboxylic Acid Ligands and Application to Catalytic Reactions
SUGIURA, Masaharu, Faculty of Life Sciences, Kumamoto University
Host in JURC NAKAMURA, Masaharu

EXPANDING SUBJECTS (ON-DEMAND FROM RELATED COMMUNITIES)

Prevention of NASH-induced Cancer Progression by SREBP Inhibitors
NAKAGAWA, Hayato, The University of Tokyo Hospital
Host in JURC UESUGI, Motonari

Developments of Novel Spintornics Materials with Ferrimagnetic Spinel Ultrathin Films
NAGAHAMA, Taro, Laboratory of Advanced Materials Chemistry, Graduate School of Engineering, Hokkaido University
Host in JURC ONO, Teruo

Electric Field Induced Magnetic Domain Wall Motion
CHIBA, Daichi, School of Engineering, The University of Tokyo
Host in JURC ONO, Teruo

Relationship between Molecular Motions and Triplet Lifetime in Amorphous Materials
HIRATA, Shuzo, Department of Materials Science and Engineering, Tokyo Institute of Technology
Host in JURC KAJI, Hironori

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

Functional Analysis of the Bound D-Amino Acids in Food Proteins
OHMORI, Taketo, Department of Biomedical Engineering, Osaka Institute of Technology
Host in JURC KURIHARA, Tatsuo

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

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

Exploration of Novel Functional Properties of Transition Metal Oxides Using Ionic Liquid Gating
HATANO, Takafumi, Department of Crystalline Materials Science, Nagoya University
Host in JURC KAN, Daisuke

Research on Physical Properties and Functions of Complex Iron Oxide Thin Films
FUJII, Tatsuo, Graduate School of Natural Science and Technology, Okayama University
Host in JURC SAITO, Takashi

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

Toward Long Spin Coherence Time of NV Center by High Quality Diamond Growth
TOKUDA, Norio, Faculty of Electrical and Computer Engineering, Institute of Science and Engineering, Kanazawa University
Host in JURC MIZUOCHI, Norikazu

Electrical Control of Spin of NV Center
YAMASAKI, Satoshi, Power Electronics Research Center, National Institute of Advanced Industrial Science and Technology
Host in JURC MIZUOCHI, Norikazu

Development of Nanoarchitectures Formed from Composites of Magnetic Metal Complexes with Diblock Copolypeptitde Amphiphiles and Their Application for Magnetic Probes
KUROIWA, Keita, Department of Nanoscience, Sojo University
Host in JURC SASAMORI, Takahiro

Structural Analysis of Chiral Lithium Binaphtholate Complex and Development of Novel Catalysts
NAKAJIMA, Makoto, Faculty of Life Sciences, Kumamoto University
Host in JURC KAWABATA, Takeo

Mechanistic Studies of Hydrogen Transfer Ability of Aliphatic Amines and Application to Related Reactions
KOTANI, Shunsuke, Priority Organization for Innovation and Excellence, Kumamoto University
Host in JURC FURUTA, Takumi

SUBJECTS FOCUSING OF JOINT USAGE OF JURC/ICR FACILITIES

Correlation between Melting Point and Crystalline Structure of Ionic Liquid-polymer Gel Electrolyte Dependent on Concentration of Lithium Salt
OSAKA, Noboru, Department of Chemistry, Graduate School of Science, Okayama University of Science
Host in JURC TOSAKA, Masatoshi

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

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

Synthesis and Structural Elucidation of Unsaturated Compounds of Group 14 Elements
MATSUO, Tsukasa, Faculty of Science and Engineering, Kindai University
Host in JURC TOKITOH, Norihiro

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

Studies on Structure-property Relationship of Pyrylium Salts
NAGAHORA, Noriyoshi, Department of Chemistry, Faculty of Science, Fukuoka University
Host in JURC SASAMORI, Takahiro

STEM-EELS Measurement of a Plasmonic Full Bandgap and Cavity Modes
HATA, Satoshi, Interdisciplinary Graduate School of Engineering Sciences, Kyushu University
Host in JURC KURATA, Hiroki

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

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

Study on Novel Supramolecular Assemblies Using High-resolution Mass Spectrometry
YAMANAKA, Masamichi, Faculty of Science, Department of Chemistry, Shizuoka University
Host in JURC TAKAYA, Hikaru

Novel Synthesis of Metal Clusters Protected with Organic Ligands and Determination of Their Compositions
KOYASU, Kiichirou, Department of Chemistry, Graduate School of Science, The University of Tokyo
Host in JURC TAKAYA, Hikaru

Development of Direct Visualization Methods of Steroid Hormones by Imaging Mass Spectrometry
HATANO, Osamu, Department of Anatomy and Cell Biology, Nara Medical University
Host in JURC ISOZAKI, Katsuhiro

SUBJECTS ENCOURAGING JOINT PROGRAM

Research Collaborations Aiming for a New Paradigm in Oxide Electronics
HITOSUGI, Taro, School of Materials and Chemical Technology, Tokyo Institute of Technology
Host in JURC KAN, Daisuke

Modification of Cell-penetrating Peptides for the Effective Delivery of Molecules into the Cells
BÁNÓCZI, Zoltán, Department of Organic Chemistry, Eötvös Loránd University of Sciences, Hungary
Host in JURC FUTAKI, Shiroh I

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

Clarification of the Relationship between Layered Oxide Structure and Its Magnetic Property
SUZUKI, Furitsu, School of Chemical Sciences, The University of Auckland
Host in JURC KAJI, Hironori I

JURC Publications (Selected Examples)

(until 31 May 2016)

Purely Organic Electroluminescent Material Realizing 100% Conversion from Electricity to Light

Kaji, H.; Suzuki, H.; Fukushima, T.; Shizu, K.; Suzuki, K.; Kubo, S.; Komino, T.; Oiwa, H.; Suzuki, F.; Wakamiya, A.; Murata, Y.; Adachi, C., *Nat. Commun.*, **6,** [8476-1]-[8476-8] (2015).

Abstract

Efficient organic light-emitting diodes have been developed using emitters containing rare metals, such as platinum and iridium complexes. However, there is an urgent need to develop emitters composed of more abundant materials. Here we show a thermally activated delayed fluorescence material for organic light-emitting diodes, which realizes both approximately 100% photoluminescence quantum yield and approximately 100% up-conversion of the triplet to singlet excited state. The material contains electron-donating diphenylaminocarbazole and electron-accepting triphenyltriazine moieties. The typical trade-off between effective emission and triplet-to-singlet up-conversion is overcome by fine-tuning the highest occupied molecular orbital and lowest unoccupied molecular orbital distributions. The nearly zero singlet–triplet energy gap, smaller than the thermal energy at room temperature, results in an organic light-emitting diode with external quantum efficiency of 29.6%. An external quantum efficiency of 41.5% is obtained when using an out-coupling sheet. The external quantum efficiency is 30.7% even at a high luminance of 3,000 $\mathrm{cd\,m^{-2}}$.

Photoluminescence of Monovalent Indium Centres in Phosphate Glass

Masai, H.; Yamada, Y.; Okumura, S.; Yanagida, T.; Fujimoto, Y.; Kanemitsu, Y.; Ina, T., *Sci. Rep.*, **5,** 13646 (2015).

Abstract

Valence control of polyvalent cations is important for functionalization of various kinds of materials. Indium oxides have been used in various applications, such as indium tin oxide in transparent electrical conduction films. However, although metastable In^+ ($5s^2$ configuration) species exhibit photoluminescence (PL), they have attracted little attention. Valence control of In^+ cations in these materials will be important for further functionalization. Here, we describe In^+ species using PL and X-ray absorption fine structure (XAFS) analysis. Three absorption bands in the UV region are attributed to the In^+ centre: two weak forbidden bands (${}^1S_0 \rightarrow {}^3P_1$, ${}^1S_0 \rightarrow {}^3P_2$) and a strong allowed band (${}^1S_0 \rightarrow {}^1P_1$). The strongest PL excitation band cannot be attributed to the conventional allowed transition to the singlet excited state. Emission decay of the order of microseconds suggests that radiative relaxation occurs from the triplet excitation state. The XAFS analysis suggests that these In^+ species have shorter In–O distances with lower coordination numbers than in $\mathrm{In_2O_3}$. These results clearly demonstrate that In^+ exists in a metastable amorphous network, which is the origin of the observed luminescent properties.

Catalytic Discrimination between Formyl Groups in Regio- and Stereoselective Intramolecular Cross-aldol Reactions

Baba, T.; Yamamoto, J.; Hayashi, K.; Sato, M.; Yamanaka, M.; Kawabata, T.; Furuta, T., *Chem. Sci.*, **7,** 3791-3797 (2016).

Abstract

Catalytic discrimination between inequivalent formyl groups was achieved using an aniline-type acid–base catalyst for the regio-, diastereo-, and enantioselective intramolecular cross-aldol reactions of enolizable dials. Although L-proline gave a mixture of the regio- and stereoisomeric products in the presence of an *N*-containing 1,6-dial, the aniline-type catalyst afforded *anti*-3,4-disubstituted pyrrolidine in high regio-, and stereoselectivity beyond the background reaction, which led to the regioisomeric 2,3-disubstituted products. The mild reactivity of the aniline-type amine facilitated catalytic discrimination between the inequivalent formyl groups. Kinetic isotope effect studies and reductive amination experiments suggested that the regioselectivity was controlled under the enamine-forming steps.

Rhombic Coulomb Diamonds in a Single-electron Transistor Based on an Au Nanoparticle Chemically Anchored at Both Ends

Azuma, Y.; Onuma, Y.; Sakamoto, M.; Teranishi, T.; Majima, Y., *Nanoscale*, **8,** 4720-4726 (2016).

Abstract

Rhombic Coulomb diamonds are clearly observed in a chemically anchored Au nanoparticle single-electron transistor. The stability diagrams show stable Coulomb blockade phenomena and agree with the theoretical curve calculated using the orthodox model. The resistances and capacitances of the double-barrier tunneling junctions between the source electrode and the Au core (R_1 and C_1, respectively), and those between the Au core and the drain electrode (R_2 and C_2, respectively), are evaluated as 4.5 MΩ, 1.4 aF, 4.8 MΩ, and 1.3 aF, respectively. This is determined by fitting the theoretical curve against the experimental Coulomb staircases. Two-methylene-group short octanedithiols (C8S2) in a C8S2/hexanethiol (C6S) mixed self-assembled monolayer is concluded to chemically anchor the core of the Au nanoparticle at both ends between the electroless-Au-plated nanogap electrodes even when the Au nanoparticle is protected by decanethiol (C10S). This is because the R_1 value is identical to that of R_2 and corresponds to the tunneling resistances of the octanedithiol chemically bonded with the Au core and the Au electrodes. The dependence of the Coulomb diamond shapes on the tunneling resistance ratio (R_1/R_2) is also discussed, especially in the case of the rhombic Coulomb diamonds. Rhombic Coulomb diamonds result from chemical anchoring of the core of the Au nanoparticle at both ends between the electroless-Au-plated nanogap electrodes.

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

Yoshimura, Y.; Kim, K.-J.; Taniguchi, T.; Tono, T.; Ueda, K.; Hiramatsu, R.; Moriyama, T.; Yamada, K.; Nakatani, Y.; Ono, T., *Nat. Phys.*, **12,** 157-161 (2016).

Abstract

Topological defects such as magnetic solitons, vortices and skyrmions have started to play an important role in modern magnetism because of their extraordinary stability, which can be exploited in the production of memory devices. Recently, a type of antisymmetric exchange interaction, namely the Dzyaloshinskii–Moriya interaction (DMI; refs), has been uncovered and found to influence the formation of topological defects. Exploring how the DMI affects the dynamics of topological defects is therefore an important task. Here we investigate the dynamics of the magnetic domain wall (DW) under a DMI by developing a real time DW detection scheme. For a weak DMI, the DW velocity increases with the external field and reaches a peak velocity at a threshold field, beyond which it abruptly decreases. For a strong DMI, on the other hand, the velocity reduction is completely suppressed and the peak velocity is maintained constant even far above the threshold field. Such a distinct trend of the velocity can be explained in terms of a magnetic soliton, the topology of which is protected during its motion. Our results therefore shed light on the physics of dynamic topological defects, which paves the way for future work in topology-based memory applications.

VISITING PROFESSORS' ACTIVITIES IN ICR

Vis Prof
MATSUO, Yutaka
(D Sc)

Laboratory of Polymer Controlled Synthesis

Project Professor, School of Engineering, The University of Tokyo
(7-3-1 Hongo, Bunkyo-ku,Tokyo 113-8656)

Lecture at *ICR*
Materials Science of Organic Semiconductor Functionalization of Fullerene/Carbon Nanotube and Development of Organic Thin Film Solar Cell

Vis Prof
MURAYAMA, Masafumi
(D Sc)

Laboratory of Hydrospheric Environment Analytical Chemistry

Professor, Center for Advanced Marine Core Research, Kochi University
(Monobeotsu, Nankoku, Kochi 783-8502)

Lecture at *ICR*
What occurred on the Shallow and Deep Seafloor by the Great East Japan Earthquake 2011?

Vis Prof
SUGIOKA, Koji
(D Eng)

Laboratory of Laser Matter Interaction Science

Unit Leader, RIKEN-SIOM Joint Research Unit, RIKEN
(2-1 Hirosawa, Wako, Saitama 351-0198)

Lecture at *ICR*
High-performance Materials Processing by Using Manipulated Laser Beams

Vis Prof
AKIYAMA,Yutaka
(D Eng)

Laboratory of Mathematical Bioinformatics

Professor, Department of Computer Science School of Computing, Tokyo Institute of Technology
(2-12-1 Ookayama, Meguro-ku, Tokyo 152-8552)

Lecture at *ICR*
Massively Parallel Bioinformatics Computing on K-computer, TSUBAME, and Azure: Metagenome Analysis and Exhaustive Protein-protein Interaction Prediction

Vis Prof
DE LA HIGUERA, Colin Manuel
(Ph D)

Laboratory of Mathematical Bioinformatics

Professor, UFR de Sciences et Techniques, University of Nantes
(2 rue de la Houssinière, BP 92208, 44322 Nantes Cedex 03, France)

Lecture at *ICR*
Machine Learning is about Intelligent Forgetting

Vis Assoc Prof
FURUKAWA, Ko
(D Sc)

Laboratory of Structural Organic Chemistry

Associate Professor, Centre for Instrumental Analysis, Niigata University
(Nishi-ku, Niigata 950-2181)

Lecture at *ICR*
Spin Dynamics Study for Functional Materials by Advanced ESR Spectroscopy

Vis Assoc Prof
KAWANO, Ryuji
(D Eng)

Laboratory of Biofunctional Design-Chemistry

Associate Professor, Tokyo University of Agriculture and Technology
(2-24-16 Naka-cho, Koganei-shi, Tokyo 184-8588)

Lecture at *ICR*
Construction and Application of Artificial Cell Membranes Using Micro-Sized Processing Techniques

Vis Assoc Prof
TAKAHASHI, Yoshiaki
(D Eng)

Laboratory of Molecular Rheology

Associate Professor, Institute for Materials Chemistry and Engineering, Kyushu University
(6-1 Kasuga Koen, Kasuga, Fukuoka 816-8581)

Lecture at *ICR*
Dissolution Condition of Cellulose into Ionic Liquids and Characterization of the Solutions by Rheological Measurement

Vis Assoc Prof
OGAWA, Yoshihiro
(D Sc)

Laboratory of Nanophotonics

Associate Professor, Graduate School of Education, Joetsu University of Education
(1, Yamayashiki-machi, Joetsu-shi, Niigata 943-8512)

Lecture at *ICR*
Coherent Spectroscopy and its Application to the Coherent Control of Quantum States in Semiconductors

Vis Assoc Prof
ZHU, Shanfeng
(D Eng)

Laboratory of Bio-knowledge Engineering

Associate Professor, Fudan University
(No.825, Zhangheng Road, Shanghai, China)

Lecture at *ICR*
DeepMeSH and MeSHLabeler: Recent Progress in Large-scale MeSH Indexing
DrugE-Rank: Improving Drug-target Interaction Prediction of New Candidate Drugs or Targets by Ensemble Learning to Rank

Prof Em KANEHISA, Minoru (D Sc)

Appointed as Res (pt) at ICR,
1 April 2012–31 March 2017

PERSONAL

Awards

MIZUHATA, Yoshiyuki

Progress Award in Silicon Chemistry, Japan

"New Progress in the Chemistry of Aromatic Compounds Containing a Group 14 element"

The Society of Silicon Chemistry, Japan

8 October 2016

SUZUKI, Yuko

ICR Award for Graduate Students

"Isolation and Ambident Reactivity of a Chlorogermylenoid"

Institute for Chemical Research, Kyoto University

2 December 2016

SUGAHARA, Tomohiro

Best Presentation Award

The 4th Presentation of the Master's Thesis

"Synthesis and Reactivity of Stable Multiple-bond Compounds between Germanium Atoms"

Grant-in-Aid for Scientific Research on Innovative Areas, New Polymeric Materials Based on Element-Blocks

4 March 2016

ZHANG, Rui

ICR Award for Graduate Students

"Synthesis of a Distinct Water Dimer inside Fullerene C_{70}"

Institute for Chemical Research, Kyoto University

2 December 2016

UEDA, Yoshihiro

The Pharmaceutical Society of Japan, Kinki Branch

Award for Young Scientists

66th Annual Meeting of the PSJ Kinki-Branch

"Final-Stage Site-Selective Acylation for the Total Synthesis of Natural Glycosides"

The Pharmaceutical Society of Japan, Kinki-Branch

8 January 2016

LU, Wenjie

Best Presentation Award

The 136th Annual Meeting of the Pharmaceutical Society of Japan

"Preparation of Functionalized Rh Carboxylate Catalyst and Its Catalytic Activity"

The Pharmaceutical Society of Japan

31 March 2016

KASAMATSU, Koji

Best Presentation Award

The 136th Annual Meeting of the Pharmaceutical Society of Japan

"Long-Lived C-N Axially Chiral Enolate Generated from Amino Acid Derivatives"

The Pharmaceutical Society of Japan

31 March 2016

TSUJI, Yoshinobu

The Cellulose Society of Japan Award

"Fabrication of Functional Cellulosic Materials through Interfacial Chemical Approach"

The Cellulose Society of Japan

14 July 2016

SAKAKIBARA, Keita

The Young Researcher Award of The Society of Fiber Science and Technology, Japan

"Development and Application of Polymer Monolith Materials with Well-Defined Morphology and High Performance"

The Society of Fiber Science and Technology, Japan

8 June 2016

NAKAMURA, Yasuyuki

ICR Award for Young Scientists

"Termination Mechanism in the Radical Polymerization of Methyl Methacrylate and Styrene Determined by the Reaction of Structurally Well-defined Polymer End Radicals"

Institute for Chemical Research, Kyoto University

2 December 2016

MASAI, Hirokazu

International Exchange Encouragement Award: The Motoharu Kurata Award

The Ceramic Society of Japan

3 June 2016

TORIMOTO, Aya

Presentation Award for Young Scientists

Workshop on Next-generation Optical Materials and their Applications

"Emission Properties of Ce in Alkaline Earth Borate Glasses"

20 December 2016

YOSHIMURA, Yoko

President Prize of Kyoto University

"Study of Spin Dynamics in Ferromagnetic Nanowire"

Kyoto University

14 March 2016

MURAYAMA, Tomo

Travel Grant

The 34th European Peptide Symposium and the 8th International Peptide Symposium

"Membrane-remodeling Amphipathic Peptides Enhance Direct Penetration of Octaarginine"

The European Peptide Society

22 June 2016

OHKANDA, Junko

The 21st Incentive Award

"Rational Design of Synthetic Molecules that Control Protein-protein Interactions"

The Society of Japanese Women Scientists

6 April 2016

KATSUDA, Yousuke

The Best Presentation Award

The 10th Symposium on Biorelevant Chemistry

"Exploration of RNA G-quadruplex Structures by an RNA G-quadruplex Ligand"

The Chemical Society of Japan

8 September 2016

WADA, Yoshimasa

The Best Presentation Award for Young Scientists

The 22nd Regular Meeting of Japan OLED Forum

"Solution-Processable Small Molecule TADF Emitters for Highly Efficient (Host-Free) Organic Light-Emitting Diodes"

Japan OLED Forum

17 November 2016

SOHRIN, Yoshiki

2016 The Oceanographic Society of Japan Prize

The 2016 Spring Meeting of the Oceanographic Society of Japan

"Development of Precise Analytical Methods for Trace Elements and Its Application to Marine Chemistry"

The Oceanographic Society of Japan

1 April 2016

SHIMOAKA, Takafumi

2016 Young Scientist Presentation Award of The Spectroscopical Society of Japan

2016 Annual Meeting of the Spectroscopical Society of Japan

"Structural and Quantitative Analysis of Three Water Species Involved in Nafion Membrane by Using Infrared and NMR Spectroscopy"

The Spectroscopical Society of Japan

2 June 2016

SHIOYA, Nobutaka

CSJ Student Presentation Award 2016

The 96th CSJ Annual Meeting

"Experimental Optimization of IR pMAIRS by Using an Optically Isotropic Thin Film Exhibiting Berreman's Effect"

The Chemical Society of Japan

13 April 2016

Young Scientist Presentation Award

The 63rd JSAP Spring Meeting, 2016

"Structure Analysis of an Organic Semiconductor Thin Film Using IR pMAIRS"

The Japan Society of Applied Physics

13 September 2016

MORI, Kazuaki

Award for the Presentation of an Excellent Paper

The 36th Annual Meeting of the Laser Society of Japan

“Terahertz Wave Generation in the Interaction of Two-pulse Laser with Clusters”

The Laser Society of Japan

31 May 2016

Award for the Presentation of an Excellent Paper

“THz Waves Generation in the Interaction between Two-pulse Lasers and Cluster Plasmas”

The Institute of Electric Engineers of Japan

5 September 2016

TERAMOTO, Kensuke

Award for the Presentation of an Excellent Paper

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

The Institute of Electric Engineers of Japan

5 September 2016

FURUKAWA, Yuki

Award for the Presentation of an Excellent Paper

The 36th Annual Meeting of the Laser Society of Japan

“Formation of LIPSS on Titanium Irradiated by Femtosecond Double Pulse Laser~Features of Structures Produced at Delay Time from 100fs to Sub Nanosecond~”

The Laser Society of Japan

31 May 2016

HARUTA, Mitsutaka

ICR Award for Young Scientists

“Determination of Elemental Ratio in an Atomic Column by Electron Energy Loss Spectroscopy”

Institute for Chemical Research, Kyoto University

2 December 2016

YOSHIDA, Ryota

Student Presentation Award

The 61st Lignin Symposium

“Ruthenium Complex-Bound Amino Acid-Catalyzed Oxidative Degradation of Lignin and Model Compounds”

Research Institute for Sustainable Humanosphere, Kyoto University

28 October 2016

SHIMAKAWA, Yuichi;
SAITO, Takashi

Daiwa Adrian Prizes 2016

“Materials Discovery using Extreme Conditions”

Daiwa ANGLO-JAPANESE FOUNDATON

15 November 2016

HOSAKA, Yoshiteru

The Best Student Presentation Award

2016 E-MRS Fall Meeting and Exhibit

“A New Layered Double Perovskite Ca$_2$FeMnO$_6$ Showing Charge Disproportionation of Unusually High Valence Fe^{4+}”

European Materials Research Society

21 September 2016

TAHARA, Hirokazu

NF Foundation R&D Encouragement Award

“Highly Sensitive Photocurrent Spectroscopy Using Femtosecond Phase-locked Pulses and Photocurrent Generation Dynamics in Semiconductors”

NF Foundation

25 November 2016

YAMADA, Takumi

ICR Award for Graduate Students

“Dynamic Optical Properties of CH$_3$NH$_3$PbI$_3$ Single Crystals As Revealed by One- and Two-Photon Excited Photoluminescence Measurements”

Institute for Chemical Research, Kyoto University

2 December 2016

AKUTSU, Tatsuya

Fellow

2016 General Meeting of Information Processing Society of Japan

“Studies on Mathematical Models and Algorithms for Bioinformatics”

Information Processing Society of Japan

3 June 2016

NAKAJIMA, Natsu

IPSJ Yamashita SIG Research Award

“Genetic Network Completion for Static Gene Expression Data”

The Information Processing Society of Japan

10 March 2016

Paper Awards




SUGAHARA, Tomohiro;
GUO, Jing-Dong;
SASAMORI, Takahiro;
TOKITOH, Norihiro *et al.*

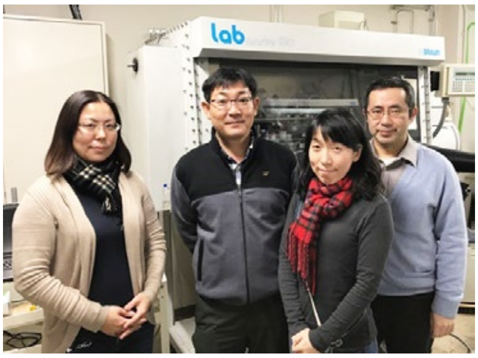
BCSJ Award Article

"Reaction of a Stable Digermyne with Acetylenes: Synthesis of a 1,2-Digermabenzene and a 1,4-Digermabarrelene"

Sugahara, T.; Guo, J.-D.; Sasamori, T.; Karatsu, Y.; Furukawa, Y.; Espinosa Ferao, A.; Nagase, S.; Tokitoh, N.

The Chemical Society of Japan

15 November 2016



WAKAMIYA, Atsushi *et al.*

The Innovative PV Award

"Perovskite Solar Cells: Elucidation of Structures and Properties of Intermediates in Solution Process and Development of Fabrication Method for Highly Efficient Cells"

Wakamiya, A.; Shimazaki, A.; Nakaike, Y.; Rafieh, A.; Jung, M.; Maruyama, N.; Aharen, T.; Murata, Y.

JSPS 175 Committee on Future Direction of Photovoltaics

20 May 2016


MORISHITA, Hiroki;
MIZUOCHI, Norikazu

38th Paper Award of the Japan Society of Applied Physics

"Perfect Selective Alignment of Nitrogen-vacancy Centers in Diamond"

Fukui, T.; Doi, Y.; Miyazaki, T.; Miyamoto, Y.; Kato, H.; Matsumoto, T.; Makino, T.; Yamasaki, S.; Tokuda, N.; Hatano, M.; Sakagawa, Y.; Morishita, H.; Tashima, T.; Miwa, S.; Suzuki, Y.; Mizuochi, N.

The Japan Society of Applied Physics

13 September 2016






KAJI, Hironori;
WADA, Yoshimasa;
SHIZU, Katsuyuki;
KUBO, Shosei;
SUZUKI, Katsuaki;
FUKUSHIMA, Tatsuya;
ADACHI, Chihaya[1]

Best Paper Award

The 23rd International Display Workshops in Conjunction with Asia Display 2016

"Design of Emitters and Charge Transporters for Highly Efficient Organic LEDs"

International Display Workshops

22 December 2016

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[1] Department of Applied Chemistry, Faculty of Engineering, Kyushu University

HASHIDA, Masaki;
MIYASAKA, Yasuhiro;
SHIMIZU, Masahiro[1];
SAKAGAMI, Hitoshi[2];
INOUE, Shunsuke;
SAKABE, Shuji

LSJ Award for Distinguished Achievements in Research

"Periodic Surface Structures Self-organized on Solid Materials Ablated by Femtosecond Laser Pulses"

The Laser Society of Japan.

31 May 2016

[1] Department of Material Chemistry, Graduate School of Engineering, Kyoto University

[2] National Institute for Fusion Science

YAMADA, Makoto

The Best Paper Award

The 9th ACM international Conference on Web Search and Data Mining (WSDM)

"Beyond Ranking: Optimizing Whole-Page Presentation"

ACM (Association for Computing Machinery)

22 February 2016

Poster Awards

FUJIMORI, Shiori

Best Poster Award

The 27th International Conference on Organometallic Chemistry (ICOMC 2016)

"Reaction of Germabenzenylpotassium with $[Cp^*RuCl]_4$: Unexpected Formation of Ruthenium-substituted Germabenzene"

21 July 2016

SUGAHARA, Tomohiro

Chemical Communications Poster Prizes

The 20th Symposium of the Society of Silicon Chemistry Japan

"Synthesis and Structure of Cyclic Compounds Containing Germanium Atoms Utilizing a Digermacyclobutene Derivative"

Royal Society of Chemistry/The Society of Silicon Chemistry Japan

8 October 2016

FUTAGOISHI, Tsukasa

27th Symposium on Physical Organic Chemistry

"Synthesis and Properties of an Open-Cage C_{60} Derivative Encapsulating Molecular Oxygen"

The Society of Physical Organic Chemistry

3 September 2016

OZAKI, Masashi

Best Poster Award, 2nd Prize

AEARU 6th Energy and Environmental Workshop

"Development of $CH_3NH_3PbI_3{\cdot}DMF$ as a Perovskite Precursor for Highly Efficient Perovskite Solar Cells"

The Association of East Asian Research Universities

27 August 2016

Best Poster Award, First Place

The 1st Frontier Solar Cells Seminar

"Fabrication of Highly Efficient Perovskite Solar Cells Using Highly Purified Precursor Material"

The 1st Frontier Solar Cells Seminar Executive Committee

18 November 2016

TSUKAO, Masahiro

Chemistry Letters Young Awards

The 10th Symposium of Organic π-Electron Systems

"Synthesis and Properties of Aluminum Complexes with π-Extended Quinolinol Ligands"

The Japanese Association for Organic π-Electron Systems

17 December 2016

KASAMATSU, Koji

Best Poster Award

42nd Symposium on Progress in Organic Reactions and Synthesis -Application in the Life Science-

"Asymmetric α-Fluorination of Amino Acid Derivatives via Racemization-Resistant C-N Axially Chiral Enolates"

Organizing Committee of 42nd Symposium on Progress in Organic Reactions and Synthesis -Application in the Life Science-

7 November 2016

OTSUKI, Haruka

Best Poster Award

Molecular Chirality Asia 2016

"Mechanistic Investigation of Stereochemical Diversity in Asymmetric Cyclization via Memory of Chirality "

Molecular Chirality Research Organization (MCRO)

23 April 2016

Best Poster Award

110th Symposium on Organic Synthesis

"Investigation of Stereochemical Diversity in Asymmetric Intramolecular Alkylation via Memory of Chirality"

The Society of Synthetic Organic Chemistry, Japan

11 November 2016

EGUCHI, Daichi

Poster Award

"Investigation of the Photochemical Behavior Between Semiconductor Quantum Dots and Porphyrin Derivatives"

The 14th Annual Meeting of The Society of Nano Science and Technology

The Society of Nano Science and Technology

15 June 2016

YAMASHITA, Kohei

Annual Meeting Poster Award 2016

65th SPSJ Annual Meeting

“Dispersibility of Polymer-brush-afforded Particles in Liquid Crystals”

The Society of Polymer Science, Japan

27 May 2016

FUJIMORI, Tomoya

The Society of Polymer Science, Japan Symposium on Macromolecules Poster Award 2016

65th Symposium on Macromolecules

“Modification of Capillary-inner Surface with Thick and Concentrated Polymer Brushes for Control of Microfluidic Flow”

The Society of Polymer Science, Japan

16 September 2016

SEKI, Toyomitsu

The Best Poster Award

The 10th International Symposium on Integrated Synthesis (ISONIS-10)

“Development of an Efficient Method for Tellurium Recovery and Recycling from Polymer-end by Using Fluorous Tellurol and Fluorous Extraction”

Organizing Committee of The 10th International Symposium on Integrated Synthesis (ISONIS-10)

19 November 2016

TORIMOTO, Aya

The Best Poster Presentation Award

The Ceramic Society of Japan Fall Meeting 2016

“Emission Properties of Ce-doped Barium Borate Glasses Prepared from Different Starting Materials”

Random Materials Session, The Ceramic Society of Japan

9 September 2016

The Best Poster Presentation Award

JSAP 77th JSAP Autumn Meeting 2016

“Study of Emission Properties of Cerium-doped Barium Borate Glasses Depending on the Starting Materials”

JSAP Ionization Radiation Division

15 September 2016

KAWANO, Kenichi

Poster Prize

The 14th Chinese International Peptide Symposium & The 5th Asia-pacific International Peptide Symposium

“Facilitated Cell Penetration of Dipicolylamine-modified R8 by Metal Complex Formation”

CPS2016 Committee

7 July 2016

AKISHIBA, Misao

Poster Prize

The 14th Chinese International Peptide Symposium & The 5th Asia-pacific International Peptide Symposium

“Modification of Natural Hemolytic Peptide Achieving Intracellular Delivery of Antibodies”

CPS2016 Committee

7 July 2016

MASUDA, Toshihiro

Award for Excellence at Poster Presentation

The 53rd Japanese Peptide Symposium

“Novel Peptide Tool to Induce Cell Movement by Affecting Membrane Tension”

The Japanese Peptide Society

27 October 2016

TAGUCHI, Hiro-omi

Poster Award

5th JACI/GSC Symposium

“Hydrosilylation of CO_2 Catalyzed by Noninnocent PNP-Pincer Type Phosphaalkene Complex with Iridium(I)”

Japan Association for Chemical Innovation (JACI)

3 June 2016

Poster Award

20th International Symposium on Homogeneous Catalysis (ISHCXX)

“Synthesis of Ir(I) and Rh(I) Complexes Bearing a Noninnocent PNP-Pincer Type Phosphaalkene Ligand (Eind-PPEP) and Their Application for Catalytic Hydrosilylation of CO_2”

ISHCXX Organizers

15 July 2016

HIROSHIGE, Nao

Region5 Poster Awards

The Physical Society of Japan 2016 Autumn Meeting

"Cascade-emission Spectroscopy on Single Giant CdSe/CdS Nanocrystals: Enhancement of Biexciton Emission through Coulomb Interaction"

The Physical Society of Japan

15 September 2016

PUBLICATIONS

INTERNATIONAL RESEARCH COLLABORATIONS

SELECTED GRANTS

THESES

PUBLICATIONS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

Agou, T.; Ikeda, S.; Sasamori, T.; Tokitoh, N., Synthesis and Structure of Lewis-Base-Free Phosphinoalumane Derivatives, *Eur. J. Inorg. Chem.*, 623-627 (2016).

Sasamori, T.; Franco, J. M. V.; Guo, J.-D.; Sugamata, K.; Nagase, S.; Streubel, R.; Tokitoh, N., Selenium-Substituted Phosphaalkenes Obtained through 1,2-Elimination of Chlorosilanes from Selenenylchlorophosphines, *Eur. J. Inorg. Chem.*, 678-684 (2016).

Klein, M.; Schnakenburg, G.; Ferao, A. E.; Tokitoh, N.; Streubel, R., Reactions of Li/Cl Phosphinidenoid Complexes with 1,3,4,5-Tetramethylimidazol-2-ylidene: A New Route to *N*-Heterocyclic Carbene Adducts of Terminal Phosphinidene Complexes and an Unprecedented Transformation of an Oxaphosphirane Complex, *Eur. J. Inorg. Chem.*, 685-690 (2016).

Guo, J.-D.; Sasamori, T.; Yamamoto, Y.; Matsubara, H.; Nagase, S.; Yorimitsu, H., Computational Picture of Silyl Transfer from Silylsilatranes to Arylpalladium Chloride, *Bull. Chem. Soc. Jpn.*, **89,** 192-194 (2016).

Tokitoh, N.; Agou, T.; Wasano, T.; Sasamori, T., Synthesis and Properties of Stable Alumoles, *Phosphorus, Sulfur and Silicon and the Related Elements*, **191,** 584-587 (2016).

Agou, T.; Nagata, K.; Sasamori, T.; Tokitoh, N., Reactivities of a Barrelene-type Dialumane as an Equivalent of an Al=Al Doubly-bonded Species, *Phosphorus, Sulfur and Silicon and the Related Elements*, **191,** 588-590 (2016).

Suzuki, Y.; Sasamori, T.; Guo, J.-D.; Nagase, S.; Tokitoh, N., Isolation and Ambident Reactivity of a Chlorogermylenoid, *Chem. Eur. J.*, **22,** 13784-13788 (2016).

Yamaguchi, K.; Murai, T.; Guo, J.-D.; Sasamori, T.; Tokitoh, N., Acid-Responsive Absorption and Emission of 5-*N*-Arylaminothiazoles: Emission of White Light from a Single Fluorescent Dye and a Lewis Acid, *ChemistryOpen*, **5,** 434-438 (2016).

Nagata, K.; Murosaki, T.; Agou, T.; Sasamori, T.; Matsuo, T.; Tokitoh, N., Activation of Dihydrogen by Masked Doubly Bonded Aluminum Species, *Angew. Chem. Int. Ed.*, **55,** 12877-12880 (2016).

Agou, T.; Yanagisawa, T.; Sasamori, T.; Tokitoh, N., Synthesis and Structure of an Iron-Bromoalumanyl Complex with a Tri-Coordinated Aluminum Center, *Bull. Chem. Soc. Jpn.*, **89,** 1184-1186 (2016).

Mizuhata, Y.; Yanagisawa, T.; Sasamori, T.; Tokitoh, N., [K(18-crown-6)][FeCp*$(CO)_2$] data, *IUCrData*, **1,** x160881 (2016).

Sugahara, T.; Guo, J.-D.; Sasamori, T.; Karatsu, Y.; Furukawa, Y.; Ferao, A. E.; Nagase, S.; Tokitoh, N., Reaction of a Stable Digermyne with Acetylenes: Synthesis of a 1,2-Digermabenzene and a 1,4-Digermabarrelene, *Bull. Chem. Soc. Jpn.*, **89,** 1375-1384 (2016).

— Structural Organic Chemistry —

Makuta, S.; Liu, M. N.; Endo, M.; Nishimura, H.; Wakamiya, A.; Tachibana, Y., Photo-Excitation Intensity Dependent Electron and Hole Injections from Lead Iodide Perovskite to Nanocrystalline TiO_2 and Spiro-OMeTAD, *Chem. Commun.*, **52,** 673-676 (2016).

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

Lee, J.; Jung, H.; Shin, H.; Kim, J.; Yokoyama, D.; Nishimura, H.; Wakamiya, A.; Park, J., Excimer Emission Based on the Control of Molecular Structure and Intermolecular Interactions, *J. Mater. Chem. C*, **4,** 2784-2792 (2016).

Kamimoto, N.; Nakamura, N.; Tsutsumi, A.; Mandai, H.; Mitsudo, K.; Wakamiya, A.; Murata, Y.; Hasegawa, J. Y.; Suga, S., Facile Synthesis of 1,4-Bis(diaryl)-1,3-butadiynes Bearing Two Amino Moieties by Electrochemical Reaction-Site Switching, and Their Solvatochromic Fluorescence, *Asian J. Org. Chem.*, **5,** 373-379 (2016).

Tahara, H.; Endo, M.; Wakamiya, A.; Kanemitsu, Y., Experimental Evidence of Localized Shallow States in Orthorhombic Phase of $CH_3NH_3PbI_3$ Perovskite Thin Films Revealed by Photocurrent Beat Spectroscopy, *J. Phys. Chem. C*, **120,** 5347-5352 (2016).

Zhang, R.; Murata, M.; Aharen, T.; Wakamiya, A.; Shimoaka, T.; Hasegawa, T.; Murata, Y., Synthesis of a Distinct Water Dimer inside Fullerene C_{70}, *Nat. Chem.*, **8,** 435-441 (2016).

Nishimura, H.; Fukushima, T.; Wakamiya, A.; Murata, Y.; Kaji, H., The Influence of Quasiplanar Structures of Partially Oxygen-Bridged Triphenylamine Dimers on the Properties of Their Bulk Films, *Bull. Chem. Soc. Jpn.*, **89,** 726-732 (2016).

Hashikawa, Y.; Murata, M.; Wakamiya, A.; Murata, Y., Synthesis and Properties of Endohedral Aza[60]fullerenes: $H_2O@C_{59}N$ and $H_2@C_{59}N$ as Their Dimers and Monomers, *J. Am. Chem. Soc.*, **138,** 4096-4104 (2016).

Satou, M.; Nakamura, T.; Aramaki, Y.; Okazaki, S.; Murata, M.; Wakamiya, A.; Murata, Y., Near-infrared Emissive Donor-Acceptor-type Molecules Containing Thiazole-fused Benzothiadiazole as an Electron-acceptor Moiety, *Chem. Lett.*, **45,** 892-894 (2016).

Murata, M.; Kaji, S.; Nishimura, H.; Wakamiya, A.; Murata, Y., Efficient Synthesis of One- and Two-Dimensional Multimetallic Gold-Bis(dithiolene) Complexes, *Eur. J. Inorg. Chem.*, **2016,** 3228-3232 (2016).

Hashikawa, Y.; Murata, M.; Wakamiya, A.; Murata, Y., Water Entrapped inside Fullerene Cages: A Potential Probe for Evaluation of Bond Polarization, *Angew. Chem., Int. Ed.*, **55,** 13109-13113 (2016).

Wang, F. J.; Endo, M.; Mouri, S.; Miyauchi, Y.; Ohno, Y.; Wakamiya, A.; Murata, Y.; Matsuda, K., Highly Stable Perovskite Solar Cells with an All-Carbon Hole Transport Layer, *Nanoscale*, **8,** 11882-11888 (2016).

Yamada, Y.; Yamada, T.; Shimazaki, A.; Wakamiya, A.; Kanemitsu, Y., Interfacial Charge-Carrier Trapping in $CH_3NH_3PbI_3$-Based Heterolayered Structures Revealed by Time-Resolved Photoluminescence Spectroscopy, *J. Phys. Chem. Lett.*, **7,** 1972-1977 (2016).

Le, P. Q.; Yamada, Y.; Nagai, M.; Maruyama, N.; Wakamiya, A.; Kanemitsu, Y., Free Carriers versus Excitons in $CH_3NH_3PbI_3$ Perovskite Thin Films at Low Temperatures: Charge Transfer from the Orthorhombic Phase to the Tetragonal Phase, *J. Phys. Chem. Lett.*, **7,** 2316-2321 (2016).

Yamashita, D.; Handa, T.; Ihara, T.; Tahara, H.; Shimazaki, A.; Wakamiya, A.; Kanemitsu, Y., Charge Injection at the Heterointerface in Perovskite $CH_3NH_3PbI_3$ Solar Cells Studied by Simultaneous Microscopic Photoluminescence and Photocurrent Imaging Spectroscopy, *J. Phys. Chem. Lett.*, **7,** 3186-3191 (2016).

Ishida, N.; Wakamiya, A.; Saeki, A., Quantifying Hole Transfer Yield from Perovskite to Polymer Layer: Statistical Correlation of Solar Cell Outputs with Kinetic and Energetic Properties, *ACS Photonics*, **3,** 1678-1688 (2016).

Wakamiya, A.; Nishimura, H.; Murata, Y., Partially Oxygen-Bridged Triphenylamines with a Quasiplanar Structure as a Key Scaffold for Hole-Transporting Materials, *J. Synth. Org. Chem. Jpn.*, **74,** 1128-1135 (2016).

Bottari, G.; Trukhina, O.; Kahnt, A.; Frunzi, M.; Murata, Y.; Rodriguez-Fortea, A.; Poblet, J. M.; Guldi, D. M.; Torres, T., Regio-, Stereo-, and Atropselective Synthesis of C_{60} Fullerene Bisadducts by Supramolecular-Directed Functionalization, *Angew. Chem., Int. Ed.*, **55,** 11020-11025 (2016).

— Synthetic Organic Chemistry —

Ueda, Y., Final-stage Site-selective Acylation for The Total Synthesis of Natural Glycosides, *YAKUGAKU ZASSHI*, **136,** 1631-1639 (2016) (in Japanese).

Alezra, V.; Kawabata, T., Recent Progress in Memory of Chirality (MOC) : An Advanced Chiral Pool, *Synthesis*, 2997-3016 (2016).

Tomohara, K.; Kasamatsu, K.; Yoshimura, T.; Furuta, T.; Kawabata, T., Asymmetric Synthesis of Multisubstituted Dihydrobenzofurans by Intramolecular Conjugate Addition of Short-Lived C-O Axially Chiral Enolates, *Chem. Pharm. Bull.*, **64,** 899-906 (2016).

Yamada, T.; Suzuki, K.; Hirose, T.; Furuta, T.; Ueda, Y.; Kawabata, T.; Omura, S.; Sunazuka, T., Organocatalytic Site-Selective Acylation of Avermectin B2a, a Unique Endectocidal Drug, *Chem. Pharm. Bull.*, **64,** 856-864 (2016).

Mishiro, K.; Takeuchi, H.; Furuta, T.; Kawabata, T., A Concise Access to C_2-Symmetric Chiral 4-Pyrrolidinopyridine Catalysts with Dual Functional Side Chains, *Chem. Pharm. Bull.*, **64,** 1073-1077 (2016).

Imayoshi, A.; Yamanaka, M.; Sato, M.; Yoshida, K.; Furuta, T.; Ueda, Y.; Kawabata, T., Insights into the Molecular Recognition Process in Organocatalytic Chemoselective Monoacylation of 1,5-Pentanediol, *Adv. Synth. Catal.*, **358,** 1337-1344 (2016).

Baba, T.; Yamamoto, J.; Hayashi, K.; Sato, M.; Yamanaka, M.; Kawabata, T.; Furuta, T., Catalytic Discrimination Among Formyl Groups in Regio- and Stereoselective Intramolecular Cross-Aldol Reactions, *Chem. Sci.*, **7,** 3791-3797 (2016).

Hyakutake, R.; Gondo, N.; Ueda, Y.; Yoshimura, T.; Furuta, T.; Kawabata, T., Catalyst-Controlled Regiodivergent Vinylogous Aza-Morita-Baylis-Hillman Reactions, *Tetrahedron Lett.*, **57,** 1321-1324 (2016).

Yanagi, M.; Ninomiya, R.; Ueda, Y.; Furuta, T.; Yamada, T.; Sunazuka, T.; Kawabata, T., Organocatalytic Site-Selective Acylation of 10-Deacetylbaccatin III, *Chem. Pharm. Bull.*, **64,** 907-912 (2016).

Furuta, T.; Kawabata, T., Chiral Imidazole and Pyridines as Asymmetric Organocatalysis, *RSC Green Chemistry, Sustainable Catalysis, M. North, Ed., The Royal Society of Chemistry*, 351-380 (2016).

Ueda, Y.; Kawabata, T., Organocatalytic Site-Selective Acylation of Carbohydrates and Polyol Compounds, *Top. Curr. Chem.*, **372,** 203-231 (2016).

Yoshida, K.; Suzuki, H.; Inoue, H.; Fujino, Y.; Itatsu, Y.; Takao, K., Organocatalytic Regioselective Chlorosilylation of Oxiran Derivatives: Mild and Effective Insertion of the Bulky Silyl Chloride by Using 4-Methoxy Pyridine *N*-oxide, *Adv. Synth. Catal.*, **358,** 1886-1891 (2016).

Yoshida, K.; Itatsu, Y.; Fujino, Y.; Inoue, H.; Takao, K., Enantioselective Organocatalytic Construction of Spiroindane Derivatives by Intramolecular Friedel-Crafts-type 1,4-Addition, *Angew. Chem. Int. Ed.*, **55,** 6734-5738 (2016).

Miyazaki, S.; Sasazawa, Y.; Mogi, T.; Suzuki, T.; Yoshida, K.; Dohmae, N.; Takao, K.; Simizu, S., Identification of Seco-clavilactonoe B as a Small-molecule Actin Polymerization Inhibitor, *FEBS Letters*, **590,** 1163-1173 (2016).

Yoshida, K.; Fujino, Y.; Itatsu, Y.; Inoue, H.; Kanoko, Y.; Takao, K., Amine Free Silylation of Alcohols under 4-Methylpyridine *N*-Oxide-Catalyzed Conditions, *Tetrahedron Lett.*, **57,** 627-631 (2016).

Kawabata, T., *Site-Selective Catalysis*, Gewerbestrasse 11 CH-6330 Cham (ZG) Switzerland: Springer Interntional Publishing (2016).

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Ueda, Y.; Kawabata, T., D-2-Naphthylalanine *N*, *N*'-[[(2*S*,5*S*)-1-(4-pyridinyl)-2,5-pyrrolidinediyl]dicarbonyl]bis-3,3'-dioctyl Ester, *e-EROS Encyclopedia of Reagents for Organic Synthesis; John Wiley & Sons, Ltd.*, DOI: 10.1002/047084289X. rn01986 (2016).

Koeduka, T.; Kajiyama, M.; Furuta, T.; Suzuki, H.; Tsuge, T.; Matsui, K., Benzenoid Biosynthesis in The Flowers of *Eriobotrya Japonica*: Molecular Cloning and Functional Characterization of *p*-Methoxybenzoic Acid Carboxyl Methyltransferase, *Planta*, **244,** 725-736 (2016).

Koeduka, T.; Kajiyama, M.; Furuta, T.; Suzuki, H.; Tsuge, T.; Matsui, K., Characterization of An O-Methyltransferase Specific to Guaiacol-type Benzenoids from The Flowers of Loquat (*Eriobotrya Japonica*), *J. Biosci. Bioeng.*, **122,** 679-684 (2016).

— Advanced Inorganic Synthesis —

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INTERNATIONAL RESEARCH COLLABORATIONS

[Australia]
RMIT University, School of Aerospace, Mechanical and Manufacturing Engineering

The University of Sydney, Key Centre for Polymers & Colloids

Monash University, Faculty of Pharmacy and Pharmaceutical Sciences

[Canada]
Université Laval, Département de Chimie

University of Waterloo, Department of Chemical Engineering

[China, P.R.]
Peking University, College of Life Science

Fujian Agriculture and Forestry University, Haixia Institute of Science and Technology

Chinese Academy of Science, Institute of Genetics and Developmental Biology

National Plant Gene Research Center

Fudan University, School of Computer Science

Fudan University, Shanghai Key Lab of Intelligent Information Processing

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Université de Renne, Sciences Chimiques de Rennes

Aix Marseille University, Mediterranean Institute of Oceanography

CNRS

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Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Chemistry and Pharmacy, Interdisciplinary Center for Molecular Materials (ICMM)

The European Molecular Biology Laboratory

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University of Bergen, Department of Biology

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Universitat Rovira i Virgili, Departament de Química Física i Inorgànica

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John Innes Centre for Plant Science Research, Department of Cell and Developmental Biology

The University of Edinburgh, Centre for Science at Extreme Conditions (CSEC) and School of Chemistry

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Columbia University, Department of Chemistry

University of Pennsylvania, Department of Materials Science and Engineering

University of Massachusetts, Department of Polymer Science and Engineering

The Ohio State University, Department of Microbiology

Boston University, Department of Mathematics and Statistics

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

SELECTED GRANTS

DIVISION OF SYNTHETIC CHEMISTRY

— Organoelement Chemistry —

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

Tokitoh, N.
Electron-state Control of Aromatic Compounds Containing Heavier Group 14 Elements by Substituent introduction and Element Substitution
Grant-in-Aid for Scientific Research (B)
1 April 2013–31 March 2016

Tokitoh, N.
Synthesis and Properties of Alumoles Having an Aluminum–Halogen Bond
Grant-in-Aid for Challenging Exploratory Research
1 April 2014–31 March 2016

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

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

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

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

— Structural Organic Chemistry —

Murata, Y.
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.
Spherical π-Figuration Based on Functionalization of Sub-Nano Space
Grant-in-Aid for Scientific Research on Innovative Areas “π-System Figuration”
1 April 2015–31 March 2017

Murata, Y.
Functional Molecular Systems Based on Dynamic Behavior of Active Species
Grant-in-Aid for Scientific Research on Innovative Areas “Stimuli-responsive Chemical Species for the Creation of Functional Molecules”
1 April 2015–31 March 2017

Murata, Y.
Creation of New Reactive Chemical Species by the Ultimate Steric Protection
Grant-in-Aid for Challenging Exploratory Research
1 April 2015–31 March 2017

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

Abbreviations and acronyms

JST : Japan Science and Technology Agency
MEXT : Ministry of Education, Culture, Sports, Science and Technology
METI : Ministry of Economy, Trade and Industry
NEDO : New Energy and Industrial Technology Development Organization

Wakamiya, A.
Creation of Wireless Electric Power Supply
Center of Innovation Program (COI)
1 October 2013−31 March 2022

Wakamiya, A.
High Dimensional Structural Control of π-Conjugated Systems and Their Functionalization
Grant-in-Aid for Scientific Research (B)
1 April 2014−31 March 2017

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

Murata, M.
Organization of Nanocarbon Molecules Based on Metal Coordination
Grant-in-Aid for Challenging Exploratory Research
1 April 2014−31 March 2016

Murata, M.
Development of Neutral Thermoelectric Materials Based on π-Extended Metal-Bis(dithiolene) Complexes
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 October 2016−31 March 2020

Murata, M.
Exploratory Studies on Materials for Energy Conversion Based on Efficient Synthesis of π-Conjugated Multimetallic Complexes
Grant-in-Aid for Challenging Exploratory Research
1 April 2016−31 March 2018

Murata, M.
Development of Functional Materials Based on Efficient Synthesis of PAHs Containing Pentagon Rings
Grant-in-Aid for Scientific Research (B)
1 April 2016−31 March 2019

Murata, M.
Exploration of Functions of Cyclopenta-Fused Polycyclic Aromatic Hydrocarbons CP-PAHs
Research Encouragement Grants, The Asahi Glass Foundation
1 April 2016−31 March 2018

— Synthetic Organic Chemistry —

Kawabata, T.
Regioselective Molecular Transformation Based on Organocatalytic Molecular Recognition
Grant-in-Aid for Scientific Research on Innovative Area
1 October 2011−31 March 2015

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

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

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

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

Yoshida, K.
Total Synthesis of Natural Products by Using Organocatalytic Asymmetric Construction of All-carbon Quaternary Stereocenter
Grant-in-Aid for Young Scientists (B)
1 April 2016−31 March 2019

— Advanced Inorganic Synthesis —

Teranishi, T.
Establishment of Deeply Penetrating Photoacoustic Imaging Technology Based on Fucntional Probes: Design and Synthesis of Activatable Probes and Development of in vivo Imaging Technology
Industry-Academia Collaborative R&D Programs, Japan Agency for Medical Research and Development
1 December 2011−31 March 2017

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

Teranishi, T.
Research on Nanoscale Phase-Controlled Nanocomposite Magnets
Mirai Kaitaku Research Project, NEDO
1 October 2012−31 March 2022

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

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

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

Sakamoto, M.
Investigation on the Gain-of-function Process by the Formation of Nanoparticle Assemblage Using DNA Origami
SPIRITS (Supporting Program for Interaction-based Initiative Team Studies)
1 April 2015–31March 2017

Sato, R.
Development of The Novel and Versatile Alloying Process via Nanosized Phosphorus Compounds
Grant-in-Aid for Challenging Exploratory Research
1 April 2015–31March 2017

Saruyama, M.
Orientational Control and Structure-specific Properties of Heterostructural Nanoparticles
Grant-in-Aid for Research Activity Start-up
1 October 2015–31March 2017

DIVISION OF MATERIALS CHEMISTRY

— Chemistry of Polymer Materials —

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

Tsujii, Y.
Super Lubrication of Novel Nano-Brushes
Advanced Environmental Materials of Green Network of Excellence (GRENE) program, MEXT
6 December 2011–31 March 2016

Tsujii, Y.
Development of High-Performance Li-ion Batteries using High-capacity, Low-cost Oxide Electrodes
NEDO Project for Development of Novel Technology in Li-ion Batteries
1 October 2012–27 February 2017

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 Cellulosic Bottlebrushes with Regioselectively Substituted Side Chains
Grant-in-Aid for Young Scientist (B)
1 April 2016–31 March 2018

— Polymer Controlled Synthesis —

Yamago, S.
New Organic Chemistry and Material Science of Curved π-Conjugated Molecules
Grant-in-Aid for Scientific Research (S)
1 April 2016–31 March 2021

Yamago, S.
Highly Value-added Polymer Material Created by New Living Radical Polymerization Agent
Next Generation Technology Transfer Program (NexTEP), JST
1 April 2014–31 March 2020

— Inorganic Photonics Materials —

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

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

Mizuochi, N.
Research on Diamond Quantum Information Device
TORAY Science and Technology Research Grant
1 January 2016–31 March 2018

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

— Nanospintronics —

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

DIVISION OF BIOCHEMISTRY

— Biofunctional Design-Chemistry —

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

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

— Chemistry of Molecular Biocatalysts —

Watanabe, B.
Synthesis of γ-Glutamyl Transpeptidase-Specific Chemical Probes and Their Application to Cancer Immunotherapy
Grant-in-Aid for Young Scientists (B)
1 April 2015–31 March 2017

— Molecular Biology —

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

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

— Chemical Biology —

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

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

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

Kaji, H.
Adachi Molecular Exciton Engineering Project
ERATO (Exploratory Research for Advanced Technology), JST
1 April 2014−31 March 2018

Fukushima, T.
Solid-State NMR Analysis of Bulk Heterostructures toward High-efficiency Organic Solar Cells
Grant-in-Aid for Young Scientists (B)
1 April 2014−31 March 2016

Fukushima, T.
Study on Weather Resistance of Solution-Processable Organic Solar Cells
Suga Weathering Technology Foundation
1 April 2015−31 March 2016

Shizu, K.
A Method of Visualizing Radiative and Non-Radiative Decays and Its Applications to Design for Deep-Blue Organic Emitters
Grant-in-Aid for Young Scientists (B)
1 April 2015−31 March 2017

Kaji, H.
Analysis of Organic Photovoltaics Materials by Solid-State Dynamic Nuclear Polarization
SPIRITS (Supporting Program for Interaction-based Initiative Team Studies)
1 April 2015−31 March 2017

Fukushima, T.
A Fundamental Study on Weather Resistance of Solution-Processed Organic Solar Cells by Solid-State NMR
Grant-in-Aid for Scientific Research (C)
1 April 2016−31 March 2018

— Hydrospheric Environment Analytical Chemistry —

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

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

— Solution and Interface Chemistry —

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

Hasegawa, T.
Development of Novel Analytical Techniques for Revealing Molecular Orientation of Adsorbed Molecules on a Rough Surface or on Nano Particles
Grant-in-Aid for challenging Exploratory Research
1 April 2014−31 March 2016

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

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

— Molecular Microbial Science —

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

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

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

Ogawa, T.
Research on Acyltransferases that Create Heterogeneity of Bacterial Biomembranes
Grant-in-Aid for Research Activity Start-up
23 August 2015–31 March 2017

DIVISION OF MULTIDISCIPLINARY CHEMISTRY

— Polymer Materials Science —

Takenaka, M.
Photon and Quantum Basic Research Coordinated Development Program, JST
1 September 2013–31 March 2018

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

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

— Molecular Rheology —

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

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

ADVANCED RESEARCH CENTER FOR BEAM SCIENCE

— Particle Beam Science —

Iwashita, Y.
Quantum Improvement of the Superconducting Acceleration Cavity Performance by the Laminated Film Structure
Grant-in-Aid for Challenging Exploratory Research
1 April 2014–31 March 2016

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

— Laser Matter Interaction Science —

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

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

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

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

— Electron Microscopy and Crystal Chemistry —

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

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

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

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

INTERNATIONAL RESEARCH CENTER FOR ELEMENTS SCIENCE

—Synthetic Organotransformation—

Nakamura, M.
Synthesis of Nitrogen-Containing Polycyclic Aromatic Compounds via Iron-catalyzed C-H Amination
Grant-in-Aid for Challenging Exploratory Research
1 April 2015–31 March 2016

Takaya, H.
Solution-Phase Characterization of Paramagnetic Metal Complex by X-ray Absorption Spectroscopy
Grant-in-Aid for Challenging Exploratory Research
1 April 2015–31 March 2017

Isozaki, K.
Development of Catalytic Multi-photon-excited Photoreactions in the Reaction Field Localizing Substrates and Excitation Sources
Grant-in-Aid for Scientific Research on Innovative Areas "Application of Cooperative Excitation into Innovative Molecular Systems with High-Order Photofunctions"
1 April 2015−31 March 2017

Iwamoto, T.
Development of Aromatic C-H Functionalization Base on Cation-π Interaction
Grant-in-Aid for Young Scientists (B)
1 April 2015−31 March 2017

— Advanced Solid State Chemistry —

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

— Organometallic Chemistry —

Ozawa, F.
Synthesis and Catalytic Properties of Stimulus-responsible Transition Metal Complexes Bearing Low-coordinate Phosphorus Ligands
Grant-in-Aid for Scientific Research on Innovative Areas "Stimuli-responsive Chemical Species for the Creation of Functional Molecules"
1 April 2012−31 March 2017

Ozawa, F.
Synthesis and Catalytic Applications of Non-innocent Phosphaalkene Ligands
Grant-in-Aid for Scientific Research (B)
1 April 2014−31 March 2017

Wakioka, M.
Development of Highly Efficient Catalytic Systems for Direct Arylation Polymerization based on Equilibrium between Active and Dormant Species
Grant-in-Aid for Young Scientists (B)
1 April 2015−31 March 2017

Ozawa, F.
Development of Highly Efficient Catalysts for Synthesizing of π-Conjugated Polymers via Direct Arylation
ACT-C, JST
1 October 2012−31 March 2018

— Nanophotonics —

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

BIOINFORMATICS CENTER

— Chemical Life Science —

Ogata, H.
Neo-virology, the Raison D'être of Viruses – Deciphering the Mechanisms of Virus-host Co-existence in Aquatic Environments
Grant-in-Aid for Scientific Research on Innovative Areas
30 June 2016−31 March 2021

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

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

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

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

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

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

— Bio-knowledge Engineering —

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

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

Yotsukura, S.
Feasibility Study of Allergen Genes Identification and Prediction of the Gene Expression Level Associated with Cultivation Conditions
Specific Project Investigation, JST
1 October 2016−31 March 2017

Yamada, M.
Nonlinear Feature Selection for Ultra-High Dimensional Data
Grant-in-Aid for Young Scientists (B)
1 April 2016−31 March 2018

Yamada, M.
Nonlinear Feature Selection for Science Discovery
PRESTO (Precursory Research for Embryonic Science and Technology), JST
1 December 2016−31 March 2020

THESES

BABA, Tomonori
D Pharm Sc, Kyoto University
“Development of Aniline-type Acid Base Catalysts for Asymmetric Direct Aldol Reactions”
Supervisor: Prof KAWABATA, Takeo
23 March 2016

CHEN, Lihui
D Sc, Kyoto University
“Synthesis and Plasmonic Properties of Copper-based Nanocrystals”
Supervisor: Prof TERANISHI, Toshiharu
23 March 2016

HSU, Shu-Yao
D Eng, Kyoto University
“Fabrication of Well-Defined Architectures of Ultrahigh-Molecular-Weight Polymers by Living Radical Polymerization”
Supervisor: Prof TSUJII, Yoshinobu
23 March 2016

HYAKUTAKE, Ryuichi
D Pharm Sc, Kyoto University
“Selective Reactions in Conjugate Addition to Unsaturated Carbonyl Compounds”
Supervisor: Prof KAWABATA, Takeo
23 March 2016

IMAYOSHI, Ayumi
D Pharm Sc, Kyoto University
“Discrimination of Mobile Supramolecular Chirality: Acylative Molecular Transformation by Organocatalysis”
Supervisor: Prof KAWABATA, Takeo
23 March 2016

JIRA, Jindalertudomdee
D Inf, Kyoto University
“Chemical Compound Enumeration and Host-Pathogen Protein Interaction Prediction By Graph-Based Approaches”
Supervisor: Prof AKUTSU, Tatsuya
23 September 2016

KAWAGUCHI, Masashi
D Sc, Kyoto University
“Current Induced Effective Magnetic Field in Ferromagnetic Multilayers”
Supervisor: Prof ONO, Teruo
12 January 2016

KAWAGUCHI, Yoshimasa
D Pharm Sc, Kyoto University
“Identification of an Octaarginine Receptor for Its Intracellular Uptake Using Photocrosslinking and Elucidation of the Intracellular Uptake Pathway”
Supervisor: Prof FUTAKI, Shiroh
23 March 2016

MOHAMED, Ahmed Mohamed
D Pharm Sc, Kyoto University
“Development of Computational Analysis Tools for Natural Products Research and Metabolomics”
Supervisor: Prof MAMITSUKA, Hiroshi
23 March 2016

NAGATA, Koichi
D Sc, Kyoto University
“Synthetic Studies on the Al=Al Doubly Bonded Species and Elucidation of Their Reactivity”
Supervisor: Prof TOKITOH, Norihiro
23 March 2016

NISHIMURA, Hidetaka
D Eng, Kyoto University
“Development of Functional Organic Materials Using Oxygen-Bridged Triarylamine Skeleton as Quasiplanar Structure”
Supervisor: Prof MURATA, Yasujiro
23 March 2016

OKU, Akihiko
D Pharm Sc, Kyoto University
“Peptide-Scientific Approaches for Intracellular Delivery of Biological Macromolecules”
Supervisor: Prof FUTAKI, Shiroh
23 March 2016

SEKI, Hayato
D Sc, Kyoto Uiversity
“High Pressure Synthesis of Heavily Substituted Perovskite Oxides and Explorations of their Physical Properties”
Supervisor: Prof SHIMAKAWA, Yuichi
23 March 2016

TAKAYA, Junichiro
D Med Sc, Kyoto University
“A Potent and Site-selective Agonist of TRPA1”
Supervisor: Prof UESUGI, Motonari
23 March 2016

TAKEUCHI, Hironori
D Pharm Sc, Kyoto University
“Novel Synthetic Strategy for Natural Glycosides based on Catalytic Sequential Functionalization of Unprotected Glucose”
Supervisor: Prof KAWABATA, Takeo
23 March 2016

YANAGI, Masanori
D Pharm Sc, Kyoto University
“Novel Strategy for Acceleration of Nucleophilic Catalysis via Counter-anion Control and Catalytic Site-selective Functionalization of Polyols”
Supervisor: Prof KAWABATA, Takeo
23 March 2016

YOSHIMURA, Yoko
D Sc, Kyoto University
“Spin Dynamics in Ferromagnetic Nanowire”
Supervisor: Prof ONO, Teruo
12 January 2016

YOTSUKURA, Sohiya
D Pharm Sc, Kyoto University
“Computational Framework for the Dissection of Cancer Genomic Architecture and Its Association in Different Biomarkers”
Supervisor: Prof MAMITSUKA, Hiroshi
23 September 2016

THE 116TH ICR ANNUAL SYMPOSIUM

SEMINARS

MEETINGS AND SYMPOSIA

THE 116TH ICR ANNUAL SYMPOSIUM

(2 December 2016)

ORAL PRESENTATIONS

TAKAYA, Hikaru (Synthetic Organotransformation)
“Solution-Phase Structure Analysis of X-ray Absorption Spectroscopy”

MIZUHATA, Yoshiyuki (Organoelement Chemistry)
“The Chemistry of ‘Heavy Phenyl Anions’ ”

WAKIOKA, Masayuki (Organometallic Chemistry)
“Direct Arylation Polymerization: A New Synthetic Method of π-Conjugated Polymers”

SAITO, Takashi (Advanced Solid State Chemistry)
“High-pressure Syntheses of Transition Metal Oxides Containing Unusually High Valence Cations”

FURUTA, Takumi (Synthetic Organic Chemistry)
“Direct Asymmetric Cross-aldol Reaction of Aliphatic Carbonyl Compounds via Catalytic Discrimination of Carbonyl Groups”

— ICR Award for Young Scientists —
NAKAMURA, Yasuyuki (Polymer Controlled Synthesis)
“Termination Mechanism in the Radical Polymerization of Methyl Methacrylate and Styrene Determined by the Reaction of Structurally Well-Defined Polymer End Radicals”

— ICR Award for Young Scientists —
HARUTA, Mitsutaka (Electron Microscopy and Crystal Chemistry)
“Determination of Elemental Ratio in an Atomic Column by Electron Energy Loss Spectroscopy”

— ICR Award for Graduate Students —
SUZUKI, Yuko (Organoelement Chemistry)
“Isolation and Ambident Reactivity of a Chlorogermylenoid”

— ICR Award for Graduate Students —
ZHANG, Rui (Structural Organic Chemistry)
“Synthesis of a Distinct Water Dimer inside Fullerene C_{70}”

— ICR Award for Graduate Students —
YAMADA, Takumi (Nanophotonics)
“Dynamic Optical Properties of $CH_3NH_3PbI_3$ Single Crystals As Reveald by One- and Two-Photon Excited Photoluminescence Measurements”

— ICR Grants for Promoting Integrated Research —
IWAMOTO, Takahiro (Synthetic Organotransformation)
“Mechanistic Study of Iron Fluoride-Catalyzed Cross-Coupling Reaction”

KATO, Mariko (Molecular Biology)
“Development of Cell-permeable Probes for Phosphatidylinositol 4,5-bisphosphate in Arabidopsis”

SAKAMOTO, Masanori (Advanced Inorganic Synthesis)
“Investigation on Photoinduced Carrier Dynamics at Nano-hetero Interfaces Using Multiple Laser Pulses”

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 OZAKI, Masashi; SHIMAZAKI, Ai; JUNG, Mina; NAKAIKE, Yumi; MARUYAMA, Naoki; AHAREN, Tomoko; RAFIEH, Alwani; SASAMORI, Takahiro; TOKITOH, Norihiro; WAKAMIYA, Atsushi; MURATA, Yasujiro
“Fabrication Protocol of Highly Efficient Perovskite Solar Cells Using Purified Precursor Materials”

GE OKAZAKI, Shuhei; MURATA, Michihisa; WAKAMIYA, Atsushi; MURATA, Yasujiro
“Synthesis of Polymers Containing Imidazole-Fused Benzothiadiazole Unit”

— Synthetic Organic Chemistry —

LW “Current Topics of Fine Organic Synthesis”

GE ARAI, Kenta; UEDA, Yoshihiro; FURUTA, Takumi; KAWABATA, Takeo
“Dirhodium-Catalyzed Chemo- and Regioselective C(sp^2)-H Amination”

— Advanced Inorganic Synthesis —

LW “Current Research Activities in Advanced Inorganic Synthesis”

GE CHEN, Lihui; SAKAMOTO, Masanori; TERANISHI, Toshiharu
“Tin Ion Directed Morphology Evolution of Copper Sulfide Nanoparticles”

GE KIMURA, Masato; SAKAMOTO, Masanori; FURUBE, Akihiro; ADACHI, Hiroyuki; SUGIMOTO, Toshiki; WATANABE, Kazuya; MATSUMOTO, Yoshiyasu; TERANISHI, Toshiharu
“Visible Light-induced Charge Separation in Heterostructured Au_xS/ZnS Nanoparticles”

GE MATSUMOTO, Kenshi; SATO, Ryota; TRINH, T. Thuy; SAKUMA, Noritsugu; TERANISHI, Toshiharu
“High-Performance $L1_0$-FePd/α-Fe Nanocomposite Magnets with Well-Controlled Nanostructures”

— Chemistry of Polymer Materials —

LW “Research Activities in Chemistry of Polymer Materials”

GE KINOSE, Yuji; SAKAKIBARA, Keita; TSUJII, Yoshinobu
“Conformation of Well-defined Janus-type Bottle Brush with Cellulosic Main Chain in Solution”

GE SHIMIZU, Yoshihiko; SAKAKIBARA, Keita; TSUJII, Yoshinobu
“Preparation of Bacterial Cellulose-reinforced Elastomers Using Percolation Structure”

— Polymer Controlled Synthesis —

LW “Research Activities in Polymer Controlled Synthesis”

GE SEKI, Toyomitsu; YU, Mengmeng; NAKAMURA, Yasuyuki; YAMAGO, Shigeru
“New Fluorous Organotellurium Compound for Living Radical Polymerization and Efficient Recovery and Recycle of the Organotellurium Group”

GE HUASHEN, Zhiren; NAKAMURA, Yasuyuki; YAMAGO, Shigeru
“Synthesis of Organoheteroatom Chain Transfer Agent via Radical Trapping Reaction and Their Uses for Living Radical Polymerization”

— Inorganic Photonics Materials —

LW “Introduction of Research Topic of Inorganic Photonics Materials Group”

— Nanospintronics —

LT TANAKA, Kensho; MORIYAMA, Takahiro; KAMIYA, Michinari; MIZUNO, Hayato; ONO, Teruo
“Spin Hall Effect in Ferromagnets Measured by Spin-torque FMR”

GE TANIGUCHI, Takuya; KIM, Kab-Jin; KOYAMA, Tomohiro; CHIBA, Daichi; ONO, Teruo
“Observation of Discrete Jump of Domain Wall Segment among Quenched Disorders”

— Biofunctional Design-Chemistry —

LW “Research Activities in Biofunctional Design-Chemistry”

GE SAKAMOTO, Kentarou; AKISHIBA, Misao; FUTAKI, Shiroh
“A Statistical Research on Structure-activity Relationships between Antimicrobial Peptides Derived from a Spider Toxin”

GE SAKAGAMI, Koki; FUTAKI, Shiroh
“Mechanism of Cellular Uptake of Cell-penetrating Peptides with Stapled α-Helix”

— Chemistry of Molecular Biocatalysts —

LW “Research Activities in Laboratory of Chemistry of Molecular Biocatalysts”

— Molecular Biology —

LW “Research Activity in Laboratory of Molecular Biology”

— Chemical Biology —

LW “Create New World of Bioactive Synthetic Small Molecules”

— Molecular Materials Chemistry —

LW “Molecular Materials Chemistry”

GE MIURA, Tsutomu; FUKUSHIMA, Tatsuya; KAJI, Hironori
“High Performance Bulk Heterojunction Organic Thin Film Solar Cells with Halogen Free Solutions”

GE OGATA, Isamu; KUBO, Shosei; SUZUKI, Katsuaki; KAJI, Hironori
“Synthesis and Photophysical Properties of a Deuterated Thermally Activated Delayed Fluorescence Material”

— Hydrospheric Environment Analytical Chemistry —

LW “Studies in Laboratory of Hydrospheric Environment Analytical Chemistry”

GE OKITA, Shutaro; UMETANI, Shigeo; SOHRIN, Yoshiki
“Solid Phase Extraction and Separation of 13 Group Metal Ions with Acylpyrazolones Loaded XAD7 Resin”

— Solution and Interface Chemistry —

GE IZUMI, Naoki; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
“Structural Analysis of Polymer Thin Films of Fluoroacrylate Having an Rf Side Chain with Various Lengths Using IR Spectroscopy”

GE UKAI, Hironori; SHIMOAKA, Takafumi; HASEGAWA, Takeshi
“Study on an Aggregation Factor of Amphiphiles Involving a Perfluoroalkyl Group Using IR Spectroscopy”

— Molecular Microbial Science —

LW “Research of Molecular Microbial Science Laboratory”

GE TOYOTAKE, Yosuke; CHO, Hyun-Nam; OGAWA, Takuya; KAWAMOTO, Jun; KURIHARA, Tatsuo
“Characterization of a Novel Enzyme for Membrane Phospholipid Biosynthesis from a Cold-adapted Bacterium”

— Polymer Materials Science —

LW “Introduction of Polymer Materials Science Laboratory”

GE NAGANO, Yoshiki; TAKENAKA, Mikihito; JANG, Junhyeok
“The Study of Heterogeneous Structure of Acrylonitrile-butadiene Random Copolymer (NBR)”

GE HIGASHINO, Naruhisa; TAKENAKA, Mikihito; YAMAGUCHI, Kaoru; Aisyah
“Alignment of Ferritin Protein by Using Nano Pattern of Block Copolymers”

GE MIYATAKE, Yuki; OGAWA, Hiroki; NISHIDA, Koji; YAMADA, Norifumi; KANAYA, Toshiji
“Phase Separation and Dewetting of Deuterated Polystyrene/poly-2-chlorostyrene Blend Thin Films”

— Molecular Rheology —

LW “Research Activities in Laboratory of Molecular Rheology”

— Molecular Aggregation Analysis —

LT MURDEY, Richard
“Introduction to Nonlinear Photocurrent Spectroscopy”

— Particle Beam Science —

LW “Status of Accelerator Laboratory, Advanced Research Center for Beam Science”

GE MIYAWAKI, Eisuke; FUWA, Yasuhiro; TONGU, Hiromu; IWASHITA, Yoshihisa
“Study of Ion Sources for Future Accelerators”

GE FUWA, Yasuhiro; IWASHITA, Yoshihisa
“Beam Focusing System for Klystrons with Permanent Mangets”

GE KITAHARA, Ryunosuke; IWASHITA, Yoshihisa; NOP Group
“Measurement of ^{14}N(n, p)^{14}C Cross Section Using Cold Neutron Beam at J-PARC”

— Laser Matter Interaction Science —

LW “Research Activities in Laboratory of Laser Matter Interaction Science”

GE FURUKAWA, Yuki; TERAMOTO, Kensuke; MORI, Kazuaki; NAKAMIYA, Yoshihide; INOUE, Shunsuke; HASHIDA, Masaki; SAKABE, Shuji
“Creation of Nanostructures on Metal Surface by Double-pulse Femtosecond Laser Irradiation”

GE MORI, Kazuaki; HASHIDA, Masaki; NAGASHIMA, Takeshi; LI, Dazhi; TERAMOTO, Kensuke; INOUE, Shunsuke; SAKABE, Shuji
“THz Waves Generation from Interaction between a Target of Argon Clusters and Intense Double-pulse Laser”

GE TERAMOTO, Kensuke; INOUE, Shunsuke; TOKITA, Shigeki; YASUHARA, Ryo; TERAO, Tokinori; KAWANAKA, Junji; NAGASHIMA, Takeshi; HASHIDA, Masaki; SAKABE, Shuji
“Generation of Intense THz Surface Waves on a Metal Wire by Intense Laser”

— Electron Microscopy and Crystal Chemistry —

LW “Research Activities in Division of Electron Microscopy and Crystal Chemistry”

GE YAMAGUCHI, Atsushi; HARUTA, Mitsutaka; NEMOTO, Takashi; KURATA, Hiroki
“Detecting the Directionality of Local Electronic States in $SrTiO_3$ by Momentum-selected STEM-EELS”

— Structural Molecular Biology —

LW “Introduction of Structural Molecular Biology Laboratory”

— Synthetic Organotransformation —

LW “Introduction of Synthetic Organotransformation Laboratory”

GE OKUZONO, Chiemi; IWAMOTO, Takahiro; ADAK, Laksmikanta; JIN, Masayoshi; TAKAYA, Hikaru; NAKAMURA, Masaharu
“Iron-Catalyzed Enantioselective Cross-Coupling of Haloester with Aryl Boron Reagent”

GE UENO, Ryo; ISHIBASHI, Kosuke; ISOZAKI, Katsuhiro; TAKAYA, Hikaru; NAKAMURA, Masaharu
“Synthesis and Photocatalytic Property of Peptide Dendron Thiolate-Functionalized Gold Clusters”

— Advanced Solid State Chemistry —

LW “Introduction of Advanced Solid State Chemistry Laboratory”

GE YUU, Hou; SEKI, Hayato; KAKU, Kaisen; HOSAKA, Yoshiteru; SAITO, Takashi; SHIMAKAWA, Yuichi
“Geometrical Spin Frustration of Unusually High Valence Fe^{5+} in the Double Perovskite La_2LiFeO_6”

— Organometallic Chemistry —

LW “Activity Report: Organometallic Chemistry Laboratory”

— Nanophotonics —

LW “Recent Research Topics of Nanophotonics Group”

— Chemical Life Science —

LW “Research Activities in Laboratory of Chemical Life Science”

GE LI, Yanze; WATAI, Hiroyasu; HINGAMP, Pascal; YOSHIDA, Takashi; OGATA, Hiroyuki
“Amplicon Analysis of Megaviridae DNA Polymerase Gene”

— Mathematical Bioinformatics —

LT JIRA, Jindalertudomdee
“Enumeration Method for Structural Isomers Containing User-Defined Structures Based on Breadth-First Search Approach”

GE BAO, Yu
“LBSizeCleav: Improved Support Vector Machine (SVM)-based Prediction of Dicer Cleavage Sites Using Loop/Bulge Length”

— Bio-knowledge Engineering —

GE YAMADA, Makoto; WIMALAWARNE, Kishan
“Nonlinear Feature Selection for Biological Data”

— ICR Grants for Promoting Integrated Research —

MURATA, Michihisa; TSUKAO, Masahiro; WAKAMIYA, Atsushi; MURATA, Yasujiro; SUZUKI, Katsuaki; KAJI, Hironori
“Elucidation of Solid-state Structures and Functions of Metal Complexes with 3D π-Systems”

KAYAHARA, Eiichi; FUKUSHIMA, Tatsuya
“Application of Cyclic π-Conjugated Moleculars to Oraganic Electronics”

CHO, Hyun-Nam; KAWAMOTO, Jun
“Analysis of the Fatty Acid-Recognition Mechanism of an Anti-Fatty Acid Antibodies and Their Application”

NGUYEN, Hao Canh
“Advanced Computational Tools for Knowledge Discovery in Ecology and Biology”

SEMINARS

Prof AJAYAGHOSH, Ayyappanpillai
CSIR-NIST, India
“Self-Sorted Donor-Acceptor Assemblie”
19 October 2016

Prof AKIYAMA, Yutaka
Tokyo Institute of Technology, Tokyo, Japan
“Massively Parallel Bioinformatics Computing on K-computer, TSUBAME, and Azure: Metagenome Analysis and Exhaustive Protein-Protein Interaction Prediction”
1 July 2016

Assoc Prof AU, Kin Fai
University of Iowa, U.S.A.
“Transcriptome Analysis at the Gene Isoform Level Using Hybrid Sequencing”
11 October 2016

Prof BERKESSEL, Albrecht
Department of Chemistry, University of Cologne, Cologne, Germany
“Carbene Catalysis and the Breslow Intermediate”
1 March 2016

Dr BURLINA, Fabienne
Laboratoire des Biomolécules, UMR 7203, Université P. et M. Curie - CNRS – ENS, Paris, France
“Design and Study of Cyclic Cell-Penetrating Peptides”
25 October 2016

Prof CHEN, Hongyu
Nanyang Technological University (Nanjin Tech University), Singapore (China, P.R.)
“Exploiting Polymer in Nanosynthesis”
19 December 2016

Dr CHEN, Sophia
Laboratoire D’utilisation des Lasers Intenses, Ecole Polytrchnique, France
“What Would You Do with 10^{22} W/cm^2 Laser Intensities?”
1 July 2016

Mr. CHENG, Didier
Laboratoire des Biomolécules, UMR 7203, Université P. et M. Curie - CNRS – ENS, Paris, France
“Comparative Studies between Antimicrobial Peptides and Cell-Penetrating Peptides”
25 October 2016

Prof CLAYDEN, Jonathan
School of Chemistry, University of Bristol, Bristol, U.K.
“Unconventional Reactivity from Organolithium Compounds”
25 April 2016

Dr CONWAY, Timothy
Institute of Geochemistry and Peterology, Department of Earth Sciences, ETH Zürich, Switzerland
“Investigating the Role of Dust in the Marine Iron Cycle Using Iron Isotopes”
8 July 2016

Prof DE LA HIGUERA, Colin Manuel
University of Nantes, Nantes, France
“Machine Learning is about Intelligent Forgetting”
14 April 2016

Senior Researcher ENAMI, Shinichi
National Institute for Environmental Studies, Ibaraki, Japan
“Physical Chemistry on an Interfacial Phenomena: (1) Mechanism of a Chemical Reaction at an Air/Liquid Interface”
19 December 2016

Dr ENDO, Hisashi
Hokkaido University, Hokkaido, Japan
“Contrasting Biogeography and Diversity Patterns between Diatoms and Haptophytes in the Central Pacific Ocean”
22 December 2016

Dr FUCHS, Julien
LULI, Ecole Polytechnique, CNRS, CEA, UPMC, France
“Intense Laser Pulses and Strong Magnetization as Tools for Investigating Astrophysical Phenomena”
1 July 2016

Assoc Prof FURUMI, Seiichi
Faculty of Science Division I, Department of Applied Chemistry, Tokyo University of Science, Tokyo, Japan
“Soft Photonic Devices Using Polymeric Self-Organization”
27 October 2016

Dr GOLOVKO, Vladimir
Department of Chemistry, Canterbury University, New Zealand
“Uncovering Structure-property Relationship: From Studies of Pure and Supported Metal Clusters Colloids to Their Use in Catalysis and Sensing”
6 July 2016

Assoc Prof GROMIHA, M. Michael
Indian Institute of Technology Madras, India
“Protein Interactions: Integrating Computational Methods and Experimental Data for Understanding the Binding Specificity”
24 November 2016

Assist Prof HAMA, Tetsuya
Institute of Low Temperature Science, Hokkaido University, Hokkaido, Japan
“Physical Chemistry on an Interfacial Phenomena: (2) Hydrogen-bonding Dynamics of H_2O Molecules at a Cryogenic Temperature”
19 December 2016

Prof HAMADA, Hiroki
Department of Life Science, Okayama University of Science, Okayama, Japan
"Organic Synthesis by Plant Cell Culture"
16 April 2016

Prof HASSAGER, Ole
Technical University of Denmark, Denmark
"Applications of Controlled Filament Stretching in Extensional Rheology"
5 February 2016

Researcher HENDEL, Gregor
Zuse Institute Berlin, Berlin, Germany
"How to Solve Integer Optimization Problems with SCIP"
21 June 2016

Dr HERVE, Marie
Karlsruhe Institute of Technology, Germany
"Spin Polarized Scanning Tunneling Microscopy: From Probing Non Collinear Magnetic Configuration to the Investigation of Their High Frequency Dynamic Properties"
18 August 2016

Prof HOVEYDA, Amir H.
Department of Chemistry, Boston College, U.S.A.
"New Concepts, Catalysts and Methods for High-Impact Chemical Synthesis"
4 November 2016

Dr ILLIEN, Françoise
Laboratoire des Biomolécules, UMR 7203, Université P. et M. Curie - CNRS – ENS, Paris, France
"A New Method to Quantify Cell-Penetrating Peptides Translocation in Cells Based on Fluorescence: Application to Penetratin, R9 and Tat"
25 October 2016

Dr INGLESON, Michael
The University of Manchester, U.K.
"Direct Electrophilic Borylation for the Synthesis of Emissive Boron Materials and C(sp^2)-Boronate Esters"
11 March 2016

Mr. ISHIDA, Toshinori
Division of Quantum Science and Engineering Faculty of Engineering, Hokkaido University, Hokkaido, Japan
"Development and Measurement of The Small-Angle Scattering Device in The Neutron Source with The Compact Accelerator"
20 September 2016

Prof ITO, Kimihito
Hokkaido University, Hokkaido, Japan
"Combining Population Genetics of Pathogens and Epidemiology of Infectious Diseases"
4 October 2016

Prof JANEŽIČ, Dušanka
University of Primorska, Slovenia
"Protein Binding Sites Dynamics in Drug Discovery"
16 November 2016

Dr JOHNSON, Brett C.
School of Physics, The University of Melbourne, Australia
"Single Photon Sources in Silicon Carbide"
23 September 2016

Dr JUNGFLEISCH, Benjamin
Argonne National Laboratory, U.S.A.
"Spin-torque Driven Magnetization Dynamics"
30 November 2016

Assist Prof KAGEYAMA, Yoshiyuki
Department of Chemistry, Faculty of Science, Hokkaido University, Hokkaido, Japan
"Mimic of Nature-Interdisciplinary Research between Mechanical Property and Dissipative Ordered Structure"
5 August 2016

Senior Researcher KINO, Koichi
Research Institute for Measurement and Analytical Instrumentation, National Institute of Advanced Industrial Science and Technology, Ibaraki, Japan
"Pulse Neutron Beam Imaging of The Lithium Ion Rechargeable Battery"
20 September 2016

Prof KLAUI, Mathias
University of Mainz, Germany
"Topology in Magnetic Materials"
25 November 2016

Prof KNAPP, Ernst-Walter
Free University of Berlin, Germany
"ProPairs: A Data Set for Protein−Protein Docking"
4 August 2016

Prof LEMIÈGRE, Loïc
Ecole Nationale Supérieure de Chimie de Rennes, France
"Chemical and Chemoenzymatic Synthesis of Glycolipids"
7 November 2016

Prof MURAYAMA, Masafumi
Center for Advanced Marine Core Research, Kochi University, Nankoku, Japan
"What Occurred on the Shallow and Deep Seafloor by the Great East Japan Earthquake 2011?"
2 December 2016

Dr MUROOKA, Yoshie
Laboratory for Ultrafast Microscopy and Electron Scattering, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland
"Filming Plasmonic Field and Magnetic Dynamics in Real Space and Time using ultrafast TEM"
12 July 2016

Dr NAKANISHI, Waka
MANA, National Institute for Materials Science, Ibaraki, Japan
"Control of Molecular Structure at Interfaces"
28 June 2016

Assist Prof OTANI, Misato
Graduate School of Biological Sciences, Nara Institute of Science and Technology, Nara, Japan
"Regulation of RNA Metabolism Related with Efficient Plant Regeneration"
22 January 2016

Prof OZAWA, Takeaki
School of Science, The University of Tokyo, Tokyo, Japan
"Luminescent Sensors and Optical Switches for Single Cell Analysis"
28 January 2016

Dr RUBIO, Vicente
Centro Nacional de Biotecnología-CSIC, Madrid, Spain
"ABA Strikes Back: Inhibition of Plant CRL4 Ubiquitin Ligases Mediated by ABA"
28 November 2016

Assoc Prof SAEKI, Takayuki
High Energy Accelerator Research Organization, Ibaragi, Japan
"Production of the Superconducting Cavity"
10 October 2015

Prof SANDAA, Ruth-Anne
Bergen University, Norway, Norway
"Marine Viruses: Small but Important"
26 September 2016

Dr SCHAPER, Andreas Karl
Philipps University of Marburg, Germany
"Microscopy of Distortion in Crystals and of Hierarchical Ordering in Macromolecular Systems"
14 October 2016

Prof SCHWECHHEIMER, Claus
Plant Systems Biology, Technische Universität München, Freising, Germany
"PIN-ning Down the Function of D6PK Protein Kinases in Auxin Transport"
28 November 2016

Prof SHIMIZU, Hirohiko M.
Laboratory for Particle Properties, Department of Physics, Nagoya University, Aichi, Japan
"The Transmission Imaging by Stable Neutron Source"
15 January 2016
"Construction of the Core Technology of a Compact Neutron Source for the Industrial Application"
11 March 2016

Dr SHINANO, Yuji
Zuse Institute Berlin, Berlin, Germany
"Towards Using over a Million CPU Cores to Solve Previously Unsolved Mixed Integer Programming Problem Instances"
21 June 2016

Dr SONG, Jiangning
Monash University, Clayton, Australia
"Systematic Identification of Secreted Effector Proteins of Bacterial Secretion System IV: A Bioinformatics Study"
30 November 2016

Prof STANG, Peter J.
The Universit of Utah, U.S.A.
"Abiological Self-Assembly: Predesigned Metallacycles and Metallacages via Coordination"
22 April 2016

Dr TESILEANU, Ovidiu
Extreme Light Infrastructure - Nuclear Physics, Czech R.
"Project of Extreme Light Infrastructure for Nuclear Physics in Czech Republic"
25 May 2016

Prof WANG, Yuan
College of Chemistry and Molecular Engineering, Peking University, China, P.R.
"Molecular Engineering of Functional Systems based on Nanoparticles"
16 September 2016

Dr YAMAMOTO, Kei
University of Mainz, Germany
"Spin Torque and Fluctuation-dissipation at FM-AFM Tunneling Junctions"
18 November 2016

Dr YAMAMOTO, Noboru
Eisai Co., Ltd., Ibaraki, Japan
"Drug Discovery Created by Chemists-From Drug Design to Biomarker"
20 May 2016

Prof YAMANAKA, Masahiro
Department of Chemistry, Rikkyo University, Tokyo, Japan
"Investigation of Stereoselectivity in Organocatalysis: Toward Rational Design Based on Transition-State Model"
8 December 2016

Prof YANG, Jinn-Moon
National Chiao Tung University, Hsinchu, Taiwan
"NetPharmalogs for Drug Discovery and Applications"
20 April 2016

Dr YASUDA, Nobuyoshi
Merck Research Institute, MERCK&CO., INC., U.S.A.
"The Art of Process Chemistry"
8 November 2016

Assoc Prof ZHU, Shanfeng
Fudan University, China, P.R.
"DeepMeSH and MeSHLabeler: Recent Progress in Large-scale MeSH Indexing"
29 August 2016
"DrugE-Rank: Improving Drug-target Interaction Prediction of New Candidate Drugs or Targets by Ensemble Learning to Rank"
2 September 2016

Dr ZINOVYEV, Andrei
Computational Systems Biology of Cancer group, Institut Curie, France
"The Shortest Path is not the One You Know: Application of Biological Networks in Precision Oncology Research"
13 December 2016

MEETINGS AND SYMPOSIA

Asian Chemical Biology Initiative 2016 Jakarta Meeting
Organized by UESUGI, Motonari
29 January−1 February 2016 (Jakarta, Indonesia)

The 11th International Workshop for East Asian Young Rheologists (IWEAYR-11)
Co-organized by WATANABE, Hiroshi
4−7 February 2016 (Shenzhen, China, P.R.)

7th Thin-film Solar Cells Seminar
Organized by YOSHIDA, Tsukasa; WAKAMIYA, Atsushi
13−15 May 2016 (Yonezawa, Japan)

The 11th Organoelement Chemistry Seminar
Organized by TOKITOH, Norihiro; SASAMORI, Takahiro; MIZUHATA, Yoshiyuki
3−4 June 2016 (Uji, Japan)

The 5th Main Group Element Chemistry Seminar
Organized by WAKAMIYA, Atsushi
3 August 2016 (Mie, Japan)

17th International Congress on Rheology
Chaired by WATANABE, Hiroshi
8−13 August 2016 (Kyoto, Japan)

Catalyst Society of Japan
"The 44th Organometallic Seminar"
Organized by OZAWA, Fumiyuki; NAKAMURA, Masaharu
24 October 2016 (Uji, Japan)

2016 JSME Annual Meeting
"Symposium S4: Would You Like to Discuss the Raison D'être for Viruses?"
Organized by OGATA, Hiroyuki; NAGASAKI, Keizo
24 October 2016 (Yokosuka, Japan)

The 1st Frontier Solar Cells Seminar
Organized by WAKAMIYA, Atsushi
17−18 November 2016 (Uji, Japan)

Workshop on pMAIRS: Innovative Analytical Technique for an Amorphous Thin Film Device with a Surface Roughness
Organized by HASEGAWA, Takeshi
2 December 2016 (Tokyo, Japan)

The 39th Annual Meeting of the Molecular Biology Society of Japan
"Symposium 3AS11: Where Did They Come From? Where Do They Habit? and What Do They Do in Our World?"
Organized by OGATA, Hiroyuki; TAKEMURA, Masaharu
2 December 2016 (Yokohama, Japan)

The 8th Asian Conference on Organic Electronics (A-COE 2016)
Organized by KAJI, Hironori
5−7 December 2016 (Uji, Japan)

INDEX

NAME INDEX

KEYWORD INDEX

2016

ICR ANNUAL REPORT

Volume 23

Institute for
Chemical
Research

Kyoto University